JMC

Journées de la Matière Condensée 2024

28-31 octobre 2024

Marseille

Le plus grand congrès de physique de la matière condensée en France

amU IMI Aix Marseille Université
amU ISFIN Aix Marseille Université
amU AMUTECH Aix Marseille Université
AFM Association Française de Mécanique
cea
CINaM
CPT Centre de Physique Théorique
FR FCM
irphé Institut de Recherche sur les Phénomènes Hors Équilibre
Centrale Méditerranée
ISEN Méditerranée
L'ÉCOLE DES INGÉNIEURS DU NUMÉRIQUE
GENSURF Recherche & Ingénierie
ORSAY PHYSICS TESCAN GROUP
PIIM
imanp Institut Matériaux Microélectronique Nanosciences de Provence
MADIREL
INSTITUT FRESNEL
IRSN Institut de Radioprotection et de Sûreté Nucléaire
UNIVERSITÉ DE TOULON
VILLE DE MARSEILLE
scientaomicron 1984-2024

Société Française de Physique

amU Aix Marseille Université

Lundi 28 Octobre

Accueil 10h - 13h30

Ouverture 13h15-14h00
Grand Amphi

Plénière 14h00 - 14h50
Denis Bartolo
Grand Amphi

Plénière 15h00 - 15h50
Ivan Favero, prix Ancel
Grand Amphi

Café 16h00 - 16h40
Salle de conférence

Mini - colloques 1
16h45 - 18h45

SMMP1_1 Charve	**NN1_1** 405	**MP3_1** 201
SMMP4_1 Massiani	**BAM2_1** 407	
SMMP6_1 SciencesNat	**2DMS2_1** 205	
	2DMS4 207	

Mardi 29 Octobre

Plénière 8h30 - 9h20
Ludovic Berthier
Grand Amphi

Plénière 9h30 - 10h20
MP Besland, L Cario, B Corraze, E Janod, J Tranchant, Prix Félix Robin
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

Posters et Exposants 11h10 - 12h00
Salle de conférence

Déjeuner 12h00 -13h20
Salle de conférence

3 Semi-plénières
13h20 - 14h10

Anne Tanguy SciencesNat	**Martien Den-Hertog** Charve	**Cécile Sykes** Massiani

Mini - colloques 2
14h30 - 16h30

SMMP1_2 Charve	**NN1_2** 405	**MP3_2** 201
SMMP4_2 Massiani	**NN4** 408	**2DMS2_2** 205
SMMP6_2 SciencesNat	**BAM2_2** 407	**2DMS1_1** 207

Café 16h30 - 17h15
Salle de conférence + 204 + 404

Mini - colloques 3
17h15 - 18h45

SMMP1_3 Charve	**NN1_3** 405	**NN3** 408
SMMP4_3 Massiani	**BAM3_1** 407	**2DMS2_3** 205
SMMP6_3 SciencesNat	**BAM5** 413	

Mercredi 30 Octobre

Plénière 8h30 - 9h20
Benoît Roman
Grand Amphi

Plénière 9h30 - 10h20
Frédéric Mila, prix Charpak-Ritz
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

3 Semi-plénières
11h10 - 12h00

Thomas Cornélius SciencesNat	**Christopher Bäuerle** Charve	**Cécile Monteux** Massiani

Déjeuner 12h00 - 13h20
Salle de conférence

3 Semi-plénières
13h20 - 14h10

Amélie Juhin, prix Ancel SciencesNat	**Freek Massee** Charve	**Véronique Lazarus** Massiani

Mini - colloques 4
14h30 - 16h30

SMMP4_4 Massiani	**NN2_1** 405	**2DMS1_2** 207
SMMP5_1 Charve	**BAM3_2** 407	**2DMS3_1** 208
SMMP6_4 SciencesNat		**IA2** 206

Café 16h30 - 17h15
Salle de conférence + 204 + 404

Mini - colloques 5
17h15 - 18h45

SMMP3 Massiani	**NN2_2** 405	**MP1** 201
SMMP5_2 Charve	**NN5_1** 408	**2DMS5_1** 205
	BAM1_1 SciencesNat	**PSI2** 203
	BAM4_1 407	**2DMS3_2** 208

GALA 19h30 - 23h00

Jeudi 31 Octobre

Plénière 8h30 - 9h20
Emmanuelle Tsitrone
Grand Amphi

Plénière 9h30 - 10h20
Annie Viallat
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

3 Semi-plénières
11h10 - 12h00

Magali Putero SciencesNat	**Wiebke Drenckhan** Charve	**Laurent Lombez** Massiani

Déjeuner 12h00 - 13h20
Salle de conférence

2 Semi-plénières
13h20 - 14h10

Michel Hehn SciencesNat	**Vincent Bouchiat, Behnaz Djoharian prix Yves Rocard** Grand Amphi

Mini - colloques 6
14h30 - 16h30

SMMP2_1 Massiani	**NN2_3** 405	**MP2_1** 201
SMMP5_3 Charve	**NN5_2** 408	**2DMS5_2** 205
IA1 206	**BAM1_2** SciencesNat	**BAM4_2** 407
	PSI1 203	

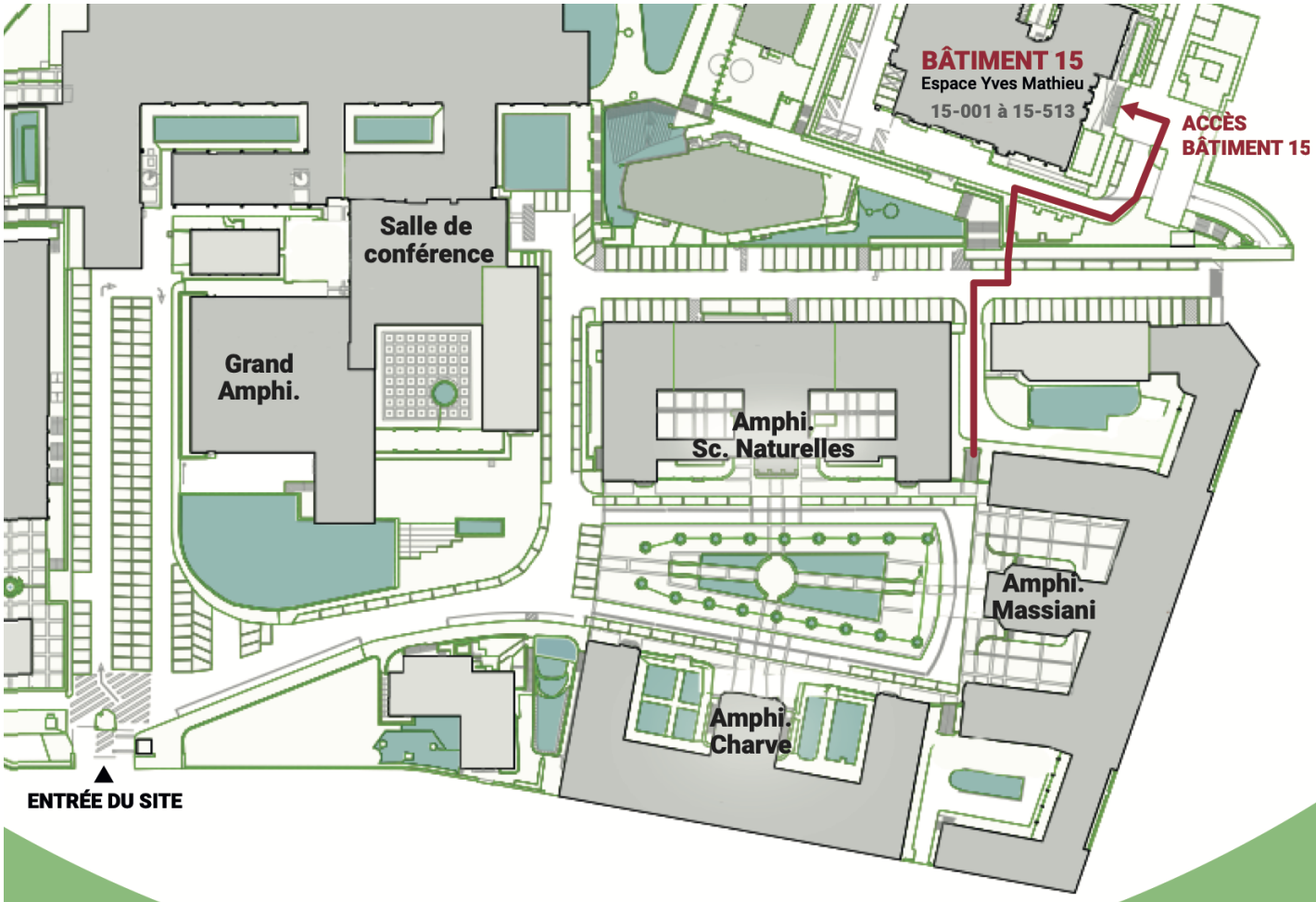
Café 16h30 - 17h00
Salle de conférence + 204 + 404

Mini - colloques 7
17h00 - 18h30

SMMP2_2 Massiani	**NN5_3** 408	**MP2_2** 201
SMMP5_4 Charve	**BAM1_3** SciencesNat	**2DMS5_3** 205

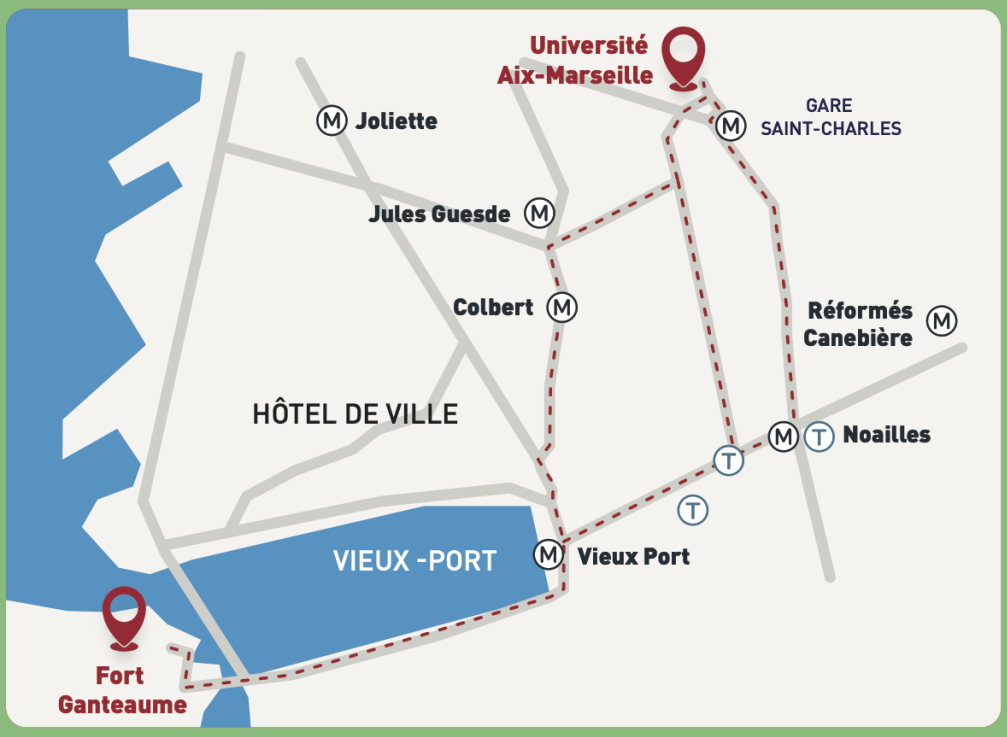
PSI3 - PSI4
413

*TOUTES LES SALLES AVEC UN NUMÉRO SONT LOCALISÉES DANS LE BÂTIMENT 15.



JMC 2024 – Infos et liens

LIEU : Campus St Charles, Aix-Marseille Université
GALA : Fort Ganteaume - Ouverture des lieux à 19h30, dernière entrée 20h30



40 minutes

25 minutes
(M1 St Charles-Vieux port puis 20min de marche)

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28 October 2024

Ouverture 13h15-14h00
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SMMP6_1 SciencesNat	**2DMS2_1** 205	
	2DMS4 207	

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*All rooms with a number are located in building 15

Plenary

Denis Bartolo

Laboratoire de Physique ENS Lyon

Emergence of collective oscillations in massive crowds.

Building upon a combination of quantitative observations and theoretical insights, I will illustrate and elucidate the emergence of collective oscillations within densely packed pedestrian crowds. Our understanding of massive crowds has long been limited by the lack of quantitative measurements. I will demonstrate that the San Fermin Festival in the city of Pamplona, Spain, provides an opportunity to circumvent this limitation. For decades, every year, at the same day and exact hour, thousands of individuals gather in the same square to await the festival's opening within a secure environment, where crowd density can, nevertheless, exceed five people per square meter. Our data reveal that beyond a critical density, crowds of pedestrians waiting for the festival's opening undergo a dynamic transition from a quiesent to a dynamic state, in which the entire crowd oscillates with a period of approximately fifteen seconds. This emergent dynamics echoes the correlated motion of goups of hundreds of individuals along chiral trajectories. I will then explain how our observations constrain the description of dense crowds as active matter and show that dense crowds are odd frictional solids.

Plenary

Ivan Favero

Matériaux et Phénomènes Quantiques, Université Paris Cité, CNRS

Optomechanics deals with the interaction between light and mechanical vibrations.

An optomechanical body has a dual optical and mechanical nature, enabling it to interact with its environment in a variety of ways. If this object is transformed into a mesoscopic probe, a number of advantages emerge: extreme sensitivity, previously unattainable temporal resolution, responsivity to several types of force, as well as high spatial selectivity. I will discuss original devices and instruments born of this optomechanical approach, which today enables us to measure matter in almost any state: solid, soft or liquid. Applications will cover atomic force microscopy, nanophysics of fluids, and dynamical measurement of individual biological objects.

SMMP1 - Fracture and Friction across Materials and Scales

Unraveling the Dynamics of Supershear Mode I Crack Growth

David Kammer * [1], Mohit Pundir [1], Mokhtar Adda-Bedia

[1] ETH Zurich – Switzerland

Linear elastic fracture mechanics (LEFM) theory has long postulated that the speed of crack growth is constrained by the Rayleigh wave speed. While numerous experimental and numerical studies have generally supported this prediction, some exceptions have raised questions about its validity and the underlying factors influencing dynamic crack behavior. In this work, we present new numerical results showing that tensile (mode I) cracks can surpass the Rayleigh wave speed and exhibit propagation at supershear velocities. The key to this finding lies in incorporating geometric non-linearities into the material model. While such non-linearities are inherent in most materials, their effects on dynamic fracture growth have been largely overlooked in previous work. Our results reveal that accounting for geometric non-linearities is sufficient to enable supershear crack propagation. In addition, we show that these non-linearities induce modifications in the crack-tip singularity, leading to unconventional crack-tip opening displacements, cohesive zone behavior, and altered energy flow dynamics toward the crack tip. These observations suggest that the elastic fields and energy budgeting in the vicinity of the crack tip of geometrically non-linear materials have a completely different behavior than that of linear elastic materials, which is commonly assumed in LEFM theory. Consequently, this provides a novel perspective on dynamic crack growth that challenges existing theoretical frameworks.

Keywords: fracture, supershear, propagation, speed

*Speaker

The stick-break instability of extended fractures

Gabriele Albertini * [1], Thomas Cochard [2], Ilya Svetlizky [3], Robert Viesca [4], David Weitz [2]

[1] University of Nottingham – United Kingdom
[2] Harvard University – United States
[3] Technion - Israel Institutie of Technology – Israel
[4] Tufts University – United States

Fractures can lead to catastrophic failure of materials. Although crack propagation in a two-dimensional plane is well understood, all cracks are extended in a three-dimensional (3D) space, through which they propagate. When cracks slowly move forward in a 3D brittle material, they do so in a discontinuous way with long pauses of no motion followed by rapid forward jumps. We call this a stick-break instability. These forward jumps are short-lived dynamic ruptures propagating perpendicular to the main direction of motion at velocities as high as the Rayleigh-wave speed. We study the crack propagation experimentally in a circular geometry that achieves an uninterrupted extended fracture front and use a fluid to control the loading conditions that determine the amplitude of the forward jump. We find that this amplitude correlates with the transverse velocity. Here we further investigate this observation with dynamic rupture simulations to shed light on the underlying mechanics. These results emphasize the importance of transverse dynamics in the forward propagation of extended fractures.

Keywords: Keywords: dynamic fracture, instability, crack, stick slip

*Speaker

A finite geometry, inertia assisted coarsening-to-complexity transition in homogeneous frictional systems

Thibault Roch * [1], Efim Brener [2], Jean-François Molinari [3], Eran Bouchbinder [4]

[1] University of Amsterdam [Amsterdam] = Universiteit van Amsterdam – Netherlands
[2] PGI 2, Forschungszentrum Juelich – Germany
[3] Ecole Polytechnique Fédérale de Lausanne – Switzerland
[4] Weizmann Institute of Science – Israel

The emergence of statistical complexity in frictional systems (where nonlinearity and dissipation are confined to an interface), manifested in broad distributions of various observables, is not yet understood. We study this problem in velocity-driven, homogeneous (no quenched disorder) unstable frictional systems of height $\boldsymbol{H}$. The latter are described at the continuum scale within a realistic rate-and-state friction interfacial constitutive framework, where elastofrictional instabilities emerge from rate-weakening friction. For large $\boldsymbol{H}$, such frictional systems were recently shown to undergo continuous coarsening until settling into a spatially periodic traveling solution. We show that when the system's height-to-length ratio becomes small - characteristic of various engineering and geophysical systems -, coarsening is less effective and the periodic solution is dynamically avoided. Instead, and consistently with previous reports, the system settles into a stochastic, statistically stationary state. The latter features slip bursts, whose slip rate is larger than the driving velocity, which are non-trivially distributed. The slip bursts are classified into two types: predominantly non-propagating, accompanied by small total slip and propagating, accompanied by large total slip. The statistical distributions emerge from dynamically self-generated heterogeneity, where both the non-equilibrium history of the interface and wave reflections from finite boundaries, mediated by material inertia, play central roles. Specifically, the dynamics and statistics of large bursts reveal a timescale $\backsim \boldsymbol{H/c}$, where $\boldsymbol{c}$ is the shear wave-speed. We discuss the robustness of our findings against variations of the frictional parameters, most notably affecting the magnitude of frictional rate-weakening, as well as against different interfacial state evolution laws. Finally, we demonstrate a reverse transition in which statistical complexity disappears in favor of the spatially periodic traveling solution. Overall, our results elucidate how relatively simple physical ingredients can give rise to the emergence of slip complexity.

Keywords: frictional systems, statistical complexity, rate, weakening, self, generated heterogeneity, wave reflections

*Speaker

Ultrasonic triggering of shear instabilities in stressed granular layers

Xiaoping Jia * [1]

[1] Institut Langevin - Ondes et Images (UMR7587) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Sorbonne Université, Centre National de la Recherche Scientifique – France

In this work, we investigate experimentally mechanical responses in dry and wet granular layers under quasi-static shear with constant normal stress. The associated structure changes are monitored with passive (acoustic emission) and active acoustic detections (wave velocity and coda correlation), accompanied by the optical tracking of particle motions through a transparent wall. Both avalanche-like dynamics (power-law scaling) and quasi-periodic stick-slip (mainshocks or laboratory earthquakes), are observed under various loading condition and interparticle interaction. Significant foreshocks (percussors) were detected with increasing rate before rupture while aftershocks were comparatively small.
The acoustic fluidization of granular layers has been investigated by applying relatively high-amplitude ultrasound ($\backsim$ 10 nm). In the case of stable sliding, the ultrasound reduces abruptly the critical steady-state stress and triggers the stick-slip instability, while in the case of instable frictional sliding, this wave vibration decreases the magnitude of stress drops. We show that such acoustic triggering of macroscopic shear instability originates from the reduction of shear contact stiffness and interparticle friction between grains by the *acoustic lubrication* (4,5), playing a role of effective temperature.
We believe that these laboratory experiments help to better understand the mechanism of dynamic triggering of earthquake by seismic waves.

Keywords: Granualr fault gouges, acoustic probing and pumping, stick slip behavior

*Speaker

Rupture collision

Soumaya Latour * [1], François Passelègue [2], Federica Paglialunga [2], Corentin Noël [2], Jean-Paul Ampuero [2]

[1] IRAP, Toulouse – Université Toulouse III-Paul Sabatier, Observatoire Midi-Pyrénées - OMP (FRANCE) – France
[2] Géoazur, Sophia Antipolis – Université Côte d'Azur, CNRS, Observatoire de la Côte d'Azur, IRD, Géoazur – France

We study the interaction between two rupture fronts as they propagate toward each other and ultimately collide. We first observe this phenomenon during laboratory experiments, at the frictionnal interface between two sliding PMMA samples. The mode II rupture fronts, as well as the radiated waves, are monitored with a fast camera.
Then, through numerical simulations, we elucidate key aspects of these observations and develop broader conclusions. We show that the collision of the rupture fronts generates interface waves that propagate on the sliding interface at the Rayleigh wave speed. The rupture fronts also interact with starting and stopping S-wave phases radiated by the opposite rupture fronts, which can modify their velocity and generate additional interface waves. We discuss the significance of these results for earthquake source phenomena.

Keywords: Dynamic rupture, interface wave, friction

*Speaker

Fracture of an ice sheet by waves: experimental model

Baptiste Auvity * [1], Sébastien Kuchly [1], Laurent Duchemin [1], Dany Dumont [2], Antonin Eddi [1], Stéphane Perrard [1]

[1] Laboratory PMMH – PMMH, CNRS, ESPCI Paris, Université PSL, Sorbonne Université, Université Paris Cité – France
[2] L'Université du Québec à Rimouski (UQAR) – Canada

The North Pole is covered by an ice sheet of about 1m in thickness, generated by sea ice freezing during the winter. At the edges of the polar ice region, ocean waves can break this ice sheet, over 200km, creating a mixed area of ice fragments and open water, called the Marginal Ice Zone (MIZ). What determines the breaking of ice sheet by waves and how does it depend on wavelength and ice thickness?

In the lab, we design a model experiment to study at a smaller scale the fracture of a thin, brittle, elastic sheet under surface wave mechanical loading. We use a varnish that forms a thin (100μm), cohesive, granular material which is brittle enough to be broken by waves of millimetric amplitude. We first show that this material mimics the wave elastic response of an ice sheet and we measure the effective Young's modulus of our heterogeneous material. Then, we determine the physical mecanisms behind the fracture of the varnish by waves,and we study the breaking threshold as a function of the amplitude and the wavelength of the incident waves.

Concomitantly, a larger scale experiment was conducted in February 2024 in the Saguenay river, in Canada. After a mechanical characterization of ice (Young modulus, thickness), we used an icebreaker to generate large enough waves to break the ice on about 100m wide. From the experimental data, I will discuss what would be the best fracture criterion at play.

Keywords: Ice sheet, Fracture, Surface waves, Waves

*Speaker

Emergence of scale effects in dynamic damage under impact loading

Alizée Dubois * [1], Paul Bouteiller *

, Yves-Patrick Pellegrini *

[1] CEA, DAM, DIF – CEA – France

Impact loading induces damage as shock waves reflect off free surfaces, creating tension and leading to the initiation, growth, and coalescence of damage. Typically, this is simulated by examining the behavior of a spherical shell under an isochoric approximation. This shell is derived from a model of porous materials, simplifying the analysis by excluding potential pore interactions. Although various inertial and visco-inertial models in this domain exist, uncertainties persist regarding the loading range and initial pore configuration that lead to the dominance of inertial over viscous terms.
Behavioral patterns within the solution of the spherical shell growth equation are investigated using both analytical and numerical approaches, employing a simplified viscoplastic model for the pore matrix. The adjustable parameters critical to damage evaluation include the initial porosity, loading deviation from the cavitation threshold, initial external radius of the hollow sphere (indicative of spatial pore density), and the loading rate. These parameters can be gauged against material properties that collectively define a viscous time scale, a typical velocity, and an 'inertial' length scale, contingent upon the viscoplastic parameters and material density.

The key factor determining the transition from a viscosity- to an inertia-dominated regime is the initial external radius of the hollow sphere relative to the inertial length scale, observed across a wide range of loading rates. Surprisingly, this transition exhibits minimal susceptibility to loading rate under typical dynamic conditions. Nevertheless, the experimental sensitivity to the loading rate strongly suggests the influence of another factor, potentially linked to the nucleation step process.

Keywords: damage, shock loading, spall fracture

*Speaker

SMMP4 – Soft and architected structures

Bending properties of kirigami sheets

Lucie Domino * , Joel Marthelot [1]

[1] Institut Universitaire des Systèmes Thermiques et Industriels – Centre National de la Recherche Scientifique, Aix-Marseille Université - AMU – France

'Kirigami' is a Japanese art form that comes from the words 'kiri' (to cut) and 'kami' (paper). While in the traditional art the goal is to obtain very intricate objects that can pop out beautifully, in the scientific literature it usually designates thin sheets that are pre-cut using a staggered pattern of slits. These kirigamis have been widely studied because of their very rich mechanical response when stretched as well as their numerous applications in adaptable solar panels (1) or shape morphing structures (2, 3) for instance.
Despite this extensive scrutiny, the bending properties of kirigami sheets have so far been overlooked. Here, we study thin sheets pre-cut with a staggered pattern of slits and measure their deflection due to gravity. We model their shape using a heavy elastica equation, and from this, extract the effective bending modulus of the kirigami sheets. We then study how the bending modulus depends on the geometric properties of the kirigami (size of the slits and spacing of the pattern).

Our work provides new insights into the mechanical behavior of kirigami structures, and opens up possibilities for their application in areas where controlling the bending properties is critical.

(1) A. Lamoureux *et al.* Dynamic kirigami structures for integrated solar tracking, Nat. Com., **2015**
(2) Y. Zhang et al., Shape-morphing structures based on perforated kirigami, EML, **2022**
(3) P. Celli *et al.*, Shape-morphing architected sheets with non-periodic cut patterns, Soft Matter, **2018**

Keywords: elasticity, slender structures, bending, kirigami

*Speaker

Mechanics of ribbon gridshells

Joo-Won Hong * [1], José Bico [1], Etienne Reyssat [1], Benoît Roman [1]

[1] Physique et mécanique des milieux hétérogenes (UMR 7636) – ESPCI Paris - PSL Research University - CNRS – France

Any surface is characterized by its field of Gaussian curvature, i.e. the product of its two principal curvatures. Bumps, saddle points or locally flat surfaces correspond to respectively positive, negative and zero Gaussian curvature. Variations of Gaussian curvature imply changes in the distances along the surface. As a classical example, drawing a flat map of the spherical Earth requires to distort continents. In practice, many mechanisms may lead to shape change through effective surface stretching: folding, cutting, inhomogeneous growth are a few.

Gridshells are structures composed of sets of beams crossing eachother. While the distances between consecutive crossing points are constant, the crossing angles may be free. The exotic geometry and mechanics of such structures result from the physical properties of its constitutive beams and their joints.

We are interested in gridshells formed by to crossed families of ribbons, which have the particular property of preventing bending in their own plane. We first describe gridshells where both families of ribbons have their normal in the plane of the overall structure. As one restricts to deformation in the plane, this Chebyshev net is fully described by the shapes of one line of each family. As we probe out-of-plane deformations, only the restricted set of uniform and negative Gaussian curvature shapes is reachable. Designing gridshells with ribbons whose normal points out of the average plane of the structure enables deployment into other shapes, with locally positive Gaussian curvature for instance.

Keywords: Mechanics, Gridshell, Shape morphing

*Speaker

Morphoplastic cellular metamaterials

Victor Charpentier [1], Ignacio Andrade-Silva [1], Trevor Jones [2], Tom Marzin [2], Stéphane Bourgeois [3], P.-T. Brun [2], Joel Marthelot * [1]

[1] IUSTI – CNRS, Aix-Marseille Université - AMU – France
[2] Department of Chemical and Biological Engineering, Princeton University – United States
[3] LMA – CNRS, Centrale Marseille, Aix-Marseille Université - AMU – France

We introduce cellular metastructures capable of morphing into structurally functional and programmable shapes obtained when pulling and releasing its boundaries. Our structures demonstrate permanent 1D to 2D and 2D to 3D morphing capabilities. We rationalize the physics at play in our morpho-plastic structures and establish design guidelines to solve the inverse design problem and obtain complex shapes by embedding the complexity of the final shape in the initial form. We forecast that our work will have an impact wherever structural functionality and deployablity are needed, e.g., consumer goods, health, and architecture.

Keywords: metamaterials, plasticity

*Speaker

Non-reciprocal transport in driven solids

Justine Parmentier * [1], Aaron Winn [2], Eleni Katifori [2], Martin Brandenbourger [1]

[1] Institut de Recherche sur les Phénomènes Hors Equilibre – UMR Université Aix-Marseille – France
[2] Department of Physics and Astronomy, University of Pennsylvania – United States

Non-reciprocal or directional transport, observed for, e.g., electrons, photons or phonons under external excitations applied to non-symmetrical crystalline structures, enable scalable and robust transport of particles and information. However, due to the nature of these systems, achieving fine control over the amplitude of undirectional transport is challenging. We apply this concept to fluid transport in vessels and demonstrate the crucial role of the coupling between external excitations and nonlinearities. Inspired by the lymphatic system, we study fluid transport in a vessel containing distributed valves. We characterize the valve contraction mechanisms and resulting unidirectional fluid transport from active contraction waves. The vessel, constructed from hyperelastic soft polymer, comprises identical valves consisting of pairs of symmetric, semi-circular, inclined leaflets. Their orientation allows liquid to flow through a preferential direction. Peristaltic waves, generated by externally induced mechanical contractions between the valves, enable variable valve closure time, thereby modulating the flow rate. The phase difference between active contraction points along the vessel stimulates peristaltic waves with directional flow. We show that, regardless of the wave direction, the presence of valves always yields forward-flow transport, the valves acting thereby as a classical continuous rectifier robust against any pressure gradient or contraction modes. Yet, the direct coupling between contractions and nonlinearities enable unexpected regimes in which backward-oriented waves maximize forward flow that can even sustain negative pressure gradients. These results are supported by theoretically computing the flow in a vessel subject to nonlinear resistances and peristaltic waves. By decreasing the leaflet efficiency so that they can no longer perfectly shut, we further demonstrate the critical coupling between the contraction amplitude and the nonlinearity of the system. These insights into valve dynamics and fluid transport mechanisms advance our understanding of non-reciprocal mechanical transport and offer new ways to tune non-reciprocal transport by coupling nonlinearities with external excitations.

Keywords: nonreciprocal transport, lymphatic system, fluid transport, nonlinearities

*Speaker

Periodic homogenization of a pressurized bioinspired cellular material in large deformation

Paul Lacorre * [1], Louison Fiore [1], Jean-Marc Linares [1], Loïc Tadrist [1]

[1] Institut des Sciences du Mouvement Etienne Jules Marey – Aix Marseille Université, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7287 / UMR6233 – France

When flowers or other plants with soft stems lack water, they lose the rigidity that allowed them to stand upright. These important changes in stiffness are mainly caused by variations in osmotic pressure within the intracellular liquid. However, these variations of apparent stiffness have not been quantified in living plants. To study the influence of pressure on the apparent mechanical properties of plants, we propose a model of these tissues with simplified geometry. Plant cells are represented by cubic cavities within a massive polymer block and air tubes in each cell allow for individual control of their internal pressure.

The effective mechanical properties of the medium are obtained by periodic homogenization of a representative volume element. The finite element simulation takes into account geometric and material nonlinearities. The elasticity tensor is reconstructed to track the evolution of material coefficients as a function of pressure and wall properties. The anisotropy of the tissue can be controlled by changing the distribution of pressure. Counter-intuitively, the apparent Young's modulus decreases with increasing pressure. A linear analytical model shows this is mostly due to volume changes upon inflation while the "true" stiffness remains constant.

Our work aims to provide fundamental answers about plant stiffness using a rigorous methodology that applies to all pressurized cellular solids. This artificial tissue is also a programmable metamaterial that could serve as a resilient actuator for robotics.

Keywords: periodic homogenization, pressurized cellular material, plant cells, large deformation, finite element simulation

*Speaker

Trainable and resettable nitinol-composites metamaterials

Paul Baconnier * [1], Martin Van Hecke [1,2]

[1] AMOLF, Amsterdam – Netherlands
[2] Leiden Institute of Physics, University of Leiden (LION) – LION, Leiden University, P.O. Box 9504, NL 2300 RA Leiden, Netherlands

We create building blocks for adaptable and resettable metamaterials by embedding nitinol wires within silicone rubber springs. Memory is encoded in the building block via plastic deformations of the wires, but can be erased by heating the nitinol wires above the so-called activation temperature through external electrical currents. Our "nitinol springs" are adaptative, non-linear, and resettable, providing ideal building blocks for adaptable and reprogrammable metamaterials. Combining multiple "nitinol springs" into simple geometries and harnessing drive/reset protocols, we enable the material to undergo shape-morphing and to encode multiple memories.

Keywords: Physical learning, Metamaterials, Memory, Shape morphing

*Speaker

Path dependency in multi-dimensionally driven multistable materials

Colin Meulblok * [1,2], Matthieu Labousse [3,4], Amitesh Singh , Martin Van Hecke [1,2]

[1] AMOLF, Amsterdam – Netherlands
[2] Leiden Institute of Physics, University of Leiden (LION) – Netherlands
[3] Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris – Université Paris sciences et lettres – France
[4] Gulliver (UMR 7083) – ESPCI Paris - PSL Research University - CNRS – France

While most studies have focussed on homogeneous driving conditions, multi-dimensional driving can elicit path-dependent behaviour. Here, we introduce a model system of coupled, precurved elastic beams and develop a systematic approach to investigate and describe such path-dependent responses. Together, our work opens avenues to leverage the response of multistable systems to spatially textured drive protocols, paving the way for memory and computing *in materia*.

Keywords: multistability, path dependency, metamaterials, singularities

*Speaker

SMMP6 – Statistical physics of disordered matter

Active hydraulic laws from frustration principles

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Viscous flows are laminar and deterministic. Robust linear laws accurately predict their streamlines in structures as complex as blood vessels, porous media and pipe networks. However, biological and synthetic active fluids defy these fundamental laws. Irrespective of their microscopic origin, confined active flows are intrinsically bistable, and therefore non-linear. As a consequence, their emergent patterns in channel networks are out of reach of available theories, and lack quantitative experiments. In this talk, I will lay out the basic laws of active hydraulics. I will show that active hydraulic flows are non-deterministic and yield degenerate streamline patterns ruled by frustration at nodes with an odd coordination number. More precisely, colloidal-roller experiments in trivalent networks reveal how active-hydraulic flows realize dynamical spin ices. The resulting streamline patterns split into two distinct classes of self-similar loops, which reflect the fractionalization of topological defects at the subchannel scales. Informed by our measurements, we formulated the laws of active hydraulics as a double spin model. A series of mappings on loop O(n) models then allow us to predict the geometry of the degenerate streamlines in two different regimes. Our fundamental understanding may help to provide design rules for active microfluidic devices, and to offer avenues to understand the motion of living cells and organisms in complex habitat. (Jorge, Chardac, Poncet & Bartolo, Nat. Phys. 2024)

Keywords: active matter, frustration, topological defects, spin systems

*Speaker

Enhanced stability and chaotic condensates in multi-species non-reciprocal mixtures

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Random non-reciprocal interactions between a large number of conserved densities are shown to enhance the stability of the system towards pattern formation. The enhanced stability is an exact result when the number of species approaches infinity and is confirmed numerically by simulations of the multi-species non-reciprocal Cahn-Hilliard model. Furthermore, the diversity in dynamical patterns increases with increasing number of components and novel steady states such as pulsating or spatiotemporally chaotic condensates are observed. Our results may help to unravel the mechanisms by which living systems self-organise via metabolism. We have studied the multicomponent NRCH model for a large number of species and illustrated the role of non-reciprocity in regulating complex phase behaviour. The self-averaging nature of the most unstable eigenvalues in our application of RMT has enabled us to make robust predictions.

*Speaker

Socio-economic agents as active matter

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We will focus on a socio-economic occupation model in the spirit of the Sakoda-Schelling model, historically introduced to shed light on segregation dynamics among human groups. For a large class of decision rules adopted by our interacting agents, the system undergoes an Ising-like phase separation (liquid-gas) while remaining out of equilibrium. Within a mean-field approximation I will show how the model can be mapped, to some extent, onto an active matter field description, paving the way for a unifying framework which considers population and price dynamics within a field theoretic approach on a territory.

Keywords: active matter, phase transitions

*Speaker

Fluctuations in dense active matter

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Active matter is a broad class of materials within which individual entities consume energy in order to perform movement. These are thus out of thermodynamic equilibrium and display a wealth of surprising phenomena which challenge our conception of equilibrium phases and dynamics. Our interest lies in the emergence of collective motion, which has been studied in systems as diverse as crowds, flocks, schools, or swarms, yet with common characteristics. More specifically we focus on dense cell tissues and bacterial suspensions, which are archetypical systems where active forces compete with crowding effects. We demonstrate, using a combination of analytical and numerical tools, how the microscopic symmetries of the active forces transfer to the macroscopic behaviour of the system. Our analytical predictions, which rely on linear elasticity theory, are validated numerically; first in athermal isotropic particles, which provide at large density a good first approximation of confluent tissues; then on vertex models, which are able to capture non-isotropic cell-cell interactions, and are thus more realistic. In the case of degree-of-freedom-wise stochastic noise against substrate friction, i.e. self-propulsion, the system exhibits remarkable velocity correlations. For carefully tailored parameters, we show these lead to irregular turbulent-like flows even in the presence of aligning interactions. In the case of pair-wise stochastic noise in the absence of pair-wise dissipation, we show that this picture is inverted, with velocities becoming anti-correlated at short range. At low noise amplitude, we show how this stabilises long-range translational order in one and two dimensions. Finally, we introduce mechanical feedback as a way to amplify fluctuations from the individual to the tissue level.

Keywords: nonequilibrium statistical mechanics, active matter, collective motion

*Speaker

Non-Reciprocal Interactions Reshape Topological Defect Annihilation

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We show how non-reciprocal ferromagnetic interactions between neighbouring planar spins in two dimensions, affect the behaviour of topological defects. Non-reciprocity is introduced by weighting the coupling strength of the two-dimensional XY model by an anisotropic kernel. As a consequence, in addition to the topological charge q, the actual shape of the defects becomes crucial to faithfully describe their dynamics. Non-reciprocal coupling twists the spin field, selecting specific defect shapes, dramatically altering the pair annihilation process. Defect annihilation can either be enhanced or hindered, depending on the shape of the defects concerned and the degree of non-reciprocity in the system. We introduce a continuous description – for which the phenomenological coefficients can be explicitly written in terms of the microscopic ones – that captures the behaviour of the lattice model.

Keywords: Active Matter, Non reciprocity, Non reciprocal interactions, Topological Defects, XY Model, Lattice Model

*Speaker

Bacterial glass transition in Pseudomonas aeruginosa

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Motile bacteria self-organize in numerous collective phases, such as orientationally ordered phase or swarming state. These collective phases result from properties and activities at the single cell scale, such as growth rate, swimming speed and cell-cell interactions. Understanding how individual properties can trigger emergence of long range order is a crucial aspect of biological and physical studies on bacteria, and can lead to better understanding of the mechanisms of colonies and biofilms formation. Here we study the properties of the 2D swarming state of an elongated motile bacteria, *Pseudomonas aeruginosa*, in growing colonies. We are able to obtain large and dense bacterial monolayers at the edge of 3D colonies expanding on agar gels. We perform the detection of bacterial trajectories from high-speed movies through the use of DistNet2D, an innovative deep learning technique that compute segmentation and tracking altogether, taking advantage of temporal information. As density increases in bacterial monolayers, *P. aeruginosa* undergoes kinetic arrest, and collectively transitions from a liquid-like state to a glassy state. We show that this transition does not only affect the scales of the system's relaxation times, but also the very nature of the dynamics at play. We reproduce the analysis to several *P. aeruginosa* mutants of different shapes and single-cell motion properties, and show that all flagellated mutants exhibit a similar glass transition. The critical surface density to trigger the transition does not depend on single-cell motion properties, and seems to only depend on the aspect ratio of cells.

Keywords: Active matter, Bacteria, Glass transition

*Speaker

BAM2 - Mechanics and microstructure of living matter across length scales

From Sequence to Mechanics: Decoding the Motifs Behind the Mechanical Stability of Proteins

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Mechanical forces are involved in various biological processes such as muscle function, hearing, and cell adhesion. Proteins adopt specific structures that enable them to support mechanical forces before unfolding. Therefore, it is essential to study the relationship between protein structure and mechanics to understand function . While β-sheet proteins are generally regarded as more mechanically stable than α-helix proteins, predicting unfolding forces based on specific protein folds remains a challenge.
In this study, we aimed to identify short sequence motifs that contribute to the mechanical stability of proteins. We focused on four protein domains with similar folds: the immunoglobulin domain 27 of titin (I27), the 4th domain of intercellular adhesion molecule 1 (ICAM1), the 2nd domain of vascular cell adhesion molecule 1 (VCAM1), and the first extracellular domain of cadherin-23 (Cdh23EC1).
Using the Distance Matrix Alignment (DALI) algorithm, we compared the 3D structures of these proteins, allowing for their spatial superimposition and the extraction of sequence alignments based on structural features. Through this alignment, we identified the sequence motif (NE)(LI)(KQR)V in the last β-strand (G) of all four domains, a stretch known to be critical for the mechanical stability of titin I27. To assess the mechanical significance of this motif in the other domains, we performed Steered Molecular Dynamics simulations (SMD) on both wild-type proteins and point mutants. SMD simulations offer an atomistic view of the unfolding process by fixing one end of the protein and pulling the other, tracking the applied force and the position of each atom over time. These simulations revealed that hydrophobic amino acids of the motif are crucial for mechanical stability. To validate these computational findings, we are currently conducting high-speed atomic force microscopy (AFM) based force spectroscopy experiments.

Keywords: protein unfolding, atomic force microscopy, steered molecular dynamics, mechanical stability

*Speaker

Actin Cortex Mechanics Probed in Live Cells

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Among the cytoskeletal components, the actin cortex is key to understand cell mechanics. Its interaction with myosin II microfilaments makes it a contractile material, and the gradients of tension thus generated across the cortex controls an important part of the cell shape changes. To probe the actin cortex mechanical properties, we developed a novel tool called Magnetic Pincher, based on superparamagnetic microbeads that can be ingested by cells and tracked in 3D using bright field microscopy with a precision of ≈20 nm. When applying an external magnetic field, beads inside the cell and free beads added to the medium attract each other to form pairs pinching the cell cortex with a known force. At low forces (≈ 50 pN), this works as a magnetic caliper, probing the cortical thickness and its fluctuations with a high time resolution (> 1 Hz). When applying ramps of higher forces (up to 1 nN), the pinching force increases and the beads acts as indenters, allowing us to access the mechanical properties of the cortex. We used 3T3 fibroblasts adhering on 20 um fibronectin discs as our model system, and applied a model describing thin-films compressions to fit our force-indentation curves on definite intervals of stress. Thus we demonstrated that the cortex has a non-linear stress-strain relation, with a tangent elastic modulus ranging from a few kilopascals to more than 10kPa at high stress. We also identified a robust, negative correlation between cortical thickness and stiffness. We explored the effects of many different perturbations of the cortex on its mechanics. Finally we combined this technique with a Nano-Indenter, enabling successive measurements of mechanical properties at both the whole cell and cortex scales within the same cell. Overall these novel results are a step toward an integrated model of single-cell mechanics.

Keywords: actin, actin cortex, cell mechanics, cytoskeleton, cell biology

*Speaker

Mechanical Polarity of the Actin Cortex

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As they divide, differentiate and migrate, cells establish a polarity by asymmetrically distributing cellular components. They also undergo striking morphological changes during polarisation. These morphological changes, often triggered by certain polarity cues, are associated with the remodeling of the actin cortex: a dynamic, thin network of actin filaments underlining the plasma membrane. While the molecular components of the actin cortex have been studied in detail, an investigation into its mechanical properties is still lacking in literature.
To study this, we use a tool developed in the team known as the Magnetic Pincher to mechanically characterise the actin cortex, in combination with optogenetics to induce cell polarisation. The Pincher uses superparamagnetic beads that self-assemble in an external magnetic field, forming linear chains. Cells ingest a small quantity of the beads a priori, following which more beads are then added to their environment. The pair of beads, i.e. one inside the cell and one outside, attract each other to 'pinch' the cortex. A 3D tracking of the beads is performed to obtain measurements on the local thickness and elasticity of the cortex.

We use genetically-modified 3T3 fibroblasts that activate the RhoA signalling pathway – a well-known polarity cue - at the cortex upon blue light-stimulation. By illuminating roughly half the cell, we can create a 'polarized rear' – a highly contracted region as a downstream effect of RhoA – and a 'polarized front' corresponding to actin protrusions. Maintaining the cell in this polarized state, we use the Pincher to characterize cortex mechanics at the cell rear and front.
Our research reveals important features of the cortex such as elasticity, non-linearity and thickness locally, inaccessible with other existing tools. Understanding these properties in the light of cell polarization can further elucidate underlying polarity-establishment mechanisms, emphasizing the link between cell signalling, cortical mechanics and its microstructure.

Keywords: actin cortex, mechanobiology, polarity, non, linear mechanics

*Speaker

Consequences of actin network architecture on its visco-elastic scaling laws

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Actin networks generate large forces at the cellular scale. In this talk, we will use a combination of simulations and analytical models to understand how macroscopic mechanics emerge from microscopic elements. In particular, we will be interested in contractile actin-myosin networks, that are usually represented as active gels. However, the link between the microscopic structure of actin gels and their macroscopic properties remain tenuous.
We show that; provided relevant terms are kept, active gels are indeed a good description of contractile actin networks. Previous work identified the active contractile unit of actin-myosin networks ; we managed to expand these results to predict how the contractile stress scales with actin density, but also with motor protein properties. We also find that, surprisingly, the effective viscosity strongly depends on motor properties, rather than on crosslinker detachment.
Overall, we derived new scaling laws for large-scale mechanics of actin-myosin networks from network architecture and the microscopic properties of their components, and we could confirm these results by numerical simulations.

Keywords: Active gel, actin, biophysics, scaling, viscosity, elasticity

*Speaker

Virtual Cages: The Collective Behavior of Active Filaments

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Motility coupled to responsive behavior is essential for many microorganisms to seek and establish appropriate habitats.
One of the simplest possible responses, reversing the direction of motion, is believed to enable filamentous cyanobacteria to form stable aggregates or accumulate in suitable light conditions.
Here, we demonstrate that filamentous morphology in combination with responding to light gradients by reversals has consequences far beyond simple accumulation:
Entangled aggregates form at the boundaries of illuminated regions, harnessing the boundary to establish local order.
We explore how the light pattern, in particular its boundary curvature, impacts aggregation.
A minimal mechanistic model of active flexible filaments resembles the experimental findings, thereby revealing the emergent and generic character of these structures.
This phenomenon may enable elongated microorganisms to generate adaptive colony architectures in limited habitats, or guide the assembly of biomimetic fibrous materials.

Keywords: Active filament, Collective behavior, Cyanobacteria

*Speaker

Molecular modulation of Drosophila muscle mechanics

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The sarcomere, a fundamental structural and functional unit of muscles, is arranged in series within myofibrils along the length of the muscle. It comprises primarily of actin and myosin filaments, which generate force by sliding past one another, as well as titin, the elastic protein that experiences mechanical tension. Actin filaments are anchored at the Z-discs of the sarcomere pointing and overlapping with the centrally located myosin filaments. This overlap forms the A-band, while the myosin-free region of actin forms the I-band. Mammalian titin spans half the sarcomere, linking actin to myosin filaments, and is the main source of passive muscle tension by storing elastic energy. Sallimus (Sls), the I-band titin homolog in *Drosophila* extends across the I-band, with its N-terminus anchored at the Z-disc and its C-terminus at the start of the A-band. Sls contains large, spring-like elastic PEVK regions that likely contribute to muscle elasticity. Our recent research has shown that deleting PEVK parts of the Sls I-band reduces both the I-band and A-band lengths of the sarcomere. This indicates a biomechanical feedback mechanism between sarcomeric components, allowing proportional scaling of filament lengths and potentially influencing both active and passive forces of the sarcomere. Our work focuses on how the Sls PEVK domain mediates this biomechanical feedback. We are analysing the mechanical properties of wild-type and Sls PEVK mutant sarcomeres during various developmental stages and in adult flies across different muscle types, by performing force-length measurements and mechanical mapping by atomic force microscopy. We have successfully mapped the mechanical properties of wild-type and mutant sarcomeres of the adult flight muscles. The identified differences suggest that structure and sequence of titin modulates the mechanical response of sarcomeres, shedding light to muscle function.

Keywords: Sarcomere, Mechanics, Drosophila, Muscle, Atomic Force Microscopy

*Speaker

Emergent morphologies of active surfaces

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Many force-generating structures in developing organisms, including the actomyosin cortex of cells and organ-lining epithelial tissues, are organised on effectively two-dimensional surfaces. A key challenge for the shape transformations such living materials are undergoing during morphogenesis is to organise locally generated active forces such that a desired global geometry robustly emerges. A popular theoretical framework that leads to the self-organisation of forces in an active material is mechano-chemical feedback, in which some "patterning agent", e.g. a concentration or order parameter field, tunes local active stress and is itself changing due to the generated flows or deformations. While this feedback ultimately leads to self-organised shape changes of an active surface, surprisingly little is known about the potential impact of active stresses that directly depend on the local curvature and, in particular, what role curvature-driven active stresses could play in guiding the robust generation of a desired surface geometry. Importantly, such a scenario eliminates the need for a separate patterning agent. Instead, surface curvature itself becomes the patterning agent and stationary states of curvature patterns correspond to emergent stationary surface geometries. Investigating this idea using a novel numerical approach to solve the force-and moment-balance equations of deforming active surfaces, we show in this work that the fully self-organized formation of stationary tubular, ellipsoidal and biconcave surfaces, as well as global shape transformations akin to cell division, can be controlled by homogeneous active processes that respond only to the local curvature.

*Speaker

MP3 – Emerging Majorana materials : towards topological quantum computing

From Majorana to Andreev and Back

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Majorana zero modes (MZM)s follow non-Abelian exchange statistics wich, together with their topological protection against local noise, holds promise for applications in fault-tolerant topological quantum computing (1). However, after more than ten years of intense experimental effort towards their unambiguous detection in hybrid semiconductor-superconductor devices, it has become evident that distinguishing MZMs from subgap Andreev bound states (ABS)s near zero energy, which are ubiquitous in such devices due to various physical mechanisms, is extremely difficult. Interestingly, this Majorana versus Andreev controversy (2) has helped us to understand that, far from being a disadvantage, the presence of ABSs can be used to design new qubit concepts. One promising route is to encode a qubit in the spin of a quasiparticle occupying an ABS in a quantum dot-based Josephson junction (3). Embedding such superconducting spin qubit in a superconducting transmon circuit, allows an intrinsic spin-supercurrent coupling providing an optimal interface with circuit quantum electrodynamics for coherent control, readout and strong coherent qubit–qubit coupling (4). By extending this idea to Josephson junctions based on a minimal chain of four quantum dots one could demonstrate a minimal Majorana-Transmon qubit based on non-local fermion parity (5).

(1) *Majorana qubits for topological quantum computing,* Ramón Aguado, Leo P Kouwenhoven, Physics Today 73, 44 (2020).

(2) *From Andreev to Majorana bound states in hybrid superconductor-semiconductor nanowires,* Elsa Prada et al, Nature Review Physics,2, 575–594 (2020).

(3) *Spectroscopy of Spin-Split Andreev Levels in a Quantum Dot with Superconducting Leads,* Arno Bargerbos et al, Phys. Rev. Lett. 131, 097001 (2023)

(4)Direct manipulation of a superconducting spin qubit strongly coupled to a transmon qubit, Marta Pita-Vidal et al, Nature Physics, 19, 1110 (2023)

(5) *Minimal Kitaev-transmon qubit based on double quantum dots,* D Michel Pino et al, Phys. Rev. B, 109, 075101 (2024)

*Speaker

Experimental realisation of 2d electron gas for the investigation of "exotic" particles

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2-dimensional electron gases (2DEGs) in GaAs-based heterostructures is the principal constituent of choice for a number of quantum devices that have allowed novel studies of " exotic " quasiparticles. These includes investigations of anyonic properties in the fractional quantum Hall effect (anyonic statistics as well as scaling dimensions) and of exotic quantum critical points resulting from frustrated Kondo interactions using the charge-Kondo effect. I will discuss the realisation of the III-V heterostructures and devices, which allows us to conduct these studies: how to achieve the necessary properties of the 2DEGs as well the components of the devices. In particular the requirements of the requisite global gates, quantum point contacts and micrometer sized ohmic contacts will be presented, as well as studies highlighting the problems and solutions for future, more complex devices for the investigations of these quasiparticles.

Keywords: 2DEGs, anyonic statistics, charge, Kondo effect, epitaxy, device fabrication

*Speaker

Topological quantum computation using spin polarized Majorana zero modes of hexagonal and pentasilicene nanoribbons

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We study the emergence of spin-polarized Majorana zero modes (MZMs) at the ends of two different finite zigzag nanoribbons: honeycomb and pentasilicene (1,2). In both cases, we consider a minimal model composed of the first nearest neighbor hopping term, Rashba spin-orbit coupling, p-wave superconducting pairing, and an applied external magnetic field. As that double nanoribbon structure mimics two parallel Kitaev chains connected by the hopping t, their energy spectrum profiles reveal regions with two or four spins up or down MZMs that can be accessed by tuning the chemical potential.
Connecting a gated quantum dot (QD) at the end of those ribbons in the limit of high local correlation, we follow the method presented in reference (3) to study the coherent transfer of quantum information between topological qubits at the ends of the nanoribbon and conventional spin qubits at the QD. Due to the spin discrimination of the MZMs, the electron transfer translates spin superposition states into superposition states of the Majorana system and vice versa, with the possibility of the realization of long-distance quantum information transfer and entanglement between spatially separated spin qubits. On the other hand, by connecting metallic leads between the QD, we can probe the conductance of the system as a function of the chemical potential. In that case, we obtain a more complex "signature" of conductances consistent with the more complex distribution of MZMs on the top or the bottom of the nanoribbon. There is no possibility of confusion with disorder, magnetic impurities, or other sources of conductances.

(1) R. C. Bento Ribeiro *et al.*, Phys. Rev. B 105, 205115 (2022); Scientific Reports 13:17965 (2023)
(2) M. Minissale *et al.*, Journal of Physics: Materials, in press (2024)
(3) M. Leijnse *et al.*, Phys. Rev. Lett. 107, 210502 (2011)

Keywords: Majorana zero modes, Quantum computation, pentasilicene nanoribbons, Spin polarization

*Speaker

Gate-tunable topological superconductivity in a supramolecular electron spin lattice

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Topological superconductivity emerges in chains or arrays of magnetic atoms coupled to a superconductor. However, the external controllability of such systems with gate voltages is detrimental for their future implementation in a topological quantum computer. Here we showcase the supramolecular assembly of radical molecules on Pb(111), whose discharge is controlled by the tip of a scanning tunneling microscope (1). Charged molecules carry a spin-1/2 state, as confirmed by observing Yu-Shiba-Rusinov in-gap states by tunneling spectroscopy at millikelvin temperature. Low energy modes are localized at island boundaries with a long decay towards the interior, whose spectral signature is consistent with Majorana zero modes protected by mirror symmetry (2). Our results open up a vast playground for the synthesis of gate-tunable organic topological superconductors.

(1) C. Li *et al. Nat. Comm.* **14,** 5958 (2023)

(2) R. Pawlak *et al.* https://doi.org/10.48550/arXiv.2310.18134

(3) C. Li *et al.* in preparation

Keywords: Scanning tunneling microscopy, radical molecule, Yu, Shiba, Rusinov state, superconductor, Majorana zero modes

*Speaker

From moiré to moiré-of-moiré states and their topologies in helical twisted trilayer graphene

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The success in twisted bilayer graphene (TBG) opened a new domain in modern physics, now called "twistronics". Such 2D vdW heterostructures offer various platforms for strudying strongly correlated materials and topological superconductivity, paving the way to future topological quantum computation and information. A close cousin to TBG is the twisted trilayer graphene (TTG). With only an additional graphene layer, TTG exhibits significantly different properties than TBG, with higher tunability and distinct symmetries and topologies. The helical twisted trilayer graphene (hTTG) is especially interesting, whose top and bottom layers are rotated in opposite directions with respect to the middle layer, forming two moiré patterns between neighboring layers that are general incommensurate. The mismatch between the two moiré periodicities gives rise to a higher-level moiré pattern on top of them, called "moiré-of-moiré" or "supermoiré" patter. With proper approximations, we can access the moiré electronic states. Interesting topological phase transition induced by twist angles and layer stacking is identified. To evaluate the supermoiré states, a theoretical framework is devised to treat it in the context of perturbed periodicity. This framework is general and can be applied to other physical systems. A pseudomagnetic field effect due to the supermoiré modulation is revealed, which is otherwise invisible by the trivial average of moiré properties over the supermoiré length scale.

References:

(1) Mao, Y., Guerci, D., & Mora, C. (2023). Supermoiré low-energy effective theory of twisted trilayer graphene. *Physical Review B*, **107**(12), 125423.
(2) Guerci, D., Mao, Y., & Mora, C. (2024). Chern mosaic and ideal flat bands in equal-twist trilayer graphene. *Physical Review Research*, **6**(2), L022025. (3) Guerci, D., Mao, Y., & Mora, C. (2024). Nature of even and odd magic angles in helical twisted trilayer graphene. *Physical Review B*, **109**(20), 205411.

Keywords: twisted multilayer graphene, topology, moiré material, quasicrystal

*Speaker

2DMS2 – Growth of 2D materials: structural, optical and electronic properties

Structural transformations in two-dimensional noble chalcogenides

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Platinum chalcogenides have received great attention among layered materials due to their peculiar physical properties. The strong layer-dependent electronic properties cause a band gap opening in monolayer PtTe2, while the system is (semi)metallic otherwise.(1) Here we show that starting with PtTe2 films, other compositions such as Pt3Te4 and P2Te2 can be obtained by a post-growth desorption of tellurium or vapor-deposited Pt atoms.(2) The experiments combined with DFT calculations provide insights into these transformation mechanisms and the stabilization of the new phases. The partially converted monolayer flakes exhibit PtTe2-Pt2Te2 heterojunctions, which enable the formation of the in-plane semiconductor-metal interface.(3) We further studied the electronic structure of edges and point defects in PtSe2 monolayer where metallic 1D states with spin-polarized bands were found.(4) In addition to stoichiometry, combining different Pt-chalcogenides in vertical heterostructures provides an additional degree of engineering of materials properties.(5) Our results showed the variation of the interlayer interaction within the moire structure locally modulates the electronic structure of PtSe2/PtTe2 heterostructures.

References

(1) Adv. Mater 28, 853 (2016); ACS Nano 15, 13249 (2021)
(2) ACS Nano 16, 9908 (2022).
(3) Nano Lett. 22, 9571 (2022).
(4) Adv. Funct. Mater. 32, 2110428 (2022).
(5) ACS Nano 17, 5913 (2023).

Keywords: two dimensional materials, platinum tellurides, quantum confinement, defects, heterostructure

*Speaker

Graphene growth mechanisms during propane/hydrogen CVD on SiC

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Propane/hydrogen CVD growth of graphene on SiC consists simply to grow graphene from propane in a hydrogen/argon atmosphere. The presence of hydrogen in the gas phase promotes Si excess on the surface, hence making impossible graphene growth without propane flow. While graphene monolayers prepared by propane/hydrogen CVD have been widely used for applications in electrical metrology or as a substrate for van der Waals epitaxy, a complete growth study for these specific growth conditions was still missing. Our contribution will discuss the growth and hydrogenation mechanisms occurring both during the growth step and cooling down. In order to study the different steps of graphene formation, we have grown samples with different growth times in conditions leading to the formation of graphene on a buffer layer. Surprisingly, incomplete graphene layers presented hydrogenated interfaces, suggesting hydrogenation of the interface during cooling down. This led us to optimize the cooling down to minimize changes in the graphene interface during this last step. The new set of graphene samples with different growth times allows us to observe the different steps of graphene formation: first, the rapid (less than 1 minute) formation of a buffer layer fully covering the SiC and the nucleation of graphene ribbons and islands, followed by their lateral growth leading to a coalescence a few minutes later. Surprisingly, the growth of the graphene can be self-limited, leading to the formation of a single layer for different growth times or propane flow. More generally, the study of graphene nucleation under different conditions will allow us to discuss the origin of carbon forming the graphene and its orientation.

Keywords: Graphene SiC CVD growth epitaxy mechanisms

*Speaker

Epitaxial growth of few layers NbSe2 on graphene

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2H-NbSe2 is a layered superconductor of Tc=7.2K that hosts a 3x3 charge density wave (CDW) under 33K **(1,2)**. By decreasing the thickness of this TMD, the CDW survives but the superconducting critical temperature shrinks **(2,3)**. Superconducting critical temperatures between 0.65K and 2.6K have been reported for monolayer 1H-NbSe2 on bilayer graphene on SiC grown by MBE, alongside Ising superconductivity that is due to a broken in-plane inversion symmetry, spin-orbit coupling and in-plane confinement of the electrons **(3,4,5,6,7,8)**. We investigate the growth of graphene on 4H-SiC(0001) substrates and the subsequent synthesis of few-layer NbSe2 by MBE on graphene. In particuliar, the growth temperature and rate of NbSe2 control the morphology and size of the islands, their roughness, and their polytype **(9)**. Investigations of superconductivity and charge density wave in sub-monolayers to trilayers NbSe2 will provide additional information to establish a comprehensive growth diagram for NbSe2, and the superconducting properties will be compared to the various values found in the literature.
(1) B. Guster *et al.*, *Nano Lett.* 19, 2019 **(2)** X. Xi *et al.*, *Nature Physics* 12, 2016 **(3)** M. Ugeda *et al.*, *Nature Physics* 12, 2015 **(4)** S Onishi *et al.*, *Phys. Status Solidi B* 253, 2016 **(5)** P. Dreher *et al.*, *ACS Nano* 15, 2021 **(6)** W. Wan *et al.*, *Adv. Mater.* 34, 2022 **(7)** H. Zhang *et al.*, *Nature Physics* 18, 2022 **(8)** Y Chen *et al.*, *Adv. Quantum Technol.* 6, 2023 **(9)** M Liu *et al.*, *Science Advances* 7, 2021

Keywords: NbSe2, graphene, MBE, superconductivity, charge density wave

*Speaker

Anomalous growth of epitaxial 2D Si: a kinetic Monte-Carlo approach

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Two-dimensional materials are renowned for their remarkable properties. Their production by exfoliation has spurred extensive research. However, their production by epitaxy, which is more paradigmatic and a priori more controlled, is still underdeveloped. This is the case in particular for silicene, which cannot be produced by exfoliation.

The a priori promising deposition of Si on a metallic substrate such as Ag(111) revealed unexpected growth modes at high temperatures and low flux where Si is inserted into the first atomic plane of the substrate and forms the inserted islands. In order to rationalize this anomalous growth, we develop an out-of-equilibrium description of an epitaxial growth model using kinetic Monte-Carlo simulations. The model incorporates several effects revealed by the experiments. It is parametrized thanks to an approach in which we show that relatively precise estimates of energy barriers can be deduced by meticulous analysis of atomic microscopy images. This analysis enables us to reproduce both qualitatively and quantitatively the anomalous growth patterns of Si on Ag(111) .

The epitaxy of Si on a van der Waals graphene layer is expected to be a promising alternative. Experiments revealed the growth of large silicene flakes over 100nm in size, surrounded by a ring and coexisting with three-dimensional dendritic islands, 3 to 4 monolayers thick. This anomalous growth mode is again not described by conventional epitaxial models. We derive a model incorporating the essential atomic processes at step edges and between different layers, and adsorption energies on the different islands' layers. Thanks to kinetic Monte-Carlo simulations, we reproduce the flakes growth mode, main morphological characteristics (ringed 2D flakes), densities, but also the long-time evolution resulting in non-coalescent dendritic pyramids for large deposits. The main thermodynamic ingredients of the model enable us to rationalize the growth process and move towards controlling it.

Keywords: KMC simulation, out of equilibrium, epitaxial growth, anomalous growth mode, silicene

*Speaker

Non van-der-Waals epitaxy of germanene on Ag(111)

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Two-dimensional (2D) honeycomb lattices beyond graphene, such as germanene, appear very promising due to their outstanding electronic properties, such as quantum spin hall effect. While there have been many claims of germanene growth, experimental evidence for a honeycomb structure has only been obtained indirectly, from STM observations or electronic properties measurements.

Among all potential substrates for germanene growth, Ag(111) which is known to be well suited for the growth of silicene, is undoubtedly the most discussed one today. On this substrate, the structures observed have been either described as honeycomb germanene or surface alloys. Using scanning tunneling microscopy (STM), surface X-ray diffraction and density functional theory, we have studied the growth of germanium layers on Ag(111) in the 400K-450K temperature range, and determined their structure and energetics (1-3). Unlike van der Waals epitaxy, we show that upon increasing coverage, a series of alloyed phases forms. Two of these phases correspond to highly ordered reconstructions for which we determined precisely the atomic structure. The first one is a c(31x$\sqrt{3}$) reconstruction corresponding to a Ag_2Ge surface alloy with an atomic density 6.45% higher than the Ag(111) atomic density. It is formed by stripes associated with a face-centered cubic top-layer alignment, alternating with stripes associated with a hexagonal close-packed top-layer alignment, in great analogy with the (22x$\sqrt{3}$) Au(111) reconstruction (2). The second one is a ($\sqrt{109}$x$\sqrt{109}$) reconstruction, composed of a periodic arrangement of Ge pentagons, hexagons and heptagons with a small concentration of Ag atoms (3). Our result opens new perspectives related to the understanding of the complex structures observed after growth of 2D Ge or Si layers on metal surfaces.

*Speaker

(1) K. Zhang, *et al*, Phys. Rev. B 102 (2020) 125418
(2) K. Zhang, *et al.*, Phys. Rev. B 104 (2021) 155403
(3) K. Zhang *et al.*, ACS Nano, 1 (2023) 15687

Keywords: germanene, surface x ray diffraction, scanning tunneling microscopy, DFT

Determining by Raman spectroscopy the average thickness and N-layer-specific surface coverages of MoS_2 thin films with domains much smaller than spot size

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Molybdenum disulfide, MoS_2, is of particular interest in optoelectronic applications due to its transition to a direct bandgap semiconductor when thinned down to a monolayer. Because the properties of MoS2 flakes are firstly a function of their thickness, or layer number (N), it is of a primary importance to determine the N of MoS_2 samples prepared by different routes.
Raman spectroscopy is a widely used technique to characterize nanomaterials due to its convenience, non-destructiveness, and sensitivity to materials change. The primary purpose of this work is to determine using Raman spectroscopy the average thickness of MoS_2 thin films synthesized by direct liquid injection pulsed-pressure chemical vapor deposition (DLI-PP-CVD). (1) Such samples are constituted of nanoflakes (with a lateral size of typically 50 nm, *i.e.* well below laser spot size), with possibly a distribution of thicknesses and twist angles between adjacent layers of multilayer domains. As an essential preliminary, we reassess first the domains and limits of application of different Raman criteria which allow determining the thicknesses of MoS2 flakes from measurements performed on reference samples, namely well characterized mechanically exfoliated and standard chemical vapor deposition MoS_2 large flakes deposited on 90 ($\pm$6) nm SiO_2 on Si substrates. Then, we discuss their application for significantly different DLI-PP-CVD MoS_2 samples with average thicknesses ranging from sub-monolayer up to three layers. Finally, an original procedure based of the measurement of the intensity of the layer breathing modes is proposed to evaluate the surface coverage for each N (*i.e.* the ratio of the surface covered by exactly N layers and the total surface) in DLI-PP-CVD MoS_2 samples.(2)
(1) V. Astié et al., *Direct liquid injection pulsed-pressure MOCVD of large area MoS_2 on Si/SiO_2*, submitted
(2) F.Wasem Klein et al., *Beilstein J. Nanotechnol.* 2024, *15,* 279–296.

Keywords: Molybdenum disulfide, Chemical vapor deposition, Raman spectroscopy, number of layers

*Speaker

2DMS4 - Optical spectroscopies and plasmons

Gold nanoparticle networks in topological defects of smectic liquid crystal

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A liquid crystal (LC) is a mesophase where the molecules are free to move as in a fluid, but show a certain degree of order as in a crystal lattice. Under specific conditions, a thin film of LC can form a pattern of flattened hemicylinders that present different kinds of topological defects (1D and 2D defects) strictly oriented along the hemicylinders direction. These defects are able to confine nanoparticles (NPs), leading to the formation of specific networks that are well oriented along the defects. Our aim is to exploit the intrinsic order of this LC matrix to ensure a good orientation and alignment of gold nanoparticles, in order to enhance their optical properties, creating a plasmonic composite. We are currently interested in using gold nanorods coated with thiol-ended polystyrene. Absorption measurements performed with POM reveal that these nanorods can form chains in the 1D defect and ribbons in the 2D defect. The unique orientation of these networks provides the composite with polarized plasmonic properties. The chains are associated with an end-to-end configuration of the nanorods parallel to the hemicylinder axis, leading to the formation of hot-spots between the rods' tips. The ribbons present instead a side-by-side configuration of the rods, which appear perpendicular to the hemicylinder axis. We show that playing with the LC's thickness and nanorod concentration we can act on the composite structure, selecting which kind of network to create. Either we form nanorod chains or nanorod ribbons or both coexisting, the three structures being associated with different kinds of activation of plasmonic properties by light polarization. To better understand the organization of these nanoparticles, the absorption measurements are coupled with numerical simulations that seem to suggest a more complex structure than the side-to-side aggregation, strongly dependent on the number of interacting rods.

Keywords: gold nanoparticles, liquid crystal, POM, simulations

*Speaker

Heavily Phosphorus-Doped Silicon Nanocrystals for Infrared Plasmonics: the Role of Nanocrystal Size on the Localized Surface Plasmon Resonance.

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Plasmonic nanoparticles have generated a strong research activity due to their rich potential and applications in nanophotonics, sensors and enhanced spectroscopy. Noble metals, especially Au and Ag, have received a strong attention because of the high quality-factor of the localized surface plasmon resonance (LSPR) they exhibit, but above all for their substantial free-electron concentration (1022-1023cm-3) which leads to plasmon resonance in the visible spectral range. The high free-electron density leads to some limitations to address infrared and terahertz domains. To overcome these limitations, highly-doped semiconductors have emerged as a promising alternative because of the lower free-carrier concentration as compared to metals and to the possibility to control the doping concentration. The existence of LSPR in semiconductors nanostructures especially in silicon as well as the role of dopant type and dopant concentration on the plasmon resonance has already been demonstrated. However, the LSPR size dependence remains poorly understood, mostly due to the complexity of physical phenomena and experimental challenges to overcome. Here the influence of the nanocrystal (NC) size on the LSPR is investigated in phosphorus-doped Si-NCs embedded in a silica matrix. Plasmonic nanocrystals were obtained from annealed P-doped SiO/SiO2 multilayers produced by evaporation in ultrahigh vacuum. The P content, equal to 0.85 at.%, is kept constant and the NC diameter is varied from 7 to 16 nm. The infrared absorption measurements revealed that the LSPR energy and quality factors are increasing functions of Si-NCs size. The plasmonic response is modeled in the framework of the Mie theory considering the Drude model. Calculated free-carriers mobility and density range between 17 and 28 cm2V-1s-1 and from 1.89×1020cm-3 to 2.6×1020 cm-3, respectively. The origin of these behavior is discussed in relation with the interaction of the plasmon with the NC/SiO2 interface and with the ionization efficiency of P atoms at the nanoscale.

Keywords: phosphorus doping, infrared absorption, LSPR, fermi velocity, silicon nanocrystals, activation energy.

*Speaker

Rapid ellipsometric imaging characterization of alloy and nanocomposite films with an artificial neural network

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Spectroscopic ellipsometry (SE) is one of the most powerful techniques for investigating the opto-geometrical properties of materials. SE is based on the measurement of the change of polarization state of light reflected from a sample. However, the trends of device miniaturization require the development of an ellipsometric setup with microscopic scaled resolution. Imaging ellipsometry was recently introduced to address this issue. Two images representing the ellipsometric angles are recorded for each wavelength. As SE is an indirect characterization tool, the extraction of physical parameters of the sample from the recorded spectra requires a modeling step. However, the analysis of this huge data-cube remains challenging. To reduce the data size, pixels can be gathered into a region of interest (ROI) by using the binning process. However, this approach assumes that opto-geometrical properties are homogeneous inside a ROI. On the other end, the fitting of the full ellipsometric map by using a classical optimization algorithm such as the Levenberg–Marquardt algorithm (LM) is often time-consuming. Even the interpolation of the Ψ and Δ values limits the power of the analysis to one-parameter optical models. In this context, we have introduced an original imaging ellipsometric characterization tool based on the used of an artificial neural network (ANN). Our technic is used to characterized plasmonic films . We demonstrate that imaging ellispometry can be use to determine the spatial variation of film thickness, NP volume fraction, NP shape distribution, dielectric function and plasmonic properties of nanocomposite films. The computing time required for the analysis of the 842460 spectra of Ψ and Δ which composed the ellipsometric map decreases from 15 days for the LM to 1 s for the ANN.is about 1 s by using ANN. This can be considered as a real drastic improvement for in-line SE imaging characterization.

Keywords: Imaging ellipsometry, neural network, plasmon

*Speaker

Dressed dipole model for a 1D chain of spherical metallic nanoparticles

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Plasmonic nanoparticle arrays enable the concentration of electromagnetic energy below the sub diffraction limit. The optical response of such materials depend on the geometry of the particles and on the geometry of the array itself. In these arrays, the localised surface plasmon resonances located on each particle interact through the long range Coulomb interaction. The simplest model for calculating the optical properties of such a nanoparticle array is the point dipole model. In which only the fundamental dipolar mode is retained at each site. This model works provided the particles are sufficiently far apart, for a grating parameter d/R > 3 (1). For denser lattices, the contribution of higher-energy modes is no longer negligible (2). To take these into account, we propose a dressed dipole model for a 1D chain of spherical nanoparticles. In this model, the dipoles are dressed with quadrupolar modes. This correction enables the first plasmonic band to be faithfully reproduced up to a lattice parameter of d/R $\approx$ 2.7. After this limit, the quadrupolar modes represent the main contribution of the lower energy bands.

Keywords: plasmons, hybridation, 1D chain, theoretical

*Speaker

Lattice modes engineering based on bi-material arrays of metallic nanoparticles

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In this work, we study the spectral response and more precisely the lattice modes supported by gold (Au), aluminum (Al) and quincunx gold-aluminum (Au-Al) gratings in the visible range. The goal is to understand the role played by gold and aluminum nanoparticles (NPs) in bi-material arrays and how they contribute to the coupling between Localized Surface Plasmon Resonances and Rayleigh Anomalies to form Surface Lattice Resonances. Finally, the work delves into fundamental mechanisms governing the optical behavior of plasmonic bi-material NPs arrays, with a specific emphasis on their application to fluorescence enhancement. By understanding these interactions, we aim to optimize the design of bi-material NP arrays to enhance both the excitation and the emission performance of fluorescence quantum dots.

Keywords: Lattice resonances, plasmon, fluorescence enhancement

*Speaker

Hybrid Chiral Plasmonic Assemblies for Sensing

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Circular dichroism spectroscopy is widely used to detect chiral molecules. However, conventional CD spectroscopy suffers from weak signals at the molecular level and limited sensitivity. Recent studies have shown that the chiral properties of (bio)molecules can be determined using plasmonic chiral metasurfaces (PCM) consisting of noble metal nanoparticles. PCM are good candidates for biosensors due to their low cost, adaptability, and miniaturized form. Recent studies have reported the design and fabrication of various plasmonic chiral metamaterials, mainly for the detection of enantiospecific interactions, based on plasmonic-driven amplification of naturally occurring CD signals. There is limited work on chiral plasmonic elements, mostly with chiral nanoparticles dispersed in solution, that detect changes in the surrounding medium resulting from the presence of the target analyte. However, instead of dispersing chiral nanoparticles in solution, chip-based sensing of chiral nanoparticles organized in long-range order that can be integrated into photonic circuits is more suitable for point-of-care devices. It will offer great advantages in terms of repeatability, miniaturization, integration with microfluidic components, selective binding, improved optical properties, enhanced sensitivity, real-time monitoring, better control and stability against different solvent and salt concentrations, that can cause precipitation when colloidal nanoparticles are used instead. Chip-based format would allow for simple washing steps during analytical procedures, even with complex biological samples, rather than simpler protein solutions.
In our research, we use silver nanowires to construct plasmonic chiral metasurfaces. To achieve precise alignment of the silver nanowires, we use Grazing Incidence Spraying (GIS). Additionally, we use Layer-by-Layer (LbL) assembly to build multilayer structures. Recently, we have integrated a flow cell on our PCM. Using microfluidics, we have performed tests to evaluate the stability, sensitivity and repeatability of our system. As a result, we have achieved a highly sensitive, reusable and stable system.

Keywords: chirality, sensing, circular dichroism, silver nanowires, plasmonic assemblies

*Speaker

Bottom Up Chiral Optical Cavities

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Designing chiral optical cavities that serve to both preserve and enhance the chirality (helicity) of the electromagnetic field is a major goal in light-matter interactions, opening doors for fields such as high-resolution chiroptical sensing, polaritonic physics, chiral quantum optics, and quantum materials. Designing such cavities has proven challenging because optical helicity reverses at each mirror reflection, nullifying chiralities in the field. This creates a demand for handedness-preserving mirrors, particularly across UV-vis wavelengths. Most current chiral mirrors are produced by costly top-down techniques, like e-beam lithography, making scalability difficult.
Structures consisting of helically assembled silver nanowires were shown to act as semi-reflective chiral mirrors, capable of maintaining the chirality of one handedness of the reflected field, and absorbing the other handedness. We prepare cavities consisting of such mirrors and characterize these structures using Mueller matrix polarimetry. We supplement these results with numerical simulations using a 4x4 transfer matrix formalism capable of handling the anisotropies inherent to these assemblies. Such simulations also allow us to also investigate the chiral nature of the electromagnetic field intra-cavity through quantities such as chiral density.
Polarimetric and numerical investigations reveal the ability to modify the chiral reflectance of such structures through a control on the thickness of the cavities. Furthermore, the performed simulations seem to suggest that the field intra-cavity is indeed chiral.

Keywords: Chirality, cavity, numerical, Polarimetry

*Speaker

NN1 - Optomechanics and nanomechanics

Gravitational-wave astronomy with ground-based interferometric detectors: from birth to the future

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Gravitational-wave astronomy, born in 2015 with the first detection of a gravitational wave (GW) produced by the merger of two black holes, has now entered a mature phase with more than a hundred events detected to date. The network of detectors, comprising the two LIGOs in the USA, Virgo in Europe and KAGRA in Japan, is currently performing its fourth observation period (O4), detecting a few GW candidates every week. In this presentation, after an overview of the physics and technology of the detectors, I will describe the main scientific results obtained so far, ranging from general relativity to astrophysics and cosmology. Finally, I will discuss plans for next-generation detectors, and their scientific potential.

Keywords: Gravitational waves interferometry, Ultra, sensitive Measurement, Interferometry, Lasers, Sub quantum measurement

*Speaker

Towards quantum thermometry using optomechanics

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The redefinition of the SI with regard to the kelvin opens up new possibilities for realising and disseminating thermodynamic temperature, especially through the development of long-term practical primary thermometry approaches. One of the most innovate ways to provide such traceability is an approached based on photonic/optomechanical technologies. Photonic/optomechanical temperature sensors can offer micrometer spatial resolution, large temperature range (from few K up to room temperature) and additionally can be self-calibrated with noise-thermometry and even provide a path towards primary temperature standards using quantum measurements.

We will present recent progress on the development of the temperature sensor based an phoxonic crystal: optomechanical resonator with co-localizsed optical (1550nm) and mechanical (few GHz) modes. The operation in different regimes will be presented: photonics thermometry (exploring the frequency displacement of the optical resonance with the temperature) and optomechanical noise thermometry (technique with an optical readout in which the thermal noise of the mechanical oscillator is used to measure temperature using the equipartition theorem relating the mean squared displacement of a mechanical resonator to its temperature). Further developments towards quantum correlation thermometry (technique which uses a laser probe whose phase noise furnishes a quantum standard used to scale the Brownian motion of an optomechanical resonator) will be discussed.

Keywords: optomechanics, thermometry, metrology, quantum sensors

*Speaker

Ultra-sensitive strain detection in a rare-earth-doped crystal

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[3] Laboratoire Lumière, Matière et Interfaces – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Ecole Normale Supérieure Paris-Saclay, UMR9024 / FRE2036, – France

Cryogenically-cooled rare-earth ion-doped crystals are unique solid-state systems that combine exceptional coherence properties in the optical domain (with applications ranging from signal processing to quantum technologies), with an inherent optomechanical coupling between the optical lines and the strain in the crystal matrix.
Several years ago, we proposed and demonstrated an original method building upon these two properties to design a cryogenic vibration sensor. This sensor is based on the real-time interrogation of a narrow spectral hole (A. Louchet-Chauvet at al., Rev. Sci. Inst. 2019). While this method showed promising bandwidth and sensitivity, it was not fully quantitative.
In this contribution we address our recent progress towards achieving directionality and quantitativeness in our measurement. We develop a strategy that allows for a more direct measurement of stress based on the off-resonance probing of the spectral hole. We focus our study on the dynamic response of the spectral hole and its connection with the spectroscopic parameters of the thulium ions. Aside from representing a significant step forward in making the sensor a reliable tool for practical applications, this work will enhance our understanding of the fundamental physics of strain-coupling in rare-earth ion-doped crystals.

Keywords: rare earth ion doped crystals, optomechanics

*Speaker

High-Order Nanowire Resonances for High-Frequency, Large-Coupling-Strength Quantum Dot Hybrid Nanomechanics

Hajer Tlili * [1], Rana Tanos [1], Yoann Curé [1], Matteo Finazzer [1], Alberto Artioli [1], Saptarshi Kotal [1], Yann Genuist [2], Pierre Verlot [3], Joël Bleuse [1], Jean-Michel Gérard [1], Julien Claudon [1]

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Hybrid nanomechanical systems embedding a quantum light emitter, such as a quantum dot (QD) are actively investigated both for their fundamental interest and for potential applications to quantum information technologies. Strain-coupling an InAs QD to the fundamental flexural vibration mode of a conical GaAs microwire enabled many pioneering contributions to the field (1,2). However, further developments call for a massive increase of the resonator frequency, from the sub-MHz range up to the GHz range.
In this work, we explore the potential of high-order mechanical resonances for high-frequency hybrid nanomechanics (3). Mechanical drive is provided by a recently developed on-chip electrostatic actuation technique (4). We show here that the on-chip electrodes generate a 3D force field that can excite flexural and longitudinal vibration modes. Wire vibrations are detected optically by measuring the QD photoluminescence spectrum. Interestingly, the ensemble of QDs probes the strain distribution in the wire cross section, thereby providing a fingerprint of the mode nature. We conduct a comprehensive characterization of flexural vibrations over the 200 kHz–200 MHz frequency span. In particular, we identify a low-loss mode (mechanical quality factor of 800) that resonates at 190 MHz. This frequency exceeds the QD radiative rate, marking a significant step toward the resolved-sideband regime. Furthermore, the hybrid coupling strength increases with the mode order. For the above-mentioned 190 MHz mode, it reaches 3.9 MHz when the QD is located at the stress maximum; this is the highest value reported so far for a QD-hybrid system.

Overall, these results establish the potential of the QD-nanowire platform for high-frequency hybrid nanomechanics.

(1) Yeo, et al., Nat. Nanotechnology 9, 106 (2014)
(2) Kettler, et al., Nat. Nanotechnology 16, 283 (2021)
(3) Tanos, et al., ACS Photonics 11, 1352 (2024) (4) Finazzer, et al., Nano Letters 23, 2203 (2023)

Keywords: quantum dot, nanowire, mechanical strain, hybrid nanomechanical systems, electrostatic actuation

*Speaker

Recursive optimization of optomechanical coupling at the nanoscale: Towards new fundamental limits

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Nano-optomechanical systems have recently been considerably developed. These devices combine unmatched transduction properties, due to their very low mass, as well as extremely high coupling to the confined electromagnetic field, enabling the detection of their vibration with extreme sensitivity. While these detection methods have now become widely used, the question of their quantum efficiency remains open, as the complexity of the nano-optical interaction may a priori require complex shaping of the transmitted wavefront in order to exploit the entirety of the information. We propose and demonstrate a new single-arm multimode optomechanical feedback device, allowing to optimize the deflection measurement of nanomechanical systems. We demonstrate an improvement in sensitivity by a factor greater than 100. The nature of the fundamental limits and their consequences for nano-optomechanics are also discussed. Our work demonstrates the need to integrate new multimode information processing methods in the perspective of operating nano-optomechanical transducers at the quantum limit.

Keywords: optomechanics, nano, optomechanics, Cramér, Rao, wave, front shaping

*Speaker

NMR with a levitating particle

Julien Voisin * , Gabriel Hétet [1]

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Nuclear Magnetic Resonance (NMR) spans diverse fields from biology to quantum science. Employing NMR on a floating object could unveil novel possibilities beyond conventional operational paradigms. In our study, we observe Nuclear Magnetic Resonance (NMR) within a levitating microdiamond. Specifically, we employ the nuclear spins of nitrogen-14 atoms in a diamond held in a Paul trap. By tightly confining the three angular degrees of freedom of diamonds in micro-traps, we observe efficient hyperfine interaction between optically polarized electronic spins of nitrogen-vacancy centers with the 14N nuclear spin, enabling nuclear spin polarization and state read-out. This represents the longest lifetime recorded for a controlled two-level system in a levitated system, surpassing the previously measured coherence time in electronic spins by three orders of magnitude. Our results hold promise for various applications, including cooling macroscopic particles to their motional ground state and exploring geometric phases crucial for gyroscopy.

Keywords: Spin, défaut cristallin, lévitation, RMN

*Speaker

Synchronized opto-mechanical oscillators for reference frequency generation and distribution

Gregorio Beltramo * [1], Robert Horvat [2], Giuseppe Modica [1], Rémy Braive [1]

[1] Centre de Nanosciences et de Nanotechnologies – CNRS, Université Paris Cité – France
[2] Centre de Nanosciences et de Nanotechnologies – CNRS, Université Paris Sud, Université Paris Saclay, – France

Integrated optomechanical devices strongly localize, within the same microscale cavity volume, an optical and a mechanical mode thus enhancing their mutual interaction. With a weak, on resonance optical field, the thermal motion of the mechanical mode can be read. By increasing power, the radiation pressure pumps energy into the mechanical oscillation arriving at a point in which the pump overcomes the mechanical losses. Under these specific conditions, the mechanical mode starts lasing. This regime of self-sustained oscillations is characterized by a very high and narrow peak in the RF spectrum at the mechanical mode frequency.
Our cavities are made of one-dimensional Gallium Phosphide photonic crystal nanobeams suspended on top of a silicon waveguide. For our structures, a power of few hundreds μW around λ=1550 nm allows to achieve self-sustained oscillations close to 3.3 GHz. Furthermore, this architecture allows us to locate several cavities on top of the same waveguide such that, when their optical and mechanical resonances are close enough, they can couple through light showing synchronization regimes.
Thanks to a controlled thermal-optical shift of the first fundamental optical modes, we control their relative detuning till a point where they overlap. Simultaneously, the mechanical modes evidence synchronization for a given pump wavelength range. With an additional low power probe laser, addressing the second order cavity optical resonance of each oscillator, we independently read the oscillations of both, verifying the synchronized regime. Finally, we demonstrate an all-optical integrated platform to generate and distribute an in-phase reference frequency at two different wavelengths which are the second order optical resonance wavelengths of the two oscillators. These two low power signals show stability performances, in terms of phase noise, comparable to ones of the high-power pump signal.

Keywords: integrated optomechanics, synchronization, pump and probe, photonic crystals

*Speaker

29 October 2024, morning

Plénière 8h30 - 9h20
Ludovic Berthier
Grand Amphi

Plénière 9h30 - 10h20
MP Besland, L Cario, B Corraze, E Janod, J Tranchant, Prix Félix Robin
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

Posters et Exposants 11h10 - 12h00
Salle de conférence

Déjeuner 12h00 -13h20
Salle de conférence †

†All rooms with a number are located in building 15

Plenary

Ludovic Berthier

Laboratoire Charles Coulomb, Montpellier

Statistical mechanics of dense disordered matter.

I will present a rapid and pedagogical overview of on-going research efforts in the broad field of dense disordered materials in various contexts, from dense fluids undergoing glass and jamming transitions to transport and mechanical properties of amorphous solids, with applications from molecular systems to biological active matter. These problems involve computational and theoretical challenges that I would like to explain, and recent developments involving advanced Monte Carlo techniques and machine learning approaches.

Plenary

Marie-Paule Besland, Laurent Cario, Benoît Corraze, Etienne Janod, Julien Tranchant

Nantes Université, Institut des Matériaux de Nantes Jean Rouxel (IMN), UMR CNRS 6502, NANTES, FRANCE

Mottronics: towards a novel electronic based on Mott insulators

After half a century of miniaturization, microelectronics is facing two major issues related to the down-scaling limit and the energy consumption. To overcome these challenges, exploration of new strategies includes the search for new materials, new physics and new architectures.
In this context, quantum materials have attracted much attention. In particular, Mott insulators standing as a broad class of quantum materials are expected to be metallic according to conventional band theory, but are insulating due to on-site electron-electron repulsions. In such systems, electronic doping or external pressure may drive insulator to metal transitions (IMT) and lead to remarkable properties such as high Tc superconductivity or giant magnetoresistance. During the last decades, filling or bandwidth control IMT in Mott insulators (i.e. the Mott transition) have been the subject of intense fundamental researches [1]. However, the use of these IMT in applications remains quite scarce for a very simple reason. Indeed, pressure or doping are not easily controllable parameters in real devices. Our group at IMN demonstrated that the electric field is an efficient parameter to destabilize the Mott insulating state and induce an insulator to metal transition [2]. We first evidenced the non-volatile and reversible switching on single crystals and further validated it on polycrystalline thin layers for several members of the Mott Insulator family [3]. This phenomenon, coined as "Electric Mott Transition" (EMT), is promising for microelectronic applications and could open the door to a novel electronics based on Mott insulators, called Mottronics [4]. Further studies highlighted that this EMT is induced by the massive creation of hot electrons leading to an electronic avalanche within a filamentary conductive path [5]. We demonstrated that this mechanism is driving EMT?s in many Mott insulators with different chemical compositions, such as the chalcogenides AM_4Q_8 (A=Ga,Ge; M=Nb,V,Ta,Mo; Q=S,Se,Te) and $Ni(S,Se)_2$, the oxides $(V_{1-x}Cr_x)_2O_3$ and the molecular system $Au(Et\text{-}thiazdt)_2$ [6].
The characteristics of the non-volatile EMT are suitable for information storage: "Mott memories?" display significant advantages compared to ReRAM based on metal oxides (OxRAM) or phase change materials (PCRAM) [7]. Furthermore, we have shown that a Mott insulator, subjected to a train of electric pulses, may display a Leaky-Integrate-and-Fire behavior based on the volatile EMT. Mott insulators therefore reproduce the main functionalities of neurons in human brain that make them potentially suitable to build up artificial neurons and hardware artificial neural networks [8]. An interesting disruptive solution would be indeed to replace the energy-intensive software networks with energy-efficient "hardware" networks of artificial neurons and synapses, i.e. building blocks based on Mott insulators.
In the longer term, our recent works based on the use of ultrafast lasers shows that ultimate switching times in the picosecond range are achievable in electro-optical or all-optical devices based on Mott insulators [9].
This presentation will first review the electric Mott transition and the new functionalities enabled by this property. It will then present some examples of Mottronics devices in particular for data storage and artificial intelligence applications.

[1] D. B. McWhan and J. P. Remeika, Phys. Rev. B, 2, 3734 (1970); A. Georges et al., Rev. Mod. Phys. 68, 13 (1996); A. Milloch et al., arXiv:2409.04154.
[2] L. Cario et al., Adv. Mater., 22, 5193, (2010) ; E. Janod et al., Adv. Funct. Mater. 25, 6287, (2015).
[3] E. Souchier et al. Phys. Stat. solidi-RRL 5, 53 (2011); J. Tranchant et al. Thin Solid Films 533, 61 (2013); M. Querré et al., Thin Film Solids 617, 56 (2016); M. Rodriguez-Fano et al., ACS Appl. Mat. Interfaces, 15, 54611, (2023).
[4] Y. Tokura et al., Nature Physics 13, 11 (2017).
[5] V. Guiot et al., Nature Commun. 4, 1722 (2013).
[6] P. Diener et al., Phys. Rev. Lett. 121, 016601 (2018); P. Stoliar et al., Advanced Mater. 25, 3222 (2013).
[7] L. Laborie et al., 52th IEEE SISC San Diego (CA) (2021); J. Tranchant et al., IEEE IMW, 1-4 (2018).
[8] P. Stoliar et al. Adv. Func. Mater. 27, 1604740 (2017); C. Adda et al. J. Appl. Phys. 124, 152124 (2018).
[9] D. Babich et al., Phys. Rev. Applied 17, 014040 (2022); T. Amano et al., Nature Physics (2024), doi: 10.1038/s41567-024-02628-4.

29 October 2024, afternoon

3 Semi-plénières
13h20 - 14h10

Anne Tanguy SciencesNat	**Martien Den-Hertog** Charve	**Cécile Sykes** Massiani

Mini - colloques 2
14h30 - 16h30

SMMP1_2 Charve	**NN1_2** 405	**MP3_2** 201
SMMP4_2 Massiani	**NN4** 408	**2DMS2_2** 205
SMMP6_2 SciencesNat	**BAM2_2** 407	**2DMS1_1** 207

Café 16h30 - 17h15
Salle de conférence + 204 + 404

Mini - colloques 3
17h15 - 18h45

SMMP1_3 Charve	**NN1_3** 405	**NN3** 408
SMMP4_3 Massiani	**BAM3_1** 407	**2DMS2_3** 205
SMMP6_3 SciencesNat	**BAM5** 413	

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[‡] All rooms with a number are located in building 15

Semi plenary

Anne Tanguy

INSA Lyon and ONERA

About the vibrational response to the thermo-mechanical behaviour of glasses: theory and applications

I will present a rapid and pedagogical overview of on-going research efforts in the broad field of dense disordered materials in various contexts, from dense fluids undergoing glass and jamming transitions to transport and mechanical properties of amorphous solids, with applications from molecular systems to biological active matter. These problems involve computational and theoretical challenges that I would like to explain, and recent developments involving advanced Monte Carlo techniques and machine learning approaches.

Semi plenary

Bruno Cesar da Silva [1], Zahra Sadre Montaz [1], Alexis Wartelle [1] Yiran Lu [1], Pascale Gentile [2], Eva Monroy [2], David Copper [4], Jean-Luc Rouviere, [3] and

Martien I. den-Hertog [1 §]

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[2] Univ. Grenoble-Alpes, CEA, Grenoble INP, IRIG, PHELIQS, Grenoble, France
[3] Univ. Grenoble-Alpes, CEA-IRIG, MEM, Grenoble, France
[4] CEA, LETI, MINATEC, Grenoble, France

Characterizing electrical properties of semiconducting materials at nm length scales by Transmission Electron Microscopy

Various transmission electron microscopy-based techniques have the potential for quantitative characterization of the electric properties of a material at nm length scales. For example, off axis electron holography enables measuring the phase change of the electron wave, that can be directly related to the projected electrostatic potential. Four-dimensional scanning transmission electron microscopy (4D-STEM) has gained in popularity rather recently, thanks to the development of fast pixelated detectors over the last years, enabling the assessment of internal electric fields with high spatial resolution [1,2] in experiments that would be too slow or noisy to be feasible in the past. However, the measurement of long range built-in electric fields present in semiconductor devices, for example p-n junctions, are typically three orders of magnitude smaller than atomic electric fields, making the 4D-STEM experiments in such systems challenging. The main difficulty for both methods is that the electrical information is combined with material contrast (for example due to chemical gradients, thickness gradients or diffraction contrast) and the challenge resides in reliably separating these two. One possibility to facilitate this task it to use in-situ biasing, in order to increase (decrease) only the electrical part of the signal, and allow subtraction of a reference measurement to remove all material related contrast, see Figure 1.

In this presentation we will show recent results we obtained using 4D STEM on semiconducting lamellae as well as nanowires containing a p-n junction. We will show a study on how the quantification, sensitivity and spatial resolution of electric field mapping in a silicon p-n junction are influenced by the acquisition parameters in a momentum resolved 4D-STEM experiment [3,4], also comparing two different TEM equipment?s. It was observed that the electric field precision is improved decreasing the semi-convergence angle. The results were invariable even using an electron dose as low as 24 e-/A^2 and a detection limit as good as 0.01 MV/cm was possible. In addition, in-situ electrical biasing coupled to momentum resolved 4D- STEM measurements were performed, see Figure 2, allowing to study the junction abruptness, to asses phenomena like dopant segregation or interdiffusion [5]. Finally, recent results on a p-n junction in a Ge nanowire will be presented. This work paves the way for the development of advanced STEM based techniques able to provide imaging and quantification of built-in electric fields, potentials and charge densities in semiconductor devices with high spatial resolution, providing crucial feedback to improve growth/device fabrication processes.

[§]Corresponding author

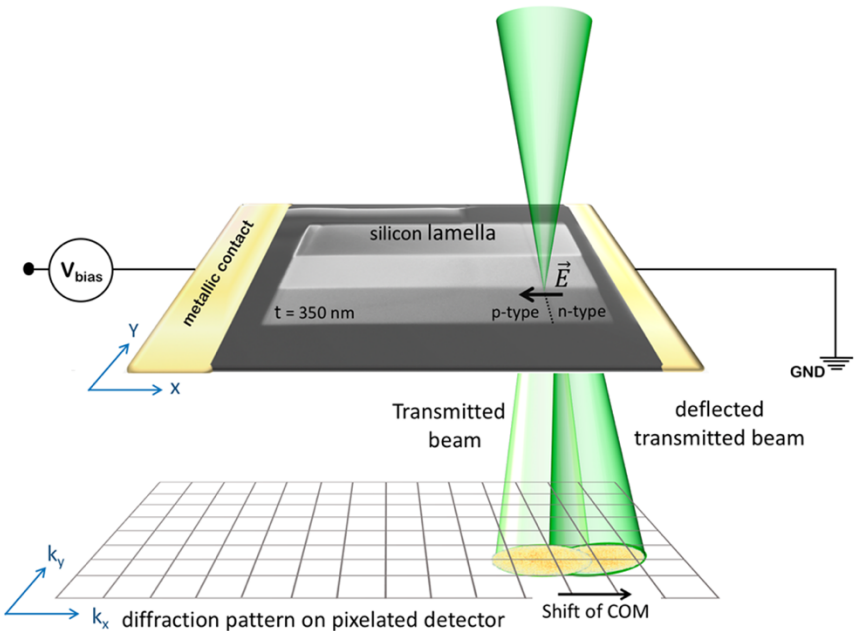

Figure 1 Schematic of the momentum-resolved 4D-STEM experiment performed in a silicon p-n junction. Reverse bias is obtained by applying a negative bias ($-V_{bias}$) to the p-side while the n-side is grounded [5].

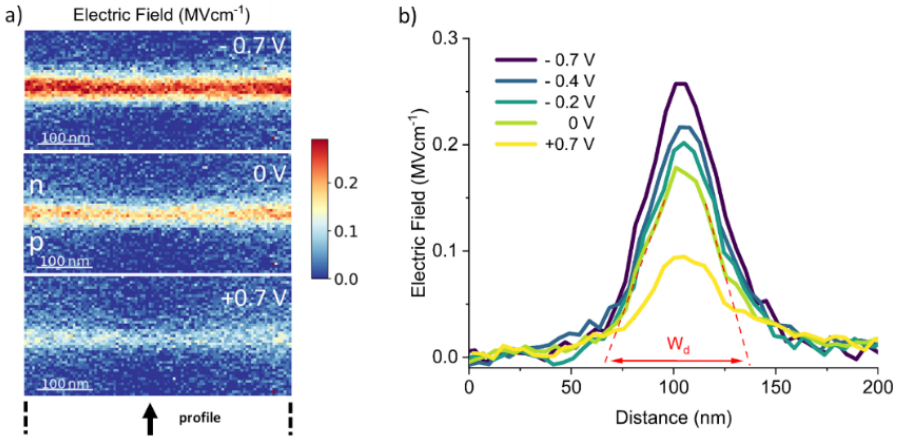

Figure 2 In-situ biasing momentum resolved 4D-STEM electric field measurements in a silicon p-n junction [5].

[1] L. Bruas, V. Boureau, A.P. Conlan, S. Martinie, J.-L. Rouviere, and D. Cooper, J. Appl. Phys. 127, 205703 (2020).
[2] A. Beyer, M.S. Munde, S. Firoozabadi, D. Heimes, T. Grieb, A. Rosenauer, K. Mller-Caspary, and K. Volz, Nano Lett. 21, 2018 (2021).
[3] S. Pllath, F. Schwarzhuber, and J. Zweck, Ultramicroscopy 228, 113342 (2021).
[4] B.C. da Silva, Z.S. Momtaz, L. Bruas, J.-L. Rouviére, H. Okuno, D. Cooper, and M.I. den-Hertog, Appl. Phys. Lett. 121, 123503 (2022).
[5] B.C. da Silva, Z. Sadre Momtaz, E. Monroy, H. Okuno, J.-L. Rouviere, D. Cooper, and M.I. Den Hertog, Nano Lett. 22, 9544 (2022).

Keywords: Transmission electron microscopy, in-situ, 4D-STEM, direct electron detector, p-n junction, nanowire

Semi plenary

Sykes, Cecile

"Active Cell Matter" team, Laboratoire de Physique de l?Ecole Normale Supérieure, 24 rue Lhomond, 75005 Paris, France

Cell biophysics : phase diagrams, phase portraits and trajectories

Stripped-down experimental systems that contain a limited number of purified proteins allow for deciphering the mechanisms of cell division and motility as well as cellular functions based on membrane deformation. Such controlled conditions allow us to propose and challenge physical modelling where physical parameters can be varied. For example, cytoskeletal dynamics, reproduced on liposome membranes, generate inward and outward membrane deformations (Figure 1) that depend on membrane tension and the structural details of cytoskeletal architecture [i]. Besides, a static study of buckling/wrinkling of actin-covered liposomes under osmotic deflation demonstrates the elastic nature of the actin cytoskeleton [ii]. My new project at LPENS addresses how the cytoskeleton interacts with the nucleus during cell motility through narrow constrictions [iii]. We apply an inference method derived from a Langevin equation approach to learn the dynamical equations describing nuclear trajectories and shape changes.

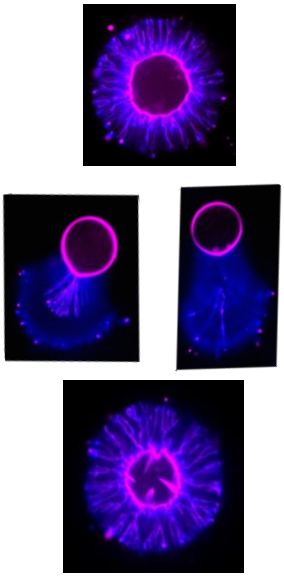

Figure 1: The dynamic actin cytoskeleton (marked by the presence of capping proteins, *Alexa Fluor 488 C5-maleimide, green*) is able to deform the membrane (*TexasRed-DHPE, red*) inward (spikes towards the liposome center) and outward (tubes emanating from the liposome membrane) and propel them through the formation of a comet-like structure. Liposomes have a diameter of 10 to 20 microns.

References

[i] C. Simon, R. Kusters, V. Caorsi, A. Allard, M. Abou-Ghali, J. Manzi, A. Di Cicco, D. Lévy, M. Lenz, J.-F. Joanny, C. Campillo, J. Plastino, P. Sens, **C. Sykes** " Actin dynamics drive cell-like membrane deformation " *Nature Physics*, https://doi.org/10.1038/s41567-019-0464-1 (2019)

[ii] R. Kusters, C. Simon, R. Lopes Dos Santos, V. Caorsi, Sangsong Wu, J.-F. Joanny, P. Sens, **C. Sykes**, "Actin shells control buckling and wrinkling of biomembranes" *Soft Matter,* **15**, 9647 – 9653 doi: 10.1039/c9sm01902b (2019)

[iii] P.M. Davidson, A. Battistella, T. Déjardin, T. Betz, J. Plastino, N. Borghi, B. Cadot, **C. Sykes** "Actin accumulates nesprin-2 at the front of the nucleus during confined cell migration" *EMBO Reports* DOI 10.15252/embr.201949910 (2020)

SMMP1 - Fracture and Friction across Materials and Scales

The Role of Grain-Scale Properties in Fault Gouge Behavior: Insights from Numerical and Laboratory Experiments

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[3] Sapienza - University of Rome – Italy

Fault zones are characterized by wear products, such as fault gouge (granular material), resulting from frictional sliding during successive slip events. Within this gouge, strain localizes onto specific shear bands, which are crucial for the onset of slip instabilities. To upscale the physics of shear deformation, small-scale experiments are essential for studying friction and uncovering the physical parameters and micro-mechanisms governing shear localization. We first conducted biaxial shear experiments on quartz fault gouges with varying initial grain sizes under constant normal stress and shearing velocity, continuously recording Acoustic Emissions (AE). Our findings indicate that the AE rate and amplitudes depend on both the average grain size and the evolution of the gouge layer. Furthermore, the different AE amplitudes observed throughout gouge shearing can be directly related to distinct micromechanical processes occurring at various stages of shearing. To further investigate the role of grain-scale properties on slip behavior and fault rheology, 2D numerical simulations of quartz fault gouges were performed in a direct shear configuration using the Discrete Element Method. Results revealed that slight changes in gouge characteristics, such as interparticle friction, bulk shear modulus, or the number of particles within the gouge, significantly impact shear localization through their orientation angle and the type localization patterns formed. However, comparing numerical results with laboratory ones is challenging due to differences in boundary conditions and certain assumptions. Indeed, our results suggest that incorporating a fragmentation algorithm in the simulations is necessary to successfully reproduce the progressive formation of shear localization observed in laboratory microstructures. The combination of numerical and laboratory experiments is complementary and provides valuable insights into the connection between microscale mechanisms and emergent macroscopic behaviors.

Keywords: Granular material, Shear Localization, Acoustic Emissions, Discrete Element Method, Micromechanical Processes

*Speaker

The effect of stress barriers and distal weakening on seismic rupture with applications to Enhanced Geothermal Systems

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Stress barriers in the subsurface significantly influence earthquake propagation and can potentially halt earthquake ruptures. Theoretical arguments have previously suggested that manipulating pore pressure to create stress barriers could reduce seismic hazards during the shear stimulation of Enhanced Geothermal Reservoirs. This concept, known as preconditioning, is experimentally demonstrated using a 40-cm-long fault model. Three pistons apply a normal load while a fourth piston applies a shear load, creating a heterogeneous stress state. Loading the fault to a near-critical state and then unloading one normal-load piston triggers dynamic events that propagate into the heterogeneous stress fields. Preconditioning reduces the mechanical energy flux to the crack tip (G) and increases the fracture energy (Gc). The reduction in G is due to a decrease in stress drop, resulting from an increase in residual shear stress associated with higher normal stress. Preconditioning can arrest seismic rupture and reduce co-seismic slip, slip velocity, and seismic moment at stress levels achievable in the field. Similarly, heterogeneous pore pressure fields in some seismic swarms can explain changes in stress drop without relying on material or total-stress heterogeneity. The studied ruptures are driven by unconventional singularities, characterized by increasing breakdown work with slip, and do not align with the assumptions of Linear Elastic Fracture Mechanics (LEFM). These experimental stress barriers inhibit slip and reduce breakdown work outside the cohesive zone. Therefore, considering distal weakening, far from the crack tip, is crucial for accurately predicting rupture arrest length.

Keywords: Unconventional singularity driven rupture, long, tailed weakening, seismic rupture

*Speaker

Interaction between slowly slipping and locked frictional interfaces

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What happens at the interface between two solid bodies in contact when they start sliding? This problem has important implications to various fields such as engineering, where the challenge is to control friction, or earthquake dynamics, where prediction of earthquakes occurrence and magnitude is crucial. A frictional interface is composed of an ensemble of discrete contacts that resist to shear. Sliding motion is mediated by the propagation of an interfacial rupture, breaking the micro-contacts, that has been shown to be a true shear crack (1). Seismic faults are known to release the stress accumulated during tectonic movement through these interfacial rapid ruptures, giving rise to earthquakes, or via slow slip events, called aseismic slip (2).
In this talk, we present model laboratory experiments in which we study the interaction mechanisms between a slowly slipping region of a frictional interface and neighboring locked regions that are destabilized by rapid interfacial ruptures, i.e., earthquakes (3). We emulate slow-slip regions by introducing a granular material patch along a portion of the frictional interface. By measuring the response of the fault to shear and performing interfacial slip measurements, we show that the slow-slip region acts as a nucleation center for seismic rupture, thereby increasing the frequency of earthquakes. The slow-slip region destabilizes into a rapid rupture, following the same rules as a crack in a homogeneous solid. These findings are important for unraveling the role of slow slip in the seismic cycle of a fault.

(1) I. Svetlizky and J. Fineberg, *Classical shear cracks drive the onset of dry frictional motion*, Nature **509**, 205-208 (2014).

(2) Peng, Z. and Gomberg, J, *An integrated perspective of the continuum between earthquakes and slow-slip phenomena*, Nature Geoscience **3**, 599-607 (2010).
(3) Y. Faure and E. Bayart, *Experimental evidence of seismic ruptures initiated by aseismic slip,* arXiv:2312.17511 (2023)

Keywords: friction, slow slip, rupture, interface, granular material

*Speaker

Phase field modeling of crack propgation in heterogeneous materials: effect of the nature of the disorder.

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While the motion of fracture is well understood in homogeneous materials, most materials are heterogeneous at various scales (from meters for brick and mortatr structure to fraction of micrometers for materials such as phase spearated glasses). In all these cases elastic modulus can be computed through homogenization techniques. However when it comes to crack propagation the small size of the process zone where the breaking takes place implies that the structure of the material must be taken into account explicitly. In this context phase field models are good candidates to describe crack propagation in heterogeneous materials since they allow to predict crack propagation in a material whose properties vary. Here the fracture behaviour of a material composed of spherical soft inclusions in a matrix is studied numerically while the fracture energy is kept uniform.
To this purpose a phase field model of dynamic crack propagation is used and the statistical nature of the disorder is varied (from a random distribution to a more uniform distribution of inclusions). Close to the propagation threshold, the motion of crack front is composed of slow and fast propagation phases. This is reminiscent of the motion of a moving contact line in the presence of disorder. It is seen that the nature of the disorder can have significant effects: The more uniform the inclusion distribution the lower the apparent fracture energy.

Keywords: phase field, fracture, disordered materials

*Speaker

Effect of surface roughness on adhesion

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Surface roughness reduces the area of intimate contact between solids and thereby considerably decreases their net attractive interactions caused by van der Waals forces. These forces remain nevertheless substantial at the small scales of MEMS, dusts and colloids, and in the contact of soft solids such as rubber.
In soft contacts, surface roughness can trigger elastic instabilities which dissipate energy, leading to adhesion hysteresis and friction without material-specific irreversibility.
However, the role of these instabilities remains poorly understood because we lack theoretical and numerical models accounting for realistic roughness. Our work focuses on the adhesion of soft elastic spheres with low roughness, where the indentation process can be described as a Griffith-like propagation of a nearly circular external crack. The equilibrium position of the contact perimeter results from the competition between elastic deformation energy and local adhesion. Local fluctuations of the elastic deformation energy (resulting from roughness) create energy barriers leading to local instabilities. Local fluctuations of the work of adhesion (or fracture toughness) have a similar effect and we map the surface topography into an equivalent fracture toughness heterogeneity using weight-function theory. This mapping allows us to describe the contact of rough spheres using efficient crack-perturbation simulations. The crack-front model describes the adhesion of rough spheres as the pinning of an elastic line by a random potential, a generic problem that has already been studied in other contexts such as contact angle hysteresis and fracture of heterogeneous materials. These previous theoretical results and our simulations show that the adhesion hysteresis is proportional to the elastic energy needed to flatten the self-affine random roughness, as long as this elastic energy is small enough for the contact area to be simply connected. We compare our theoretical predictions to the hysteresis measured in the adhesion of soft rubber spheres with rough surfaces.

Keywords: adhesion, friction, fracture, roughness, heterogeneity, disorder

*Speaker

Memory Effects in a Crack Front Driven in a Heterogeneous Material

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A slowly driven crack front in a heterogeneous material can exhibit various propagation dynamics, ranging from gentle smooth motion to abrupt jerky jumps, depending on the loading conditions. The dynamics associated with these regimes, and more broadly the behavior of the crack front, are closely related to how the system remembers its previous states. However, the statistical understanding of how a breaking sample "forgets" its initial conditions or "learns" its steady state remains limited. In this study, we examine two distinct scenarios: (i) a crack front modeled as a circular elastic line propagating in the revolution direction of a torus covered with a random potential, and (ii) a crack front subjected to cyclic loading and unloading, oscillating along a cylinder. Regardless of the driving speed, loading stiffness, interaction range, frozen noise amplitude, or system dimensions, we investigate how long it takes for the front to forget its initial conditions and converge to a cyclic behavior.

Keywords: memory effect, numerical simulation, crackling

*Speaker

Resonant slippage of glycerol on mica hints at phononic liquid friction

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The fundamental understanding of friction of liquids on solid surfaces remains one of the key knowledge gaps in the transport of fluids. While the standard perspective emphasizes the role of wettability and commensurability, recent works have unveiled the crucial role of the solid's internal excitations, whether electronic or phononic, on liquid-solid dissipation. In this work, we take advantage of the considerable variation of the molecular timescales of supercooled glycerol under mild change of temperature, in order to explore how friction depends on the liquid's molecular dynamics. Using a dedicated tuning-fork-based AFM to measure the hydrodynamic slippage of glycerol on mica, we report a 2-order of magnitude increase of the slip length with decreasing temperature by only $30C$. However the solid-liquid friction coefficient is found to be a non monotonous function of the fluid molecular relaxation rate, fα, at odd with an expected Arrhenius activated behavior. In particular we report a linear increase of friction with glycerol's molecular relaxation rate at high temperature, which cannot be accounted for by existing models which treat the solid surface as a static corrugated potential. We show that this unconventional scaling of friction can be explained by a contribution of the solid's vibrations which resonate with high frequency density fluctuations in the liquid. Such a resonance allows efficient momentum transfer and boosts friction. This dynamical contribution to friction relies on the overlap of the phononic structure of mica with the vibrational modes of the liquid. As a consequence, it opens new perspectives to control hydrodynamic flows by properly engineering phononic excitation spectra in channel walls and industrially relevant membrane materials.

Keywords: slippage, liquid, friction, glycerol, supercooled, glass, glass transition, friction, AFM

*Speaker

Temperature fluctuations effects on crack nucleation and propagation in fracture and decohesion phenomena

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Fracture and decohesion phenomena are extensively studied across various fields due to both their theoretical interest and numerous applications. One of the most recognized and utilized frameworks in this domain is the energetic approach represented by Griffith's energy criterion.
Despite analytical studies and experimental findings validating the effectiveness of this criterion for the propagation of a pre-existing crack, it remains inadequate for incorporating several critical phenomena for structural design. For instance, it fails to predict crack nucleation and presents difficulties in accounting for temperature effects in a rigorous analytical way.

This study aims to elucidate the influence of temperature on crack nucleation and propagation in decohesion and material failure. Building on the Griffith energy criterion, we have developed a simplified model focused on mode I fracture, extending the established criterion to incorporate crack nucleation and the influence of thermal fluctuations. By employing tools from equilibrium statistical mechanics, we integrate entropic effects into the overall energy balance. Furthermore, we implement a multiscale paradigm by concurrently formulating both discrete and continuum (limit) models. This approach enables us to gain a more comprehensive understanding of the complex phenomena of fracture and decohesion, providing insights into how microscopic-scale events influence meso- and macroscopic response.

Although the developed models are intentionally simplified, this approach allows for analytical results and deeper insights into the underlying physics. Our energetic approach captures the competition between external loading, elastic deformation, fracture energy, and entropic effects. Specifically, our model can predict crack nucleation and quantify the impact of thermal fluctuations on this phenomenon.
Interestingly, our approach reveals a classical critical behavior, with the critical load decreasing as temperature increases. Consequently, we demonstrate that at the critical temperature, the system undergoes a phase transition leading to complete rupture without the application of any mechanical load.

Keywords: temperature effects, fracture, decohesion

†Speaker

Analysis of the relaxation time in subcritical rupture of heterogeneous materials

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Predicting subcritical rupture of heterogeneous materials is an important subject in physics of materials. Subcritical rupture happens when a material is loaded at a constant force below its ultimate tensile strength for a long time. This process ends with the ultimate failure that defines the lifetime of the sample,
tauc. The lifetime is a scattered and hard to predict parameter. If we stop maintaining the target force before the final rupture, we observe a relaxation of the force in the sample. This relaxation can be fitted using a visco-elastic rheological model (1) which predicts a logarithmic decay of the force with a characteristic time
tau . The aim of our experiment is to measure the evolution of the relaxation time,
tau , during the subcritical rupture process. For this purpose, we use paper samples held in a tensile stress apparatus controlling elongation and we impose a constant force with a feedback loop. In addition to this constant force, we apply tiny force steps to probe the relaxation locally. The time between two steps is proportional to the characteristic relaxation time. Experimentally, for paper samples, we observe that this time
tau increases linearly, indicating a slowing down in the subcritical rupture dynamics, then fastly decreases at about 80% of the lifetime
tauc(2). This behavior can be qualitatively explained by the fiber bundle model (3) that describes the phenomenological rupture of a heterogeneous fibrous material. Considering the strain of our sample, we recover behaviors already observed in other soft materials such as protein gels (4). When a constant force is applied, the strain rate first decreases with a power law then increases sharply before the final rupture.
References

(1) Journal Chemical Physics 11.3, 1943
(2) Phys. Rev. E.94.023002
(3) Phys. Rev. Materials 7, 033601
(4) Phys. Rev. Lett. 113, 038303

Keywords: subcritical rupture, heterogeneous material, predictability

*Speaker

Poromechanical coupling in the rupture of saturated geomaterials

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Understanding crack development in porous rocks is crucial for applications such as permeability enhancement and leakage prevention in reservoir engineering. The interaction between surrounding water in rock pores and the advancing crack front introduces complex physical phenomena, including lubrication, chemical reactions, and mechanical effects. Theoretical models suggest a significant coupling between fluid flow and matrix deformation, indicating that rapid crack propagation can generate underpressurized zones ahead of the crack tip, thereby critically influencing crack growth.
Using a novel testing setup, we investigate these induced poromechanical effects that have remained unexplored experimentally. We employ a controlled crack propagation test, the wedge splitting test (WST), within a triaxial cell. This setup allows for measuring fracture energy, the resistance to crack propagation, while observing pore pressure fluctuations in a cement-based rock analogue during rupture.

Our tests reveal that pore pressure fluctuations are highly dependent on the crack propagation velocity, showing distinct regimes from fully drained to nearly undrained conditions. Indeed, we observe that the faster the crack advances, the more localized and stronger is the underpressurized zone. This effect may critically affect the micromechanisms at stake during material breakdown at the crack tip, which we investigate from fracture energy variations.

Keywords: Poromechanics, fracture, geomaterials

*Speaker

The impact of Mn and Al on the trapping and diffusion of hydrogen in γ-Fe: An atomistic insight

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Common alloying elements such as Mn and Al can significantly influence the local dynamics of Hydrogen in steel, promoting or attenuating the mechanisms associated with Hydrogen induced embrittlement. In experiments, the local chemical composition might significantly deviate from the grain-averaged composition due to segregation effects and local ordering. It is a unique advantage of first principles simulations that these individual physical effects can be separated and their influence on the microstruture can be studied in a well-controlled and hierarchical manner. Here, we propose a first principles-based framework to systematically unlock the physical underpinnings of such influence in Mn/Al-alloyed γ-Fe. Our framework can be readily adapted to analyse H behaviour in the bulk phase of any face-centred cubic (FCC) Fe-X-Y alloy, provided that solutes X and Y substitute the Fe sites. In our scheme, all thermodynamically stable substitutional solute sites were identified ($<=$ 5.4 wt% Mn; $<=$ 4 wt% Al) up to the third nearest neighbour (NN) shell of a single H atom. The impact of Mn/Al on H-binding was quantitatively evaluated, indicating a surprisingly strong correlation with the local Al distribution regardless Mn content, and indirect stabilization by Al when present in the 2nd NN shell. Nonetheless, Al strongly repels H bonding. The contradictory role of Al was explained in terms of bonding/anti-bonding orbitals occupancy in H-M interactions (M = Al, Mn, Fe). The barriers to H hopping between adjacent local environments and the corresponding jump frequencies were subsequently calculated, providing insights into the limits imposed by the presence of Al and Mn on H mobility in Mn/Al-alloyed γ-Fe. Most notably, presence of Al in the 2nd NN shell of H severely reduces the H jump frequency, leading to irreversible trapping at high Al contents. Such behaviour may critically contribute to mitigate H-induced delayed fracture in Al-rich austenite steel.

Keywords: Hydrogen embrittlement, Steel, Hydrogen trapping, Density Functional Theory

*Speaker

SMMP4 – Soft and architected structures

Architected materials and instabilities: a journey towards uniformity

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Soft matter architected materials exhibit intriguing buckling modes that reside at the unit cell scale and can occur uniformly across the sample. These modes were first observed by Papka &Kyriakides (1999) during bicompaction experiments on polycarbonate honeycombs. They experimentally identified 3 patterns, but without precise measurements of their critical loads. In addition, these patterns did not appear uniformly in the samples. Later experiments by Shan et al. (2014) on silicone rubber honeycombs reported the same patterns, but this time the patterns were uniform across the specimen. Subsequent modelling by Combescure & al. (2020), assuming periodicity and an infinite specimen, also confirmed the existence of these 3 modes, while establishing the theoretical critical loads at which they appear.
In order to take advantage of these patterns, which exhibit interesting and different wave propagation properties, a faithful prediction of the appearance of bifurcated modes in architected materials subjected to mechanical loading requires both the ability to predict the possible buckling patterns, and the critical loads that cause them as well as ensuring the uniformity of the modes in the material.

The present study therefore has a dual role. On the one hand, to carry out numerical simulations of bicompaction tests in order to understand the influence of various experimental parameters on the buckling uniformity: behavior and homogeneity of the specimen material, honeycomb geometry, type of boundary, loading conditions and friction coefficient. Secondly, to carry out better instrumented tests (camera tracking and multiple force measurements) in order to quantify the buckling uniformity actually achieved, and to compare theoretical and experimental critical loads.

Keywords: architected materials, instabilities, experimental, simulation

*Speaker

Design of optimal architectures for ultra-light isotropic microtruss-based metamaterials

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Microtruss-based architectured materials offers an unprecedented range of mechanical properties, expanding their potential applications. Their remarkable stiffness-to-weight ratio has attracted significant attention in transportation research. However, in most cases, the proposed architectures are anisotropic on a large scale, making it difficult to characterize their response to fracture, in particular (1) In our work, we designed a new class of microtruss-based metamaterials, the structure of which have the particularity to be isotropic at small scales. This led us to develop a new set of numerical tools to create such structures and their digital twins to predict each of their mechanical properties (2). We will see that these novel microtruss-based materials of locally isotropic structures can reach an unprecedented stiffness-to-density ratio, closely approaching the theoretical upper bounds established by Hashin-Shtrikman for isotropic porous solids (3). Conversely, they exhibit rather weak compression strength and we will discuss an on-going approach to increase this strength by introducing a statistical spatial modulation of the local microbeam features (diameter, shape, constituent material...) in an appropriate manner. We statistically introduce those properties using scale-invariant factors. Hence, the material remains isotropic and we can fine-tune the local autocorrelation of each property, using only a couple of control parameters.
References:

(1) Shaikeea, A. J. D., Cui, H., O'Masta, M., Zheng, X. R., & Deshpande, V. S. (2022). The toughness of mechanical metamaterials. Nature materials, 21(3), 297-304.

(2) A. Montiel, T. Nguyen, C. L. Rountree, V. Geertsen, P. Guenoun, and D. Bonamy Effect of architecture disorder on the elastic response of two-dimensional lattice materials (2022), Phys. Rev. E 106, 015004

(3) Z. Hashin, Shtrikman A variational approach to the theory of the elastic behaviour of multiphasematerials, S. J Mech Phys Solid (1963) 127e140.

Keywords: metamaterial, isotropic, stiffness, compression

*Speaker

Stability analysis of a class of tensegrity modules

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Tensegrities are structural systems that can be stabilized by the internal tensile members connected to rigid bodies. Tensegrity structures have been used in a wide range of applications, including artistic and architectural projects, robotics and biological systems. When solicited by external forces, tensegrity structures often present large displacements and rotations, while the tensile members are subjected to large strains. In this scenario, the stability of the system is not guaranteed and bistable behavior can be observed. The goal of the present contribution is to verify the stability of a class of tensegrity modules while identifying key geometrical and material parameters. Initially, the equilibrium equations of the system are obtained via an energy approach. Next, the evolution of the system's state as a function of the external sollicitations is obtained. Finally, the influence of the geometrical and material parameters on the stability of the system is studied.

Keywords: Tensegrity, Unstability, Bistable, Nonlinear

*Speaker

Is disorder enough to enhance material stiffness and strength?

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Geometry governs the response of materials at almost all scales. In this talk, I will discuss recent results in the context of 3D-printed random cellular and porous polymers. The present work introduces a novel and versatile computer-aided design (CAD) and experimental strategy to obtain random Voronoi-type geometries, called M-Voronoi (from mechanically grown), with smooth void shapes and variable intervoid ligament sizes that can reach very low relative densities. This is achieved via a numerical, large strain, nonlinear elastic, void growth mechanical process. Originally small circular voids embedded in a cell of arbitrary shape (triangle, circle, rectangle, trapezoid) grow when subjected to displacement (Dirichlet) boundary conditions. The deformed voids evolve into smooth Voronoi-type geometrical shapes leading to macroscopic isotropy or anisotropy depending on the prescribed boundary conditions. The void growth process is a direct consequence of mass conservation and the incompressibility of the surrounding nonlinear elastic matrix phase and the final achieved relative density may be analytically estimated in terms of the determinant of the applied deformation gradient. We show by experiments that, when compared with classical periodic or random metamaterial designs, the features present in M-Voronoi such as random and smooth void shapes as well as variable intervoid ligaments is beneficial to achieve enhanced stiffness and more importantly strength and hardening after an initial bifurcation when in compressive loads.

Keywords: porous materials, architected materials, instabilities, 3D, printing, buckling

*Speaker

Soft architected biological materials: from the hierarchical structure to the impact behavior

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The interest in mimicking the structure of biological materials for engineering purposes is growing. However, biological materials have complex 3D structures arranged hierarchically. In the case of cellular materials like cork, wood, bone or citrus peel, its goes from the single cell wall to large scale density gradient. Spatial relationships, 3D morphology and interaction within and across these length scales collectively provide a basis for mechanical function. Thus, mapping the spatial organization and morphology of individual cells up to the scale of intact biological materials is fundamental to understanding system-level mechanical behaviors in these materials. Without it, it is difficult to propose convincing bioinspired structures.

Among the structure of interest, citrus peel is looked into for mechanical energy absorption purposes under impact loads. Several researches have highlighted gradient in the citrus peel by 2D observations. Some cone beam x-ray tomography has also been used. However quantitative and qualitative questions remain especially concerning the density gradient and the geometry of the cells inside the peel. Furthermore, the link between the hierarchical structuration of Citrus peel and its mechanical behaviour need to be unveiled.

This work aims at exploring the 3D structure of the Citrus Maxima at different scales thanks to the new possibilities offered by the development of phase contrast synchrotron tomography on the new beamline BM18 at ESRF and to link it to the mechanical properties of the peel through in-situ quasi-static compressive tests, dynamic compressive tests (fly wheel, drop tower).

Keywords: architected materials, visco, elasticity, bio, inspiration, impact

*Speaker

Liquid crystalline suspensions of high aspect ratio 2D clay nanosheets with photonic properties

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Suspensions of high-aspect ratio 2D clay nanosheets, have been investigated using Small Angle X-ray Scattering (SAXS) combined with reflection spectrometry in the visible range. The high aspect ratio of synthetic fluorohectorite clays allows for investigation of liquid crystalline orientational order for relatively large nanosheets spacings, in a range which also produce structural coloration. Various clay and salt concentrations have been investigated. Particular attention is given to the confinement caused by container geometry, such as cylindrical (capillary), flat (cuvette), and spherical (droplet) confinements . The SAXS characterization suggest coherent regions that have a nematic orientational distribution that is linked to the container geometry and suspension packing. References:
1. *Liquid crystalline structuring in dilute suspensions of high aspect ratio clay nanosheets*, Osvaldo Trigueiro Neto, Sabine Rosenfeldt, Paulo Henrique Michels-Brito, Konstanse Kvalem Seljelid, Andrew Akanno, Bruno Telli Ceccato, Rini Padinjakkara Ravindranathan, Tomás S. Plivelic, Leander Michels, Josef Breu, Kenneth D. Knudsen & Jon Otto Fossum, **Colloid and Polymer Science May**, (DOI: 10.1007/s00396-024-05268-5) (2024)

2. *Bright, noniridescent structural coloration from clay mineral nanosheet suspensions*, Paulo H. Michels-Brito, Volodymyr Dudko, Daniel Wagner, Paul Markus, Georg Papastavrou, Leander Michels, Josef Breu, Jon Otto Fossum, **Science Advances 8(4)**, DOI: 10.1126/sciadv.abl8147 (2022)

Keywords: Lamellar liquid crystals, clay colloids, structural colors

*Speaker

Effect of in-plane electric field on the microphase separation in thin films of diblock and triblock copolymers

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Electric fields of 10 V μm and higher are able to align microphase-separated patterns in block copolymers along the field lines. In this work, the structure of a thin film of diblock and triblock copolymer melts in an in-plane DC or AC electric field is studied theoretically. The situation is considered when the copolymer forms a hexagonal morphology of standing cylinders in bulk in the absence of an external field. Self-consistent field theory calculations are carried out to determine the most thermodynamically favorable thin film structure. The results are presented as phase diagrams with the film thickness and electric field energy on the axes and as distributions of the local composition, which serve as an order parameter in the system. It is concluded that electric fields only weakly affect the spinodal curves of block copolymers but they can reorient or markedly modify microphase-separated morphologies in those systems. In particular, a transformation of standing cylinders into long threads aligned in the field direction on the tens of microns scale observed in the recent experiments on polystyrene–*block*–poly(4-vinyl pyridine) copolymers can be interpreted as a phase transition from the perpendicular to parallel hexagonal phase. This transition takes place in a certain range of film thicknesses, provided the electric field strength exceeds a certain threshold value. Such reordering can lead to a coexistence of different phases that appear in the film areas with different local thicknesses. The morphological rearrangements under an in-plane field, which preserve connectivity between the film surfaces through the domains of the minor copolymer block, can be important for practical applications.

Keywords: microphase separation, electric field, block copolymer, thin film, phase coexistence

*Speaker

Characterization of a bistable buckling unit cell under quasi-static and dynamic forcing

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In recent years, bi-stable systems, as for instance a buckled beam, are gaining a lot of interest due to their wide field of applications in the quasi static regime, for instance mechanical fuses and mechanical actuators in soft robotics, and in the dynamic regime, for instance energy harvesting devices and nonlinear energy sinks. Bistable systems typically present a double well potential with an unstable state in between two stable regions, which results in an energy barrier able to store mechanical energy. Such potential is inherently nonlinear, leading to amplitude dependent stiffness, which can even be negative. In this context, we focus on the mechanical behaviour of a buckling beam made of a 3D printed soft material in both static and dynamic regime. The static response is determined using traction compression test machine to measure the force, the deflection and input energy, coupled with camera-based displacement field measurement to resolve the local deformation of the beam. These two measurements are connected through von Kármán beam model, relating the deformation to the bending and compressive energies. In addition, we aim at describing the deformation in terms of decomposition over the stable and unstable buckling modes. The dynamic response, which relies on a typical Duffing-like softening behaviour in the weakly nonlinear regime, is determined via amplitude dependent frequency response function using a shaker and accelerometers, in addition to the camera-based instantaneous local deformation measurement of the beam. We aim at getting better understanding by relating the static and dynamic observations via the camera-based field measurement, in particular.

Keywords: Bistability, nonlinearity, buckling, video processing, vibration

*Speaker

Dynamic behavior of elastic beams near shape transitions

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Many elastic structures exhibit rapid shape transitions between two possible equilibrium states: umbrellas become inverted in strong wind and hopper popper toys jump when turned inside out. This snap-through is a general motif for the storage and rapid release of elastic energy, and it is exploited by many biological and engineered systems from the Venus flytrap to mechanical metamaterials.

Here we use an elastic beam as a model system to realize different snap-through instabilities that are reminiscent of instabilities observed in more intricate elastic structures. We present numerical and theoretical work that shows that all the dynamic characteristics of these transitions depend solely on the nature of the underlying bifurcation the system undergoes at the transition. Importantly, we show that these dynamic characteristics can be anticipated from symmetry considerations.

These findings explain some surprising features observed in more intricate elastic structures and open new opportunities to design mechanical metamaterials that exploit these shape transitions.

Keywords: snap, through, elastic instabilities, bifurcations

*Speaker

Surprising stiffening regimes of curved sheets under loads

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In this presentation, we investigate a practical construction problem: what is the optimal structure to support a force F at a distance L of a rigid wall?
Over the very wide variety of possible structures, we restrict our problem to the structures obtained by curving a thin and flat sheet onto a circular cylinder. We use transparency sheets held with a clamp on a cylinder of diameter 5 cm. In this configuration, the sheet is much stiffer than its flat equivalent because of the imposed transverse curvature. In a typical loading experiment, we use the hook near the free end of the curved sheet to hang a mass m and we identify the maximal load mg before the sheet collapse.

In recent experiments, we have identified various unexpected regimes that we would like to report in this presentation:
- non-monotonic dependence with the length (some longer sheet can be more resistant)
- stiffer sheets with imperfect (ie non-rigid) boundary condition for the clamping
- stiffer sheets with a structure that is longer than the distance L for the applied force
- open sheets that can be stiffer than their equivalent closed cylinders

None of these effects are predicted by the Euler-Bernoulli beam theory and they are all the result of non-linear coupling in the thin-shell regime. The collapse of the structure comes from a buckling instability due to a compression at the bottom of the sheet because of the applied force. However, and because the force is locally applied, the force modifies the sheet shape by increasing its transverse curvature and therefore reinforcing its global bending rigidity.

Keywords: buckling, curvature, induced rigidity, geometry

*Speaker

The Y-rod test

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We study the mechanical and geometrical behavior of two ribbons that are joined together at one extremity in the form of a dowsing Y-rod. The ribbons are pulled apart at their free ends in opposite directions. We consider the angle θ made by the connected end with the normal to the direction of the pulling forces.
If both ribbons are identical, the connected end is oriented normal to the pulling direction, $\theta = 0$. Breaking the symmetry of the system with different bending stiffnesses modifies that angle, with the joined end pointing towards the pulling force on the weaker ribbon. Surprisingly, over a wide range of forces, this angle is independent of the load and is a function of the stiffness asymmetry alone.

We rationalize this observation with a boundary layer analysis in the framework of two coupled Kirchhoff beams. The analytical solution found for the shape of the boundary layer allows us to use this simple test as a quite accurate measurement of relative
bending stiffness. We present this model, as well as its limits for forces large enough to violate hypotheses, introducing either plasticity or three-dimensional effects in the boundary layer.
Finally, by allowing an inhomogeneous cross-section of one of the ribbons along its length, and thus a curvilinear variation of its bending stiffness, we prevent the angle from being load-independent. The dependence of the angle θ with the applied force can be chosen by figuring out the corresponding spatial evolution of the beam's cross-section. We formulate this inverse problem in the framework of the tapered Elastica, and present a direct application to a visual linear force sensor made with two thin pieces of Mylar and one piece of double-sided tape.

Keywords: Slender structures, boundary layer, solid mechanics, elasticity

*Speaker

Tristability and hysteresis in beams with slits

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Buckling and snapping instabilities form the backbone of many mechanical metamaterials. Here we show that beams with a slit show both reversible buckling and hysteretic snapping under axial load, and for a given load can become tristable. Using multiple slits or beams, we realize complex responses with potential applications for mechanical metamaterials with computing and memory.

Keywords: Multistability, Hysteresis, Hysteron, Buckling

*Speaker

Effective Path Analysis of Transmitted Waves in Fractal Porous Media.

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This research investigates the acoustics of porous media characterized by fractal, or self-similar, structures. Utilizing a fractal approach, we employ differential operators in non-integer dimensional spaces to address the fundamental equations of acoustics in such media. Our primary objective is to examine the transmission of ultrasonic waves within a fractal porous medium. Our findings reveal that the fractal dimension significantly influences wave transmission. In fractal porous materials, waves travel along more complex and intricate paths, resulting in increased tortuosity and attenuation. We introduce the concept of an effective path length, which depends on the fractal dimension, to describe the actual trajectory of wave propagation. Additionally, we define an effective tortuosity, directly proportional to the effective path length, to quantify the additional tortuosity brought about by the fractal structure.

The insights gained from this study are crucial, as they enhance our understanding of wave behavior in self-similar porous media, which are prevalent in various natural settings and have multiple practical applications, including sound insulation and the design of acoustic materials. Furthermore, understanding the impact of fractal dimensions on wave behavior is vital for developing more efficient acoustic solutions. This research also sets the stage for further theoretical and experimental work on applying fractal geometry to analyze wave propagation in porous structures.

Keywords: Porous media, Acoustics, Fractal, Non integer dimensions

*Speaker

SMMP6 – Statistical physics of disordered matter

How do relaxations proceed in swap Monte Carlo dynamics?

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The swap Monte Carlo method is a powerful sampling technique for slow dynamics near the glass transition.
The development of a continuous polydisperse particle model suitable for this technique has revealed that the relaxation is accelerated by more than 10 orders of magnitude compared to the standard molecular dynamics or Monte Carlo.
With this technique allowing equilibration at very low temperatures, equilibrium relaxation in the time evolution of molecular dynamics has been studied in detail and features such as dynamic facilitation have been clearly identified.
However, it is not clear how the relaxation proceeds in swap dynamics with varying particle diameters.
Here, we have performed swap Monte Carlo simulations for polydisperse particles in 2D and 3D.
In the presentation, we will report detailed characterizations on dynamical heterogeneities in swap Monte Carlo dynamics.

Keywords: glass transition, dynamical heterogeneity, numerical simulations

*Speaker

Fracture of Polymeric Double Networks via Coarse-Grained Molecular Dynamics Simulations

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Network-forming polymeric materials are ubiquitous, from industrial products (tires, food,...) to living organisms (cytoskeleton, extracellular matrix,...). This widespread presence necessitates the development of robust and long-lasting polymeric materials (1). Recently, the synthesis of multi-network systems has shown promise in creating networks with remarkably enhanced mechanical properties (2,3). In these systems, a first isotropically pre-stretched brittle network is coupled to a second or more floppy ductile networks that only break at later stages. The synergistic interaction between these networks significantly increases the overall toughness (4). However, the physical mechanisms underlying this enhancement remain poorly understood, which led to a trial-and-error synthesis approach to optimize the mechanical properties of these new polymeric materials. In this study, we employ coarse-grained molecular dynamics simulations to investigate the mechanical response of double networks at the monomeric level, from synthesis to uniaxial stretch testing. By tuning the synthesis parameters we are able to replicate the key features of the experimental response. The detailed insights provided by numerical simulations allows us to quantify several quantities inaccessible experimentally (5). By this means, we show how the preparation protocol influences the microstructure of both networks and their coupling, affecting the mechanical response of the polymeric network.

(1) Creton, C. "50th anniversary perspective: Networks and gels: Soft but dynamic and tough." Macromolecules 50.21 (2017).
(2) Gong, J. P., et al. "Double-network hydrogels with extremely high mechanical strength." Advanced materials 15.14 (2003).
(3) Webber, R. E., et al. "Large strain hysteresis and mullins effect of tough double-network hydrogels." Macromolecules 40.8 (2007).
(4) Slootman, J., et al. "A molecular interpretation of the toughness of multiple network elastomers at high temperature." PNAS 119.13 (2022).
(5) Le Goff., et. al. "A coarse-grained molecular dynamics study of damage localization during the fracture of double polymer networks". In preparation.

Keywords: Fracture Mechanics, Double Networks, Molecular Dynamics

*Speaker

A microscopic view of failure in multiple polymer networks

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Network-forming materials are ubiquitous and appear in industrial products such as tires, food, and cosmetics as well as composing the cytoskeleton within the cells of living organisms. They are lightweight and display desirable properties such as optical transparency and reversible deformability up to large strains. However, the microscopic mechanisms protecting a network against macroscopic fracture and the processes that control crack growth are still poorly understood. A deeper understanding is needed to fully exploit the potential of polymer networks in advanced and novel material design. In recent years a general phenomenon has emerged where materials composed of an interpenetrated stiff filler network and a soft matrix network display toughness far greater than either constituent (1,2). Herein we adapt photon correlation imaging (3) (PCI), a dynamic light scattering method, to reveal the microscopic rearrangements within poly(ethyl acrylate), PEA, networks (4) during deformation by extension and fracture. We examine how such rearrangements differ in a simple PEA network and in double network composed of two interpenetrated PEA networks, one stretched and stiffer with respect to the other. We find that rearrangements in the double networks occur over larger distances from the fracture tip, thereby serving to reduce stress at the crack tip and hinder its propagation.
References

(1) J. P. Gong, Y. Katsuyama, T. Kurokawa, and Y. Osada Adv. Mater., 2003 15, 1155.

(2) E. Ducrot, Y. Chen, M. Bulters, R. P. Sijbesma, and C. Creton Science, 2014 344, 186.

(3) A. Duri, D. A. Sessoms, V. Trappe, and L. Cipelletti Phys. Rev. Lett., 2009 102(8), 085702.

(4) P.Millereau, E. Ducrot, J. M. Clough, M. E. Wiseman, H. R. Brown, R. P. Sijbesma, and C. Creton, PNAS, 2018 115(37), 9110–9115.

Keywords: gels, polymer, dynamic light scattering, fracture

*Speaker

Glassy transition in a family of oligomers: influence of the length of the chain

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The glass transition has already been subject to many studies in the past decades (1). However, the understanding of this phenomenon is far from complete. It seems now well established that the relaxation of supercooled liquids is a non-homogeneous phenomenon. The material is a patchwork of small regions presenting a wide dispersion of size and relaxation times, both increasing when the temperature decreases. These small regions, the dynamic heterogeneities (DH), have a typical mean size of some nanometers or tens of nanometers. A large number of simple molecules, like for example glycerol, have been measured (2).
In this study, we consider a simple molecule, 1-Propylene Glycol (PG) and its oligomer, N-PG. Varying the value of N from 1 to 20, we have a set of molecules with the same dielectric contributors at both end (-OH groups), no other significant contribution inbetween (in our experimental conditions) and a molecular length increasing with N, around the DH dimensions. Our aim was to investigate the influence of the length of the chain on the glassy transition by linear and non-linear dielectric spectroscopy.

The 3rd order susceptibilities, chi_3, follow Bouchaud-Biroli predictions (3): —chi_3— present a hump for all values of N with a maximum decreasing when N increases. The phase curves are superimposed for all N as a mastercurve.
The value of the maximum of the reduced value of chi_3 being proportional to the mean number Ncorr of correlated particles in the DH, we are able to show that the evolution of Ncorr as a function of the alpha relaxation time is independent of N.

References

(1) R. Richert, *J. Phys.:Condens. Matter,* 2017, 29, 363001-363026. doi: 10.1088/1361-648X/aa7cc4.
(2) S. Albert at al., *Science,* 2016, 352 (6291), 1308-1311. doi: 10.1126/science.aaf3182.
(3) J.-P. Bouchaud, G. Biroli, *J. Chem. Phys.*, 2004, 121, 7347–7354,

Keywords: glass transition, oligomer, dielectric spectroscopy

*Speaker

Crossing the Frontier of Validity of the Material Time Approach in the Aging of a Molecular Glass

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Physical aging corresponds to the evolution of out-of-equilibrium material properties caused by structural rearrangements. For glassy materials, which are in practice forever stuck in an out-of-equilibrium state, it can have important consequences on long-term material performances such as mechanical strength or optical properties.A simple aging experiment is a temperature step for which the liquid's response is usually non-linear due to the strong temperature dependence of the relaxation time. The concept of material time introduced by Narayanawasmy quantitatively explains this effect well for relative temperature step amplitude below a few percent (1). The fact that it links equilibrium and aging dynamics has physical implications that were recently explored in the literature (2). This justifies the still lacking precise characterization of the limit of validity of this approach when the system is set far from equilibrium.
We performed aging experiments on glycerol in response to ideal upward temperature steps of amplitude ranging from 0.3 to 18 K. Large temperature steps are notoriously difficult to achieve and we used a specially designed experimental setup that allows fast heating and thermal equilibration while giving access to the dielectric response (3). The 40 ms heating time that we obtained is 50 times faster than state of the art setup and 2000 times faster than commercial setups. For small step amplitude, we checked the validity of the material approach in its simplest form, namely the Single Parameter Anzatz (SPA). By increasing the step amplitude, we showed that the SPA show its limits simultaneously with the more general material time framework. These results help setting the bounds beyond which new theoretical arguments are needed to quantitatively describe aging.

(1) Riechers et al., Science advances (2022).
(2) Böhmer et al., Nat. Phys. (2024).
(3) Hénot et al., J. Phys. Chem. Lett. (2024).

Keywords: out, of, equilibrium, aging, supercooled liquid

*Speaker

Simultaneous memory effects in the stress and in the dielectric susceptibility of a stretched polymer glass

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We study by Dielectric Spectroscopy the molecular dynamics of relaxation processes during plastic flow of glassy polymers
up to the strain hardening regime, for 3 different protocols of deformation. The measured dielectric spectra cover 4 decades in frequencies and allow us to measure the evolution as a function of the applied strain of the dominant relaxation time τ_α and of the width w_τ of the distribution of relaxation times. The first protocol is performe
We confirm that for increasing strain both τ_α and w_τ first decrease reaching a minimum in the stress softening regime be
In the second protocol we stop the deformation at some point λ_w in the strain hardening regime and we let the sample age for a
during which the applied stress remains high. Upon resuming the deformation at constant $\dot{\lambda}$, $stress - strain$ displays a yield stress and a stress softening regime comparable in magnitude to that of the reference protocol before re
$stress$.
In the third protocol the stress is canceled during t_w. In this case after recovering the constant $\dot{\lambda}$ the dielectric spectrum and the stress-strain curve rejoin almost immediately the reference curve.
Our interpretation for the results of the third protocol is that aging dynamics is frozen when the stress is removed, as it is known for polycarbonate at room temperature. Our experiments set precise conditions for a theory of strain hardening.

Keywords: Polymer glass, plastic flow, memory effects

*Speaker

Experimental identification of topological defects in 2D colloidal glass

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Topological defects are ubiquitous in various physical systems, generally appearing in the form of singularities in the order parameter space that are mathematically described by topological invariants and cannot be removed by continuous transformations. Such defects play a crucial role in different fields, ranging from cosmology to solid-state physics and biological matter. Since, these irregularities are defined with respect to an ordered reference configuration, their existence in disordered systems has been debated for a long time. Recent observations of well-defined topological defects in glassy systems (1-3) and establishing their close connection with the plasticity of the material has motivated further exploration in this direction. We have investigated a two-dimensional glassy system composed of colloidal particles interacting via an effective magnetic attraction. Our study (4) confirms the presence of topological defects in the eigenspace of the vibrational frequencies of this experimental 2D amorphous solid. These defects strongly correlate with the vibrational features and spatially correlate with each other and structural "soft spots", more prone to plastic flow. This sheds light on the complex interplay between topology, disorder, and vibrational behavior in amorphous systems, paving the way for a deeper understanding of the nuanced relationship between mathematical topology and material behavior.

References:

(1) Z. W. Wu, Y. Chen, W.-H. Wang, W. Kob, and L. Xu; Nat. Commun. **14,** 2955 (2023).

(2) M. Baggioli, I. Kriuchevskyi, T. W. Sirk, and A. Zaccone; Phys. Rev. Lett. **127,** 015501 (2021).

(3) P. Desmarchelier, S. Fajardo, and M. L. Falk; Phys. Rev. E **109**, L053002 (2024).
(4) V. Vaibhav, A. Bera, A. C. Y. Liu, M. Baggioli, P. Keim, A. Zaccone; arXiv:2405.06494 (2024).

Keywords: Colloidal glass, Topological defects, Vibrational properties, Plasticity

*Speaker

Nanoparticle Taylor Dispersion Near Charged Surfaces with an Open Boundary

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The dispersive spreading of microscopic particles in shear flows is influenced both by advection and thermal motion. At the nanoscale, interactions between such particles and their confining boundaries become unavoidable. We address the roles of electrostatic repulsion and absorption on the spatial distribution and dispersion of charged nanoparticles in near-surface shear flows, observed under evanescent illumination. The electrostatic repulsion between particles and the lower charged surface is tuned by varying electrolyte concentrations. Particles leaving the field of vision can be neglected from further analysis, such that the experimental ensemble is equivalent to that of Taylor dispersion with absorption. These two ingredients modify the particle distribution, deviating strongly from the Gibbs-Boltzmann form at the nanoscale studied here. The overall effect is to restrain the accessible space available to particles, which leads to a striking, tenfold reduction in the spreading dynamics as compared to the noninteracting case.

Keywords: Brownian motion, diffusion, nanofluidics, evanescent waves, electrostatic double layer forces

*Speaker

Non linear transport of ions in 2D nanochannels: Effect of the long-range electrostatic correlations

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Recent experimental advances in nanofluidics have allowed to explore ion transport across molecular-scale pores. Such subnanometric channels are of particular interest for iontronic applications, as they enable a fine control of ionic properties. Carbon-based 2D nanochannels – where a single molecular layer of electrolyte is confined between solid walls – are a promising platform to implement this strategy, but a precise description of ion transport in these structures is lacking.

In this work, we investigates the consequences of ionic pairing, on charge transport, in a 2D nanochannel using molecular dynamics simulations. We show that the nature of this ionic association undergoes a drastic change when the strength of electrostatic interactions – controlable through temperature or channel height – reaches a certain threshold, corresponding to the aggregation of ions into clusters.

We fully describe this phenomenology both at equilibrium and in the presence of an electric field. In particular, we observe that considering strong anisotropic correlation between ion is necessary to explain our conductance measurements obtained in simulations. Eventually, we analyze how ionic association is affected by water molecules, and how it impacts electrical conduction. Our results shed light on nanoscale ion transport underlying many nanofluidic experiments.

Keywords: Confinement, Ionic correlations, Non linear transport, Molecular dynamics, Brownian dynamics, Phase transition

*Speaker

Visualization of plastic events in colloidal gels

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The yielding of colloidal gels is a gradual process where the transition from microscopic elastic to plastic deformations accompanies changes in the rheological properties. Whereas for glassy, disordered systems this is relatively well understood, for lower volume fraction systems with more open - or even fractal - structures our understanding on how stress is distributed over the particle networks and how plastic events are generated is less understood, in particular in relation to the physical chemistry of the particles used. To study this in real space, we report on high speed confocal studies of the yielding transition of depletion flocculated colloidal particles. PMMA-g-PHSA particles are used in an index and density matched suspending medium and the response to simple shear deformations is studied. The parameters studied are the volume fraction and the strength of the depletion force. Non affine motions or discontinuities identified with the optical flow method are measured as a function of strain for stresses in the vicinity of what is typically described as the rheological yield stress. We quantify the number of events per unit volume and the number of particles participating in such plastic events as a function of the different parameters. The goal is to get insights into the stress activated kernels which dictate plastic flow.

Keywords: yielding, colloidal gels, plasticity

*Speaker

Mechanism of Delayed Collapse in Colloidal Gels Revealed by Multiscale Confocal Microscopy

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The delayed collapse of colloidal gels vexing problem. Although the equilibrium behaviour of colloid-polymer-mixtures is well understood, that of far-from-equilibrium gels is astoundingly complex, especially when solvent-mediated hydrodynamic interactions play a role (1). As the gels age, they become stronger due to coarsening. Quite counterintuitively for a material whose strength increases with time, gels undergo sudden, catastrophic failure by collapsing under gravity, sometimes months or even years after preparation. An understanding of such delayed collapse has long remained elusive, but recently, we have made two breakthroughs which have uncovered the mechanism of gel collapse. Firstly, we have revealed the basic mechanism of failure with a novel imaging method that reveals the forces between emulsion droplets (2). We have gone on to develop a second new method which has led to a step change in our understanding of delayed collapse in gels: Mulltiscale Confocal Microscopy.

Evidence has been found that, prior to collapse, channels, or "streamers" emerge in the gel. However, determining the nature of these streamers has proven challenging. Understanding gel collapse boils down to identifying microscopic failure in a macroscopic (larger than 1cm) sample. Finding such a needle in a haystack has now become possible by imaging such large samples with a microscopic level of detail, ie Multiscale Confocal Microscopy. This new experimental approach has revealed the mechanism by which the streamers form.

(1) Royall CP, Faers MA, Fussell SL and Hallett JE, "Real Space Analysis of Colloidal Gels: Triumphs, Challenges and Future Directions", J. Phys.: Condens. Matter, 33 453002 (2021).
(2) Dong J, Turci F, Jack RL, Faers MA and Royall CP, "Direct Imaging of Contacts and Forces in Colloidal Gels", J. Chem. Phys. 156 214907 (2022).

Keywords: Colloids, Gel, Microscopy, Confocal

*Speaker

Composition effect of the thermo-mechanical behavior of glasses

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We employed molecular dynamics simulations to extensively explore the thermo-mechanical behavior of two glass materials-an oxide silica glass (SiO2) and a binary Cu-Zr-based metallic alloy (Cu50Zr50)-during shear deformation cycles. By calculating the energy balance and tracking the temperature evolution of both glasses under deformation cycles, we proposed a constitutive law that accurately reproduces the self-heating process generated for each glass due to plastic defor-motion. We performed simulations at different shear rates to verify the validity of our model. Both glasses were equilibrated at a very low temperature (10 K) and two independent deformation rates were applied to each sample. Using a precise atomic description of the instantaneous deformation, combined with an exact coarse-graining procedure, we show that self-heating is supported by strain gradient plasticity with nanometric characteristic lengthscales.

Keywords: Glasses, thermo, mechanical couplings

*Speaker

NN4 - Nanoparticles for energy

Heater@luminescent nanoplatforms based on Prussian blue core@silica shell nanoparticles for photothermia and thermometry

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Photothermia, which involves the generation of heat by a photothermal agent following exposure to light irradiation, is a phenomenon of great interest in medical and catalytic fields,1 and for the stimulation of chemical and biological reactions.2,3In the realm of photothermal heat generation, a significant challenge lies in accurately regulating temperature not only at the macroscopic level but also in the immediate proximity of the surface of the nano-heater. In this context, considering that conventional temperature measurement instruments are ineffective at the nanoscale due to limitations in sensitivity, accuracy, and spatial resolution, precise tools for temperature measurements are needed.

In this work, we studied the design and investigation of new multifunctional heater/thermometer nano-objects containing (i) Prussian blue (PB) nanoparticles heater core, characterized by the general formula A1-xFeIII(FeII(CN)6)1-x (where A denotes an alkaline ion), possessing promising photothermal properties, and (ii) Tb3+/Eu3+ based luminescent coordination compound as emissive thermometer for its demonstrated excellent thermometric capacity4. The obtained hybrid nano-objects present both, a heating ability under irradiation at 808 nm and a bright luminescence in the visible region characteristic of Tb3+ and Eu3+ ions, which make them multifunctional. Moreover, the observed emission is temperature-dependent allowing to use these nanoparticles as temperature nanoprobe in the close proximity of the PB core with a satisfactory maximal relative sensitivity of 0.75 %·∘C-1 at 20 ∘C.

(1) Duan. S et al. *RSC Adv*, **2023**, 13, 14443-14460

(2) Mateo. D et al. *Chem. Soc. Rev*, **2021**, 50, 2173-2210

(3) Pallavicini. P et al. *Chem. – Eur. J.* **2021**, 27, 15361–15374
(4) T. Pelluau et al. *Nanoscale*, **2023**, 15, 14409

Keywords: nanoparticles, luminescence, thermometry, photothermia, lanthanide complex

*Speaker

Iron oxide multifunctional nanoplatforms: towards temperature control in photothermia and magnetothermia

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Over the past decades, inorganic nano-objects capable of generating significant heat when remotely activated by external *stimuli* have garnered considerable attention. For this reason, numerous nano-heaters with diverse compositions, sizes, and morphologies activated either by light irradiation (photothermal agents) or by the application of an alternating current magnetic field (magnetothermal agents), have extensively been reported1.
Among these, iron oxide nanoparticles received a particular attention due to their capacity of generating heat when it is exposed to external stimuli. This characteristic offers promising applications in hyperthermia treatment, catalysis, and radical release2. Yet, a better understanding and control of the temperature rise at the surface of the nanoparticles remains challenging.

The current study aims to expand the investigation into the development of multifunctional nanoplatforms based on iron oxide materials. We will first discuss the use of the generated heat on a magnetite nanoparticle with thermosensitive radical initiators, alkoxyamines R1R2NOR3, anchored to its surface2. The magnetic core exhibits a high intrinsic loss power of 4.73 nHm2.kg–1 providing rapid heating of their surface under the action of an alternating magnetic field. This causes the homolysis of the alkoxyamine C–ON bond and triggers the formation of radicals3,4.

1. Guardia, P. *et al. ACS Nano* **6**, 3080–3091 (2012).

2. Bouvet, B. *et al. Nanoscale* **15**, 144–153 (2022).

3. Pelluau, T. *et al. Nanoscale* **15**, 14409–14422 (2023).
4. Adam, A. *et al. Colloids and Surfaces A: Physicochemical and Engineering Aspects* **640**, 128407 (2022).

Keywords: Magnetic nanoparticles/ Hyperthermia/ Radical release/ Luminescence

*Speaker

Control on the formation of colloidal crystals of uniform populations of cubic maghemite nanoparticles with tunable size and surface chem-istry

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Iron oxide nanoparticles with controlled size, shape, and magnetic properties have attracted considerable attention due to their unique magnetic properties and potential applications in various fields, including biomedicine, biosensing, and energy storage(1). The thermal decomposition organometallic precursors in the presence of surfactants has been widely studied to synthesize iron oxide nanoparticles with controlled size and shape (2). There are different parameters such as reaction temperature, reaction time, solvent, concentration of the reactants, and the ligands, which can influence the size, shape, and properties of the resulting nanoparticles (3). Besides the development of strategies for cubic IONPs synthesis with tunable size and shape, the control of their interaction with various environments is of great importance and required to adjust the surface chemistry. This is the case for example to improve: (1) the dispersion of the NPs in a given solvent; (2) their surface activity; (3) their biocompatibility. In this study we investigated the synthesis of uniform cubic maghemite NPs with two different coating agents, dodecanoic acid (C12) and oleic acid (C18). This study has been done to form colloidal crystals from cubic maghemite and verify their collective properties. For these two types of ligands, the synthesis conditions are adjusted to promote three sizes of NPs, identical from one ligand to another.

- Park, Jongnam, et al. "One-nanometer-scale size-controlled synthesis of monodisperse magnetic Iron oxide nanoparticles." *Angewandte Chemie* 117.19 (2005): 2932-2937.
- Baaziz, Walid, et al. "Magnetic iron oxide nanoparticles: reproducible tuning of the size and nanosized-dependent composition, defects, and spin canting." *The Journal of Physical Chemistry C* 118.7 (2014): 3795-3810.
- Wetterskog, Erik, et al. "Precise control over shape and size of iron oxide nanocrystals suitable for assembly into ordered particle arrays." *Science and Technology of Advanced Materials* 15.5 (2014): 055010.

Keywords: Maghemite Cubic shape Thermal decomposition Tunable surface chemistry Magnetism

*Speaker

Reactor design and heating agent for magnetically induced catalysis

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Climate change is a major worldwide challenge, with the energy and industrial sectors being responsible for the majority of GHG emissions. A variety of solutions are being studied, such as the electrification of industrial heating and power-to-gas storage solutions. In this study, we aim to study an innovative magnetically heated pilot-scale methanation reactor. Induction heating presents a unique advantage in this context, offering rapid and localized heating directly to the catalytic bed via the heating agent, which improves reaction kinetics, energy efficiency and reactor control. The heating agent is Iron wool, a commercially available, low cost and versatile material that has been successfully used by our group for a variety of magnetically induced heterogeneous catalytic reactions. Our study investigates both the magnetic heating of our catalytic bed as well as the advantages in terms of high conversion rates of CO into methane, low power consumption, and a dynamic reactor control which is suitable for PtG applications. First, the effect of packing and geometrical factors on the heating were studied, and the heating mechanisms were defined. In addition, the pilot reactor showed extremely fast start-up times compared to current industrial methanation reactors, with the possibility to dynamically control the heating. High CO2 conversion rates ($> 90\%$) and high CH4 selectivity ($> 98\%$) were obtained. The experimental results were then replicated with the developed numerical model and further simulations and operating conditions were explored. This research not only highlights the feasibility of using induction heating in the methanation process but also underscores its broader implications for the future of industrial process electrification, aiming to contribute to more sustainable and flexible energy systems.

Keywords: Magnetic heating, Power to gas, Methanation, Reactor design

*Speaker

BAM2 - Mechanics and microstructure of living matter across length scales

A nuclear jamming transition in embryonic tissues

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The regulation of tissue physical states and rigidity transitions is crucial for embryonic development and tissue morphogenesis. While distinct cellular properties, such as cellular density and mechanics of cell-cell contacts, are known to control emergent tissue properties, the role of sub-cellular organelles on tissue physical states has not been studied. Combining theoretical modeling and in-vivo experiments, we discover a novel type of rigidity transitions, nuclear jamming transition, governed by nuclear volume fraction and nuclear aspect ratio. By implementing nuclei as repulsive soft particles that interact with cell junctions in the Active Foam model, we study how nuclei alter emergent tissue structure and dynamics. For isotropic nuclei, tissue dynamics progressively slow down while tissue structure becomes more ordered as nuclear volume fraction increases, a signature of fluid-to-solid transition. As the nuclear aspect ratio increases, the nuclear jamming transition occurs at a smaller nuclear volume fraction because anisotropic nuclei start to touch cell junctions at a smaller nuclear volume fraction. For a large nuclear volume fraction and a large nuclear aspect ratio, we observe a formation of nematic domain that leads to anisotropic cell shapes as well as enhanced cell movement. Analysis on tissue structures, nuclear movements, and mechanical properties of developing eye tissues in zebrafish embryo shows that retinal tissues undergo a nuclear jamming transition with increasing nuclear volume fraction and decreasing nuclear aspect ratio. Our result highlights a novel rigidity transition governed by nuclear-to-cytoplasmic ratio and nuclear geometry, which can be an important mode of phase transitions during embryonic development.

Keywords: Phase transition, Morphogenesis, Nucleus

*Speaker

Healing Regimes for Microscopic Wounds in the Vertex Model of Cell Tissues

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Wounds in epithelial tissues compromise their vital role in homeostasis. A rapid and efficient wound healing encompasses different mechanisms, which includes the formation of a contractile actin-myosin cable around its edge, known as the purse-string mechanism(1,2). We combine mean-field calculations and numerical simulations of the Vertex model to study the interplay between tissue properties and the purse-string mechanism and its impact on the healing process. We find different regimes, where the wound opens, closes partially or completely. We also derive an analytic expression for the closure time which is validated by numerical simulations. This study establishes under which conditions the purse-string mechanism suffices for closure, providing an analytical mean-field expression for the respective thresholds.

Keywords: wound healing, vertex model, mean field, purse, string

*Speaker

Cell shape elongation and alignment during convergent-extension of biological tissues

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Morphogenesis of biological tissues relies on a complex interplay between the constituent cells. A key morphogenetic process is anisotropic tissue deformation, also called convergent-extension (CE), which can be driven either by externally applied forces, internally generated active forces, or by a combination of both. Our work is in part motivated by Xenopus embryo explants, which undergo CE without any externally applied force. During this process, we observe cell shape alignment perpendicular to the axis of explant elongation. To better understand such cell shape alignment, we study convergent extension using vertex model simulations. We find that cells always align parallel to the direction of CE for purely external driving. However, for active internally driven CE, cells can also align perpendicular to CE, in particular if CE is resisted by external forces. Our results demonstrate that whether CE is driven externally or internally can in part be inferred from imaging data alone.

*Speaker

Medium-assisted tumbling as a control of bacteria exploration in a complex fluid

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In nature, many fluids hosting bacteria populations or protecting against microbial contamination, display non-Newtonian rheology. To study the 3D spatial exploration of motile E.coli bacteria in a model complex environments, we design a motility medium with tunable macroscopic rheology. By increasing the solid charge in soft carbomer grains, the rheology goes from a Newtonian viscous suspension to a jammed yield-stress fluid. Using a novel 3D Lagrangian tracking device, we monitor many bacteria (together with its flagella) tracks and characterize changes in their motility features up to the making of a motility barrier at higher carbomer concentration. We show that the presence of local mechanical disorder and the resistance to penetration, override the biologically borne run-andtumble navigatHi ion process. This "medium-assisted" exploration scenario, characterized by a stop and go kinematics, is deeply related to the flexibility of the flagella bundle that insures the swimming propulsion.

*Speaker

SUBSTRATE STIFFNESS IMPACTS EARLY BIOFILM FORMATION BY TUNING BACTERIAL SURFACE MOTILITY

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Most bacteria live in surface-associated communities called biofilms. These spatially-organized communities are essential to the survival of bacteria in harsh environments, and are closely linked to antibiotic resistance in pathogenic strains. Biofilms stem from the colonization of substrates by bacteria, a promiscuous process that takes place on a wide range of living tissues and inert materials. Here, we have studied experimentally the impact of substrate rigidity on bacterial adhesion and early biofilm development. By imaging and tracking adhering bacteria in situ, on polyacrylamide hydrogels of defined stiffness (1-100 kPa), we demonstrate that the opportunistic promiscuous pathogen Pseudomonas aeruginosa explores substrates differently based on their rigidity. This leads to striking variations in microcolony structure, strain mixing during co-colonization and phenotypic expression. Using simple kinetic models, we propose that these phenotypes arise through a purely mechanical interaction between the elasticity of the substrate and the type IV pilus (T4P) machinery, a contractile surface appendage that mediates surface-based motility ("twitching"). Our 1D model is based on a force balance between (i) a pilus that extends, attaches and retracts with a defined frequency; (ii) the deformation of the underlying substrate at the pilus tip upon retraction; and (iii) the friction force due to adhesion of the bacterial body when it is dragged across the surface at the other end of the pilus. The efficiency of pili activity is thus modulated by the deformability of soft substrates (1). Together, our findings reveal a new role for substrate softness in the spatial organization of bacteria in complex microenvironments, with far-reaching consequences on efficient biofilm formation by P. aeruginosa, and possibly other microorganisms. (1) Sofia Gomez, Lionel Bureau, Karin John, Elise-Noëlle Chêne, Delphine Débarre, Sigolene Lecuyer (2023) Substrate stiffness impacts early biofilm formation by modulating Pseudomonas aeruginosa twitching motility eLife 12:e81112

Keywords: bacteria, surface motility, microcolonies, biofilms

*Speaker

Control of active patterns through communication between self-propelled particles in microstructured environments

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The collective movement of motile bacteria is an example of active matter, and is one of the simplest systems with a large number of interacting particles exhibiting non-trivial macroscopic behavior. Communication-based reciprocal control of motility has been shown to generate self-organized spatial structures, positioning it as a mechanism for pattern generation without external cues. However, the habitats in which bacteria live are spatially structured at multiple scales, and the physical constraints of the environment have a strong effect on their collective behavior. In this work we address the effects of spatially structured habitats on the self-organization of active patterns based on communication between motile particles. We used CRISPRi methodology and quorum-sensing communication system to construct synthetic strains of *Escherichia coli* whose motility depends on the concentration of a chemical signal produced by a complementary strain. We tracked individual bacteria to understand the behavior of these systems at the single-cell level and observed a dependency of the velocity and persistence time on the concentration of signaling molecules and the presence of the complementary strain. To study how physical barriers modify the collective behavior that emerge due to interactions mediated by chemical signals between motile particles, we fabricated spatially structured habitats using microfluidic devices. In a long channel without spatial features, we observed that a mixture of complementary strains remains mixed in space. However, in a linear array of habitat patches connected by corridors, an ecosystem that simulates the patchy environment where populations coexist, we observed the spatial segregation of the same mixture of complementary populations. These results shows that changing the habitat landscape has a direct impact on bacterial motility, generating a change in the scale of the patterns that emerge. Studying how bacteria interact with their physical environment provides a deeper understanding of how ecological processes operate at different scales.

Keywords: Active patterns, Synthetic biology, Motile bacteria, Quorum, sensing

*Speaker

Growth, death, and resource competition in sessile organisms

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Population-level scaling in ecological systems arises from individual growth and death with competitive constraints. We build on a minimal dynamical model of metabolic growth where the tension between individual growth and mortality determines population size distribution. We then separately include resource competition based on shared capture area. By varying rates of growth, death, and competitive attrition, we connect regular and random spatial patterns across sessile organisms from forests to ants, termites, and fairy circles. Then, we consider transient temporal dynamics in the context of asymmetric competition, such as canopy shading or large colony dominance, whose effects primarily weaken the smaller of two competitors. When such competition couples slow timescales of growth to fast competitive death, it generates population shocks and demographic oscillations similar to those observed in forest data. Our minimal quantitative theory unifies spatiotemporal patterns across sessile organisms through local competition mediated by the laws of metabolic growth, which in turn, are the result of long-term evolutionary dynamics.

Keywords: ecology, spatial dynamics, competition, metabolic scaling

*Speaker

Conformal phase transition in active fluids

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Many biological systems such as bacterial monolayers and human cells are characterised as active fluids. Recently, vorticity isolines have been used to show conformal invariance in active turbulence and place it in the percolation universality class, which was confirmed for several experimental systems (Andersen et al. 2024). To understand how this invariance emerges, we look at the transition to active turbulence by varying the strength of the activity. We find that the fractal dimension of zero vorticity contours changes from 1 to 7/4, the expected value for percolation, thereby reflecting the appearance of scale invariant structures. We also use the vortex shape anisotropy to pinpoint the transition. This work takes a step towards understanding the universality in active turbulence and could lead to a fundamental understanding of emergence of conformal symmetry in biological fluids as a new type of active phase transition.

Keywords: active matter, active nematics, percolation

*Speaker

BAM3 - Physics of Morphogenesis in Living Organisms

A mechanical transition from tension to buckling underlies the jigsaw puzzle shape morphogenesis of histoblasts in the Drosophila epidermis

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The polygonal shape of cells in proliferating epithelia is a result of the tensile forces of the cytoskeletal cortex and packing geometry set by the cell cycle. In the larval Drosophila epidermis, two cell populations, histoblasts and larval epithelial cells, compete for space as they grow on a limited body surface. They do so in the absence of cell divisions.
We report a striking morphological transition of histoblasts during larval development, where they change from a tensed network configuration with straight cell outlines at the level of adherens junctions to a highly folded morphology. The apical surface of histoblasts shrinks while their growing adherens junctions fold, forming deep lobules. Volume increase of growing histoblasts is accommodated basally, compensating for the shrinking apical area.
The folded geometry of apical junctions resembles elastic buckling, and we show that the imbalance between the shrinkage of the apical domain of histoblasts and the continuous growth of junctions triggers buckling. Our model is supported by laser dissections and optical tweezer experiments together with computer simulations. Our analysis pinpoints the ability of histoblasts to store mechanical energy to a much greater extent than most other epithelial cell types investigated so far, while retaining the ability to dissipate stress on the hours time scale.
Finally, we propose a possible mechanism for size regulation of histoblast apical size through the lateral pressure of the epidermis, driven by the growth of cells on a limited surface. Our work indicates that in growing non-dividing cells, compressive forces, instead of tension, can also drive cell morphology.

*Speaker

Collective Dynamics Underlying Embryoid Reductional Division

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How do collectively organized multi-cellular life forms emerge from the exchange of individual mechanical and morphogenetic cues? Deciphering multiscale population dynamics poses a fundamental challenge to understanding the mechanism whereby embryonic growth is coordinated on larger scales. Establishment and maintenance of asymmetric pre-patterning in the *C. elegans* embryo is an ideal subject for statistical exploration of self-assembly, however a physical theory of development from germ layer specification through morphogenesis is lacking. Coupling high-resolution optical imaging with non-equilibrium statistical analysis provides phenomenological insight into the role of mechanics and shape on macroscopic ordering during embryogenesis. Analyzing stochastic trajectories according to cell fate distinctions and using a particle-based reductional division model with generation dependent control was found to be a robust statistical strategy for probing the relationship between growth rate, adhesion, volume, and diffusivity in generating collective space-time morphological patterns. Significantly, oscillations in anomalous diffusion during gastrulation suggest that periods of relaxation accompany waves of collective motion and an increase in super diffusive behavior from differentiated cells suggests that non-equilibrium activity shifts from being driven by proliferation to directed motion. Our data-driven theoretical approach identifies self-organization principles governing proliferation in confinement and yields a new perspective about the embryo as active matter.

Keywords: embryogenesis, confinement, living active matter, self, organization, collective dynamics

*Speaker

Temperature scaling of sub-cellular to tissue-level properties in a developing embryo

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During its development, the zebrafish embryo undergoes somitogenesis and antero-posterior elongation. The developmental speed of this process depends on temperature, a phenomenon that occurs in many other organisms (1).
At 25∘C, it is established that body axis elongation relies on a fluid-to-solid transition at the tip of the tail, during which the area that will give rise to somites solidifies progressively to stabilize durably the tail shape (2). During this developmental progression, cell-cell interactions can be connected to the tissue-scale physics using an active foam model (3).
To explore how temperature affects this fluid-to-solid transition and in turn impacts developmental speed, we have designed a temperature-controlled stage to explore how sub-cellular dynamics and tissue-level properties depend on temperature. This stage minimizes gradients over large samples, such as embryos, and can be used to study the thermal tolerance of several physiological processes in the fish, including heart rate. With this new device, we can measure the rheology of embryonic tissues on a physiological temperature range (20-30∘C) using ferrofluid droplets (4). We are also able to quantify the dependance of active cellular processes on temperature changes. The ability to perform controlled changes in temperature while measuring the physical state of the tissue will help us reveal how temperature changes affect embryonic morphogenesis, from subcellular to tissue scales.
(1) Crapse et al, Mol Syst Biol (2021)

(2) Mongera et al., Nature (2017)

(3) Kim et al., Nature Physics (2021)
(4) Serwane et al., Nature Methods (2017)

Keywords: Morphogenesis, Rheology, Tissue dynamics, Zebrafish, Live Microscopy

*Speaker

Wing expansion in Drosophila melanogaster

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During their final transformation, insects emerge from the pupal case and deploy their wings within minutes. The wings deploy from a compact origami structure, to form a planar, rigid and functional blade that allows the insect to fly. The deployment is powered by a rapid increase in internal pressure, and by the subsequent flow of hemolymph into the deployable wing structure. Using a combination of imaging techniques, we characterize the internal and external structure of the wing in *Drosophila melanogaster*, the unfolding kinematics at the organ scale, and the hemolymph flow during deployment. We find that beyond the mere unfolding of the macroscopic folds, wing deployment also involves an expansion of cell surface and the unfolding of microscopic wrinkles in the cuticle enveloping the wing. A quantitative computational model, incorporating mechanical measurements of the viscoelastic properties and microstructure of the wing, predicts the existence of an operating point for deployment and captures the dynamics of expansion. This model suggests that insects exploit material and geometric nonlinearities to achieve rapid and efficient reconfiguration of soft deployable structures.

Keywords: Biomechanics, Inflatable structure, Tensile test, Micro CT, Nanoindentation, Viscoelasticity

*Speaker

Mechanics of the cellular microenvironment as probed by cells in vivo

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Tissue morphogenesis, homeostasis and repair require cells to constantly monitor their three-dimensional microenvironment and adapt their behaviours in response to local biochemical and mechanical cues. Yet the mechanical parameters of the cellular microenvironment probed by cells in vivo remain unclear. Here, we report the mechanics of the cellular microenvironment that cells probe in vivo and in situ during zebrafish presomitic mesoderm differentiation. By quantifying both endogenous cell-generated strains and tissue mechanics, we show that individual cells probe the stiffness associated with deformations of the supracellular, foam-like tissue architecture. Stress relaxation leads to a perceived microenvironment stiffness that decreases over time, with cells probing the softest regime. We found that most mechanical parameters, including those probed by cells, vary along the anteroposterior axis as mesodermal progenitors differentiate. These findings expand our understanding of in vivo mechanosensation and might aid the design of advanced scaffolds for tissue engineering applications.

Keywords: Mechanobiology, Phase transitions, Morphogenesis

*Speaker

BAM5 – Phase transitions in biology

(Micro)phase-separation in nucleo: formation and dynamics of heterochromatin compartments

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The spatial segregation of heterochromatin, the inactive part of the genome, into distinct, membraneless spatial compartments inside the cellular nuclei, involves the binding of Heterochromatin Protein 1 (HP1) to specific genomic regions. While HP1 exhibits liquid–liquid phase separation properties in vitro, its mechanistic impact on the structure and dynamics of heterochromatin condensate formation in vivo remains largely unresolved. I will present our recent work on modeling the mutual coupling between self-interacting HP1-like molecules and the chromatin polymer. In particular, how the specific affinity of HP1 for repressed regions facilitates coacervation in nucleo and promotes the formation of stable condensates at HP1 levels far below the concentration required to observe phase separation in vitro and how the dynamical cross talk between HP1 and the viscoelastic chromatin scaffold also leads to anomalously slow equilibration kinetics. Finally, I will show how the morphology of these complex coacervates is further found to be governed by the dynamic establishment of the underlying repressive landscape, which may drive their increasingly abnormal, aspherical shapes during cell development, consistently with 4D microscopy measurements of HP1 condensate formation in live Drosophila embryos performed in collaboration with the Karpen lab.

Keywords: phase separation, polymer physics, chromosome

*Speaker

Phase separation kinetics of bio-inspired condensates under passive and active conditions

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We investigate the structural dynamics and kinetics of condensates made up of cationic peptides (RRASLRRASL) and poly uracil (polyU) RNAs, serving as an ideal model system for membrane-less organelles. Employing absorbance measurements at 500 nm, the critical peptide concentration is estimated to be 400 μM at a fixed polyU concentration (0.5 g/L) in a physiological buffer (50 mM HEPES pH 7.4). Confocal microscopy images of fluorescently labelled peptide/polyU condensate at this concentration display a droplet-like morphology (1 to 5 μm). The absorbance increased rapidly (t $<$ 1s) and remained stable for 150 minutes for the sample containing 0.5 g/L polyU and 1000 μM peptide, indicating coacervation. The charge ratio was estimated to be 2.45. Preliminary experiments were carried out by performing time-resolved small-angle X-ray scattering (TR-SAXS) with a stopped-flow device for rapid mixing at 37 ∘C. TR-SAXS patterns revealed that with unphosphorylated peptides, the condensate size increased rapidly and reached a few hundred nanometers in t $<$ 400 ms. Contrary to the anticipated $\alpha \approx$ for a standard coalescence process established from the scaling law R∼t$\hat{}\alpha$, our empirical findings yielded a scaling exponent of 0.45 $\pm$ 0.03, marking a 35% deviation from the theoretical prediction. Next, we studied the dephosphorylation of double-phosphorylated peptides by Lambda Protein Phosphatase (LPP), which dephosphorylates the serine residues of the peptide, thus driving coacervation. The absorbance linearly increased by 50% within 150 minutes for the sample containing 0.5 g/L polyU, 1000 μM peptide, and 400 U/mL LPP, denoting an increase in the number and/or size of the condensates over time. When the sample concentration was doubled, the absorbance started to increase at t = 15 minutes and remained stable for the subsequent 125 minutes. This could be attributed to the higher sample concentration, which increased the condensation rate, resulting in an early equilibrium.

Keywords: Biomolecular condensates, Liquid, liquid phase separation, Kinetics, Time, resolved small, angle X, ray scattering, Confocal microscopy

*Speaker

Macromolecular crowding controls the size and concentration of chemically active droplets

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Biomolecular condensates play a central role in the spatial organization of living matter, and their formation is now well understood as a form of liquid-liquid phase separation (LLPS).It has been established that such condensates are sensitive to many physiological parameters, such as pH or ionic strength. However, little is known about the effect of macromolecular crowding on their size and on their concentration, even though excluded volume effects are known to play a prominent role on the structure and dynamics of the intracellular medium. In this work, we address this question theoretically, using Brownian dynamics simulations where biomolecular condensates are modeled by chemically active droplets, whose building blocks are represented explicitly as particles that interact with attractive or repulsive interactions, depending on whether they are in a droplet-forming state or not. In addition, our model accounts for the presence of "crowders", whose density can be varied. First, our microscopic description of the system, which goes beyond the usual continuous or field-based models, allows us to account precisely for the structure and shape of the condensates, their polydispersity, as well as their typical lifetimes – observables which are usually out of reach from previous deterministic approaches. Second, we show that increasing the density of crowders in the system tends to reduce the size of the droplets, and to increase their typical concentration. We therefore argue that the interest of this work is two-fold: (i) it provides methodological tools, that open the way to microscopic,particle-based simulations of biomolecular condensates with Brownian dynamics simulations; (ii) it sheds light on the role of macromolecular crowding on LLPS in biologically relevant conditions.

Keywords: LLPS Brownian, dynamics, simulation activite, reaction crowding droplets

*Speaker

Role of the sequence length in the coil-to-globule transition of elastin-like polypeptides

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Phase separation of disordered proteins resulting in the formation of biocondensates has received significant attention due to its fundamental role in cellular organization and functioning and is sought after in many applications. For instance, the liquid-liquid phase separation of tropoelastin initiates the hierarchical assembly of elastic fibers - key components of the extracellular matrix providing resilience and elasticity to biological tissues. Inspired by the hydrophobic domains (HDs) of tropoelastin, elastin-like polypeptides (ELPs) were derived, exhibiting a similar phase behavior. Even though it appeared certain that elastin condensates retain liquid-like properties, a recent experimental study questioned this viewpoint by demonstrating that the aggregate state of elastin-derived materials can depend on the length of HDs. (1) Here, we employ state-of-the-art atomistic modeling to resolve the conformational ensembles of a single ELP as a function of its sequence length. (2) For the first time, we report the free energy profiles of ELPs in the vicinity of conformational transitions which show more compact polypeptide conformations at higher temperatures. We access the conformations visited by ELPs through descriptors from polymer physics. We find that short ELPs always remain in coil-like conformations, while the longer ones prefer globule states. The former engages in intrapeptide hydrogen bonds temporarily retaining their liquid-like properties while the latter forms long-lived (hundreds of nanoseconds) intrapeptide hydrogen bonds attributed to ordered secondary structure motifs. Our work demonstrates the importance of the sequence length as a modulator of conformational properties at a single chain and possibly explains the change in aggregate state in elastin condensates.
(1) A. Vidal Ceballos et al., *PNAS,* 119.37 (2022)
(2) T.I. Morozova et al, bioRxiv, 2023.12. 04.569864

Keywords: disordered polypeptides, phase separation

*Speaker

Controlled liquid-like droplet formation through phase separation of the bacterial DNA segregation complex ParBS with CTP

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The bacterial DNA segregation is mainly performed with the ParABS system. It is composed of ParB, a binding protein, ParA, an ATPase and parS, a specific binding DNA sequence that ParB binds with high affinity. Hundreds of ParB are recruited around parS into a complex, called ParBS, which displays liquid-like properties.

Recently, it has been shown that ParB is using energy stored as CTP in the cells according to the clamping and sliding model. Upon specific binding onto parS, ParB binds CTP that is used to switch the ParB into a clamp that is then released DNA to perform transient 1D diffusion until it detaches and unbinds CTP. The role of the CTP is not understood: neither the time scale of the ParBS formation nor the total number of ParB into ParBS could be accounted with the clamping and sliding model.

We hypothesize that the ParB clamp leads to an increase of the ParB-ParB interactions, leading to an increased speed and specificity of the ParBS formation during a liquid-like phase separation. We offer a proof of concept via numerical simulations of ParB as a Lattice Gas displaying a discontinuous phase transition.

*Speaker

MP3 – Emerging Majorana materials : towards topological quantum computing

Atom-by-Atom Fabrication of Topological Superconductors with Associated Majorana Quasiparticles

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One of the major challenges for the future of quantum computation is the drastic reduction of the error rate associated with quantum decoherence phenomena. Robust topological qubits, as realized by Majorana states, may ultimately provide a solution and constitute a new direction of topological quantum computation. However, an unambiguous identification of Majorana states requires well defined model-type platforms and appropriate experimental tools for their atomic level characterization.
We make use of STM-based single atom manipulation techniques in order to fabricate well-defined defect-free 1D atomic chains of magnetic adatoms (Mn, Fe, Co) on s-wave superconductor substrates (Re, Ta, Nb) with high spin-orbit coupling (1). The spin structure of these low-dimensional adatom arrays is characterized by spin-polarized STM (2), while scanning tunneling spectroscopy measurements reveal the evolution of the spatially and energetically resolved local density of states as well as the emergence of zero-energy bound states at both chain ends above a critical chain length. In order to confirm the interpretation of the zero-energy states as Majorana quasiparticles, we use Bogoliubov quasiparticle interference (QPI) mapping of the 1D magnet-superconductor hybrid systems for directly probing the non-trivial band structure of the topological phases as well as the bulk-boundary correspondence. Such experiments constitute the ultimate test and rigorous proof for the existence of topologically non-trivial zero-energy modes. We will focus on recent experiments which aim at optimizing the magnitude of the topological gap and therefore the robustness of Majorana modes by heterostructure engineering involving superconducting substrates with high Tc and interfacial thin films exhibiting large spin-orbit coupling.

(1) H. Kim et al., Science Advances 4, eaar5251 (2018); L. Schneider et al., Nature Physics 17, 943 (2021); L. Schneider et al., Nature Nanotechnol. 17, 384 (2022).

(2) R. Wiesendanger, Rev. Mod. Phys. 81, 1495 (2009); L. Schneider et al., Science Advances 7, eabd7302 (2021).

Keywords: Majorana quasiparticles, topological quantum computation, atomic engineering, spin-polarized scanning tunneling spectroscopy

*Speaker

Time-domain Braiding of Anyons

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Recent experiments have evidenced anyons, quasiparticles that keep a memory of particle exchanges via a braiding phase factor. This provides them with unique dynamical properties so far unexplored. In this work, we investigate the dynamics of anyon tunneling in the time domain by using triggered anyon pulses incident on a quantum point contact (QPC) in a = 1/3 fractional quantum Hall (FQH) fluid. When an anyon excitation is emitted toward a QPC in a FQH fluid, this memory property translates into tunneling events that may occur long after the anyon excitation has exited the QPC. The dominant mechanism for particle transfer is not the direct tunneling of the incoming excitations, but rather a braiding process between the incoming excitations and particle-hole excitations created at the QPC. Anyon tunneling is then governed by the mutual braiding phase

*Speaker

The Thermoelectric Effect and Its Natural Heavy Fermion Explanation in Twisted Bilayer and Trilayer Graphene

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We study the interacting transport properties of twisted bilayer graphene (TBG) using the topological heavy-fermion (THF) model. In the THF model, TBG comprises localized, correlated f-electrons and itinerant, dispersive c-electrons. We focus on the Seebeck coefficient, which quantifies the voltage difference arising from a temperature gradient. We find that the TBG's Seebeck coefficient shows unconventional (strongly-interacting) traits: negative values with sawtooth oscillations at positive fillings, contrasting typical band-theory expectations. This behavior is naturally attributed to the presence of heavy (correlated, short-lived f-electrons) and light (dispersive, long-lived c-electrons) electronic bands. Their longer lifetime and stronger dispersion lead to a dominant transport contribution from the c-electrons. At positive integer fillings, the correlated TBG insulators feature c- (f-)electron bands on the electron (hole) doping side, leading to an overall negative Seebeck coefficient. Additionally, sawtooth oscillations occur around each integer filling due to gap openings. Our results highlight the essential importance of electron correlations in understanding the transport properties of TBG and, in particular, of the lifetime asymmetry between the two fermionic species (naturally captured by the THF model). Our findings are corroborated by new experiments in both twisted bilayer and trilayer graphene, and show the natural presence of strongly-correlated heavy and light carriers in the system. Finally, I show that the THF model not only explains the dichotomy between light and heavy electrons observed in thermoelectric transport but also offers an attractive pathway for understanding the unconventional superconductivity of TBG.

Keywords: Twisted bilayer graphene, Thermoelectric effect, Seebeck coefficient, Heavy Fermion model, Superconductivity

*Speaker

Majorana zero modes on quantum Hall edges survive edge reconstruction

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Majorana zero modes can be trapped on v = 1 quantum Hall edges proximitized by superconductors (1). Softening of the edge potential of the v = 1 quantum Hall edge allows for a narrow v =1/3 strip to be deposited near the edge by reconstruction (2). Subsequent edge renormalisation due to inter-edge interactions and disorder induced tunneling leads to a new edge structure. Such a process is typically regarded to be deleterious, leading to a breakdown of the topological bulk-boundary correspondence (3). We show here that the Majorana zero modes survive reconstruction of the quantum Hall edges (4). Moreover, the v = 1/3 strip arising due to edge reconstruction allows the existence of a second Majorana (in contrast to a parafermion, as would be expected for a v = 1/3 system), decoupled from the original Majorana. The signatures of the additional degeneracy due to the second Majorana are found in the phase shifts of the Josephson current.

(1) N. Lindner et al. Phys. Rev. X **2**, 041002

(2) U. Khanna et al. Phys. Rev. B **103**, L121302

(3) R. Bhattacharyya et al. Phys. Rev. Lett. **122**, 246801
(4) K. Iyer et al. arXiv:2308.01980v2

*Speaker

Majorana Zero Modes at proximitized self-assembled Xenes Nanoribbons for Topological Quantum Computation

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In recent decades, research in condensed matter physics shows theoretically that in certain exotic states of matter, such as topological superconductors, pairs of Majorana fermions can emerge as bound states at defects or interfaces, known as Majorana Zero Modes (MZMs). Recently, we have proposed a new platform potentially hosting anyons, which could be braided for realizing topologically protected quantum computation (1). It relies on highly perfect, high aspect ratio, massively parallel, spontaneously self-organized and self-assembled atom-thin epitaxial silicene (2) or pentasilicene nanoribbons (3) proximitized by an s-wave superconductor. They could host distant MZMs at their extremities allowing for the creation of highly stable qbits preserved against external disturbances and environmental noise, and hence, protected from decoherence. As we will show, the self-assembly of these nanoribbons could be a distinct advantage over engineered or atom-by-atom constructed nanowires (4).
(1) M. Minissale *et al.*, Journal of Physics: Materials, in press https://doi.org/10.1088/2515-7639/ad5763 (2024)

(2) R. C. Bento Ribeiro *et al.*, Phys. Rev. B 105, 205115 (2022)

(3) R. C. Bento Ribeiro *et al.,* Scientific Reports 13:17965 (2023)
(4) K. C. Li R. *et al.*, Results in Physics 56, 107322 (2024)

Keywords: Majorana, Nanowires, MZMs, Pentasilicene

*Speaker

2DMS1 - New perspectives and complementaries for electron and X-ray spectroscopies

Time-Resolved Cathodoluminescence to study the carriers dynamics in InGaN quantum wells

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The development of time-resolved Cathodoluminescence (TR-CL) in a scanning electron microscope has enabled the measurement of the lifetime of excited states in semiconductors with a sub-wavelength spatial resolution (1)–(3). These results demonstrated that TR-CL is essential to study the correlation between semiconductor optical and structural properties. While TRCL is usually done in a scanning electron microscope, the improvement of the spatial resolution and the combination with other electron-based spectroscopies offered by TEM has been a step forward for TR-CL (4), (5). Our TRCL experiment are performed in a cold-FEG electron microscope (6). This technology allows among other things to reach a spatial resolution of a few nanometers, essential for the study of III-N heterostructures. In this presentation we will discuss for example the advantage and inconvenient of TRCL in a UTEM and present our results on the study of charge carrier dynamics in In0.3Ga0.7N/GaN quantum well with a resolution below 10 nm. Comparing different heterostructure we will discuss the impact of growth conditions on the optical properties. We will study the QW emission dynamic both along and across the quantum well and correlate the results with the strain maps obtained from the high resolution HAADF-STEM images(7) and temperature dependent time-resolved photoluminescence experiments.

References

(1) P. Corfdir *et al. J. Appl. Phys.*, vol. 105, no. 4, 2009.
(2) R. J. Moerland, et al, *Opt. Express*, vol. 24, no. 21, 2016.
(3) X. Fu *et al. ACS Nano*, vol. 8, no. 4, 2014.
(4) S. Meuret *et al.*, *Appl. Phys. Lett.*, vol. 119, no. 6, p. 6, 2021.
(5) Y. J. Kim and O. H. Kwon, *ACS Nano*, vol. 15, no. 12, 2021.
(6) F. Houdellier et al *Ultramicroscopy*, vol. 186, pp. 128–138, 2018.
(7) N. Cherkashin, et al, *Ultramicroscopy*, vol. 253, p. 113778, 2023.

Keywords: Cathodoluminescence, Nitride Heterostructures

*Speaker

From fine structure to electronic 'orbital' mapping: contribution of electron energy-loss spectroscopy in the transmission electron microscope

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The concept of electronic orbitals has enabled the understanding of a wide range of physical and chemical properties of solids through the definition of, e.g., chemical bonding between atoms. In the transmission electron microscope, which is a powerful tool for high-spatial-resolution analysis of solids, the accessible quantity is the local distribution of electronic states. However, the interpretation of electronic state maps at atomic resolution in terms of electronic orbitals is far from obvious, not always possible, and often remains a major hurdle preventing a better understanding of the properties of the system of interest.
This presentation is motivated by the recent methodological and technological developments in transmission electron microscopy (TEM) that enabled atomic-resolution analysis of the electronic structure of solids, towards so-called electronic 'orbital' mapping. Although proof-of-principle experiments have been reported using CBED or STEM-EELS (1) in bulk crystals, much work remains to be achieved to enable electronic state mapping in a robust, reproducible, and interpretable fashion at specific and relevant areas of solids, like crystal discontinuities. The current state of the art of electronic state mapping in the TEM and its interpretation as electronic orbitals will be introduced by purposedly distinguishing between approaches that rely on elastic and inelastic scattering, in real and reciprocal spaces (2). The example of epitaxial graphene multilayers will be presented to illustrate some of the challenges of core-loss EELS towards the prospect of 'orbital' mapping (3). Contrast variations in fine structure maps are analyzed by means of inelastic channeling calculations, which further show the significance of theoretical support for interpreting electronic state maps.

(1) J-M. Zuo et al., Nature **401**, 49 (1999); S. Löffler et al, Ultramicroscopy **177**, 26 (2017)

*Speaker

(2) M. Bugnet et al., Journal of Microscopy, 1-19 (2024)
(3) M. Bugnet et al., Physical Review Letters **128**, 116401 (2022)

Keywords: core level spectroscopy, electron energy loss spectroscopy, electronic orbital, fine structures

Excitons in solid helium under pressure

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We have calculated the absorption and electron energy loss spectra (EELS) of solid helium at various pressures solving the first principles Bethe-Salpeter equation from many-body perturbation theory, which is the state-of-the-art approach for excitons in materials. EELS experiments in helium bubbles encapsulated in various materials and inelastic x-ray scattering measurements on helium crystals under pressure have reported contradicting trends for the He K-edge energy as a function of pressure (1,2). Our results show a distinct exciton peak that increases linearly with pressure in both its position and intensity, resolving the discrepancy between the different experiments. By investigating the exciton dispersion as a function of momentum transfer along the -M direction, we found a strong parabolic-like shape. At variance with Wannier or Frenkel exciton models, the exciton dispersion is unusually dominated by the screened Coulomb interaction. Near the Bragg reflection points, we have discovered an anomalous angular dependence of the excitonic peak in the spectra, which completely disappears with an infinitesimal change of the momentum transfer. This dramatic effect is explained in terms of crystal local fields related to inhomogeneous charge responses, similarly to what occurs for the plasmon in graphite (3).
References:

(1) M.-L. David, F. Pailloux, V. Mauchamp, and L. Pizzagalli "In situ probing of helium desorption from individual nanobubbles under electron irradiation" Appl. Phys. Lett. 98, (2011).

(2) H. K. Mao, E. L. Shirley, Y. Ding, P. Eng, Y. Q. Cai, P. Chow, Y. Xiao, Jinfu Shu, R. J. Hemley, C. Kao, and W. L. Mao "Electronic Structure of Crystalline 4He at High Pressures" Phys. Rev. Lett. 105, (2010).
(3) R. Hambach, C. Giorgetti, N. Hiraoka, Y.Q. Cai, F. Sottile, A.G. Marinopoulos, F. Bechstedt, Lucia Reining "Anomalous Angular Dependence of the Dynamic Structure Factor near Bragg Reflections: Graphite" Phys. Rev. Lett. 101, (2008).

Keywords: Helium, Pressure, eels, espectroscopy

*Speaker

X-ray optical activity beyond chirality:X-ray Natural Circular Dichroism in Chiral and Achiral Compounds

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Chirality, the absence of improper symmetry operations in a crystal, is often associated with optical activity. However, optical activity can exist without chirality in specific cases. This study aims to understand X-ray Natural Circular Dichroism (XNCD), where a sample shined with left and right circularly polarized light exhibits differences in X-ray absorption.

We investigate achiral crystals, specifically those with improper symmetry operations, which show significant XNCD signals (2). Focusing on crystals with D2d (42m) and S4 (4) symmetries, we observe that XNCD has been reported in these cases. Since S4 is a subgroup of D2d, the XNCD angular dependence for S4 crystals is more complex.

We compute the expressions for the X-ray Absorption Spectroscopy (XAS) and XNCD cross-sections and detail the geometric parameters in their definitions. Special attention is given to the symmetry properties relevant to XNCD, considering the crystal space group, the point group of the space group, and the local point group of the absorbing atom. Through an analytical study of the angular dependencies of XNCD, we demonstrate the information derived from the shape of the XNCD signal.

Finally, we present simulated XAS and XNCD spectra at the K-edges of 3d elements in chiral and achiral compounds. The calculations are performed in the DFT framework using the FDMNES code and within the Multiple Scattering theory or the Finite Difference method(1). Thanks to calculations, the various factors governing the intensity of the XNCD signals are analysed.

References

(1) Y Joly. "X-ray absorption near-edge structure calculations beyond the muffin-tin approximation". In: Physical Review B 63.12 (2001), p. 125120.

(2) C. R. Natoli et al. "Calculation of X-ray natural circular dichroism". In: The European Physical Journal B-Condensed Matter and Complex Systems 4 (1998), pp. 1–11.

Keywords: X, ray optical activity, X, ray Natural circular dichroism, X, ray absorption spectroscopy, crystallography

*Speaker

Small Matrix Approximation of Hybrid LR-TDDFT for the Calculation of Excitation Energies

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Linear Response Time Dependent Density Functional Theory (LR-TDDFT), in the adiabatic approximation, is a well-established technique to reliably obtain excitations energies and optical gaps of materials. Amongst the vast choice of density functional approximations, hybrid exchange-correlation (xc) kernels (employing a fraction of non-local Fock exchange) stand out as particularly accurate. Computational costs have, however, limited the applicability of the hybrid LR-TDDFT approach to the case of small to medium sized molecules. Here we overcome the computational bottleneck by extending the Small Matrix Approximation of LR-TDDFT, to hybrid xc kernels. As LR-TDDFT is a single excitation theory akin to configuration-interaction singles (CIS) it is suited for x-ray absorption spectroscopy, especially in the soft x-ray range where the adiabatic approximation still holds; SPA offers then the possibility as well of calculating the spectral distribution of materials within the x-ray regime in a fast and efficient way. The exceptional accuracy and computational efficiency of the approach is demonstrated by benchmark calculations on an illustrative set of ionic, covalent, molecular and semiconducting infinite periodic crystals. The approach is implemented in the publicly distributed CRYSTAL program.

Keywords: TDDFT, XRay Absorption, Optical Gap, Small Matrix Approximation, Solid State, Crystals

*Speaker

Correlative spectroscopies in van der Waals materials

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In recent years, the inelastic branch of the SEXTANTS beamline has been developing a collaborative research initiative aimed at correlating different state-of-the-art spectroscopies. We perform resonant inelastic X-ray scattering (RIXS) in the soft X-ray regime (50 eV – 1000 eV), and on the same experimental setup, we can perform X-ray excited optical luminescence (XEOL). Both spectroscopies can be conducted down to 18 K and under electric and magnetic fields, thanks to the MAGELEC sample environment. Moreover, we closely collaborate to correlate RIXS and XEOL spectroscopies with electron energy loss spectroscopy (EELS) and cathodoluminescence on various van der Waals materials and correlated systems. In my talk, I will present our recent results. Specifically, I will discuss how, on the magnetic compound CrSBr, we have used crystal field calculations to model the linear dichroism measured in RIXS to determine the chromium crystal field scheme. Additionally, to correlate magnetic properties with photoluminescence (PL) behavior, we measured both RIXS and PL under an applied magnetic field to track the antiferromagnetic-ferromagnetic transition at approximately 0.3 T. I will also present our correlative RIXS-XEOL and EELS study of hexagonal boron nitride (hBN), where the direct exciton responsible for strong luminescence at 6.4 eV was carefully characterized using these three spectroscopies. Finally, I will emphasize the usefulness of combining complementary spectroscopies like RIXS and EELS, as well as excitation and recombination techniques.

Keywords: RIXS, EELS, XEOL, vdW, magnetism, hBN, photoluminescence, exciton, RIXS, MCD

*Speaker

2DMS2 – Growth of 2D materials: structural, optical and electronic properties

Electronic properties of two-dimensional van der Waals heterostructures probed at the nanoscale: Impact of the twist angle

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Two-dimensional van der Waals (vdW) heterostructures have become very attractive in the last decade, thanks to the high tunability of their (opto)-electronic properties. In particular, the interlayer vdW interaction offers unique opportunities of transferring a given property from one layer to the other, through proximity effects (1). For example, when proximitized with a properly chosen 2D system, it is possible to induce in graphene new properties, such as magnetism or enhanced spin orbit coupling, all lacking in the pristine material (1,2). Combining magnetic properties and large SOC in graphene is a very active field, related to potential applications in (opto)-spintronics (2).
Recent theoretical works have focused on the interlayer proximity effects between graphene (Gr) and one layer (1L) of a semi-conducting transition metal dichalcogenide. From these calculations, the authors conclude that the interlayer proximity effect, which rely on the hybridization between the electronic states of each layer, is driven by the interlayer twist angle (3-5). In this talk, I shall review our STM/STS results (complemented by DFT calculations) devoted to that topic, in the case of the 1L-PtSe2/graphene vdW heterostructure (6), and more recently for the 1L-WSe2/graphene system. This work results from a collaboration with the group of M. Jamet (IRIG-SPINTEC, CEA-Grenoble).

1) I. Zutic et al., Mater. Today **22**, 85 (2019).
(2) J. F. Sierra et al., Nat. Nanotechnol. **16**, 856 (2021)
(3) T. Naimer et al., Phys. Rev. B **104**, 195156 (2021)
(4) Y. Li and M. Koshino, Phys. Rev. B **99**, 075438 (2019)
(5) A. David et al., Phys. Rev. B **100**, 085412 (2019)
(6) P. Mallet et al., Phys. Rev. Mater. **7**, L121001 (2023)

Keywords: van der Waals heterostructures, interlayer interaction, twist angle, scanning tunneling microscopy and spectroscopy

*Speaker

Microspectrometry of 2D materials using quantitative phase imaging

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Families of 2-dimensional (2D) transition metal dichalcogenides (TMD) - such as MoS2, WS2, PtSe2 - have emerged as strong candidates for applications in optics and photonics (1). Of equal importance to their intrinsic optical properties is the ability to locally modify them through various processes, either in a defined area or in a micro/nano-patterned fashion. This can be achieved using a laser (2,3), or with a focused ion beam (4,5), among other approaches. In this context, it is important to measure and image the modulated optical properties, preferably in a simple manner. To that end, we use cross-grating wavefront microscopy (CGM) (6,7), a straight-forward quantitative phase imaging technique, to characterize intrinsic and modified/patterned 2D MoS2, building on our previous work (8). Operating in wide-field mode with sub-second acquisition time and diffraction-limited resolution, we show the wealth of information that CGM brings to characterize 2D TMD nanophotonic systems, including quantitative maps of the real and imaginary parts of the refractive index and optical conductivity.

(1) A. Singh et al. *ACS Photonics* **7**, 3270–3285 (2020)

(2) X. Wang et al. *ACS Appl. Mater. Interfaces* **13**, 26143–26151 (2021)

(3) A. Enrico et al. *ACS Nano* **17**, 8041–8052 (2023)

(4) R. Mupparapu et al. *Adv. Mater. Interfaces.* **7**, 2000858 (2020)

(5) J. P. Thiruraman et al. *Adv. Funct. Materials* **29**, 1904668 (2019)

(6) G. Baffou. *J. Phys. D: Appl. Phys.* **54**, 294002 (2021)

(7) G. Baffou. *ACS Photonics* **10**, 322–339 (2023)

(8) S. Khadir et al. *ACS Photonics* **4**, 3130–3139 (2017)

Keywords: TMD, 2D material, nanophotonics, optics, phase microscopy, QPI, optical spectroscopy, metamaterials, refractive index

*Speaker

3R-2H lateral heterojunctions in bilayer WSe2 grown by CVD

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Transition metal dichalcogenides (TMDs) are a family of two-dimensional (2D) materials with chemical formula MX2 (M= transition metal, X= S/Se/Te). An interesting feature of 2D materials is the various possibilities of their vertical stacking, even between two layers of the same material. Here, we study tungsten di-selenide WSe2 obtained by Chemical Vapor Deposition at C2N, which presents the unusual characteristic of possessing two stable low-energy polytypes in its bilayer (2ML) form. As such, it can be grown either with a non-centrosymmetric orthorhombic (3R) crystal structure, extensively studied for the intriguing physics emerging from its broken inversion symmetry (1), or in the more symmetric hexagonal stacking (2H) configuration (2), characterized by a 60◦ rotation of the top layer.
We focus here on the investigation of 2ML-WSe2 crystals in which we identify possible 2H inclusions in predominantly 3R phase structures, forming 3R-2H lateral heterojunctions that are directly grown by chemical vapor deposition (CVD). With the aid of several experimental means (e.g., micro-Raman, PL, SHG, TEM), we probe the different optical and electronic properties associated with the two distinct stacking orders together with the differences in their crystal structures and associated symmetry. This study allows us to unambiguously discern the two phases in the grown heterostructures and to further investigate the boundary between them.

References:
(1) Z. Zeng, X. Sun, D. Zhang, W. Zheng, X. Fan, M. He, T. Xu, L. Sun, X. Wang, A. Pan, Adv. Funct. Mater., 2019, 29, 1806874. 10.1002/adfm.201806874
(2) K. M. McCreary, M. Phillips, H.-J. Chuang, D. Wickramaratne, M. Rosenberger, C. Hellberg, B. T. Jonker, Nanoscale, 2022, 14, 147-156 . 10.1039/D1NR06119D

Keywords: WSe2, 2D material, CVD growth, TMD, stacking order

*Speaker

Stabilization of magnetic vortices in Fe_5GeTe_2 at room temperature

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A recent work demonstrated ferromagnetic order at room temperature in a 12 nm-thick Fe5GeTe2 film grown by Molecular Beam Epitaxy (1).
A key area of exploration is the effect of patterning on its magnetic state (2), which we address here using micrometric structures of different shapes – squares, discs, and rectangles – lithographed in a Fe5GeTe2 film.

We study these microstructures with scanning NV center magnetometry, a highly effective technique for quantitative and non-perturbative imaging of magnetic textures at the nanoscale, owing to its high magnetic sensitivity of a few $mu\mathrm{T}\sqrt{\mathrm{Hz}}$ and its spatial resolution of about 50 nm. We first demonstrate the stabilization at room temperature of magnetic vortices in various micrometric structures of sizes ranging from 4 down to 1 μm, while smaller objects host a single ferromagnetic domain.
Second, we apply an external magnetic field with a magnitude of 6 mT and observe the vanishing of the vortices. We then extract the saturation magnetization Ms of the material from our images of the stray field generated by the resulting ferromagnetic state. We obtain a value for Ms of about 160 kA/m.
Finally, we observe the re-stabilization of the magnetic vortices after removing the external magnetic field.

This research highlights the potential of the van der Waals magnet Fe5GeTe2 for applications, with the demonstration of the stabilization and manipulation of magnetic vortices at room temperature.

(1) Ribeiro et al, npj 2D Mater Appl 6, 10 (2022)
(2) Li et al, Nano Letters 18, 5974-5980 (2018)

Keywords: Fe5GeTe2, MBE, magnetic vortices, scanning NV center magnetometry

*Speaker

Proximity effect between 2D ferroelectric and 2D ferromagnetic materials

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Recently, molecular beam epitaxy (MBE) has become a powerful tool to grow high quality 2D materials on large areas opening a new route for their integration in spintronic or electronic devices. As an example, the MBE growth of 2D Van der Waals ferromagnetshas been achieved with perpendicular magnetic anisotropy and room temperature Curie temperature (Tc). Those materials are made of atomically thin monolayers weakly bound to each other by van der Waals interaction. In such materials, the number of layers is a key parameter to control the magnetic properties. Post growth annealing constitutes another method to tune magnetic properties by controlling the annealing temperature and duration. Our primary candidate for exploring this effect is Cr2Te3, a 2D vdW ferromagnet. After the growth on graphene, we can modify the Curie temperature (almost 100 K of increase) with in situ annealing while keeping a similar atomic structure. We also found out that using a stable capping layer (alumina) allows us to increase the Curie temperature even higher (up to room temperature) by annealing the film in air. Another promising family of materials are 2D ferroelectrics. One recent example is the 2D layered α-In2Se3 material with polarization both in and out of plane and exhibiting a Tc above room temperature. Moreover, this material also possesses other phases (β and γ) with the same stoichiometry but different electronic properties, which is of great interest for developing new memory devices. This combination of knowledge on 2D vdW ferromagnetic and ferroelectric materials with high Tc lead us toward the development of a multiferroic heterostructure (2D ferromagnet/2D ferroelectrics) working at room temperature, by taking advantage of the proximity effects between the two materials.

Keywords: 2D materials, van der Waals, Molecular beam epitaxy, ferromagnet, ferroelectric, annealing

*Speaker

Synthesis and Decoupling of monolayer 1T FeS2 using alkali metal intercalation

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In this poster, we present the successful synthesis of a novel 2D transition metal dichalcogenide (TMDC), specifically single-layer 1T FeS, achieved through advanced techniques including synchrotron grazing incidence X-ray diffraction (GI-XRD), scanning tunneling microscopy (STM), electron diffraction, and spectroscopy. This material, which does not naturally occur as free-standing atomic layers or thicker mineral forms, has been synthesized using 2D fabrication methods. Our findings reveal that high-quality single-layer 2D FeS with grain sizes surpassing 500 nm can be produced at temperatures as low as 300∘C. The FeS layer displays a commensurate (5x5) moiré superstructure relative to the Au substrate, with a lattice parameter of 3.607 Å. The S-Fe-S layer adopts a 1T stacking arrangement with p3m1 symmetry, exhibiting periodic buckling that results in a (5x5) superlattice relative to Au. The interaction with the Au substrate induces a buckling of the top Au layer, which aligns with the periodic corrugations of the FeS sheet. This interaction not only stabilizes the FeS layer, enabling growth of larger than 500 nm size domains, limited only by step edges of the Au single crystal. Ultimately, we also demonstrate the decoupling of monolayer FeS from the Au substrate through alkali metal intercalation, proving its stability as a free-standing layer.

Keywords: single layer, TMDC, FeS2, GISXRD, STM

*Speaker

Experimental Realisation of 2D Nodal-Line Semimetals

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Topological semimetals are materials having symmetry-protected band crossings at either points (Dirac and Weyl semimetals), or along lines and loops (Dirac Nodal Line semimetal) in the reciprocal space. In the last case, the presence of Dirac nodal lines (DNLs) in a system makes it a good candidate for high-frequency electronic applications due to the possible high-velocity charges carriers arising from the linear band dispersion (1). In addition, their higher density of states near the DNLs compared to Dirac semimetals would make them superior for electronic applications.
However, if calculations have predicted the existence of DNLs in a growing number of systems these last years, the experimental realizations are still sparse, especially for 2D layers (2).

In this presentation, we will concentrate more specifically on Si/Cu and Ge/Cu 2D systems. Although studied for decades, essentially from the point of view of growth mode and surface alloy formation (3) these systems have recently regained interest due to the prediction of DNLs in Cu2Si or Cu2Ge 2D crystals. We will show how, by combining angle-resolved photoemission, scanning tunnelling microscopy and DFT calculation we could evidence the existence of linearly dispersing bands and DNLs in these layers (4). The effect of the 2D layer / substrate interaction and spin-orbit coupling will be also addressed (5).

(1) A.D. Franklin, Science, 349, 6249 (2015)

(2) B. Feng et al., Nat. Commun. **8** 1007 (2017)

(3) See for example: F. Ringeisen et al., J. Vac. Science & Techn. B 1, 546 (1983) and R. Dudde et al., Phys. Rev. B 41, 12 029 (1990)

(4) M. Cameau et al., *2D Mater.* 11 035023 (2024)
(5) M. Cameau et al., Phys. Rev. Materials 3, 4, 044004 (2019)

Keywords: 2D materials, topological semimetals, Dirac nodal lines, photoemission, ARPES, STM

*Speaker

Investigating electronics of MBE-grown 2D materials by momentum microscopy (kPEEM)

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Photoemission techniques are amongst the most powerful, yet not always easily accessible tools to investigate the electronic properties of 2D materials and related heterostructures. Lab-based instruments providing measurements at the microscopic level are becoming necessary for the optimization of the processing steps of such systems and rapid retrieval of fundamental information such as work function, spin-orbit-splitting, interface charge transfer, band offsets and carriers effective mass. Conventional micro-ARPES, often performed at synchrotron radiation facilities does not bring the necessary lateral resolution and flexibility in terms of access time. In previous investigated studies (1-4) performed with photoelectron emission microscopy demonstrated the effective investigations at the micron-scale of 2D materials band structure due to the excellent control of the analysis area and minimal radiation damage. Here, we will present recent results of kPEEM analysis on different MBE-grown 2D materials heterostructures based on graphene and selenide TMDCs, highlighting the performances in terms of size of analysis area and energy resolution close to the thermal broadening. Figure 1 shows some preliminare results obtained by kPEEM analysis on PtSe2 grown on Gr/SiC substrate.
(1) Kim, Chen, Renault, Kis *et al.*, Phys. Rev. B 94 (2016) 081401(R); npj 2D Materials & Applications 2 (2018) 2.

(2) Chen, Kim, Renault, Kis et al., ACS Nano 12 (2018) 11161.

(3) Ferrah, Renault, Bouchiat, Cunge et al., ACS Appl. Nano Mater. 2 (2019) 1356.
(4) Dau, Gay, Renault, Jamet et al., ACS Nano 12 (2018) 2319.

Keywords: TMDC, Graphene, kPEEM

*Speaker

Topological phase transition in bilayer WSe2/III-V heterostructure

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Molecular beam epitaxy (MBE) growth of bilayers two-dimensional (2D) materials on conventional 3D semiconductors gives rise to 2D/3D quasi-van der Waals heterostructures. The importance of these heterostructures depends on the properties of the 2D material used. Thus, the stacking and crystalline structure of the bilayer is an important factor that needs investigation. We report a direct observation of a controllable phase transition in bilayer tungsten diselenide (WSe2) on GaP(111) heterostructure induced by annealing temperature. The crystalline structures of 3R stacking bilayer accompanied by 1T' phase and the 2H phase were characterized using reflection high energy electron diffraction (RHEED). The phase transition mechanism is confirmed using the electronic properties by XPS and ARPES. This temperature-induced crystalline phase transition makes the WSe2 bilayer an ideal platform for controlling topological phase transitions in 2D materials.

Keywords: 2D material, phase transition, electronic band structure, ARPES

*Speaker

Superconductivity in one and two dimensional flat band systems

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Over the past years, we have been witnessing a rapidly growing interest for the physics in flat-band (FB) systems. FBs are dispersionless parts in the electronic spectrum originating from destructive quantum interferences. FBs are at the heart of a plethora of exotic and unexpected physical phenomena, such as topological states, Wigner crystals and an unconventional form of superconductivity of geometric nature. In this presentation, i will present several intriguing and counter-intuitive features associated to this unusual type of superconductivity that takes place in dispersionless bands. I will discuss in particular the connection between FB superconductivity and the concept of quantum metric (QM), which is at the origin of its geometric nature. I will show as well that in contrast to the conventional superconductivity, the FB superconductivity is robust against disorder and dilution effects.

Keywords: flat band, superconductivity, strongly correlated systems, quantum metric, disorder

*Speaker

NN1 - Optomechanics and nanomechanics

Surface Acoustic Waves and Spin Waves interaction: resonance, angle dependence and non-reciprocity

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The emerging field of magnon straintronics promises advancements in beyond-CMOS technology, enabling the design of magnonic logic devices with voltage control over spin wave (SW) amplitude and phase through strain-induced magnon-phonon coupling. Resonant coupling between phonons and magnons in heterostructures of piezoelectric and magnetostrictive materials, conceptualized in the late 1950s, leads to Ferromagnetic Resonance and SW generation, either at magnetic remanence or with a moderate magnetic field. This induces mode hybridization due to magnetoelastic coupling.
Recently, the coupling of surface acoustic waves (SAW) and SW has been observed in SAW-induced Ferromagnetic Resonance (SAW-FMR). Weiler et al. demonstrated this in Ni thin films in the GHz regime in piezoelectric media. Intriguing phenomena involving SWs and phonons are observed at magnetoelastic resonance, such as acoustically-assisted spin pumping and acoustically driven magnetization switching.

We achieved SAW-FMR in Fe epitaxially grown on a GaAs(001) substrate, a spintronic and magnonic compatible magnetoelastic and piezoelectric heterostructure. The dependence of acoustic attenuation and sound velocity on Bext is critical, particularly in the backward configuration when Bext is parallel to the Fe hard axis (110). A phenomenological approach, derived from LLG equations, interprets this dependence with calculated SW dispersion curves. Our model describes the non-reciprocity effect observed when inverting kSAW at SAW-FMR resonance.

To understand the role of magnetic anisotropy and magnetoelastic coupling in SAW-FMR, we implanted N atoms into Fe thin films at low doses, preserving the epitaxial character and manipulating SW spectra. N atom implantation impacts in-plane and out-of-plane magnetic anisotropy in a Fe thin film.

Our study envisions SAW-based magnonic devices where a single IDT provides energy to activate magnetization dynamics and SW propagation in numerous waveguides. Tailoring SW propagation and magnetic anisotropy through ion implantation opens avenues for energy-efficient advanced magnonic devices with enhanced functionalities.

*Speaker

Elliptical micropillars for efficient generation and detection of coherent acoustic phonons

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Elliptical micropillars based on GaAs/AlAs multilayer structures present two non-degenerate optical modes in orthogonal linear polarizations.(1) Due to this property, recent works have reported various applications, e.g., efficient emissions of single photon sources and polarization filtering in Brillouin scattering.(2)(3) Here, we propose using elliptical optophononic micropillars to enhance the efficiencies of coherent acoustic phonon generation and detection in pump-probe experiments. The pump pulses polarized along one axis are tuned with the corresponding optical mode. We enhance the efficiency of phonon generation by maximizing the electromagnetic field inside the cavity. At the same time, as the probe pulses are detuned from the other mode, the detection of reflectivity changes due to the presence of phonons is sensitive. We theoretically studied and experimentally compared the phonon amplitudes in four micropillars with different ellipticities.(4-5) We report an enhancement of a factor of _˜3.1 when comparing the signals from the elliptical and circular micropillars.(5) This improvement achieved by slightly changing the shape of the structures is promising for practical applications in constructing efficient optophononic transducers. (6)(7)

(1) Gayral, B. et al. Appl. Phys. Lett. 72, 1421–1423 (1998)

(2) Gerhardt, S. et al. Phys. Rev. B 100, 115305 (2019)

(3) Rodriguez, A. et al. ACS Photonics 10, 1687–1693 (2023)

(4) Lanzillotti-Kimura, N. D. et al. Phys. Rev. B 84, 064307 (2011)

(5) Xiang, C. et al. arXiv:2310.15271

(6) Castillo López de Larrinzar, B. et al. Nanophotonics 12, 1957–1964 (2023)
(7) O'Brien, K. et al. Nat Commun 5, 4042 (2014)

Keywords: Nanophononics, elliptical micropillars, time, domain Brillouin scattering, pump, probe spectroscopy

*Speaker

Bulk acoustic wave resonators as sensitive probes for solid-state spin defects

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Understanding spin-phonon interactions is essential for solid-state quantum technologies that exploit the spin degree of freedom. Experimental probes for spin-phonon interaction in the quantum regime are therefore needed. We developed a versatile technique to probe the resonant coupling of solid-state spin defects to strain in very wide range of target crystals. Our technique consists in measuring high overtone bulk acoustic wave resonators (HBAR) made out of crystals hosting spin defects, at 50 mK, within a vector magnetic field. By bonding a thin-film lithium niobate transducer onto the target crystal, we couple to its HBAR modes at GHz frequencies. Our fabrication procedure is relatively simple and robust, and yields functional HBAR on a variety of target crystals, with finesses up to 50. On CaWO4 crystals doped with Er3+ ions, we demonstrate the ability to perform acoustic paramagnetic resonance and to unveil the angular dependence of spin-phonon interactions. This technique could be instrumental to identify spin species and crystal hosts suitable to achieve coherent spin-phonon interactions.

Keywords: spin, phonon, HBAR, acoustic paramagnetic resonance, lithium niobate

*Speaker

Watching surface acoustic waves in the GHz range using ultrashort light pulses

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Laser ultrasonics consists of generating and detecting elastic waves in a sample with lasers. The knowledge of the elastic waves' propagation properties is crucial to understanding the sample's mechanical behaviour and determining its elastic properties. Surface acoustic waves (SAWs), in particular, are used in various domains ranging from nondestructive testing and filters to phononic crystals and phononic metamaterials. Laser ultrasonics is the ideal tool for observing SAWs in micrometric samples with GHz-range resonant frequencies thanks to its contactless nature and high spatial resolution.
A typical set-up involves an optical pump-probe technique, with a periodic light pulse source of subpicosecond duration, in order to work in the GHz range. The SAWs are generated by the absorption of light pulses (pump beam) focused on the sample, while they are monitored by delayed light pulses (probe beam) also focused on the sample. By scanning the focused position of the probe beam, two-dimensional imaging can be achieved. A delay line on one of the beams allows one to get time-resolved information. Usual setups are however limited in obtaining signal only at integer multiples of the repetition frequency of the laser (typically _˜80 MHz). This problem is lifted here by modulating in amplitude one of the beams.

In this presentation, we will illustrate this technique in two cases. In the first one, we will detect and image a zero-group-velocity (ZGV) Lamb mode in a silico-nitride plate coated with a titanium film. Such modes have the peculiarity of being stationary, thus locally confining energy and are associated with high quality factor.
In the second example, we will observe whispering-gallery modes in a copper disc. After obtaining the dispersion curves, we will add a spatial-light-modulator (SLM) to shape the laser source to generate chiral surface-acoustic whispering-gallery modes selectively.

Keywords: laser ultrasonics, picosecond acoustics, surface acoustic waves, whispering, gallery, modes, zero, group, velocity Lamb mode

*Speaker

Coherent acoustic phonon transport in optophononic waveguides

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Characterizing acoustic phonon transport is a fundamental step toward manipulating phonon dynamics.(1) Here, by designing a GaAs/AlAs optophononic waveguide, we investigate acoustic phonon exchange between two distinct positions on the waveguide. In the vertical direction, the Fabry-Perot cavity enables strong confinement of acoustic phonons that has been demonstrated in previous works.(2-4) In the lateral direction, the interface between the air and semiconductor acts as an acoustic mirror that reflects phonons, guiding them along the waveguides. We optically generate phonons at one position and track the phonon dynamics by probing them remotely on the waveguides. We report the observation of 20 GHz acoustic phonon transport over 20 μm. The experimental results are in good agreement with numerical simulations based on a finite element method. Our study paves the way for building complex phononic networks and has potential applications in quantum technology and data processing.(5)
(1) Priya et al. Appl. Phys. Lett. 122, 140501 (2023)

(2) Anguiano, S. et al. Phys. Rev. Lett. 118, 263901 (2017)

(3) Rodriguez, A. et al. ACS Photonics 10, 1687–1693 (2023)

(4) Xiang, C. et al. arXiv:2310.15271 (2023)
(5) von Lüpke, U. et al. Nat. Phys. (2022)

Keywords: Nanophononics, coherent phonon generation, phononic waveguides

*Speaker

Time resolved study of two-dimensional phononic crystals based on self-assembled colloidal nanospheres

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Phononic crystals, elastic analogues of photonic crystals, offer significant promise in controlling the propagation of elastic energy, pivotal for applications such as tunable filters, heat management systems, and acousto-optical devices. By directly influencing phonon flow, phononic crystals enable control over thermal conductivity. Colloidal self-assembly provides a cost-effective method to engineer phononic crystals with desired properties (1,2). Here, we investigate the hypersonic phononic properties of self-assembled two-dimensional colloidal crystals composed of polystyrene (PS) nanospheres on a silicon substrate. We demonstrate the tunability of hypersonic phononic bandgaps by varying the interactions between neighbouring PS nanospheres. Ultrafast pump-probe transient reflectivity techniques were employed to explore phononic modes across different frequency ranges (3). Phonon transport in the samples was analyzed using the pump-probe method, confirming the phonon insulating properties. The experimental observations are well-supported by a finite element method model. These findings highlight the potential of self-assembled colloidal crystals for creating tunable hypersonic phononic insulators, paving the way for advanced phononic applications.

(1) W. Cheng, J. Wang, U. Jonas, G. Fytas, and N. Stefanou, *Observation and Tuning of Hypersonic Bandgaps in Colloidal Crystals*, Nature Mater **5**, 830 (2006).

(2) B. Graczykowski, N. Vogel, K. Bley, H.-J. Butt, and G. Fytas, *Multiband Hypersound Filtering in Two-Dimensional Colloidal Crystals: Adhesion, Resonances, and Periodicity*, Nano Lett. **20**, 1883 (2020).

(3) M. Hiraiwa, M. Abi Ghanem, S. P. Wallen, A. Khanolkar, A. A. Maznev, and N. Boechler, *Complex Contact-Based Dynamics of Microsphere Monolayers Revealed by Resonant Attenuation of Surface Acoustic Waves*, Phys. Rev. Lett. **116**, 198001 (2016).

Keywords: colloidal crystals, nanophononics, pump, probe

*Speaker

A radiofrequency superconducting qubit for quantum control of ultracoherent mechanical resonators

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Superconducting qubits are a powerful platform to probe various quantum phenomena, when coupled to a different physical system, for instance a mechanical resonator mode (1). The most popular superconducting qubit-the transmon-operates at a frequency of several GHz: a microwave signal at this frequency excites transitions between the two qubit states, and can be used to implement quantum logic gates. However, the fact that most of superconducting qubits operate in the GHz frequency domain limits the class of systems they can interact with. Building upon the heavy fluxonium qubit architecture (2), we have developed a superconducting qubit with an unprecedentedly low transition frequency of 1.8 MHz (3). Notably, we have demonstrated a qubit with a coherence time exceeding 30 μs, the ability to prepare the qubit in a pure state with 97.7% fidelity, and single-shot readout capability. Moreover, by detecting a weak charge modulation by repeated qubit interrogation, we demonstrate the high-sensitivity of this qubit to a nearly resonant electric charge modulation, proving its potential in a hybrid quantum system. We will finally present our recent efforts to achieve the resonant (strong) coupling regime between this qubit and an ultra-coherent softly-clamped mechanical membrane mode. In this device, the mechanical mode is a defect mode of a high stress phononic crystal membrane, that we characterize with a motorized optical interferometer (4). It has a frequency of a few MHz, matching that of the qubit, and a quality factor reaching hundreds of millions at cryogenic temperature. This hybrid quantum system could be used to observe macroscopic quantum phenomena. (1) Y. Chu et al. *Nature* 563, 666 (2018).
(2) H. Zhang et al. *Physical Review X* 11, 011010 (2021).
(3) Najera-Santos et al. *Phys. Rev. X* 14, 011007 (2024)
(4) Ivanov et al. *Appl. Phys. Lett.* 117, 254102 (2020)

Keywords: phononic crystal, superconducting qubit, hybrid quantum system, quantum sensing

*Speaker

Micro-oscillators as Maxwell Demons

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In my talk I will present a system we developed to study thermodynamics at the scale of the fluctuations. Our system is built around a micro-cantilever in air, on which we act using a fast acting feedback loop. By changing the logic of our feedback, this provides us with a very versatile model system for the study of nanoscale thermodynamics in the underdamped regime.
Among the possible applications, this system is well-suited to the study of famous paradoxes of thermodynamics such as Maxwell Demons, where energy is extracted from a single heat bath in apparent violation of the second law. The underdamped nature of our system allows us to operate the cycles with minimal loss and find the optimal regime for energy extraction. In order to lift the paradox I will introduce the concept of information and show how it can be used to quantify the efficiency of such information engines.

Keywords: micro oscillators, stochastic thermodynamics, Maxwell Demon, information theory

*Speaker

Hyperspectral Electromechanical imaging at the nanoscale: Dynamical backaction, dissipation and quantum fluctuations

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Nanomechanical systems have tremendously developed over the past two decades, becoming essential both in science and technology. The sensing supremacy of nanomechanical systems stems from their extremely low mass, combined with a low mechanical dissipation made possible by the recent, impressive progress in nanomechanical engineering and fabrication.
Owing to their very reduced dimensions, nanomechanical devices generally display very high thermal resistances, resulting in a strongly enhanced response to thermal phenomena, that is notably suspected to represent major limitations in developing ultra-coherent nanomechanical transducers. However, the fundamental consequences of this enhanced thermal behaviour remain essentially unknown, their experimental investigation requiring an instrumentation enabling to sample the nanomechanical thermal response at the nanometre scale.
We report a new scanning thermomechanical microscopy platform enabling to both heat and acquire the fluctuations of mechanical nanostructures with nanometric resolution. We use this platform to image the nanomechanical noise response of a 40 nm diameter nanowire while scanning a localized heat source across its surface. We develop a thermal backaction model, which we use to demonstrate a close connection between the structure of the nanowire, its thermal response, its dissipation and its fluctuations. We notably identify the presence of a localized thermoelastic defect, which we demonstrate behaves as a single fluctuation hub, whose e-beam excitation yields a far off-equilibrium vibrational state, largely dominated by the quantum fluctuations of the heating source. Our platform is of interest for future development of ultra-low loss nanophononic devices, and appears as a new playground for investigating quantum thermodynamics in the strongly dissipative regime and at room temperature.

Keywords: nanomechanics, nanothermics, thermodynamics, quantum measurement, electron beam microscopy, nanowires, nanomaterials

*Speaker

Wide-band, tunable and high-efficiency microwave-to-acoustics transduction on lithium niobate

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Acoustic waves play an essential role in a wide variety of quantum systems such as microwave-to-optics transducers, quantum acoustics devices or devices using strain to couple to spin defects. For surface acoustic waves and Lamb waves, control and detection are commonly achieved using interdigital transducers (IDTs) on piezoelectric materials. However conventional IDTs are either inefficient or have narrow bandwidth and are not tunable in-situ.
Here we demonstrate an acoustic transducer showing both high efficiency ($> 50\%$) and wide bandwidth (hundreds of MHz), as well as in-situ tunability in the 4-8 GHz band. This transducer is based on IDTs fabricated on suspended lithium niobate, integrated with SQUID arrays on Si. We pattern lithium niobate structures to obtain basic acoustic networks such as waveguides and resonators for Lamb waves. On the other hand, SQUID arrays serve as tunable matching circuits for the IDTs.
This technique is directly compatible with the quantum toolbox of superconducting circuits (parametric amplifiers, photon counters, etc.) and completes it with a highly sensitive acoustic probe. Among other experiments, it could be used to perform the acoustics spectroscopy of 2D-material or to sense phonons emitted by spin relaxation.

Keywords: Superconducting quantum circuits, Acoustic transduction, impedance matching

*Speaker

NEMS reservoir computing with high memory capacity

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Physical reservoir computing is a type of artificial neural network where the dynamic of a physical nonlinear system called reservoir is exploited for information processing. Among the various physical systems proposed for the reservoir, Nano Electromechanical Systems (NEMS) have often been considered in recent studies, thanks to their intrinsic nonlinear behavior and energy efficiency.
The use of a single NEMS resonator for reservoir computing has already been demonstrated. It consists in driving the resonator in nonlinear regime and at a fixed frequency. To perform the processing, the input signal is used to modulate the amplitude of the drive force that generates the vibration of the device. We then measure its transient response, and multiply it with a trained readout function that gives the final output. To add memory, a feedback loop composed of the delayed response of the system is required in the experimental set-up.

In order to test the performance of the system, several benchmarks have been proposed in the literature. One of them called "Parity Benchmark" consists in computing from a simple training, the product of the last "n" samples of a random binary sequence (alternating between -1 and 1).
Due to the low memory capacity of the classic experimental set-up, we have always reported a decreasing success rate for this test as the level "n" increases. In order to overcome this limitation, we propose in this work a new set-up including multiple delayed feedbacks. Simulation results show that for high value of "n", only the system having "n-1" feedbacks has the highest success rate, thus proving a link between the number of feedbacks and the memory capacity.

Keywords: Reservoir computing, nanomechanical resonator

*Speaker

NN3 - From single molecule to supramolecular or polymerized layer on surfaces

Exploring synthetic carbon allotropes on surfaces: from metallated graphdiyne to nanoporous graphene structures

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Elemental carbon exists in two natural allotropes, diamond and graphite. Synthetic carbon allotropes such as fullerenes, carbon nanotubes, graphene and graphyne represent a growing family of fascinating architectures with outstanding properties (1). Several of these 2D materials can be synthesized on surfaces.
Firstly, I will report direct evidence of band formation in on-surface synthesized metallated Ag-Graphdiyne (Ag-GDY) sheets with mesoscopic regularity (2). Employing scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission spectroscopy, the formation of valence and conductions bands are observed. Furthermore, density functional theory (DFT) calculations corroborate these observations and reveal that doubly degenerate frontier molecular orbitals on a honeycomb lattice give rise to flat, Dirac and Kagome bands close to the Fermi level. DFT also indicates an intrinsic band gap for the pristine material, which is retained for a bilayer with *h*-BN, whereas adsorption-induced in-gap electronic states evolve at the synthesis platform with Ag-GDY decorating the (111) facet of silver.

Secondly, I will focus on exploring on-surface synthesized porous graphene nanoribbons (GNRs) and nanoporous graphene (NPG) structures (3). In particular, I will show that when the electronic properties are measured with STS, these measurements are subject to a wave function decay into the vacuum that masks the undisturbed electronic orbital shape. We use Au(111)-supported gulf-type GNRs and NPGs as model systems fostering frontier orbitals that appear confined along the edges and nanopores in STS measurements. DFT calculations confirm that these states originate from valence and conduction bands. The deceptive electronic orbital confinement observed is caused by a loss of Fourier components, corresponding to states of high momentum. This effect can be generalized to other 1D and 2D carbon-based nanoarchitectures.

(1) A. Hirsch *et al.* Nat. Mater. **9**, 868 (2010)

(2) I. Piquero-Zulaica *et al.* Adv. Mater. 2405178 (2024)

(3) I. Piquero-Zulaica *et al.* Nat. Commun. **15,** 1062 (2024)

*Speaker

Keywords: Nanoporous graphene, graphdiyne, STM/STS, ARPES, on surface synthesis

Self-assembled monolayer of push-pull chromophores towards the polarization modulation for controlled detection of biomolecules

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The specific detection of antibodies using antibody/antigen binding interactions has been the subject of numerous studies in the field of biosensors(1-3). Notably, a promising functional ON/OFF-system has been proposed based on the reversible modification of the conformation of a charged oligopeptide by the application of an electrical potential on the surface, thus making it possible to control the antibody-antigen interaction(4). So far, this system can only respond to a single electrical stimulus, thus limiting its use to a single antibody/antigen pair and preventing the detection of the binding interaction of several antibody/antigen pairs within a single platform. For this purpose, we are considering an original approach based on the use of "push-pull" chromophores to control the potential allowing the conformation of the oligopeptide to be switched between the OFF-state (antibody-antigen interaction not allowed) and the ON-state (interaction permitted). This structure of the push-pull chromophores forms an electrical dipole depending on the nature of the donor and attractor groups, and the π-conjugated bridge. The idea is to add push-pull chromophores presenting different electrical dipole moments -each one being associated to a specific electrical potential value- between the surface and the oligopeptide supporting a given antigen, and to insert these systems within an inert matrix of molecular compound of oligoethylene glycol(OEG). Therefore in this work we have synthesized original non-charged push-pull chromophores bearing a thiol anchroring group, and studied their self-assembled monolayers (SAMs) on gold surfaces. After having analysed the influence of the various parameters (solvent, concentration,...) on the quality of homogeneous push-pull films, we have devoted our work to the preparation of SAMs made of isolated push-pull chromophores inside the OEG inert matrix testing various approaches and parameters.

1.Casalini,*et_al.*,*ACSNano***2015**,9,5051

2.Marquette,C.A;Blum,L.J.*Biosens.Bioelectron.***2006**,*21*,1424

3.Wen,W.*et al.*,*Anal.Chem.***2017**,*89*,138

4.Santos-Gomes,B.*et_al.*,*ACSAppl.Bio.Mater.*,**2018**,*1*,738

Keywords: push, pull chromophore, ferrocene, oligopeptide, oligo(ethylene glycol), self, assembled monolayer

*Speaker

UV induced on-surface deoxygenation: the case of dibromo-sulfoxides on 2ML NaCl(100)/Au(111)

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Due to their rich in-solution chemistry, sulfoxide derivatives are promising reagents for the development of new chemical tools for on-surface synthesis. Among them, dibenzothiophene S-oxide (DBTO) is known to undergo S=O bond cleavage under UV irradiation in the solvent (1), along with the generation of dibenzothiophene and atomic triplet oxygen O(3P). This study provides evidence of on-surface deoxygenation of a dibrominated sulfoxide derivative (ortho-Br)2-DBTO under UV irradiation.
The molecules were first deposited on the Au(111) surface. Non-contact AFM intramolecular imaging of an isolated molecule with a CO-functionalized tip at 9.8 K allows identification of its configuration adsorption, which is confirmed by DFT calculations as well as particle probe models. (2)
The behavior of a supramolecular phase of molecules adsorbed on two mono-layers of NaCl / Au(111) under illumination (UV 280 nm) was then investigated. High-resolution images show that 36% of molecules were successfully deoxygenated upon 190 minutes of irradiation. The structural characterization is completed by a series of bias spectroscopies measured on top of the S atom of several molecules chosen among a statistical set of pristine/deoxygenated molecules. Deoxygenated molecules exhibit increased contact potential difference (CPD), pointing towards a more negative charge state of the S atom, consistently with a deoxygenated state. References:
(1) Mrinmoy Nag and William S. Jenks, "Photochemistry of Substituted Dibenzothiophene Oxides: The Effect of Trapping Groups", J. Org. Chem. 70 (9), 3458-3463 (2005)
(2) http://ppr.fzu.cz/

Keywords: onsurface synthesis, sulfoxide derivatives, UV induced onsurface deoxygenation, supramolecular phase, Scanning probe microscopy, CO functionalized tip .

*Speaker

Anomolous growth of ClAlPc submonolayer films on Au(111) investigated at room temperature

Edward Dunn * [1], Victor Vaillant [1], Nesrine Shaiek [1], Stéphane Lenfant [1], Nataliya Kalashnyk [1]

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Phthalocyanines are stable, optically active molecules with a core which can host a variety of metallic ions (1). As a result, the conformation of planar phthalocyanines has been widely studied for the formation of light-emitting or light-absorbing thin films where a suitable core can be chosen to select appropriate properties. In ClAlPc the Cl atom projects out of the plane of the molecule presenting two conformations on the surface, Cl-up and Cl-down, which determine the direction of the dipole between the Cl and the Al in the core. Such non-planar varieties offer the possibility to vary the potential of the surface by switching between two states using voltage pulses (2) or ultraviolet radiation (3), acting as a form of molecular switch. Previous work with low temperature (LT) scanning probe microscopy (STM) and room temperature (RT) ultraviolet photoemission spectroscopy (UPS) (4) have been used to identify the common characteristics of ClAlPc on coinage metal surfaces. In this study we show through RT STM that, contrary to existing reports (5), stable sub-monolayer films of ClAlPc can be observed at room temperature on Au (111), even at relatively low coverages. In these films ClAlPc adsorbs Cl-down, unlike the reports from cryogenic temperature studies. In addition, we identify a consistent set of frequently observed defects, a third molecular adsorption conformation and the unusual growth of a second layer before the completion of the first.

(1) Gottfried J. M. *Surface Science Reports*, **70**, 3, 259-379, 2015.

(2) Huang Y. L. et al. *Small*, **8**, 9, 1423-1428, 2012.

(3) Arumugam et al. *Applied Surface Science*. **493** 1090-1097, 2019

(4) Huang Y. et al. *Phys. Rev. B*, **87**, 085205, 2013.
(5) Matencio S. et al. *J. Phys. Chem. C*, **122**, 16033-16041, 2018.

Keywords: phthalocyanine, switch, STM

*Speaker

Bottom-Up Synthesis of Graphene Nanomeshes: Overcoming Challenges in Lateral Fusion of Nanoribbons.

Elie Geagea * [1], Daniel Medina-Lopez [2], Luca Giovanelli [1], Laurent Nony [1], Christian Loppacher [1], Stéphane Campidelli [2], Sylvain Clair [1]

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The exceptional electronic, optical, and mechanical properties of graphene inspire significant scientific interest, both fundamentally and for applications. When graphene is reduced to nanometric sizes, it forms nanoribbons or nanoparticles, which exhibit distinct properties such as a bandgap. Beyond size reduction, creating a regular network of holes in a 2D graphene structure, known as a graphene nanomesh (GNM), can also open a bandgap, forming a new 2D semiconductor. While initial GNMs were produced using a top-down approach, this method lacks precise control over hole size, spacing, and edge states. To achieve atomic-scale precision in GNMs, a bottom-up approach is necessary.
Our strategy involves two key steps: first, the growth of one-dimensional (1D) graphene nanoribbons (GNRs) with precise molecular design control; second, the lateral fusion of these ribbons to form the desired nanomesh with controlled porosity and geometry. However, this fusion reaction is highly challenging and faces constraints that result in limited fused nanomeshes with numerous defects.
In this study, we investigate the reaction mechanism of a chevron-like precursor in ultrahigh vacuum (UHV), on the Au(111), Ag(111), and Cu(111) surfaces, to elucidate the factors hindering successful lateral fusion. We aim to understand the mechanism of the reaction and the reasons behind these constraints. Based on our findings, we propose an alternative fusion route through strategic molecular design that combines Ullmann coupling reactions and deoxygenative fusion. This approach seeks to enhance the efficiency and quality of the lateral fusion process, paving the way for more effective fabrication of graphene nanomeshes with desired properties.

Keywords: Graphene Nanomesh, STM, UHV

*Speaker

Effect of dipolar interactions on the relaxation rate of ferromagnetic nanoparticles in a 1D chain : Monte Carlo investigation versus analytical approach

Denis Ledue * [1]

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The relaxation rate of ferromagnetic nanoparticle assemblies plays a key role in numerous applications, such as, for instance, magnetic hyperthermia. In this context, it has been shown that one-dimensional (1D) assemblies open promising routes. However, before developing applications, it is important to understand the underlying physics at play, and in particular, the parameters that control the dynamics of these magnetic systems. In this work, we study the relaxation rate of 1D chains of magnetic nanoparticles, with long-range dipolar interaction, thanks to time step quantified Monte Carlo (MC) simulations and compare the MC results to analytical developments based on Langer's theory. Each nanoparticle exhibits uniaxial anisotropy with an easy-axis aligned along the chain direction. Two cases, relevant to experimental situations, are inspected: the applied field is parallel to the chain (longitudinal case) or perpendicular to it (transverse case). In both cases, we obtain good qualitative agreement between analytical and numerical results, which evidence that dipolar interactions decrease the relaxation rate with a more pronounced effect in the transverse field case. As shown by the analytical formulas, such a decrease can be explained by an increase of the energy barrier in presence of dipolar interactions. The quantitative agreement between analytical and MC data is better for the longitudinal field case, as the dipolar and applied fields cooperate, whereas they compete in the transverse field case.

Keywords: Ferromagnetic nanoparticles, Relaxation rate, Dipolar interactions, Monte Carlo simulations, Langer's theory

*Speaker

Why are dipolar interactions demagnetizing in a randomly distributed assembly of nanoparticles?

Alexandre Tamion * [1], Florent Tournus [1], Véronique Dupuis [1]

[1] institut Lumière Matière – CNRS : UMR5306, Université Claude Bernard - Lyon I – France

The miniaturization and densification of magnetic objects have rendered magnetic dipolar interactions (DIs) a parameter that can no longer be neglected in various fields such as magnetic resonance imaging (MRI), nano-oscillators, hyperthermia, ferrofluids, etc. DIs between magnetic objects often present a major challenge from both fundamental and applied perspectives. The properties of magnetic objects can be drastically altered, preventing the precise determination of their intrinsic properties (e.g., anisotropy, reversal field). In an assembly, the simplest and most commonly used experiment to observe magnetic interactions involves plotting the Im parameter proposed by Wohlfarth in 1958. This Im parameter is derived from IRM and DcD measurements (Isothermal Remanent Magnetization curve and Direct Current Demagnetization curve) conducted at low temperatures when the nanoparticles (NPs) are in the blocked regime (Im = DcD - (mr - 2IRM)). A negative Im corresponds to demagnetizing interactions, while a positive Im indicates magnetizing interactions. Since the early 2000s, a consensus has formed in the scientific community: a negative Im is attributed to the presence of dipolar interactions, whereas a positive Im is attributed to the presence of exchange interactions between magnetic objects. Considering a mean dipolar field (magnetostatic theory) leads to a negative Im when the magnetic field is applied perpendicular to the plane of the assembly and positive within the plane. Experimentally, the Im measured in an assembly of macrospins is negative in both measurement directions, which is in complete contradiction with magnetostatic theory. This experiment serves as the starting point of this study, aimed at addressing the simple question: Why are dipolar interactions demagnetizing in a randomly distributed assembly of NPs?

Keywords: Nanoparticule, magnétisme, macrospin, interaction dipolaire

*Speaker

Exploring the Role of Dipole-Dipole Interactions and Assembly Shape in Magnetic Hyperthermia: Towards Optimized SAR

Abdelhamid Morjane † [1,2], Francois Vernay [1], Vincent Russier [2]

[1] Université de Perpignan Via Domitia – Laboratoire PROMES-CNRS – France
[2] Institut de Chimie et des Matériaux Paris-Est – Université Paris-Est Créteil Val-de-Marne - Paris 12, Centre National de la Recherche Scientifique – France

Magnetic hyperthermia is a process that converts electromagnetic energy into heat by applying an external alternating magnetic field to magnetic nanoparticles (MNPs). The efficiency of magnetic hyperthermia is measured by an observable known as the Specific Absorption Rate (SAR), which quantifies the power absorbed by a magnetic assembly subjected to ac magnetic field and therefore re-emitted as heat.
Several parameters are crucial for optimizing the SAR to control heat production (1). One of our aims is to clarify the role of DDI in the magnetic hyperthermia process and to determine the conditions under which the SAR is either reduced or enhanced. To achieve this, we employ two complementary approaches. The first approach is a semi-analytical method based on perturbative calculations that is only suitable for low-density samples. Yet, it allows to pinpoint what are the key parameters to tune the SAR. The second approach is Monte Carlo simulations which are used to investigate samples with high concentrations of nanoparticles.

Using semi-analytical approaches within the framework of Debye theory (2), we aim to clarify how the assembly external shape influences SAR. In particular, we explore the effect of DDI strength in different assembly shapes, understanding their role in modifying the hysteresis behavior and heat generation. We also investigate the effect of the intrinsic nanoparticle's properties by combining uniaxial and cubic magnetocrystalline anisotropies as a possible effect of the intrinsic cubic symmetry of the iron oxide NP. By comparing results from semi-analytical methods and Quantified Time Monte Carlo simulations, we aim to identify the critical parameters that synergistically optimize the (SAR).

(1) B. Mehdaoui *et al* . Adv. Funct. Mater. 2011, 21 ; H. Gavilan *et al.* Chem. Soc. Rev. **50**, 11614 (2021); J.G. Ovejero *et al.* Materials, **14**, 6416 (2021).
(2) J-L Déjardin et al Journal of Applied Physics, 2017, 121.

Keywords: Magnetic hyperthermia, Dipole Dipole interaction, Specific Absorption rate

†Speaker

Measuring AC susceptibilities of magnetic nanoparticles assemblies and quantifying time with Monte Carlo simulations.

Jean-Guillaume Malherbe * [1], Vincent Russier *

[2], Juan-Jose Alonso [3]

[1] Institut de Chimie et des Matériaux Paris-Est – Université Paris-Est Créteil Val-de-Marne (UPEC) – France
[2] Institut de Chimie et des Matériaux Paris-Est – Centre National de la Recherche Scientifique – France
[3] Departamento de Fisica Aplicada [Malaga] – Spain

Studying the response to an external AC field of magnetic nanoparticles (MNP) assemblies is of practical interest for applications such as hyperthermia as example. After evaporating the solvent the MNP agregate in frozen ordered or disordered structures. Here we consider MNP smaller than the critical size for the single domain regime. From a theoretical point of view, they can be studied through an effective one spin model including both the magnetocristalline energy and a coupling between the dipoles.
The response to the AC field is obtained from the in and out of phase susceptibilities χ'(ω) and χ"(ω). Those quantities can be computed with time quantified Monte Carlo (MC) simulations (1). In such processes, the natural time unit is a simulation time step and the frequency of the AC field is set from this reference.

Here we will discuss how it is possible to map this simulation time unit with the experimental one and how results from different MC schemes compare. Both the rule of the relaxation time of individual particles as a quantity for measuring time and the minimal set of microscopic parameters necessary to quantify time in our simulations will be discussed. Different cases will be considered ranging from independent particles to long range interacting ones. This study will give new insights for distinguishing between individual and collective behavior with regard to dynamical properties of MNP assemblies.

(1) J.-O. Andersson et al. Phys. Rev. B **56**, 13983 (1997); U. Nowak et al. Phys. Rev. Let. **84**, 163 (2000); P.V. Melenev et al. Phys. Rev. B **86**, 104423 (2012).

Keywords: Time qantified Monte Carlo, AC Susceptibilities, Magnetic Nanoparticles

*Speaker

30 October 2024, morning

Plénière 8h30 - 9h20
Benoît Roman
Grand Amphi

Plénière 9h30 - 10h20
Frédéric Mila, prix Charpak-Ritz
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

3 Semi-plénières
11h10 - 12h00

Thomas Cornélius	**Christopher Bäuerle**	**Cécile Monteux**
SciencesNat	Charve	Massiani

Déjeuner 12h00 - 13h20
Salle de conférence †

†All rooms with a number are located in building 15

Plenary

Benoît Roman

PMMH ESPCI

Shape-changing : geometry and instabilities of acctive materials

We can witness everyday in Nature the fascinating process of self- shaping systems : organs form, plants grow, leaves develop, flowers bloom with amazing control of complex shapes. This morphogenesis is due to the advent of specific spatial distribution of internal active forces (or strain).
In stark contrast, the many manufacturing techniques developed by human all rely on making sure that the materials used are homogeneous passive, and applying external forces that impose the shape from outside.
Could we mimic morphogenesis with physical systems?
This talk will discuss the physics of self-shaping, which involves geometry, instabilities and inverse problems, review examples of "programmable active materials "designed for shape- morphing, and mention possible applications.

Plenary

Milla Frédéric

Ecole Polytechnique Fédérale de Lausanne, Switzerland

New challenges in quantum magnetism

Quantum magnetism has played a very important role in the twentieth century, with milestones such as Bethe's solution of the spin-1/2 Heisenberg chain in 1931, spin- wave theory in 1952, or the discovery of the Haldane gap in spin-1 chains in 1983. The field is far from closed however, and several basic models of frustrated quantum magnetism are still heavily debated. In view of their potentially quite exotic properties, quantum magnetism has emerged as one of the favourite platforms to investigate quantum matter, with already several successes among which the discovery of new quantum phases such as spin nematics, spin supersolids, or fractional magnetization plateaus. Yet the best is still probably to come, and after a quick review of these successes, I will discuss some of the challenges the field is still facing, including the definitive solution of some paradigmatic models of frustrated quantum magnetism such as the Kagome spin-1/2 antiferromagnet or the experimental identification of quantum spin liquids with non-trivial topological properties.

Semi plenary

Thomas Cornelius

IM2NP UMR 7334 CNRS, Aix-Marseille University, Marseille, France

Functional materials in the light of *in situ* synchrotron X-ray diffraction

The functional properties of materials are strongly influenced by their crystalline state, including strain and defects. While strain and defects can sometimes be detrimental to these properties, their controlled application allows for elastic strain engineering and defect engineering. At the nanoscale, it has been shown that nanomaterials can exhibit ultra-high yield strength before entering the plastic regime, opening new possibilities for elastic strain engineering.

To better understand how crystalline structure, strain, and defects affect material properties at the nanoscale, it is essential to investigate these parameters under various external stimuli. X-ray diffraction is an ideal tool for studying the structure-property relationship due to its high sensitivity to crystalline structure, strain, and defects. Recent advancements in focusing optics at synchrotron sources now enable hard X-ray beams to be routinely focused down to the sub-100 nm scale, facilitating nanoscale or individual nanostructure characterization. *In situ* and *operando* measurements allow for real-time monitoring of structural variations in materials under mechanical stress, electrical fields, or thermal excitation. Furthermore, the current upgrades of 3^{rd} generation synchrotrons to extremely brilliant 4^{th} generation sources have increased the coherent flux by one to two orders of magnitude, significantly enhancing coherent X-ray diffraction imaging methods. This work showcases *in situ* studies of the structural properties of materials using synchrotron X-ray diffraction methods, particularly during the application of mechanical or electrical stresses to ferroelectric materials and individual micro- and nanostructures.

Semi plenary

Christofer Bäuerle

Université Grenoble Alpes, CNRS, Institut Néel, Grenoble, France

Flying interacting electrons and their potential for quantum technologies

Decades of intensive research have been devoted to the precise control of single electrons, essential for establishing the electrical current standard in the SI unit system. Recently, the concept of flying electron qubits has emerged where the charge or spin degree of freedom of an electron are used as qubits that are manipulated and transported through electronic circuits using simple electromagnetic fields. Challenges remain, including high-fidelity control and scalable quantum circuit design.
In this talk, I will present the latest advances in single electron transport [1]. We will discuss two complementary methods for transporting single charge carriers through quantum electronic circuits.
Firstly, electrons are isolated from the Fermi sea and transported using sound waves [2,3], achieving a transport fidelitiy above 99% [4,5] and enabling single particle collision experiments [6]. The partitioning statistics of the two-electron state reveals a clear antibunching effect that could be quantitatively attributed to Coulomb repulsion. This work has been recently extended to the partitioning of a multi-electron state containing up to five electrons.
Secondly, electrons propagate along the surface of the Fermi sea in the form of an ultrashort electron wave packet. We find that the coherence is enhanced compared to the DC case, paving the way for a plethora of new quantum experiments at the single electron level. By elucidating these breakthroughs, we aim to contribute to the ongoing efforts in harnessing single electrons for quantum information processing and advancing our understanding of quantum phenomena at the nanoscale.

References

[1] C. Bäuerle et al., Reports on Progress in Physics 81, 056503 (2018)
[2] H. Edlbauer et al., Applied Physics Le4ers 119, 114004 (2021)
[3] B. Jadot et al., Nature Nanotechnology 16, 570 (2021)
[4] S. Takada et al., Nature Communica:ons 10, 4557 (2019)
[5] J. Wang et al., Physical Review X 12, 031035 (2022)
[6] J. Wang et al., Nature Nanotechnology 18, 721 (2023)

Semi plenary

M. Alaa Eddine [1], S. De Chateauneuf Randon [1], D. Radajewsky [1] B. Bresson [1],

T. Salez [2], C. Lecoeur [3], C. Lorthioir [4], S. Belbekhouche, [3] and

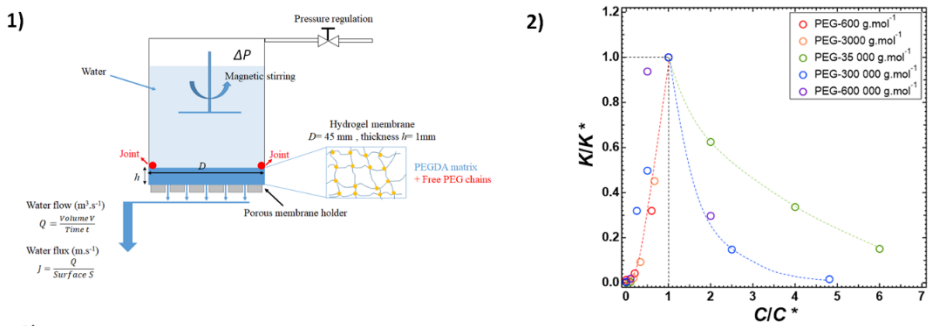
Cecile Monteux [1] ‡

[1] ESPCI Paris, France
[2] Université de Bordeaux, France
[3] ICMPE, Université Paris Est, France

[4] Phenix, Sorbonne Université, Paris, France

Filtration and selective retention through hydrogels

Pressure-driven membrane technologies, such as microfiltration, ultrafiltration, nanofiltration and reverse osmosis, have proven their effectiveness in a broad range of water treatment applications [1]. Hydrogels, which are networks of polymer chains in water, have been the subject of recent work in the context of filtration [3]. For example, thin coatings of hydrogels (<100 nm thick) deposited on classical filtration membranes allow to increase the hydrophilicity of the membranes and to decrease their fouling by hydrophobic proteins [4]. An important remaining challenge is to control the selectivity and permeability of the hydrogels. We have developed a series of hydrogels of controlled permeability obtained by a simple and robust method. We photopolymerize poly(ethylene glycol) diacrylate, (PEGDA) under UV light in the presence of non-crosslinkable PEG free chains.
We find that the PEG chains are trapped in the matrix and nevertheless enable to increase the permeability by orders of magnitude [5,6]. To account for this behavior we suggest that the PEG chains induce nanodefects in the cross-linking density that controls the permeability of water through the hydrogels. Furthermore taking advantage of the fact that the free polymer chains are trapped in the PEGDA hydrogels we vary the type of free polymer chains to functionalize our hydrogels and selectively retain solutes through hydrogel bonds or electrostatic interactions. This study opens new perspectives for the design of flexible hydrogel membranes with controlled permeability and their application in water treatment and bioseparation.



‡Corresponding author

[1] Petersen, R.J., Composite reverse osmosis and nanofiltration membranes. Journal of Membrane Science, 1993. 83(1): p. 81-150.
[2] Kayvani Fard, A., et al., Inorganic Membranes: Preparation and Application for Water Treatment and Desalination. Materials (Basel), 2018.
[3] Tokarev, I. and S. Minko, Stimuli-responsive porous hydrogels at interfaces for molecular filtration, separation, controlled release, and gating in capsules and membranes. Adv Mater, 2010. 22(31): p. 3446-62.
[4] Fu, W., et al., Highly hydrophilic poly(vinylidene fluoride) ultrafiltration membranes modified by poly(N- acryloyl glycinamide) hydrogel based on multi-hydrogen bond self-assembly for reducing protein fouling. Journal of Membrane Science, 2019. 572: p. 453-463.
[5] Large and non linear permeability variations of hydrogels by addition of polymeric additives, M. Alaa-Eddine, S. Belbekhouche, S. De Chateauneuf Randon, T. Salez, B. Bresson, C. Monteux, Macromolecules, 2022,10.1021/acs.macromol.2c01462. **hal-03767505v1**
[6] Sieving and clogging in PEG/PEGDA hydrogel membranes, ALAA EDDINE, M. De Chateauneuf Randon, S. ; Bresson, B.; Belbekhouche, S.; Monteux, C. Langmuir, 2023 **hal-04240879v1**

30 October 2024, afternoon

3 Semi-plénières
13h20 - 14h10

Amélie Juhin, prix Ancel SciencesNat	**Freek Massee** Charve	**Véronique Lazarus** Massiani

Mini - colloques 4
14h30 - 16h30

SMMP4_4 Massiani	**NN2_1** 405	**2DMS1_2** 207
SMMP5_1 Charve	**BAM3_2** 407	**2DMS3_1** 208
SMMP6_4 SciencesNat		**IA2** 206

Café 16h30 - 17h15
Salle de conférence + 204 + 404

Mini - colloques 5
17h15 - 18h45

SMMP3 Massiani	**NN2_2** 405	**MP1** 201
SMMP5_2 Charve	**NN5_1** 408	**2DMS5_1** 205
	BAM1_1 SciencesNat	**PSI2** 203
	BAM4_1 407	**2DMS3_2** 208

GALA 19h30 - 23h00

§

§All rooms with a number are located in building 15

Semi plenary

M. Alaa Eddine [1], S. De Chateauneuf Randon [1], D. Radajewsky [1] B. Bresson [1], T. Salez [2], C. Lecoeur [3], C. Lorthioir [4], S. Belbekhouche, [3] and

Amélie Juhin ¶ [1]

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How the symmetry of x-rays reveals the asymmetry of matter

X-ray spectroscopies performed at synchrotron light sources, such as X-ray Absorption Spectroscopy (XAS) and Resonant Inelastic X-ray Scattering (RIXS) are powerful tools to study complex materials, due to their chemical selectivity that allows disentangling the respective contributions of different atomic species [1]. In this talk, I will show how the use of incident polarized x-rays (either linear or circular) can allow a deeper understanding of the electronic structure and reveal emergent properties. X-ray dichroism is defined as the difference in the x-ray cross-section measured for two polarization states of the incident light (vertical vs horizontal linear polarizations or left vs right circular polarizations). There exist different types of dichroisms that depend on the symmetry of the light-matter interaction operator with respect to time-reversal symmetry and to space inversion (also called parity) symmetry. While parity is broken in non-centrosymmetric crystals, time-reversal symmetry can be broken in materials either by spontaneous magnetic ordering or by the application of an external magnetic field. Different combinations yielding to different measurable dichroisms are therefore possible, the most popular certainly being X-ray Magnetic Circular Dichroism which is measured in centrosymmetric ferro/ferrimagnetic materials and provides access to the ground state spin and orbital magnetic moments of the absorbing atom. Other types of X-ray dichroisms, such as X-ray Natural Circular Dichroism, X-ray Magnetic Linear Dichroism or X-ray Magneto-Chiral Dichroism, have been so far less explored, despite their intrinsic high potential in measuring ground state momenta that can be connected to magnetic and / or optical activity properties.

I will present some of the recent achievements made in the field of x-ray dichroisms and discuss remaining open questions and prospects. Examples will cover crystals with x-ray optical activity [2, 3] as well as remarkable magnetic materials, such as magnetite [4], single molecule magnets [5], nanoparticles [6], magnetic liquids [7] and magnetotactic organisms [8].

[1] F. M. F. de Groot et al. Resonant Inelastic X-ray Scattering. Nature Reviews Methods Primers, 4, 45 (2024).
[2] U. Serdan et al. Dilution of Racemate-Forming Fe(II) and Ni(II) Congeners into Conglomerate-Forming $[Zn(bpy)_3](PF_6)_2$. Chemistry, 5, 255-268 (2023).
[3] N. Bouldi et al. X-ray magnetic and natural circular dichroism from first principles: calcula+on of K- and L_1- edge spectra. Physical Review B 96, 085123 (2017).
[4] H. Elnaggar et al. Noncollinear Ordering of the Orbital Magnetic Moments in Magnetite. Physical Review B 96, 085123 (2017).
[5] L. Poggini et al. Engineering Chemisorption of Fe_4 Single-Molecule Magnets on Gold. Advanced

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Materials Interfaces 8, 2101182 (2021).
[6] N. Daffé et al. Nanoscale distribution of magnetic anisotropies in bimagnetic soO core-hard shell $MnFe_2O_4$@$CoFe_2O_4$ nanoparticles. Advanced Materials Interfaces 4, 1700590 (2017).
[7] N. Daffé et al. Bad Neighbour, Good Neighbour: How Magnetic Dipole Interactions Between Soft and Hard Ferrimagnetic Nanoparticles Affect Macroscopic Magnetic Properties in Ferrofluids. Nanoscale 12, 11222 (2020).
[8] D. M. Chevrier et al. Collective magnetotaxis of microbial holobionts is optimized by the three-dimensional organization and magnetic properties of ectosymbionts. Proceedings of the National Academy of Sciences 120, e2216975120 (2023).

Semi plenary

Freek Massee

Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, Orsay, France

How atomic scale current-noise gives us a deeper insight into the behaviour of electrons

A direct consequence of the discreteness of the electron charge is the presence of time- dependent fluctuations of the electronic current, called shot-noise. Since shot-noise is directly sensitive to the charge of the current carrying entities, as well as to their dynamics, shot-noise has been a powerful tool in the study of mesoscopic systems [1]. In this talk I will present how we managed to increase the spatial resolution of shot-noise measurements to the atomic level by implementing cryogenic circuitry operating in the MHz regime into our home-built scanning tunnelling microscope [2]. After discussing the technique, I will show how atomic scale noise allows us to visualize otherwise hidden interactions between electrons themselves and with the lattice in doped superconductors [3] and semiconductors.

[1] Ya. M. Blanter and M. BIker, Physics Report 336, 1 (2000).
[2] F. Massee et al., Rev. Sci. Instrum. 89, 093708 (2018).
[3] U. Thupakula et al., Phys. Rev. Le[. 128, 247001 (2022).

Semi plenary

Véronique Lazarus

IMSIA, ENSTA Paris, CNRS, EDF, Institut Polytechnique de Paris, 91120 Palaiseau, France

What is behind the diversity of crack shapes?

Whether in living organisms (cracked skin, fractured bones, etc.), in our food (cheese, caramel, etc.), in our homes (joints, walls, peeling paint, etc.), in the arts (paintings, ceramics, etc.), in geology (basaltic columns, seismic faults, septarias, etc.) or in industrial components (aircraft, phone screens, packaging, etc.), cracks are everywhere, often worry us, are sometimes deliberately provoked, but the diversity and complexity of their shapes always fascinate us. From the propagation of a single crack to multi-cracking, I will present the main physical principles underlying their formation.

PSI2 - Physical Chemistry of plastics pollution

La contamination par les microplastiques en zone littorale : la Baie de Marseille comme site pilote

Laurence Vidal * [1]

[1] CEREGE – UMR Université Aix-Marseille, CNRS, Institut de recherche pour le développement [IRD], INRAE – France

Les microplastiques (MP) contaminent tous les milieux marins, de la surface aux profondeurs. Cependant, l'estimation précise des stocks et des flux de MP dans les environnements marins reste difficile, car la colonne d'eau et les sédiments sont largement sous-étudiés. La plupart des études se concentrent uniquement sur les MP présents à la surface, ce qui entraîne un biais d'observation qui pourrait contribuer au "paradoxe du plastique manquant".
La mer Méditerranée, dont le littoral héberge 150 millions d'habitants, est soumise à des pressions anthropiques importantes et diverses. On estime qu'elle concentre environ 7% de tous les MP de surface, chiffre qui pourrait être sous-estimé si tous les compartiments marins étaient pris en compte.

Nous nous intéresserons ici au littoral Marseillais, deuxième ville de France par sa population. Sur la base d'une collecte biannuelle d'échantillons entre 2020 et 2023, nous présenterons la distribution spatio-temporelle des MP dans les eaux de surface, la colonne d'eau, et les sédiments de surface. L'ensemble de ces données permettra de proposer un suivi temporel de la pollution par les MP dans la zone. Nous montrerons comment la dispersion des particules peut être impactée par les conditions hydrodynamiques en surface et sub-surface. La caractérisation de cette pollution dans tous les compartiments marins permettra d'estimer les stocks de MP accumulés dans la Baie de Marseille. Les pistes pour améliorer notre compréhension du transfert vertical des MP et leur interaction avec les processus biologiques seront envisagées.

Keywords: Microplastiques, Observations in situ, Baie de Marseille

*Speaker

Mécanismes de dégradation de polymères vieillis artificiellement et quantification des produits de dégradation générés

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Le plastique est omniprésent dans l'environnement, notamment aquatique. Même si des estimations ont été faites des entrées de plastiques dans l'environnement1, il est difficile d'étudier l'ensemble des produits de dégradation dans les milieu naturel. Ceci peut en partie s'expliquer par leur diversité : la dégradation d'un plastique peut avoir de nombreux effets et résultats, avec parmi eux non seulement des fragments micro (< 5mm) voire nanoplastiques (< 1μm) difficiles à détecter et identifier2, mais également des molécules solubles et des composés volatils nanométriques. Si des études de certains produits de dégradation ont déjà été faites ponctuellement en utilisant le carbone3, aucune quantification complète de tous les produits de dégradation n'a été à notre connaissance proposée.
Nous proposons un protocole de quantification simultanée de l'entièreté des produits de dégradation basé sur le bilan carbone que nous appliquons à la comparaison de deux plastiques : le LDPE qui est le polymère le plus abondant dans l'environnement, ainsi que le PBAT, polymère dit biodégradable souvent utilisé pour remplacer le LDPE dans les applications de sacherie et de paillage.
Grâce à ce nouveau protocole et à l'addition de méthodes d'analyse quantitative nous quantifions l'ensemble des produits de dégradation générés par vieillissement UV et agitation dans l'eau. Nous proposons un scénario de dégradation pour chacun des deux polymères prenant en compte les différents mécanismes de dégradation ayant lieu en parallèle : fracturation, délamination, érosion. Ces scénarios illustrent le lien structure-propriétés en ce qui concerne la réaction des plastiques aux UV et à l'agitation mécanique, qu'il s'agisse de la nature ou de la quantité relative des produits. Ces résultats devraient permettre à terme de prédire quantitativement les produits de dégradation générés par tout plastique.

Keywords: Abiotic degradation, Carbon budget, Model, LDPE, PBAT

*Speaker

Etude du relargage des additifs dans l'environnement marin par spectroscopie Raman

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La spectroscopie Raman fait partie des techniques très appréciées par les chercheurs pour l'étude des plastiques. Non-destructive et facile à mettre en œuvre, elle permet une identification rapide du polymère (constituant majoritaire) et de certains additifs (pigments, ...) qui, même s'ils sont présents en très faibles quantités, sont toxiques pour notre environnement mais aussi pour la santé humaine. Au milieu de tous ces plastiques accumulés dans notre environnement marin, une question se soulève : quel est le taux de relargage des additifs dans notre environnement extérieur au cours de leur vieillissement ? Si de tels éléments de réponse peuvent être apportés, il serait alors possible d'établir un lien de causalité entre le relargage des additifs et la modification de la structure interne du polymère. Ces informations acquises donneraient accès à des données concrètes pour la gestion de ces déchets.

Keywords: Additifs, relargage, spectroscopie Raman, environnement marin, vieillissement

*Speaker

Coupling Scanning Electron Microscopy and Raman spectroscopy in a single chamber to analyse nano- and microplastics

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Microplastics (MPLs) are polluting debris originating from human activities. They are well described by their color, shape, polymer type and size (1). The size distribution is usually presented between 5 μm and 5 mm due to the diffraction limit of optical methods. However, reaching the nanoscale is of prime importance for describing the whole range of size and understanding their chemical reactivity. Moreover, it is interesting to determine the size distribution for each family of plastic present in an environmental sample. The idea was therefore to correlate a chemical analysis with the size measurements at the scale of individual particles, inspired by the methods developed in nanotechnology, We thus coupled Raman spectroscopy to Scanning Electron Microscopy in a single chamber to localize and analyse MPLs without moving the samples. Model microplastics and nanoplastics of polyethylene and polystyrene were used to model small marine debris. To prevent any damage on microplastics, the protocol of analysis was adapted, allowing the recording of Raman spectra of nano- and microplastics beads without altering them. These developments were done in the project Moustic funded by Anses (The French National Research Program for Environmental and Occupational Health of Anses (2020/01/188)).

Keywords: microplastics, Raman, electron microscopy

*Speaker

Production of polymer nanoparticles for biodegradation and ecotoxicological studies

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We developed a methodology to obtain surfactant-free polymer nanoparticles in suspension in water for ecotoxicological and biodegradation studies. Biosourced poly(lactic acid) (PLA) and oil-based polystyrene (PS) are commodity polymers used in many applications like food packaging, while polycaryophyllene (PCAR) is a biosourced polymer interesting for cosmetics formulation. The nanoprecipitation method consists in quickly adding a large proportion of water into a polymer solution in a water-miscible solvent. Control of the parameters (initial concentration, stirring and evaporation

*Speaker

rates...) allowed obtaining nanoscale particles with good repeatability. We evaluated the stability of these surfactant-free nanoparticles in deionized water. Their negative zeta potential stabilizing the particles in suspension was ascribed to HCO3- anions adsorbion at the hydrophobic polymer-water interface (arising from the dissolution of CO2 from air) already reported in literature. While there was no significant change in hydrodynamic size of the particles for PLA and PCAR, thereby confirming their temporal stability, this was not the case for PS. In a second part of this study, we developed a biodegradation methodology to compare micro- and nano plastics biodegradability. We assessed the biodegradation conditions following the OECD 301F guidelines. Colloidal stability of model nanoplastics in the mineral water used as growth medium was estimated by DLS and zetametry. We did not find significant change compared with the samples prepared by nanoprecipitation in pure DI water in the first part. First preliminary biodegradability results show that nanoparticles degrade at a lower rate than microparticles, suggesting that their biodegradation depends on the inability of the inoculated microorganisms to detect nanosized particles as compared to microparticles, on which they can adhere and produce their biofilm. This 'micro vs. nano' effect will be further studied through biotechnological analysis (qPCR assays) of bacterial populations of the biofilms as planned by the interdisciplinary consortium of the ANR project ELIMINATORS.

Keywords: nanoplastics, nanoprecipitation, biodegradation assays, ecotoxicological assays

SMMP3 – Fracture of hydrated materials

Environmental control of crack propagation in biopolymer hydrogels

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The fracture energy of hydrated biopolymer networks (gelatin, alginate...) is extremely sensitive to the nature and amount of solute or co-solvent in the process zone where extended, non-covalent crosslinks (triple helices, ion-chelating egg-boxes...) are disrupted. The micromechanics of rupture involves two distinct processes: network/solvent interaction under extreme strain state, poroelastic transport of solvent from both the bulk and the crack-tip environment. In practice, assessing the rate-dependent fracture energy change in response to an environmental modification gives deep insight into both processes (1). Examples are : embrittlement of gelatin-glycerol gels by enviromental water, weakening of calcium-alginate gels by non-binding ions, pinning of gelatin gels by network-clogging silica nanoparticles...
Tougening of gelatin hydrogels by an alcohol-water environment provides with a case study of how to decipher the free energy contribution of alcohol to the fracture energy of the protein network, out of the poroelastic dissipative background. The energy modulation of the fracture energy can then be confronted with the modulation of equilibrium properties such as the gelation temperature (2)

(1) For a review see : Baumberger, T., & Ronsin, O. (2020). Environmental control of crack propagation in polymer hydrogels. *Mechanics of Soft Materials*, *2*(1), 14.

(2) Baumberger, T., & Ronsin, O. *to be published.*

Keywords: Biopolymer hydrogels, poroelasticity, protein, solvent interaction, preferential hydration

*Speaker

Freezing hydrogels reveals a simple power-law behavior in their compressions and osmotic pressures.

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Hydrogels are particularly versatile materials that are found across a wide range of natural and industrial applications. One key reason for this versatility is their high water content, which lets them dramatically change their volume and many of their material properties – often by orders of magnitude – as they swell and dry out. To understand hydrogel behavior, we need techniques to characterize how these properties change across a range of different water contents. Here, we show that one approach is to use Gel-Freezing Osmometry (GelFrO), an extension of freezing-point osmometry(FPO), which is commonly used to characterize aqueous solutions. We re-imagine FPO to apply to hydrogels by tracking the shrinkage of a gel layer in contact with ice. We demonstrate GelFrO for several different hydrogels, by measuring their mechanical response to compression and their osmotic pressure as a function of polymer content. We compare the results with classical gel-swelling theoretical predictions, and do not find good agreement. Instead, our data is well-described by simple power-law expressions. We interpret this as a hallmark of a microscopic fractal structure of the gel's polymer network, and propose a simple way to connect the gel's fractal dimension to its mechanical properties. Finally, we use the results to derive a new, broadly applicable constitutive model for hydrogel mechanical behavior. GelFrO offers many advantages over current approaches, including the ability to work with small samples, the need for only relatively short equilibration times, and the fact that it gives access to a wide range of gel compressions.

Keywords: hydrogel, large, strain response, osmotic pressure

*Speaker

Destruction of porous media due to the swelling of silica based gels

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We report on the unexpected behaviour of an amino-functionalized silane gel upon hydration in confinement. When the gel is present, as thin films, in a porous medium such as stones, we show that the swelling pressure of the gel can be large enough to break completely the stone . We have quantitatively investigated the swelling dynamics of the gel in stones with different pore sizes and porosities and related to the microscopic swelling of thin films of gel. For that, the forces generated during swelling were measured on gel films at the microscopic scale. Our findings reveal that the swelling pressure can be sufficiently high to disintegrate consolidated sandstones, reducing them to a pile of sand grains. Remarkably, the swelling of the confined gel in the porous network of the stone is a reversible process, occurring even after repeated swelling and drying cycles. To further understand the physical processes leading to this swelling behavior, the hydration process with liquid water and water vapor is investigated using Confocal Raman microspectroscopy. Although, Amino-functionalized silanes are widely used as coupling agent across various applications, their peculiar swelling property have not been investigated yet. This could open new routes for their application in civil engineering and other fields due to its capability for easy and localized destruction of porous media, requiring only a minimal amount of energy.

Keywords: swelling, gels, porous media

*Speaker

Dehydration drives damage in the freezing of brittle hydrogels

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It is widely known that freezing breaks soft, wet materials. However, the mechanism underlying this damage is still not clear. To understand this process, we freeze model, brittle hydrogel samples, while observing the growth of ice-filled cracks that break these apart. We show that damage is not caused by the expansion of water upon freezing, or the growth of ice-filled cavities in the hydrogel. Instead, local ice growth dehydrates the surrounding hydrogel, leading to drying-induced fracture. This dehydration is driven by the process of cryosuction, whereby undercooled ice sucks nearby water towards itself, feeding ice growth. Our results highlight the strong analogy between freezing damage and desiccation cracking, which we anticipate being useful for developing an understanding of both topics. Our results should also give useful insights into a wide range of freezing processes, including cryopreservation, food science and frost heave.

Keywords: freezing damage, hydrogel fractures, dehydration, cryosuction, desiccation cracking

*Speaker

Effect of polymer ionization on hydrogel membranes composed of associating polymers

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Reversible association of polymers in solution can lead to the formation of physical gels. In particular, soft transparent self-healing membranes can be formed at liquid-liquid interfaces (Dupré de Baubigny et al. *ACS Macro Lett.* 2021, 10, 204). The growth of such membranes strongly depends on polymer ionization, which is controlled by pH, as was found for the membrane composed of poly(propylene oxide) and poly(methacrylic acid) (PMAA) at the oil-water type interface. The membrane growth can be described as an interdiffusion-controlled process at low ionization of PMMA, whereas the character of the process changes with increasing ionization. The concentration of mobile ions is high enough to provide the electroneutrality of the gel and the external solution due to Debye screening. However, the difference in concentrations of charged monomer units in the gel and solution creates an electrostatic potential barrier at the gel boundaries. The slowdown in film growth in the interdiffusion-controlled regime can be explained by a drop in the composition gradient inside the membrane caused by the entropic contribution of counterions. The effects of the electrostatic barrier on the (1) concentrations of counter ions and, as a consequence, on the polymer ionization and (2) absorption rate of the charged polymer and, therefore, on membrane growth, are discussed.

Keywords: hydrogel, membrane, associative bonds, polymer ionization

*Speaker

SMMP4 – Soft and architected structures

Atypical elastic instabilities in a soft string

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When a system is forced at a given frequency, it generally responds at the excitation frequency and, in the case of parametric forcing, at half the frequency. This effect was observed by Faraday on a vertically vibrated liquid and by Melde when he was studying string resonances.
In this presentation, we present an experiment similar to that of Melde, but here, the string is made of a soft material, *i.e.* with a low Young's modulus. We observe an original response, different from the Faraday-type sub-harmonic instability: pairs of sub-harmonic frequencies are created (for example f/3 and 2f/3 or f/4 and 3 f/4, where f is the forcing frequency). By varying f, the unstable pairs are modified. A theoretical model based on multi-scale development is used to predict these observations.

Keywords: soft string, parametric instability

*Speaker

Field measurement of sea ice elastic propreties using elastic waves multimodal propagation

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As a consequence of global warming, the Arctic ocean is warming up, leading to a fast decay and weakening of the Arctic sea ice cover. Owing to its proximity with open ocean, the ice cover is submitted to diverse stresses such as wind, oceanic currents and surface waves. All these stresses may break the sea ice cover over hundreds of kilometers leading to a complex area called the Marginal Ice Zone (MIZ). This region is covered by sea ice fragments of different sizes, from a few meters to a few kilometers. This multiscale medium has a complex yearly dynamic, which results from environmental stresses and sea ice mechanical propreties.
Sea ice can be seen as an heterogeneous brittle elastic material which presents elastic propreties that are highly varying in time but also in space. In order to measure these propreties, our team took part in two field measurement campaigns in the Saint-Lawrence estuary and on multi-year ice in the Lincoln Sea.

During these field campaigns, we generated elastic in-plane and out-of-plane waves within this floating elastic plate over several meters. Using an array of geophones, sensitive to local displacements, we have been able to record the multimodal propagation of these waves in order to infer elastic propreties such as the Young modulus, the Poisson ratio or the thickness over the whole area covered by the array of sensors.
These field measurements enable us to extract rare data on elastic propreties of ice, which are important to understand the dynamic of Arctic sea ice and can be used by climate models.

Keywords: mechanics, elastic solid, sea ice, field measurement

*Speaker

Towards reconfigurable soft acoustic metalenses

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Wavefront shaping of ultrasound is a major issue in many applications such as medical diagnosis, underwater acoustics, non-destructive testing, and many other fields. As an example, the focusing of ultrasonic waves can be achieved with traditional methods using acoustic lenses or transducer arrays and time-reversal mirrors. For two decades, many artificial structures, such as phononic crystals and acoustic metamaterials have been proposed to fabricate various new-concept focusing lenses. Recently, the concept of acoustic metasurfaces has also introduced new opportunities for wavefront shaping with effective and compact devices (1).
Here, I will report various sub-wavelength acoustic lenses made of soft porous silicone rubber. This soft porous polymer material is very interesting to achieve acoustic metasurfaces because its acoustic index, that strongly depends on the porosity and elastomer's elastic properties, can reach very high values of the order of ten. For example, we fabricated flat and soft gradient-index acoustic lenses for wavefront shaping (ultrasound focusing, vortex generation) in free space (2) by mastering emulsion templating methods and supercritical drying techniques (3). I will also show that 3D underwater ultrasound focusing is achievable thanks to quasi-flat and ultra-thin lenses with high acoustic index and very low curvature (4). Finally, I will present some perspectives about the tunability and reconfigurability of these soft acoustic metalenses by controlling the crosslinking of the soft porous polymer matrix.

References

(1) Assouar *et al.* "Acoustic metasurfaces," *Nat Rev. Mater.* **3** (2018).

(2) Jin *et al.* "Flat acoustics with soft gradient-index metasurfaces," *Nat. Comm.* **10** (2019).

(3) Kumar *et al.* "Drying kinetics and acoustic properties of soft porous polymer materials", *J. Porous. Mat* **28** (2021).
(4) Lombard *et al.* "Quasi-flat high-index acoustic lens for 3D underwater ultrasound focusing," *Appl. Phys. Lett.* **120** (2022).

Keywords: Wavefront shaping, acoustic metasurfaces, soft porous silicone rubber, crosslinking

*Speaker

Topological waves in acoustic lattices with chiral symmetry

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We discuss a particular class of architectured materials, consisting in discrete lattices of acoustic waveguides. We discuss the exotic properties that emerge when the lattice is bipartite, or equivalently, has chiral symmetry. When combined with other spatial symmetries, this can lead to various effects such as topological edge waves, or topologically protected invisibility. We will discuss the relations between symmetries and these peculiar wave phenomena, and their manifestation in explicit examples.

Keywords: Phononic crystals, topological insulators, wave scattering

*Speaker

Observation of Micropolar Modes from Transmitted Waves in a Multilayer Polystyrene Plate.

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This research investigates the behavior of sound wave propagation through a multilayer micropolar plate composed of expanded polystyrene, examining various incident angles. By integrating theoretical models with experimental methods, we analyze the changes in transmission coefficients across the frequency spectrum, highlighting the dynamic variations in vibrational modes. Using a setup that includes a loudspeaker, a microphone, and a data acquisition system (National Instruments), we precisely identified the classical Lamb modes below the critical angle and discovered new micropolar modes beyond this critical angle for a single layer of the material. For multilayer configurations with very thin air films between the layers, we observed increased attenuation as well as an augmentation of both Lamb and micropolar modes within the same frequency range of 0-60 kHz. These experimentally validated findings are consistent with theoretical predictions and significantly enhance our understanding of the engineering applications of these materials.

Keywords: acoustic, vibration, continuum, propagation, waves

*Speaker

Breaking the reciprocity of waves using time-modulated jump conditions

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The modulation of material properties in space and time is one of the paths to break the reciprocity of waves. This makes possible media with one-way band-gaps (acoustic or elastic diodes). However, practical realization of time-dependent bulk properties is difficult (especially the mass density), if not impossible.

Instead of modulating bulk properties, it seems more feasible to modulate properties at N discrete points periodically spaced, typically the jump conditions. In previous works, homogenization of periodic (in space) and constant (in time) spring-mass jump conditions has shown how the interface parameters modify the bulk properties of the effective medium. It is therefore expected that similar networks with modulated (in time) spring-mass conditions will yield effective time-dependent bulk properties.

Our contribution is then two-fold. First, scattering by a single modulated interface (N=1) is studied both analytically and numerically. Analytical methods involve harmonic balance method and exact solutions, whereas numerical modelling relies on a time-domain numerical scheme and an immersed interface method. Second, wave propagation through N1 interfaces is compared with the findings of leading-order homogenization and of Floquet-Bloch analysis. Two types of modulations are considered: all interfaces are modulated in phase, or the modulation is phase-shifted according to a function of time and space. The latter case emulates a wave-like space-time modulated medium, whose properties have been recently clarified.

Keywords: Metamaterials, time modulated jump conditions, non reciprocity, low frequency homogenization

*Speaker

Nonlinear Nonreciprocal Waves in Topological Metamaterials

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Topological and non-Hermitian (NH) systems offer promising avenues for advanced wave devices, showcasing unique phenomena such as robust topological and skin states. Recent research has increasingly focused on exploring the interplay between these two types of waves. In this context, we introduce a one-dimensional NH model: a non-reciprocal variant of the Su-Schrieffer-Heeger (SSH) chain. We first demonstrate the exceptional properties of this NH SSH chain in the low-amplitude regime. We then, look at the system's behavior as it transitions into a finite-amplitude regime where nonlinear effects cannot be neglected. We demonstrate that just by incorporating on-site Kerr effects, we can greatly enhance the range of wave phenomena achievable beyond what is observed in its Hermitian counterpart.

Keywords: Non, Hermitian systems, Non, reciprocal Networks, Nonlinear dynamics, Topological edge modes, Non, Hermitian Skin Effects

*Speaker

SMMP5 - Surface tension, soft solids and fluid-structure interactions

Magnetic pillar arrays : a way to control liquid mobility

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Superhydrophobic and slippery surfaces are two examples of non-wetting materials that have been widely studied in recent years1,2. Of all the work that has been done, only a small number involve active surfaces, whose dynamics can be adjusted by an external stimulus 3–5. In this presentation, I will show how we have taken advantage of the mobility of a network of magnetically activatable micrometric pillars to control the movement or positioning of water drops on an inclined surface. Firstly, I will review the fine characterisation of the displacement of the pillars using a magnetic field (associated with its gradient), and how the surface structuring needs to be optimised to allow optimum deflection of the pillars. Then, I will show how local anchoring at the level of the pillar has a crucial impact on drop mobility, either with static or dynamic pillar deflection. Finally, I will show how an understanding of the phenomena at the pillar scale helps to explain drop displacement, whether on a wetted surface of the Cassie-Baxter type (figure 1), or in the case of Liquid Infused Surfaces.

(1) Guan, J. H.; Wells, G. G.; Xu, B.; McHale, G.; Wood, D.; Martin, J.; Stuart-Cole, S. Langmuir 2015, 31 (43), 11781–11789.

(2) Lafuma, A.; Quere, D. Nat Mater 2003, 2 (7), 457– 460.

(3) Chen, W.; Zhang, X.; Zhao, S.; Huang, J.; Guo, Z. Chem. Commun. 2022, 58 (8), 1207– 1210.

(4) Bolteau, B.; Gelebart, F.; Teisseire, J.; Barthel, E.; Fresnais, J. ACS Appl. Mater. Interfaces 2023, 15 (29), 35674–35683.

(5) Lin, Y.; Hu, Z.; Zhang, M.; Xu, T.; Feng, S.; Jiang, L.; Zheng, Y. Advanced Functional Materials 2018, 1800163.

*Speaker

When gravity actually influences the macroscopic contact angle in partial wetting problems

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Controversy still exists as to whether the contact angle of a liquid on a solid is affected by drop size or gravity. Pethica et al. (1957) and Leja et al. (1960) suggested that the contact angle is affected by gravity. In contrast, Herzberg et al. (1970) claimed that the change in the contact angle with drop size was produced by hysteresis rather than the effect of gravity. Boruvka et al. (1977) introduced the concept of line tension to explain the change in the contact angle with drop size. Since that times, many researchers have concluded that the contact angle is not affected by gravity, but nobody has yet proved or denied this conjecture theoretically.
The present work aims to show that gravity influences partial wetting when the drop volume is such that the shape strongly deviates from a spherical cap. To uncover what happens to the macroscopic contact angle, we have implemented two complementary approaches: one experimental and the other from modeling. A sessile drop of distilled water is injected by a motorized syringe through a 1 mm hole drilled in a horizontal PMMA substrate, in an ambient air environment. In parallel, an axisymmetric macroscopic model was developed to compute the drop shape in static equilibrium, accounting for thermodynamic equilibrium and the conservation equation of total energy. This model leads to an algebraic-differential system comprising four first-order differential equations in space, and two algebraic constraint equations. As this system is highly non-linear, it is computed with the numerical asymptotic method.
This set-up exhibits the gravity influence on macroscopic contact angle over a wide range of Bond numbers. Moreover, the developed model enables us to understand how this occurs, emphasizing the dissipative role of three-phase-zone energy in its evolution, both in advancing and in receding contact lines.

Keywords: Partial wetting, macroscopic contact angle, Young's equation, Laplace's equation, Bond number

*Speaker

Dynamics and Dragging of Capillary Bridges

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A simple method for liquid transfer involves stretching a liquid bridge formed between two surfaces. When the stretching reaches a certain height, the liquid bridge breaks, allowing the transfer of a portion of the liquid from one surface to another.
This study intents to investigate the mechanisms at the origin of the drag and breakage of the liquid bridge from a liquid bath in a dynamic regime at capillary numbers Ca = ηV σ = 10–5 – 10–3 and Weber number We = ρV 2R σ < 1. We used a capillary bridge technique(1,2) consisting in a spherical surface withdrawn from the bath at a controlled velocity. We tested two hydrophobic surfaces, smooth and textured, as well as three types of liquids: deionised water, a water/glycerol mixture with 10% glycerol and a water/glycerol mixture with 50% glycerol. We observed that the contact line dynamics depends on the displacement velocity of the solid relative to the liquid, the surface properties and the viscosity of the fluid. When the spherical surface is dipped into the bath and is withdrawn from its surface, it drags a liquid bridge. As the surface is pulled-off from the liquid free surface, the contact line recedes until it reaches a critical velocity a fixed position on the surface. When this velocity reaches a critical value, the contact line becomes trapped on the surface. The latter being reached for larger radii at higher pulling speeds, we correlate this to the Landau-Levich transition(3).
Before break-up, the shape of the capillary bridge can deviates from its quasi-static shape, depending on the pull-off velocity. At low velocities, such a dynamic dewetting is well described by static laws as only capillarity and gravity control the shape of the liquid bridge. At high velocities, we identify experimentally the inertia driven dynamics before the capillary bridge breaks.
Finally, our study highlights that the rupture of the capillary bridge results from a competition between dissipative processes at the contact line and capillary-inertial processes at the neck of the liquid bridge.
1 L. Vagharchakian, F. Restagno and L. Léger, Phys Chem B, (2009).
2 C. Cohen et al., Soft Matter 15, pp. 2990-2998 , (2019).
3 L. Landau and B. Levich., Acta Physicochimica U.R.S.S. Vol. XVII, (1942).

Keywords: Capillary bridge, surface tension, wetting

[*]Speaker

Formation of homogeneous and uniform film by coalescence of drops

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Wet coatings are of great industrial interest as they allow for the protection or functionalization of surfaces by a thin film. These films can be deposited through different techniques such as spraying or inkjet printing. For these techniques, drops are deposited on a surface where they coalesce to form a continuous film. In the case of spraying, drops are distributed in sizes and positions while inkjet printing allows for a well-controlled deposition of each drop. The coalescence of drops has been widely studied for pairs of drops. However, coalescence mechanisms involving multiple drops remain an open question. In order to obtain uniform films all the drops have to merge without leaving any dry area. We present model experiments involving a small number of drops to study coalescence locally. For this purpose, an experimental set-up was designed to automatically deposit glycerol drops on a glass plate with controlled patterns. We measure the dynamics of coalescence as well as the dimensions and geometry of the liquid drops in their final state. During coalescence, liquid bridges grow between the drops. Our experiments suggest that, in a viscous regime, the width of this bridge follows an exponential relaxation up to a final state. The number of drops involved and the deposition pattern both have a strong influence on the sequence of coalescence events. Moreover we observe that contact angle hysteresis plays a major role in the geometry of the final state. It leads to contact line pinning and prevents liquid drawback after merging. Coating formation involves a large number of drops so we propose to use the experimental set-up to study the mechanisms of coalescence of an array of droplets.

Keywords: Coalescence, sessile drops, surface coating

*Speaker

Drop deformation in a planar elongational flow: impact of surfactant dynamics

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In 1932, sir G.I. Taylor published a paper about drop deformation in extensionnal flow. The drop membrane deformation is well-described by a balance between its viscous stress and surface tension; despite the influence of surfactants over the mechanical balance is admitted, exhaustive measurements of such behavior was missing. We propose an experiment to describe the deformation through the measurement of the drop size and shear stress. It is performed while changing the surfactants types or their concentration.
Our data show that the deformation is smaller that Taylor's results when the surfactant's concentration is smaller than the critical micellar concentration. Thus a new analytical model is proposed to describe the drop deformation with surfactant kinetics effects. The competition between adsorption and desorption dynamics leads to an analytical result

which is in good agreement with experiment. Taylor result for a pure liquid drop is also recovered in the limits of null surfactant concentration or a saturated drop.
The model is expanded further to provide a generalization to any linear flow up to second-order deformation by using spherical harmonics and tensorial theory including dilational and shear viscosities. Furthermore the angle deviation of a droplet under shear flow decreases from pi/4 with the capillary number depending on adsorption and desorption dynamics.

*Speaker

The separation behaviour of a monodisperse millimetric emulsion during continuous droplet generation

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In the petroleum production process, surfactants naturally present in the oil stabilize generated water-in-oil (W/O) emulsions during extraction and transport. The formation of the dense-packed zone highly concentrated in water droplets creates specific requirements for the industrial separator design and its continuous operation. A droplet size distribution varies from well-studied micrometric sizes on the separator inlet to millimetric ones near the water/emulsion interface.
This research focuses on the millimetric emulsion separation. We use a millifluidic setup with a T-junction to generate one-by-one monodisperse W/O droplets whose diameter ranges from 0.4 mm to 3 mm. The droplets are stored in a container pre-filled with water and oil. Varying the oil and water inlet flow rates results in either a steady state of one or several droplet layers or continuous emulsion accumulation. In the latter case, after droplet generation has been stopped, the emulsion separation is additionally observed at rest. The height evolution of the emulsion-water and emulsion-oil interfaces is analyzed.

The droplet size effect on emulsion separation is studied for the water-in-dodecane system with an oil-soluble surfactant added. At concentrations above the CMC (*critical micelle concentration*) value, a constant separation rate is observed for a given droplet size, which is nondependent on generation conditions. For the concentrations below CMC, the separation dynamic is more complex. The addition of a water-soluble surfactant to the studied system (containing an oil-soluble surfactant) accelerates separation to almost instantaneous coalescence. Visually, all the emulsions obtained have a highly drained polyhedral structure resembling that of a foam. Coalescence occurs mainly at the water-emulsion interface, which is the opposite of the case for a microdroplet emulsion.
The presented approach and its results on the model system can be helpful in the following studies of coalescence under flow conditions and the modelling of industrial separator units.

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

*Speaker

Mobile soap film spinning

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Liquid foams are bubble assemblies, whose neighboring bubbles share micron-thick liquid films. Foam lifetime is inherently linked to the stability of these films. Here we investigate the influence of gravity on soap film thinning and drainage. We designed a setup involving the rotation of a circular soap film along its symmetry axis. The soap film experiences a centrifugal force that mimics gravity, between 0.1 and 100 times g. We examined a solution composed of SDS surfactant, featuring mobile interfaces.

To characterise the thinning dynamics, we measured the spatio-temporal thickness evolution using interferometry. When spinning, the soap film exhibited two distinct zones marked by a thickness gradient discontinuity. The inner zone comprised concentric fringes, associated with the soap film elasticity, while the outer zone was perturbed by local thickness variations associated with the phenomenon of marginal regeneration. Thinner film elements created at the outer edge of the film migrated inwards due to buoyancy, up to the discontinuity. For each experiment, the time evolution of the thickness profile is characterized. The effects of the gravity and solution viscosity are studied systematically to confront the results with existing data and model from the literature. These results contribute to the understanding of the phenomenon of marginal regeneration and its impact on foam film drainage.

Keywords: soap film dynamics, drainage, mobile interface, experimental interferometry

*Speaker

Isolated meniscus around rings suspended in vertical soap films

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When an object is placed into a soap film, a meniscus forms at their contact. Along this meniscus, thin film elements nucleate and grow, a phenomenon known as marginal regeneration. In a vertical soap film, these elements detach from the meniscus and rise into the soap film due to effective buoyancy. While it is known that these elements play a role in soap film drainage, it is not yet understood how the dynamics of marginal regeneration affect the shape and stability of these menisci, with a possible feedback on drainage itself.

We built an experiment to create large vertical soap films (15 x 25 cm^2) with a stationary thickness profile. Fed from the top by a syringe pump, each film typically lasts from a few minutes to one hour. The thickness of the soap film is measured by interferometry. This setup allows us to introduce rings into the film that form single circular menisci. We then zoom in on the meniscus with a camera that captures the reflection of a mercury lamp and the transmission of a conventional blue lamp. We systematically varied the ring radius, the ring section diameter, and the thickness of the surrounding soap film.

We measured the extension of the meniscus as a function of the angle around the ring. This extension is of the order of 100 μm and increases from top to bottom. We show that all the curves can be rescaled with the extension of the meniscus at the top of the rings, thus providing a master curve for all the rings and parameters. We demonstrate that such profiles are compatible with a dynamic meniscus where the fluid contained in the meniscus flows downward by gravity, while the meniscus is globally fed by the surrounding soap film through film exchange by marginal regeneration.

Keywords: soap films, meniscus, marginal regeneration, buoyancy, stratified media

*Speaker

Gliding in a soap film

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Soap bubbles and soap films which are ephemeral and fragile in appearance, can sometimes be surprisingly resistant. They withstand the impact of drops and solid particles, capturing a part of their kinetic energy and spontaneously heal after their passage. In addition, films with a thickness of a few micrometers can hold objects more than a hundred times thicker than them.
We consider here the dynamics of millimeter-sized beads when deposited in a horizontal soap film. We show that a single particle is spontaneously attracted towards the center of the film. From its static equilibrium position and its motion, we model the forces that apply on it. We show that contrary to what is generally assumed, the mass of the film itself induces a small deformation which dominates over the bead-induced deformation for the particle dynamics. We also model the friction force, and show that the simple system of a marble in a soap film is a very sensitive tool to measure surface viscosities, with a precision of 10-8 Pa s/m. We finally focus on the interaction between two particles, and study the orbits that spontaneously appear when they approach each other. Depending on the distance between the particles, different forces come into play: capillarity or the film deformation, which we evidence and model.

Keywords: soap film, particle, capillarity, interfaces, friction, surface viscosity

*Speaker

Evaporation-driven buckling of a suspension drop with graphene oxide nanosheets

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We investigate experimentally the evaporation of a single water drop with graphene-oxide nanosheets. The drops are placed on a superhydrophobic substrate and observed by a camera at controlled humidity conditions. As previously observed for other colloidal suspensions, during evaporation the particles form a semi-solid shell that buckles. Prevalent studies argue that buckling is the result of particle-particle repulsion being overcome for large compressions, but a complete understanding of the phenomenon has in fact not been achieved.

It is known that graphene oxide is an amphiphilic particle, whose amphiphilicity can be tuned by changing pH. In our experiments, we observe that acidic droplets buckle at a larger radius than basic droplets for a given particle concentration. A change in pH is often associated to changes in particle-particle interactions. However, in our case observations of the shape of the fluid interface post-buckling suggest that the change in pH affects the adsorption of GO particle on the surface of the drop, in turn changing the effective surface tension. For acidic droplets, GO adsorption reduces the air-water tension to values close to zero, and the shell buckles. In contrast, for basic droplets, particle adsorption is minimal, and the surface tension remains high and the particle layer below the interface rearranges without buckling.

Changing the relative humidity, and thus the rate of evaporation, yields repeatable buckled morphologies at fixed particle concentration. The observed buckling wavelength is inversely proportional to the evaporation rate and the buckled shapes (observed by SEM) can be qualitatively described by spherical harmonics. The reason why deterministic, evaporation rate dependent buckling is observed is an open question and the subject of future investigations.

These experiments are used to better understand spray drying of 2D nanomaterials.

Keywords: buckling, surface tension, evaporation

*Speaker

Surface Bubble Accelerates Evaporation

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Liquid evaporation inside a simple circular tube is a pure diffusion process known as Stefan diffusion tube problem. However, introducing a bubble at the liquid surface remarkably changes the evaporation dynamics. Different bubble/vessel aspect ratio leads to different evaporation rates. A vapor jet erupting from the apex of the bubble generates a forced vapor convection, transporting mass away from the vicinity of the bubble into the atmosphere. Comparing the vapor jet with classic fountains, we characterize the fountain-like jet by measuring its height and foot diameter with Schlieren imaging technics. We then investigate the change in vapor jet with time, for different liquids and bubble/vessel aspect ratios. We simultaneously measure the evaporation rate, which enables us to relate the presence of the vapor jet to the evaporation efficiency. Finally, we discuss the coupling effect between the evolution of the vapor jet shape and the evaporation dynamic process.

Keywords: surface bubbles, evaporation, vapor transport, thermo induced Marangoni flows

*Speaker

The peculiar shape of air bubbles trapped in ice

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Water usually contains dissolved gases. When it freezes, these gases are expelled and form bubbles which eventually are trapped in the ice. One can easily observe such bubbles in an ice cube out of the freezer. These bubbles are never spherical; they come in a range of shapes evoking eggs or pears, elongated and asymetric. Some of these bubbles are "ice worms", micrometer-thick and centimeter-long. The peculiar shape of air bubbles trapped in ice results of a delicate balance between heat and mass transfer, freezing and surface tension. We show that these intertwined mechanisms can be modeled by a single ordinary differential equation, strongly non-linear. Its analysis explains several features of the bubble shape, such as their flat top, and provides a bifurcation diagram for the ice worms. This mathematical model is confirmed by our experiments. By matching the solutions of the differential equation to the empirical bubble shapes, we are able to estimate the gas supersaturation in the melt and the nucleation radius of the bubble at the freezing front. Our work could find applications in glaciology, but also in designing porous materials made through freezing-casting.

Keywords: Freezing, Capillarity, Bubbles, Ice

*Speaker

PHASE SEPARATION MECHANISMS OF CONCENTRATED POLYMER SOLUTIONS

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Phase separation mechanisms of concentrated polymer solutions (above 10wt%) is a key mechanism which takes place in every polymer membrane manufacturing process. As such it is an important mechanism to master and understand but the dissymetry of the separating phases in viscosity, elasticity and density could generate unusual behaviors. We report here about such an experimental study by confocal light microscopy where we investigate growth laws, morphologies and scaling behaviors as a function of polymer concentration and phase separation temperature.

Keywords: phase separation, polymer solution, scaling, growth, spinodal decomposition

*Speaker

SMMP6 – Statistical physics of disordered matter

Computer simulations of molecular liquids at the experimental glass transition

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We present a Monte Carlo algorithm which allows efficient equilibration of computer models for simple molecular glass-formers down to temperatures close and below the experimental glass transition. The algorithm builds on the recent progress achieved using swap Monte Carlo for simple atomic glass-formers, and achieves a similar speedup for simple molecules in three-dimensions. As a consequence computer simulations can now easily study the structure and dynamics of very realistic molecular liquids at temperatures matching experimental conditions, including those leading to ultrastable molecular glasses.

*Speaker

A self-consistent current response theory of jamming and vibrational modes in low-temperature amorphous solids

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Topologically disordered solids exhibit characteristic anomalies like sound atten- uation in the absence of thermal fluctuation and deviations from Debye's law in the density of states.

Employing the Zwanzig-Mori projection operator formalism and Gaussian factoriza- tion approximations, we develop a first-principles, self-consistent theory of transverse momentum correlations in athermal disordered materials, extending beyond the stan- dard self-consistent Born approximation (1). The vibrational anomalies in glass at low temperatures are recovered in the stable solid limit, and floppy modes lacking restoring forces are predicted in unstable states below the jamming transition. Near the un-jamming transition, the speed of sound vanishes. Approaching the jamming transition from below, a characteristic length scale indicating the distance over which injected momentum remains correlated, diverges. We discuss the related scaling laws. Importantly, our theory does not predict negative eigenvalues of the Hessian.

Our theory can be mapped to the schematic theory (2) of the Euclidean-random- matrix model introduced by Parisi and co-workers (3). Our predictions are in qualitative and even good quantitative agreement with its numerical solutions (4). Additionally, our predictions for the critical dynamics agree with the simulation results of Ikeda, Mizuno (5).

References

(1) Florian Vogel, Philipp Baumgartel, and Matthias Fuchs. Arxiv preprint (2405.06537): A self-consistent current response theory of jamming and vibrational modes in low-temperature amorphous solids, 2024.

(2) F. Vogel and M. Fuchs. Phys. Rev. Lett., 130:236101, 2023.

(3) M. Mezard, G. Parisi, and A. Zee. Nuclear Physics B, 559(3):689–701, 1999.

(4) P. Baumgartel, F. Vogel, and M. Fuchs, 2023.

(5) H. Mizuno and A. Ikeda. Phys. Rev. E, 98:062612, 2018.

Keywords: Amorphous solids, Jamming, Mode, Coupling Theory, Euclidean, Random, matrix

*Speaker

Correlations of tensor field components in isotropic systems with applications to stress and strain correlations in elastic bodies

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Correlation functions of components of second-order tensor fields in isotropic systems can be reduced to an isotropic fourth-order tensor field characterized by a few invariant correlation functions (ICFs). The components of this field depend in general on the coordinates of the field vector variable, e.g., the wavevector q in reciprocal space, and thus on the orientation of the coordinate system. Importantly, these angular dependencies should not be confused with those of ordinary anisotropic systems with invariant material functions depending explicitly on the direction of the field vector.

The procedure to obtain the ICFs, applicable quite generally also for non-equilibrium driven systems, is discussed for (fourth-order tensorial) correlation functions of time-averaged stress fields and instantaneous strain fields in reciprocal space and using "natural rotated coordinates" independent of the coordinate system. Since all ICFs must become constant in the large-wavelength limit all correlations (in any coordinate system) are known in terms of only three phenomenological parameters. The long-range correlations in real space observed in several recent studies for these fields are thus traced back to the known symmetries and the generic structure of isotropic tensor fields. Moreover, for equilibrium elastic bodies all phenomenological constants can be traced back (fluctuation-dissipation theorem) to
the known elastic constants. The often made additional assumption of localized plastic rearrangements ("Eshelbies") is thus not required.

Naturally, for time-dependent correlation functions of tensor fields the phenomenological constants dependent on time. This time-dependency is completely described in terms of a few invariant) material functions which may be independently measured. Depending on certain tensorial invariants of response functions strong octupolar pattern of time-dependent correlation functions of stress and strain fields are predicted.

Keywords: tensor fields, viscoelastic properties, quenched disorder, elastic properties

*Speaker

Pioneering Fluctuations in Viscoelastic Stress

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The interpretation of scattering techniques or microrheological experiments is based on our knowledge of thermal fluctuations. Yet, for flows, our understanding of fluctuations is restricted to Newtonian materials, where fluctuating hydrodynamics applies fluxes uncorrelated in time and space. This corresponds to a local-equilibrium application of the Landau and Lipshitz Ansatz of the fluctuation dissipation theorem (FDT). Thus, the noise is Gaussian.
In this work (1), we present novel insights into fluctuations in flowing viscoelastic materials. We illustrate the limits of the classical Gaussian approximation and show how, in the context of a local field theory, the most fundamental viscoelastic model, the Upper Convected Maxwell (UCM), exhibits different fluctuations depending on the underlying microscopic dynamics. Both the temporary network model and the dumbbell model, which constitute model systems for two groups of microscopic models, reproduce the Maxwellian behavior. Until now, literature pointed out the equality of the two models with respect to stress evolution. We now quantify differences when taking into account fluctuations and suggest techniques to measure them. Furthermore, we connect the scale of structural variables to the difference in the observed fluctuations.
With a novel formulation of the FDT, we point out that in a network system, Gaussian noise is doomed to lead to contradictions in the FDT's formulation (2). We outline in which cases experiments and molecular dynamics simulations should account for these findings to capture the correct microscopic dynamics of complex materials.
We thank Prof. Öttinger for his guidance and support of the project.
(1) A. Winters, H. C. Öttinger, and J. Vermant. arXiv:, 2024

(2) H.C. Öttinger et al., *Journal of Non-Equilibrium Thermodynamics*, 46,1 (2021)

Keywords: Polymer physics, Fluctuations Dissipation Theorem, Viscoelasticity, Microrheology

*Speaker

Disorder-Induced Anti-Friction in Anomalous Diffusion

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The diffusion of particles with passage times significantly slower than regular Brownian motion is observed in various systems, such as amorphous materials, living cells and rheology. This behavior is typically attributed to trapping or waiting times that are scale-free and uncorrelated. Our work demonstrates that correlated waiting times, termed quenched disorder, can redefine our understanding of transport properties.
We show that the mobility of a driven particle anomalously depends on channel width, increasing as it grows narrower. Remarkably, this effect suggests a reduction in friction for flow as the channel constricts, opposing expectations based on regular or even anomalous transport dynamics. We further reveal that modifying geometrical constraints in the presence of quenched disorder alters the statistics of rare events, notably extremely large trapping times, resulting in surprising alterations to motion dynamics.
References
(1) D. Shafir and S. Burov, arXiv:2403.01665 (2024), (accepted to PRL).

Keywords: disordered matter, Quenched disorder, Anomalous Diffusion

*Speaker

Scale-invariant phase transition of disordered bosons in one dimension

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Bosonic particles with local interactions in one dimension (1D) are described by a universal harmonic theory, known as Luttinger liquid (LL). Diagonal disorder induces an instability in LL towards a non-superfluid Bose glass (BG) phase – a compressible insulator displaying exponen- tial decay of off-diagonal correlations. The disorder-induced quantum phase transition between superfluid and non-superfluid states of bosonic particles in one dimension is generally expected to be of the Berezinskii-Kosterlitz-Thouless (BKT) type. In this work, we consider the disorder-induced localization transition in 1D superfluids of bosons with power-law hopping decaying with distance as $1/r\alpha$. Here, we show that hard-core lattice bosons with integrable power-law hopping decaying with distance as $1/r\alpha$ – corresponding in spin language to a XY model with power-law couplings – undergo a non-BKT continuous phase transition instead. We use exact quantum Monte-Carlo methods to determine the phase diagram for different values of the exponent α, focusing on the regime $\alpha > 2$. We find that the scaling of the superfluid stiffness with the system size is scale-invariant at the transition point for any $\alpha \leq 3$ – a behav- ior incompatible with the BKT scenario and typical of continuous phase transitions in higher dimension. By scaling analysis near the transition point, we find that our data are consistent with a correlation length exponent satisfying the Harris bound ≥ 2 and demonstrate a new universal behavior of disordered bosons in one dimension. For $\alpha > 3$ our data are consistent with a BKT scenario where the liquid is pinned by infinitesimal disorder.

Keywords: Superfluidity, Luttinger Liquid, Quantum Monte Carlo, BKT, Bose, Hubbard Model, Long, range interactions

*Speaker

Mutual information as a measure of mixing efficiency in viscous fluids

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Fluid mixing at the microscale is of paramount importance in biological organisms and in artificial systems. Examples range from the the uptake of oxygen, nutrients or chemical signals in aquatic organisms to microreactors and "lab on a chip" applications. In biology, mixing is frequently accomplished by cilia which drive long-range flows, but also localized regions of chaotic advection. A particular challenge to microscale mixing is posed by the time-reversibility of flows at low Reynolds numbers. Mixing therefore requires an interplay between advection (stirring) and diffusion. Here we introduce mutual information between particle positions before and after mixing as a measure of mixing efficiency. We demonstrate its application in a Couette flow in an annulus and show that the mixing efficiency depends in a non-trivial way on the time sequence of rotation. We show that under this measure, the mixing efficiency is symmetric upon time reversal of the actuation sequence. Among all sequences with the same rotation angle, the ones with optimal mixing consist of a fast rotation in the middle of the time interval, or in some cases two symmetrically arranged. We also determine mutual information from Brownian dynamics simulations using data compression algorithms and demonstrate that advanced neural network based compression algorithms can be applied to estimate mutual information to a high accuracy. Our results show that mutual information provides a universal and assumption-free measure of mixing efficiency in microscale flows. Furthermore, we expect that our formalism will also be applicable to more complex mixing situations, for example by active swimmers, natural or artificial cilia or in active materials. Our current work is to apply mutual information in studying mixing caused by different types of microswimmers.

Keywords: Fluid mixing, Information theory, Entropy production, Compression algorithms, Viscous fluids

*Speaker

BAM1 - Dynamics of biological and bio-inspired systems, from single particles to suspensions

How does mucus rheology affect mucociliary clearance ?

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The airways are protected by mucus, a complex fluid transported along the epithelial surface, from the lungs to the throat, by the coordinated beating of millions of microscopic cilia. This process is known as mucociliary clearance. Dysfunction of this essential function is associated with all chronic respiratory diseases and in particular with obstructive respiratory diseases where the accumulation of mucus leads to the airway obstruction.
The aim of this project is to study the influence of mucus rheology on mucus transport and identify conditions that result in mucus arrest. In vitro experiments are conducted on bronchial epithelium using native and synthetic mucus combined with traceable fluorescent beads. We perform in-situ microrheology measurement and explore the relationship between mucus transport and mucus rheology.
This study provides new insights into the processes involved in mucus transport. It may contribute to the development of new therapeutic approaches based on biophysical markers.

Keywords: Mucus, rheology, invitro experiments

*Speaker

E. coli in motion in clay environments

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Motion of microorganisms in Newtonian fluids is extensively studied, yet understanding their motility in environments of complex rheology remains quite challenging. This study investigates the swimming dynamics of E. coli in clay suspensions (Laponite RD) across different physical states- isotropic liquid, gel, and glass phases- achieved by varying mass concentrations. In Newtonian fluids, the exploration kinematics of E.coli results in the compound of run and tumble phases. Our measurements based on a 3D Lagrangian tracking technique that allows to follow a single bacterium over several minutes, reveals that the mechanical constraints disrupt the typical swimming dynamics and the bacteria exhibit a specific "stop & go" process due to the medium entrapment. Visualization of both the body and the flagella points on a link between tumbling and stopping frequency. Remarkably in Laponite solutions, with a pH of approximately 10, E. coli remains motile despite their usual inability to swim at such high pH hence suggesting a protective effect of the clay on the bacteria.

Keywords: E. coli, rheology, microswimmers

*Speaker

Self-propelled droplets facing a counterflow in 1D channels.

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Artificial micro-swimmers have recently become a central field of research in soft-matter. Understanding their behavior in confined environment is an important step toward a deeper understanding of the dynamics of cells and micro-organisms in complex media.

A very promising and original type of swimmer developed in our team, consists in pure water droplet swimming in an oil phase containing micelles of surfactant. The droplet's activity comes from the formation of swollen micelles at its interface which induce Marangoni stresses and thereby motion of the droplets. These droplets move at a typical velocity of few tens of micrometers per second for a few hours. In two dimensions, although their trajectories are relatively stable, their global dynamics is extremely rich as the droplets interact with their neighbors through their environment.

Here we experimentally study the swimming motion of the droplets, when they are confined in circular or square capillaries and face a well-controlled counter-flow. We observe that the droplets can swim in a direction opposed to the main flow and use PIV measurements to characterize quantitatively the counter-flow inside the capillaries and investigate its influence on the swimming behavior of the droplets.

Keywords: soft mattter, active matter, interfacial activity, microfluidics

*Speaker

Micro-organisms in aerosols

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Marine aerosols are crucial to ocean/atmosphere exchanges; they are produced during the explosion of the many surface bubbles. Some of these micro-droplets travel great distances: their content spreads over a wide area. The ocean surface is covered with surfactants, biological matter and particles. It is known that microorganisms interact with surfaces and local flows : how do they impact aerosol production ? Are they captured and subsequently propagated over long distances ?

To answer to those questions we built an experimental setup that allow us to study the aerosol formation in a solution of Chlamydomonas reinhardtii: we inject an air bubble in the solution with a syringe pump; a high-speed camera follows the bubble bursting phenomenon and we measure physical parameters as bubble size, drop size and drop velocity. We catch the first and speeder drop with a glass slide above the solution, where we eventually verify the presence the presence of micro-organisms with the microscope.

In this presentation we will discuss the size and the velocity of the first droplet, as well as the presence and mobility of microalgae in the droplet. We will draw comparisons with other kinds of contaminants, namely micro-plastics, surfactants and bacteria.

Keywords: Micro, algae, water, air surface, bubble bursting

*Speaker

Wall entrapment enhances bacterial chemotactic response to deposited aerosols in the microlayer

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The sea surface microlayer is the thin layer of water separating the atmosphere from marine waters below. This typically half-millimeter-deep laminar layer mediates all gas exchange and receives all material deposited from the atmosphere, such as aerosol particles, before any transfer to deeper water can occur. The microlayer is a harsh environment characterized by large temperature and salinity fluctuations and strong ultraviolet radiation. Yet field sampling suggests a microlayer bacterial community does indeed exist, distinct from that in deeper waters. We hypothesize that motile microlayer and near-surface bacteria can successfully exploit the transient nutrient patches produced by surface-deposited aerosols using chemotaxis-driven foraging strategies, thus obtaining privileged access to rare resources. We developed a novel millifluidic device to image a static air-water interface with falling aerosol particles and swimming bacteria, enabling tracking of individual particles and cells. We observed that marine bacteria swam to and accumulated at the surface when exposed to environmentally relevant fluxes of deposited chemoattractant aerosols. These accumulations formed within seconds to minutes in extraordinarily thin films ($<$ 0.1 mm) and were approximately an order of magnitude higher than expected from previously established chemotactic accumulations observed in bulk. Using a novel theoretical model of bacterial behavior, we demonstrated that this strong accumulation can indeed be explained by the coupling of chemotaxis to dissolved aerosol-borne attractants and 'wall entrapment' at the air-water interface – a physical mechanism by which motile bacteria reside near boundaries for longer times. Our results highlight how interfaces in the environment modify the behavior of microorganisms, and in particular demonstrate that the microlayer is an environment where motile bacteria, through both active and passive mechanisms, quickly respond to aerosol deposition and accumulate in high-nutrient regions, thus resulting in a competitive advantage for motile cells.

Keywords: chemotaxis, bacterial motility, hydrodynamic entrapment, aerosols

*Speaker

A MICROFLUIDIC DEVICE WITH BIOMIMETIC SUBMICRON SLITS TO APPREHEND RED BLOOD CELL SPLENIC FILTRATION

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Red blood cells (RBCs) in the bloodstream continuously travel through thin capillaries that are smaller than their size, and are thus highly deformable. Splenic interendothelial slits fulfil the major physiological function of periodically monitoring RBC deformability to remove abnormal and aged cells. Today, due to lack of suitable in-vitro devices the mechanisms of RBC splenic filtration are still poorly understood. Here, we developed a unique microfluidic device containing high aspect ratio slits with submicron width by using a simple, inexpensive, and highly flexible combination of standard UV lithography and anisotropic wet etching. Such device allows to quantitatively elucidate mechanisms of RBC splenic filtration. As a proof of concept, we first show that the biomimetic slits discriminate RBCs with deformability alterations induced by sickle cell disease or spherocytosis. Second, we combined the microfluidic experiments with a RBC multiscale computational model to decipher retention rates and transit times of RBCs squeezing in slits as a function of external parameters and RBC mechanical properties. Healthy RBCs are able to undergo extreme deformations to pass through 0.28-μm wide slits at body temperature. To achieve this feat, they must meet two requirements: (i) geometrically, their surface area-to-volume ratio must be compatible with a shape in two tether-connected equal spheres; (ii) mechanically, cells with low surface area-to-volume ratio must locally unfold their spectrin cytoskeleton inside the slits. Our in-vitro and in-silico approach allows to quantify splenic clearance of diseased cells and cells engineered for transfusion and drug delivery.

Keywords: Microfluidics, Red blood cell and biomechanics

*Speaker

BAM3 - Physics of Morphogenesis in Living Organisms

Growth and shape of thin living systems

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The shapes of living systems such as plants, flowers, fish, or small animals in embryonic stages are extremely diverse. If they all result from cell proliferation, their global shapes are rapidly dominated by growth processes leading to very complex and beautiful geometries. Morphogenesis and embryogenesis aim to understand this diversity, using the physical laws of soft materials, but also trying to incorporate biological information and, of course, observations. Morpho-elasticity has demonstrated its power by showing that most growth processes of soft materials destabilize shapes that are initially too symmetric, such as disks, layers, or spheres. However, elasticity is a difficult science that yields to heavy finite element simulations of partial differential equations. Focusing on thin samples, one can adopt a 2D analytical treatment, and as for Darcy or Stokes flow, one can take advantage of complex analysis. I will show how the basic equations of elasticity with growth can be treated quite easily, even analytically. As an example I will take the case of Monstera deliciosa and jellyfish

Keywords: growth, soft tissue, embryo, elasticity, instability

*Speaker

Biomechanical determinants of shape diversity in cnidarian larvae

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Cnidarians form a wide phylogenetic family including diverse marine species such as anemones, corals, and jellyfishes. During development, almost all cnidarians feature a larval stage where it organises in an axisymmetric bilayer tissue that can present or not an oral opening. The axial elongation and asymmetry of the larva shape varies during its development but also from one specie to another. Understanding the mechanical controls of this shape is then important to bring light to the specie-specific morphogenesis process but also to study evolution between species.
In this talk, I will show that quantitative imaging of myosin distribution in different cnidarian species at different developmental stages allowed us to reveal common features preserved along species. It appears that myosin concentrates essentially at the outer surface- with a myosin excess around the aboral pole facing the opening- and at the interface between the inner and outer layer where the distribution exhibits anisotropy with circumferential cables of myosin.
I will then explain how we implemented those observations in an active surface model where the larva is described as a viscoelastic open shell generating nematic torque and tension, accounting for the anisotropic interfacial myosin distribution, and an active isotropic torque around the aboral pole, accounting for the excess of outer myosin there. Using simulations of this model and experimental myosin profiles, we were able to reproduce different species shape but also to reveal four mechanical modules controlling the larva shape. While nematic effects drive axial elongation, species-specific variations in oral geometry influence the shape asymmetry, further modulated by aboral isotropic bending and tissue thickness profile. Biological perturbations of those modules confirmed this picture and show that different combination of those four modules can lead to similar shape, this mechanical redundancy being a potential source of evolutionary innovation.

Keywords: active surface model, morphogenesis, evolution

*Speaker

Transport in canal networks of the gastrovascular system during development of the jellyfish Aurelia aurita

Laureline Julien * [1], Stanislaw Zukowski [1,2], Paheli Desai-Chowdhry [3], Purba Chatterjee [3], Aaron Winn [3], Eleni Katifori [3], Annemiek Jm Cornelissen [1]

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The canal network of the gastrovascular system of the jellyfish Aurelia aurita transports nutrients and oxygen to the tissues, enabling the jellyfish to swim.
In this network, canals have a preferential flow direction followed by the majority of the nutrients. Depending on this direction, the organization of the canals varies, forming either straight canals or a reticulated network. Investigating how the flow is propelled and characterizing the pulsatility inside the network are crucial steps to understand the role of pulsatility in the formation of the network and the differentiation of flow direction.

The flow in the canals is propelled by the expansion and contraction of the deformable canals, assisted by the movements of cilia that line the inner walls of the canals. We study the relative contribution of these two mechanisms to understand how they generate an effective flow that facilitates distribution towards the circular canal at the rim of the umbrella and back to the center of the jellyfish. We perform measurements while the jellyfish, both with and without anesthetic, is lying flat on its exumbrella, and the flow inside the canals is analyzed using the PTV method.

We observe that cilia alone succeed in transporting particles. Particles are trapped by the cilia and forwarded. Muscle forcing increases the particles' time-averaged velocity in all canals. Additionally, the path of a particle becomes more oriented in the channel. Our observations confirm Southward's 1955 findings that adradial straight canals also transport food particles in the opposite direction. A rich hydrodynamic complexity emerges from circulation in this system.
The scyphomedusa Aurelia aurita is part of the phylum Cnidaria, which is the sister group to all animals with bilateral symmetry. We hope that understanding how transport is realized in this ancient phylum will provide insight into how circulatory systems evolved.

Keywords: jellyfish, gastrovascular network, flow, contractions, cilia

*Speaker

Physics of hominization

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One school of paleontologists claims that there exists a tendency towards hominins characterized by a correlation between brain growth and flexure of the head. This kind of idea has a bad reputation. However, nothing forbids that their might exist an internal correlation between different biomechanical features. A detailed study of head formation in the chicken model reveals that the early brain is a series of vesicles, separated by rings (1). Head formation can be boiled down to dilation of a tube strangled by collars of cells. A simple model shows that such an object flexes when it dilates. The early brain behaves as a stick of balloons. It flexes like a stick and dilates like a balloon. Physical experiments are able to accelerate brain dilation, which causes a forward head flexure, or conversely, to shrink the brain, which causes a retrograde rotation. This confirms the existence of an internal correlation between flexure and dilation. However, the head grows also under the influence of blood flow. A detailed study of heart formation shows that the embryo texture localizes the aortas under the midbrain, which contributes to a stronger dilation and flexure, for similar reasons (2). In summary, the process of hominization is caused by a competition between dilation of brain vesicles (2D shells), and linear contraction of cell cables or vessels (1D elements). This competition is already present in the first divisions, since cell division already proceeds by contraction of an actin ring, around a dilating cell membrane. Hence, the principle at the root of human origin (interplay between surface tension and line tension) is truly fundamental and upscaled during evolution. The origin of humans can be explained by first principles (3).

1-Fleury, V., *Sci Rep* **14**, 7250 (2024).
2-Fleury, V., *Soumis*
3-Fleury, V., *Sigila* N○Le Double, (mai 2024).

Keywords: hominisation, évolution, cerveau, coeur, morphogenèse

*Speaker

BAM4 - Physics of plants

Biomimetic leaf-on-chip to study embolism in plants

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Global warming will lead to increasingly severe droughts and threatens most forests across the globe (1). One of the main dangers of droughts for trees is the generation of air embolism, which impairs the sap conduction and can lead to their death. In leaves, embolism has been shown to spread intermittently, exhibiting catastrophic events (2). Bordered pits containing a cellulosic membrane connect neighboring vessel elements of a vein. They reduce the embolism spreading, but cannot completely avoid it, just stop it for a while. Hence, they are responsible for this intermittent propagation of air observed in real leaves. By using PDMS-based biomimetic leaves to reproduce evapotranspiration (3), it has been demonstrated in linear geometry that the presence of narrow constrictions in the network can generate this non-linear dynamic through an elastocapillary coupling between the air / water interfaces and the compliant structure of the microfluidic device (4).
We present here an extension to 2D and more complex channel systems, where different structural parameters of these constrictions are studied. By varying their dimensions and the network connectivity experimentally, we succeeded in influencing the hierarchy of the embolism propagation. Coupling deformation measurements of the experimental compliant network and numerical simulations, we demonstrate that our system behaves as a network of hydraulic capacitances. Further theoretical developments including viscous dissipation lead us to describe the system as an electrical circuit made up of capacitors and resistors. We will finally discuss the relevance of this framework and these new biomimetic tools to describe embolism propagation in real plants.

References

(1) Brodribb *et al. Science* **368,** 261-266 (2020).
(2) Brodribb *et al. PNAS* **113,** 4865-4869 (2016).
(3) Noblin *et al. PNAS* **105**, 9140–9144 (2008).
(4) Keiser *et al. J. Fluid Mech.* **948**, A52 (2022).

Keywords: Plant physics, microfluidics, bubble dynamics, biomimetics, elastocapillarity

*Speaker

Growth of a heterogeneous plant cell wall: a biomechanical model

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Plant cells are surrounded by rigid walls, which are multilayered and heterogeneous structures consisting of a soft polymer matrix reinforced with stiff cellulose microfibrils. Research has highlighted the role of mechanical forces acting on the cell wall in the regulation of plant cell growth. Microfibril reorientation during cell expansion has emerged as a key factor influencing morphogenesis through its effect on apparent wall properties. In this work, we develop a model that couples cell growth to the mechanics and synthesis of a heterogeneous and multilayered wall. To do this, we use various concepts from the literature on fibre-reinforced polymers. In particular, we use the Halpin-Tsai equations to predict elastic properties and the Tsai-Hill criterion to predict plastic yield. Our model provides insight into cell growth dynamics, wall stress profiles, apparent wall properties and the effect of key parameters such as microfibril volume fraction and aspect ratio on these results.

Keywords: Biomechanics, plant cell growth, microfibrils, modelling

*Speaker

Mechanobiology of root hair growth

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Root hairs are single cells that grow laterally from the root epidermis. They play a crucial role in the absorption of nutrients from the soil. While they keep a small typical diameter of 10μm, root hairs can reach _˜1 mm in length, thus significantly increasing the surface area of roots, enhancing their ability to uptake essential resources for plant growth and development.
Root hairs are under high internal pressure, namely turgor pressure. This pressure induces deformation (creep) of their wall at the tip of the cell, leading to cell elongation and deposition of new material in the cell wall, a process called tip growth. Measuring turgor pressure, and its potential regulation in different conditions, is thus crucial to understand plant development.

Turgor pressure varies within plants, organs and cells. Probing it on a single cell level is a challenge. Few techniques have been developed such as cell pressure probe(1) or atomic force microscopy(2). The pressure probe can even be used to control or modulate pressure inside the cells(3) but has limitations. In particular, it needs the cell to be punctured, which can lead to leaks and modify turgor pressure itself.

We developed a new setup to probe turgor pressure on single root hairs of Arabidopsis Thaliana by compressing the cell between parallel plates. As root hairs can be viewed as cylindrical pressurized pipes, the internal pressure can be deduced from force-indentation curves.

We will show here the technique, its validation and the first results obtained on pressure regulation during root hair growth, in particular in media of different rigidities, and in response to hyper-osmotic chocks.

(1) Steudle & Zimmermann (1971) *Zeitschrift für Naturforschung ;* Tomos & Leigh (1999) *Annual review of plant biology*

(2) Arnoldi *et al.* (2000), Physical Review

(3) Lew (1996) *Plant Physiology*

Keywords: root hair, turgor pressure, mechanobiology, development

*Speaker

Penetration of a granular medium by a tip-growing tube

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Anchoring a structure in the ground is a challenge that requires the application of significant external forces. However, anyone who spends a Sunday gardening knows that even young plants can develop impressive root networks without the need for external forces to anchor them. One peculiarity of roots is that they grow primarily at the tip. We mimic this growth using a soft cylindrical tube that everts on itself to understand whether this mode of penetration changes the interaction with a soil, modeled as a granular medium. The granular medium consists of a packing of beads and the penetration force of the everted tube is compared with the reference case of a rigid tube. For the rigid tube, we recover the classical quadratic dependence of the penetration force with depth, as friction is mobilized over the entire penetration depth. In contrast, the force required to penetrate with tip growth initially increases with depth before reaching a plateau, probably because friction anchors the tube in the granular medium, thereby damping the penetration force. In addition, the tube tends to bend as it penetrates, a consequence of the interactions between the mechanical behavior of the inflated tube and the mechanical stress in the granular medium. These results suggest that tip growth is an effective anchoring mechanism.

Keywords: granular medium, eversion, soft tube, penetration

*Speaker

The Biomechanics of Insect-Triggered Trichome Rupture

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Trichomes, the hair-like protrusions adorning the surfaces of many plants, serve primarily as a defense system against herbivorous insects. These microscopic appendages come in a variety of forms across plant species and have precisely-tuned architectural and mechanical properties that allow them to obstruct, immobilize or deter insects attempting to eat the plant through a combination of chemical deterrents, elasticity, and controlled fracture behaviors. Concerningly, crop domestication has resulted in a decline in the presence and variety of trichomes in many staple crops, with large-scale implications for crop loss and overreliance on harmful pesticides in the agriculture industry.
In this study, we investigated the biomechanics of trichomes in both wild and domesticated tomato species using microstructural characterization techniques from soft matter physics. Micropipette force sensing coupled with high-speed imaging enabled measurements of the various trichome types' bending moduli, as well as the critical forces required to rupture glandular trichomes in both species. Glandular rupture involves the rapid release of a pressurized solvent that is toxic to many insects. Our results show trichomes can undergo such rupture upon the application of forces as low as tens of nanonewtons - forces comparable to those exerted by insects during locomotion. We then directly observed a target pest, thrips, inadvertently triggering the rupture of trichomes and the ensuing accumulation of viscoelastic solvent on their bodies, demonstrating an effective defensive strategy.
By integrating structural analysis, mechanical testing, and ecological observations, this work reveals the ingenious biomechanical strategies employed by trichomes at the intersection of soft matter physics and plant evolutionary biology.

Keywords: plant physics, trichomes, insects, soft matter physics, micropipette force sensing, biomechanics, living matter, microstructure

*Speaker

Fast movements of Mimosa pudica: an osmotic muscle?

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Plant movements span timescales ranging from tenths of seconds to several hours, and rely on a rich variety of physical mechanisms. The "touch-me-not" plant, Mimosa pudica, folds its leaves in a couple of seconds in response to mechanical or electrical stimuli. This movement is reversible, and leaves reset within a few tens of minutes.

Purely osmotic water transport across the whole pulvinus—a flexible, hinge-like bulge at the base of each leaf—constitutes the textbook explanation of the motion. This scenario received only limited experimental evidence, however, and implies that pulvini operate near the physical limits of osmotic transport.

Here we experimentally characterise the kinematics of the movement and the mechanics of the pulvinus. We then build a simple osmotic motor model to capture the global dynamics and to estimate the microscopic quantities characterising the motor. Our preliminary results suggest that osmosis is not compatible with the motion time scale. We finally elaborate and test an alternative mechanism based on local water redistribution from cells to neighbouring air channels.

Keywords: biomechanics, soft actuation, plant movements

*Speaker

MP1 – Spin or Orbital current-induced magnetization torques and self-induced torques : how to distinguish between different contributions in magnetic materials

Large Chiral Orbital Texture and Orbital Edelstein Effect in Co/Al Heterostructure

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Recent experiments by S. Krishnia et al., Nano Lett. 23, 6785 (2023), reported an unprecedentedly large enhancement of torques in Pt/Co bilayer upon adding a well-protected Al layer on top of Co, which does not occur when Cu layer is placed instead of Al. As spin-orbit coupling is small in light elements such as Al, these experiments suggest that the enhanced torques could originate from the orbital Edelstein effect at the interface rather than from the spin Hall or spin Rashba-Edelstein effects, which are conventionally regarded as the main sources to generate spin-orbit torques. Based on first-principles calculations, we reveal the emergence of a large orbital texture at the interfacial Co layer in Co/Al heterostructure with a clear helical locking of the in-plane orbital momentum in reciprocal space, which is found to be much smaller at the Co/Cu interface. Our results demonstrate that the origin of the chiral orbital texture can be attributed to non-trivial hybridization due to the formation of the surface states at the interfacial Al layer. Importantly, the chiral orbital texture preserves itself in the absence of spin-orbit coupling, which is found to produce smaller contributions with a higher-order winding of the orbital momentum. We further employ the Kubo formalism to calculate the orbital magnetoelectric susceptibility in response to an applied electric field. Our calculations unveil that the chiral orbital texture at the Co/Al interface can give rise to the out-of-equilibrium orbital polarization producing large field-like torques, thus providing a rigorous theoretical interpretation for the experimental data and advancing the use of orbital transport phenomena in all-metallic magnetic systems with light elements.

Keywords: orbitronics, spin, orbit torques, orbital chiral texture, vorbital Edelstein effect

*Speaker

Spin Charge Interconversion in Synthetic Ferrimagnetic Co/Gd Bilayers

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Spin-orbitronics in ferrimagnets have gained a lot of traction in the field of Nanomagnetism for efficient memory and logic applications. Ferrimagnets bring together the advantages of ferromagnets and antiferromagnets in terms of control and detection of magnetization and fast dynamics. In particular rare-earth (RE)-transition metal (TM) ferrimagnetic alloys facilitate current driven operations while exhibiting exciting phenomenon such as self-torques, fast current driven domain wall motion (CDDWM) and single pulse all optical switching (AOS)(1-3). Moving towards RE-TM synthetic ferrimagnets (SFiM) enables easier tunability via thickness and interface engineering. In the past few years, wide-range single shot AOS, giant spin orbit torques (SOT) have been reported in SFiM such as Co/Gd multilayers (4). In order to understand the SOT and the role of interface effects in a bilayer RE-TM SFiM system, we fabricate bilayers of Co(2nm)/Gd(1nm and 2nm) on SiO2 substrate with different capping layers of Al, Pt and Ta along with reversal of the bilayer stacking order. We pattern Hall bars, spin-pumping and spin-torque FMR and spin Seebeck devices using UV lithography to perform spin-charge interconversion studies. We mainly rely on performing SOT studies using the harmonic Hall technique for charge to spin conversion and for spin to charge conversion we perform spin-pumping FMR experiments. Based on these studies we also aim to disentangle orbital and spin contributions in the torques. This ultimately helps us in engineering multilayer systems with high spin-charge interconversion efficiency in SFiM systems, achieving field free self-induced SOT switching and favourable static and dynamic properties of spin textures such as skyrmions.

(1) Céspedes-Berrocal et al. *Advanced Materials*, *33*(12), 2007047.
(2) Mangin et al. *Nature materials*, *13*(3), 286-292.
3)*Kimeletal.Nature Reviews Materials*, *4*(3), 189 − 200.
(4)*Lietal.Advanced Electronic Materials*, *9*(1), 2200613.

Keywords: Synthetic ferrimagnets, spin orbit torques

*Speaker

Spin- and orbital-charge conversion at the surface states of Bi1-xSbx Topological insulator

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Topological insulators are quantum materials characterized by Time-reversal protected surface states (TSS) which make them appealing candidates for the design of next generation of highly efficient spintronic devices. The very recent demonstration of large transient spin-charge conversion (SCC) and subsequent powerful THz emission from Co—Bi1-xSbx bilayers clearly demonstrate such potentiality and feasibility for the near future (1-3). Amongst the exotic properties appearing in and at the surface of such quantum materials, spin-momentum locking (SML) remains as a key ingredient to effectively convert the spin degree of freedom into a charge or a voltage signal. In that sense, in this work we will provide some clear theoretical and numerical insights implemented by multiorbital and multi-layered tight-binding methods (TB). These developments clarify our recent experimental results obtained by THz-TDS spectroscopy techniques in the time domain (2); and allows us to disentangle the various magnetic SCC contributions. Taking advantage of their spin-momentum locking property, we also postulate the occurrence of Orbital-to-charge conversion (OCC) taking place also in these aforementioned experiments at equal footing to SCC.

By extending the spin-to-charge conversion theory, we postulate the emergence of its orbital counterpart, namely the Orbital-charge conversion (OCC), covering different contributions in terms of the orbital degree of freedom. Our results unveil the interest and prospects for the use of specific materials as source of both spin and orbital current (as Ni); and we may anticipate the advantage of using lighter elements with the restricting requirement of large SOC would be avoided in the latter case. Furthermore, given that physical degrees of freedom as photons are able to also carry orbital angular momentum we comment on recent theoretical efforts to opto-electronic properties in our system.

Keywords: Spintronique, transport électronique, isolateurs topologiques

*Speaker

Exploring magnetothermal enhancement by tuning orbital and spin current

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The generation and detection of spin currents play an important role in the field of spin-orbitronics. One of the reliable methods to quantify the spin-to-charge interconversion is the spin-Seebeck effect (SSE). This effect refers to the generation of a spin current by a temperature gradient across a magnetic material and is usually detected by the voltage (1). In addition to the SSE, also the orbital-Seebeck effect can generate spin and orbital polarized currents in a ferromagnet, making it possible to observe the spin/orbital angular momentum-to-charge conversion (2-3). We carried out thermospin measurements to get the spin/orbital-to-charge interconversion. The amplitude of the thermospin voltage has two contributions, one of them is the anomalous Nernst effect (ANE) due to the ferromagnet (FM) itself, and the other is the Inverse Spin/Orbital Hall effect (ISHE/IOHE). We perform the measurement in patterned microdevices in a controlled experiment measuring the voltage detected as a function of the magnetic field with a fixed heater current between 40 mA and 100 mA. We have investigated different materials and heterostructures, ranging from single FM layers, "typical" FM/HM bilayers, to systems including Cu/MgO and Ti/MgO interfaces together with FePt and CoPt alloys. A direct comparison of the measured voltage amplitude, for the same heater input power conditions, gives a gain in magnetic alloy systems with Pt, and with Cu/MgO, and Ti/MgO interfaces. For example, the output power of Co or NiFe-based systems is below 1 pW while the output power of the new systems such as CoPt/Cu/MgO reaches as high as 7 pW. Our results show that we can benefit from efficiently combining the orbital current and orbital-charge conversion phenomena together with the spin-charge current.
(1) Phys. Rev. Materials 7, 104203 (2023)

(2) arXiv:2403.07055v1 (cond-mat.mes-hall)
(3) Phys. Rev. Applied 19, 014069 (2023)

Keywords: Orbital current, Orbital Seebeck effect

*Speaker

Theory of orbital diffusion and torque

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Recent progress in the physics of spin-charge interconversion mediated by spin-orbit coupling has shed new light on the orbital angular momentum degree of freedom. Indeed, while the orbital ordering driven by the crystal-field potential governs the interplay between crystal structure and electronic properties of strongly correlated materials such as Mott insulators, the possibility of transporting the orbital information in these materials has remained an open question so far. In the context of metallic spintronics though, it has been progressively realized that the orbital angular momentum can be generated out of equilibrium, transported, and detected, rather similarly to the spin angular momentum. In this communication, I will present a quantum theory of orbital diffusion and uncover several mechanisms governing orbital torque and magnetoresistance phenomena, including orbital diffusivity, spin-orbit polarization, orbital swapping, and orbital mixing conductance. These new concepts are crucial to the understanding of experimental results and can be computed from first principles.

Keywords: spintronique, moment orbital, courant de spin

*Speaker

IA2 - Artificial intelligence in electron microscopy

Biomolecular structure determination in post-AlphaFold era

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AI-based methods for predicting protein structure from a sequence of amino acids, such as AlphaFold2, produce similar models to those obtained experimentally, but they are still limited to static structures and the protein dynamics is still studied by experimental techniques, such as cryo electron miscopy (cryo-EM) and cryo electron tomography (cryo-ET), or using hybrid methods that combine cryo-EM/ET with modeling. AI based methods could be useful for obtaining the initial models, when such models are unavailable, but their efficiency in predicting large, multisubunit, and flexible complexes remains to be demonstrated. In this talk, I will present the methods that we have developed for extracting biomolecular structure and dynamics from cryo-EM and cryo-ET data and discuss the future work regarding this challenging problem.

Keywords: cryo electron microscopy, cryo electron tomography, learning the dynamics of biomolecular complexes

*Speaker

Data Reduction and Clustering Approaches for a Comprehensive Phase Analysis inside Na-ion battery Cathode Materials

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In the field of battery electrode materials, the presence of multiple phases undergoing structural modifications can significantly impact battery performance and durability. Understanding the contributions of these phases and their spatial distribution is crucial. Our study focuses on the chemical evolution of Na3V2(PO4)2F3 (NVPF) during charge/discharge cycles using scanning transmission X-ray microscopy (STXM) and X-ray absorption spectroscopy (XAS) at the SOLEIL Synchrotron's HERMES beamline. NVPF cathodes were cycled to achieve various Na contents, specifically Na2.5V2(PO4)2F3, Na2V2(PO4)2F3, Na1V2(PO4)2F3, and Na0.3V2(PO4)2F3.
To process the STXM-XANES data, we developed a Python-based solution incorporating machine learning and deep learning algorithms such as non-negative matrix factorization (NMF), Pearson correlation coefficient (PCC), and variational autoencoder (VAE). This approach allowed us to create detailed phase maps within individual NVPF crystals based on X-ray absorption edges of V and O, revealing insights into sodium-ion diffusion processes essential for advanced cathode material development.

In parallel, we performed a structural study using four-dimensional scanning transmission electron microscopy (4D-STEM) Automated Crystal Orientation Mapping (ACOM) on the same crystals. We developed the ePattern4 code to index diffraction spots and reduce noise in large datasets, which, combined with the ASTAR software, enabled us to generate structural phase maps.
By developing a Python solution for phase and reliability mapping, our study offers valuable insights into the confidence level of our phase identification within the samples. This combination of advanced analytical techniques and machine learning algorithms effectively characterizes phase heterogeneities in NVPF cathode material. Our findings are crucial for advancing sodium-ion battery development, aiding in the design and optimization of electrode materials with enhanced performance and durability.

Keywords: Scanning transmission X, ray microscopy, 4D, STEM, Battery material, NMF, PCC, VAE

*Speaker

Unlocking 3D nanoparticle shapes from 2D HRTEM images: Deep Learning for classification at atomic resolution

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Nanoparticles (NPs) are typically observed and analysed using High Resolution Transmission Electron Microscopy (HRTEM) for highly precise structural studies at the atomic scale. However, determining their 3D shapes from 2D HRTEM images is a tedious process. Indeed, this type of analysis is based on manual post-processing which suffers, among other issues, from experimental noise or human bias performed at post-experimental stage. In this context, the integration of artificial intelligence methodologies into data acquisition and analysis protocols is a very promising approach (1). To tackle the problem of identifying the 3D shape of NPs, we developed a Deep Learning (DL) model to automate this task ensuring reliable statistical analysis of a large number of NPs, many of which cannot be identified by conventional methods.
For this purpose, the model is trained on datasets of simulated HRTEM images of NPs, labelled according to their shapes, ranging from 4 to 8 nm. To generate a representative dataset, we constructed atomistic 3D models of NPs deposited on amorphous carbon (2), subjecting NPs to random rotations to encompass all potential observed orientations. Finally, HRTEM images were simulated using the Dr Probe code (3) based on the multi-slice method with parameters consistent with aberration-corrected transmission electron microscopes.

The objective of generating an optimal training dataset was attained through comprehensive studies evaluating the impact of various parameters, including amorphous carbon, resolution, focusing conditions, NPs' size, and NPs' orientations, on DL model predictive accuracy. This approach has resulted in the development of an efficient and accurate framework for predicting 3D NP shapes from 2D HRTEM images, validated across simulated and experimental datasets.

References
(1) S. R. Spurgeon *et al.*, Nat. Mater. 20, 274 (2021)
(2) C. Ricolleau *et al.*, J. Appl. Phys. 114, 213504 (2013)
(3) J. Barthel, Ultramicroscopy 193, 1 (2018)

Keywords: artificial intelligence, deep learning, nanoparticle, transmission electron microscopy, atomistic simulation

*Speaker

EELS Spectra classification: Machine Learning vs Neural Network

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Processing Electron Energy Loss (EELS) hyperspectral images involves mapping changes in the fine structures of core-loss edges. In the case of transition metals, these changes can reflect, for example, valence states probed at the atomic scale in STEM.
Various methods are employed for this task. Some, like Principal Component Analysis (PCA) and Non-negative Matrix Factorization (NMF), decompose each spectrum at a sub-pixel level. Others, like clustering, assign unique labels to every pixel. Clustering has been utilized in EELS data processing through algorithms like K-Means or hierarchical clustering (1-3).
Recently, Neural Networks have been used to classify EELS spectra, whether in the form of Convolutional Neural Networks (CNNs) (4), or a denoising autoencoder followed by a Dense Network for classification (5).
We evaluated a CNN approach against traditional Machine Learning (ML) methodologies. We analyzed the fine structures of the Co-L3 edge in Co3O4. This model system presents Co2+ and Co3+ valences with atomic columns purely composed of one valence along (001) zone axis (6).

We simulated a dataset with Co2+ and Co3+ L3 edges. The performances of different unsupervised clustering algorithms were compared to that of a simple CNN under varying noise levels.
We applied both the clustering method and the CNN trained on the simulated data to our experimental dataset. We found that these methods demonstrated comparable performance. While the unsupervised approach is more straightforward to implement and offers greater generalizability, the CNN accomplishes the task more rapidly.

References:

(1) Torruella, P. et al. (2018) *Ultramicroscopy*, *185*, 42-48.
(2)Blanco-Portals, J. et al. (2022) *Microscopy and Microanalysis*, *28*(1), 109-122.
(3) Cho, M. et al. (2023).*Microscopy and Microanalysis*, 29(1), 1925–1926.
(4) Chatzidakis, M., & Botton, G. A. (2019) *Scientific reports*, *9*(1), 2126.
5)$Pate, C.M.etal.(2021)Sci\ Rep\mathbf{11}, 19515.$
(6)$Teurtrie, A, PhDthesis, 2019, https://theses.fr/2019SACLS464$

Keywords: EELS, hyperspectral image, Machine learning, Deep Learning, classification

*Speaker

Machine learning appliqué à la détection de défauts et l'analyse de leur distribution

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La caractérisation d'un matériau irradié nécessite une analyse minutieuse de la population de défauts présents en son sein, tels que les bulles, les cavités et les précipités. Cette tâche, réalisée à partir d'images de microscopie électronique en transmission (TEM), est souvent laborieuse, chronophage et sujette à l'erreur humaine. Ainsi, les approches basées sur l'apprentissage profond sont de plus en plus utilisées, offrant une automatisation du comptage et de la caractérisation individuelle des défauts (1).
Cette étude se concentre sur la détection et la caractérisation des boucles de dislocation dans un alliage à haute entropie irradié, un domaine de recherche en pleine expansion, notamment dans le contexte des applications nucléaires (2). L'irradiation aux ions génère de nombreuses boucles de dislocations, qui se superposent sur les micrographies TEM. Nous présentons ici une méthode de détection basée sur un réseau neuronal de type Mask R-CNN (3), suivie d'une analyse des distributions des populations de boucles de dislocations. Cette analyse est réalisée en comparaison avec des simulations par dynamique d'amas, guidée par un algorithme génétique.

Cette approche permet d'accéder à des informations précieuses sur les mécanismes de formation et de mûrissement des boucles de dislocations dans les alliages à haute entropie sous irradiation, ouvrant ainsi de nouvelles perspectives pour la conception et l'optimisation de matériaux résistants aux environnements extrêmes. En outre, l'utilisation de l'apprentissage profond dans la caractérisation des matériaux irradiés présente des avantages significatifs, notamment en termes d'efficacité et de précision. Plus généralement, cette méthodologie pourrait être étendue à d'autres types de défauts et de matériaux, offrant ainsi un outil polyvalent pour la recherche en science des matériaux.

(1) Jacobs, R., Comput. Mater. Sci. 211, 111527, (2022).

(2) Pickering, Ed J., *et al.*, Entropy 23.1 (2021): 98.
(3) He, Kaiming, *et al.*, Proceedings of the IEEE international conference on computer vision. 2017.

Keywords: Intelligence artificielle, Microscopie électronique en transmission, HEA, Segmentation

*Speaker

TEM image processing and segmentation by thresholding and AI methods for the characterization of Xe bubbles in UO2

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During in pile irradiation, the nuclear fuel UO2 (a ceramic material) undergoes significant chemico-physical and structural modifications. The fission reaction of a 235U atom by a neutron results in the creation of fission products (FPs) of which 15% are rare gases: xenon and krypton. These gaseous fission products are insoluble in UO2, so they can precipitate as sub- to nanometric bubbles in the matrix. In order to supply and validate simulation models of the behavior of fission gases in nuclear fuel, it is necessary to experimentally characterize in detail these bubbles (size, density, pressure, shape, etc.).

Currently, this characterization is carried out manually from transmission electron microscopy (TEM) images, which represents a time-consuming task, which limits the quantity of data and therefore the statistics, and could be subject to significant measurement biases.

A semi-automatic counting method by thresholding is developed on Imagej/Fiji. This method makes it possible to determine the density as well as the size of the smallest bubbles ($<$ 2 nm) with an error of 4% compared to manual counting and a counting time divided by at least a factor five. In addition, the protocol used allows adaptability to the imaging conditions and reduces the measurement bias of manual counting by improving the statistics on the data and reducing the sensitivity on the image quality.

Regarding the counting of the largest bubbles, the thresholding method is insufficient. For this, two segmentation methods, using artificial intelligence (AI), are developed on WEKA and Ilastik. These methods produce very interesting results for the characterization of large bubbles, particularly for the determination of their shape where they are more accurate than manual characterization.

Keywords: nuclear fuel, GFP, image processing, threshold, AI

*Speaker

Towards FIB-SEM/SIMS low-dose high-speed acquisition using alternative scanning patterns boosted with ML

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Beam damage and shot noise are two factors that influence the resolution in Focused Ion Beam - Scanning Electron Microscopy (FIB-SEM) and Secondary Ion Mass Spectrometry (SIMS). Beam damage causes structural modifications, while shot noise affects the signal-to-noise ratio (SNR), leading to image distortion. The conventional raster scanning suffers from flyback distortions and can introduce additional dose to the sample, potentially damaging sensitive materials (1).
To mitigate these issues, alternative scanning patterns such as bidirectional, spiral, Hilbert curve, and Z-order have been proposed. These methods aim to reduce beam damage and improve image acquisition by maintaining continuous beam movement and eliminating flyback. Each pattern has distinct advantages and challenges, such as the bidirectional pattern's requirement for post-processing due to directional distortions, the spiral pattern's non-uniform image quality, and the Hilbert and Z-order patterns' susceptibility to distortions with small dwell times (2,3).

The sparse scan pattern, which scans only a portion of the pixels, offers reduced acquisition time but is sensitive to drift and requires complex reconstruction procedures. Implementing these patterns can be enhanced with machine learning or deep learning algorithms, which contributes to a low-dose, high-speed acquisition, adding complexity and computational demands to the system (4).

Our goal is to implement these novel scanning methods on a high-vacuum FIB-SEM platform (Scios from Thermo Fisher Scientific) equipped with a SEM column, Ga-FIB column, and a SIMS system (5). We successfully tested these patterns using a custom-built acquisition system controlled by a USB-6351 acquisition card from National Instruments. The system manages scan control and data acquisition, with a LabVIEW program overseeing operations.
These improvements in raster schemes are expected to enhance materials research by facilitating high-resolution imaging of transient processes and radiation-sensitive samples.

Keywords: FIB, SEM, High, speed low, dose acquisition, scan patterns, image reconstruction

*Speaker

Deep Learning Assisted Denoising of in situ Liquid STEM Movies of Nanoparticle Nucleation and Growth

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Understanding of the formation mechanism of metallic nanoparticles (NPs) has over recent years greatly benefitted from in situ liquid TEM that enables imaging the nucleation and growth of individual NPs in liquid media. However, these experiments pose challenges regarding both imaging and data analysis. Substantial scattering from the liquid around the nano-objects and the electron transparent SiN membranes significantly diminishes the signal quality (1). One solution would be to increase the electron dose rate, but this can lead to undesirable effects due to radiolysis.
To address this issue, we propose an innovative approach that combines artificial intelligence and scanning transmission electron microscopy kinematic simulations (2). Our approach enables the differentiation and extraction of valuable signals from unwanted background fluctuations and noises in liquid dark-field STEM sequences. Besides considering the size and shape dispersions of nanoparticles, our kinematic simulations account for a significant obstacle in studying NP growth by liquid cell TEM: the formation of NPs on the opposite membrane of the cell that contribute to the random background fluctuations because they are imaged way out-focus. Considering these challenges, our method effectively denoises low and high magnification videos, elevating the signal-to-noise ratio (SNR) from 1.56 to 8.27, above the threshold value of 5 set by the Rose criterion. Consequently, our analysis pipeline facilitates the study of NP growth mechanisms with improved statistics and fewer acquisition constraints. We will show application of this methodology to investigate surface site attractiveness on both gold nanocubes and nanorods within the context of NP synthesis.

1. N. de Jonge, *Ultramicroscopy 187*, 113–125 (2018).
2. D. S. He, Z. Y. Li, and J. Yuan, *Micron 74*, 47-53 (2015).

Keywords: in situ Liquid STEM, Denoising, Deep Learning, Gold Nanoparticles

*Speaker

2DMS1 - New perspectives and complementaries for electron and X-ray spectroscopies

Coupling of excitations. Coupling of spectroscopies.

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Signatures of electronic correlation on excitation spectra can be often interpreted in terms of coupling of excitations. A prominent example are satellites in photoemission spectroscopy that can be explained within an electron-boson coupling picture, where the bosons are the charge excitations induced by the creation of the photohole.
These ideas promote a collaborative strategy based on the coupling between the spectroscopies that independently measure the various excitations, such as photoemission, electron energy loss spectroscopy and inelastic x-ray scattering (both in the resonant and non-resonant versions).

In this talk, I will present some case studies where the tight interlinking between theory and experiment has been crucial for the investigation of electronic excitations in materials ranging from simple metals to transition metal oxides (1-4). Finally, since what is calculated and what is measured are often different, I will highlight the importance of bridging the gap between theory and experiment to uncover new physics.

The results that will be presented have been obtained thanks to fruitful collaborations with several members of the Palaiseau Theoretical spectroscopy group and colleagues from experimental groups.

(1)C. Su, K. Ruotsalainen, A. Nicolaou, M. Gatti, A. Gloter, Advanced Optical Materials, 11, (2023)
(2)F. Pressacco, D. Sangalli, V. Uhlíř, D. Kutnyakhov, J. Arregi, S. Agustsson, G. Brenner, H. Redlin, M. Heber, D. Vasilyev, J. Demsar, G. Schönhense, M. Gatti, A. Marini, W. Wurth, F. Sirotti, Nat. Commun., 12, 5088 (2021)
(3)K. Ruotsalainen, A. Nicolaou, C. Sahle, A. Efimenko, J. Ablett, J. Rueff, D. Prabhakaran, M. Gatti, Phys. Rev. B, 103, 235136 (2021).
(4)J. Zhou, L. Reining, A. Nicolaou, A. Bendounan, K. Ruotsalainen, M. Vanzini, J. Kas, J. Rehr, M. Muntwiler, V. Strocov, F. Sirotti, M. Gatti, Proc. Natl. Acad. Sci. U.S.A., 117, 28596-28602 (2020).

*Speaker

Time-resolved nanothermometry using photon-electron pump-probe spectroscopy

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Understanding the thermal transport in nanostructures is a crucial and complex phenomenon for many technologies, especially as devices shrink in size towards the nanometer scale. In this case, studying out-of-equilibrium behavior requires access to timescales from ps to μs. Existing methods (1) that provide both these temporal and spatial resolutions remain limited. However, recent advances in event-based direct detectors in electron microscopy (2) open new possibilities.
In this study, we use distinct EELS signatures to measure the temperature of 2D semiconductors, Si3N4, and Al films after focused (_˜1 μm) and pulsed (_˜20 ns) laser excitation in the visible range. By synchronizing the laser pulse with a Timepix3 detector, we introduce a novel method for measuring temperature with nanometer and nanosecond resolutions. A simple 2D diffusion model allows us to model the observed temperature dynamics. Since various spectroscopic excitations from IR to far UV are used, our approach provides a universal tool for probing nanosecond thermal dynamics in nanostructures. The temporal resolution here is limited by the technology of the Timepix3 detector and will be improved in the future. Furthermore, this method can be extended to diffraction-based techniques like 4D-STEM to detect subtle dynamical changes in crystalline lattices under different stimuli.

References

(1) A. El Sachat *et al.*, Nanomaterials **11** (2021) 175
(2) Y. Auad *et al.*, Ultramicroscopy **239** (2022) 113539

Keywords: Nanothermometry, electron/photon spectroscopy, 2D materials

*Speaker

X-ray Absorption spectroscopy by Dynamical Mean-field theory

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X-ray Absorption spectrocopy (XAS) provides rich and valuable information about the chemical state and local environment of selected elements in solids. However, the resulting spectra must be analysed through comparison with numerical XAS spectra.
Accurate and reliable theoretical description of the electronic state of the absorbing site and its surroundings is therefore crucial for the analysis of experimental data. In strongly correlated materials, the strong Coulomb interaction between electrons renders such large many-body quantum systems very challenging and they must be solved with approximate models and numerical methods. In my PhD project, I try to include in the modelling of XAS not only the absorbing atom but also a continuum of surrounding electronic states. I will present my work on Nickel Oxyde (NiO), a paradigmatic example of strongly correlated materials, using dynamical mean-field theory and a Matrix-Product-State impurity solver.

Keywords: (strong correlations) (core, level spectroscopies)

*Speaker

Recent developments in the soft X-ray RIXS and XAS program at the ESRF

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The ESRF synchrotron in Grenoble operates the soft X-ray beamline ID32 designed for XAS and RIXS studies of transition metal and lanthanide materials. Recently, the high-resolution RIXS spectrometer at ID32, the benchmark for high-resolution RIXS instruments in Europe and the world, has undergone a major upgrade which greatly further improved its resolution and through-put. At the same time, the arsenal of sample environments available to users has also been continuously developed. In addition to the standard cryogenic sample environment we can now also offer uniaxial strain, high temperatures or electric and magnetic fields to users.
In early 2024, the high-resolution RIXS instrument at ID32 was complemented with a compact, very high through-put RIXS spectrometer that is operated at the XMCD branch of the beamline. This spectrometer can be used with several end-stations: the ID32 high-field magnet for RIXS measurements in fields up to 9T and down to 4K, a compact material science end-station for materials research, and in the future a pulsed field magnet granting access to fields of 50+ Tesla. This creates unique new opportunities for materials research solely available at ID32, in particular, for magnetic dichroism studies combining XAS and RIXS.
In this talk, we will present the recent and prospective instrumental developments at ID32, discuss some of the scientific opportunities created and show some recent scientific examples.

*Speaker

Characterization of Valence Electrons Excitations in 2D Titanium Carbide Layers combining electron and X-ray spectroscopies with DFT simulations.

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Two-dimensional transition metal carbides or nitrides - so-called MXenes - are among the youngest and largest family of 2D materials, Ti_3C_2 being one of the most studied. This later compound combines high metallic conductivity with hydrophilicity, a true originality as compared to other 2D materials, and allowing cost-effective processing as thin films for a very large range of applications. In addition, because of the synthesis process, Ti_3C_2 layers are functionalized with different chemical species (*e.g.*, T = O, F or Cl) which have a strong impact on their physicochemical properties. Controlling MXene multilayers properties thus relies on the characterization of the chemistry/functionalization of the layers, but also of the number of stacked layers and the average interlayer distance which can be controlled and modified in many different ways. Focusing on valence electrons excitation spectra, we will illustrate the complementarity between monochromated Electron Energy Loss Spectroscopy (EELS) and high-resolution (HR) synchrotron X-ray photoelectron spectroscopy (XPS) in characterizing the electronic structure and architecture of Ti_3C_2 multilayers at different scales. Quantitative analysis of the experimental data is performed using Density Functional Theory simulations. In particular, we will show that the valence EELS signal in Ti_3C_2 multilayers is dominated by collective excitations, *i.e.,* surface and bulk plasmons. These modes being intrinsically delocalized, they are highly sensitive to the multilayers' architecture, allowing to determine on the nanometer scale the exact number of layers in a given multilayer, as well as the evolution of the interlayer spacing. Very complementary, valence HR-XPS spectra can be directly related to the projected electronic densities of states of the topmost MXene layers in a film. These spectra thus provide a direct picture of the valence band electronic structure with deep insights on the role of the surface functionalization, in connection with the synthesis process.

Keywords: EELS, high resolution XPS, MXenes, DFT, plasmons, electronic structure

*Speaker

2DMS3 - Electronic and optical excitations in bulk and low-dimensional materials

electronic and optical properties of close-to 30° boron nitride twisted bilayers

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We investigate the electronic structure and the optical absorption onset of hexagonal boron nitride bilayers at moderate twist angles (1) as well as twists in the vicinity of 30∘ (2). Our study is carried out with a DFT-based tight-binding model that we developed on purpose and validated against DFT simulations.
We demonstrate that approaching 30∘ (quasicrystal limit), all bilayers sharing the same twisted supercell develop identical band structures, irrespective of their stacking sequence. This band structure features a bundle of flat bands laying slightly above the bottom conduction state which is responsible for an intense peak at the onset of absorption spectra. These results reveal the presence of strong, stable and stacking-independent optical properties in boron nitride 30∘-twisted bilayers.

By carefully analyzing the electronic spatial distribution, we elucidate the origin of these states as due to interlayer B-B coupling. We take advantage of the the physical transparency of the tight-binding parameters to derive a simple triangular model based on the B sublattice that accurately describes the emergence of the bundle.
(1) S. Latil, H. Amara, and L. Sponza, "Structural classification of boron nitride twisted bilayers and ab-initio investigation of their stacking-dependent electronic structure", SciPost Phys. 14, 053 (2023).
(2) L. Sponza, V.B. Vu, E. Serrano Richaud, H. Amara, and S. Latil, "Emergence of flat bands in the quasicrystal limit of boron nitride twisted bilayers", Phys. Rev. B 109 L161403 (2024).

Keywords: hexagonal boron nitride, twisted bilayers, tight, binding, excitons

*Speaker

Electronic properties of 2D Transition Metal Dichalcogenides ternary alloys: an ab initio study

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First principles calculations are performed to investigate the properties of monolayer transition metal dichalcogenides (TMDs) ternary alloys of the form MXY, with M = Mo, W and X $\neq$ Y = S, Se. We are particularly investigating the influence of the composition of these alloys on the properties of the parents TMD materials. To have a better understanding of the composition dependent, the thermodynamic stability, structural and electronic properties of these alloy configurations at various concentrations have been comparatively studied using the density functional theory (DFT). We found that the introduction of the foreign Y atom affects the lattice constants of the 2D systems, in agreement with literature (1). From bandstructure analysis, we saw that the introduction of the Y chalcogen fine tunes the band gap of a MX2 monolayer keeping the direct band gap character at K point. In addition, the orbital-projected bandstructure reveals that the band gap is mainly due to the d orbital of M atom. Beyond these ground-state properties, the electronic density, and the Kohn-Sham structure of the studied systems are used to calculate the absorption and electron energy loss spectra, within time-dependent density functional theory (TD-DFT) using the Selected-G method (2). The spatial dependence of the response function as well as of the induced density are also analysed (3). Our results show clearly specific signature of the electronic density for each chalcogen.
References :

(1) K. Zollner, P. E. F. Junior, and J. Fabian, Physical Review B **100** (2019), 195126.

(2) N. Tancogne-Dejean, C. Giorgetti, and V. Véniard, Physical Review B **92** (2015), 245308.
(3) S. Mazzei and C. Giorgetti, Physical Review B **106** (2022), 035431.

Keywords: Transition Metal Dichalcogenides monolayer, alloying, electronic properties, DFT, TDDFT.

*Speaker

Theoretical exploration of exciton-exciton interactions in 2H-transition metal dichalcogenide bilayers

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The fundamental properties of an exciton are determined by the spin, valley, energy, and spatial wavefunctions of the Coulomb-bound electron and hole. In van der Waals materials, these attributes can be widely engineered through layer stacking configuration to create highly tunable interlayer excitons with static out-of-plane electric dipoles, at the expense of the strength of the oscillating in-plane dipole responsible for light-matter coupling. Here we show that interlayer excitons in bilayer 2H-MoX2 (X=S,Se) systems can exhibit electric-field-driven coupling with the ground (1s) and excited states (2s) of the intralayer A excitons (1). We can also demonstrate, theoretically as well as experimentally, that the hybrid states of these distinct exciton species provide strong oscillator strength, large permanent dipoles and high energy tunability (2). Thanks to GW+BSE calculations, we can address the origin of these couplings in the intimate nature of those excitations (1,3).
(1) S. Feung et al, Nature Commun. 15, 4377 (2024)

(2) N. Leisgang et al, Nature Nanotechnol. 15, 901 (2020)
(3) L. Sponfeldner et al, Phys. Rev. Lett. 129, 107401 (2022)

Keywords: TMD, GW+BSE, bilayers, excitons

*Speaker

Excited-state dynamics of electrons and phonons in semiconductors

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Nonequilibrium electron dynamics governed by electron-phonon interactions plays a central role in the operation of various electronic devices and is essential for understanding many phenomena in condensed matter. The real-time Boltzmann transport equation (rt-BTE) using scattering integrals computed from first principles can describe various dynamic phenomena involving electrons and phonons. In the first part of the talk, I will present a joint experimental and theoretical investigation of the excited-state electron and hole cooling dynamics. Combining the transient absorption (TA) measurements with unprecedented temporal resolution and the *ab initio* ultrafast electron-phonon dynamics, we show conclusive evidence in TA spectra for the asymmetric hot electron and hole cooling in nitrides and zinc-blende materials.
The second part of the talk will focus on the structural dynamics, in particular, the phonon-phonon interactions incorporated into the rt-BTE. For realistic systems and dense momentum grids, these calculations become extremely challenging because of the high computational cost of the scattering integrals. Here, we employ multirate infitesimal methods, implemented in the Sundials library (1), to split different time scales in coupled electron and phonon rt-BTE. Additionally, I will present a recently developed data-driven approach, dynamic mode decomposition (DMD), to speed up rt-BTE and learn the dominant patterns from dynamics (2). I will conclude with an overview of our Perturbo code (3), an open-source framework to study electron interactions and dynamics in materials, highlighting open problems and future directions.

References

(1) D. J. Gardner, et al., "Enabling New Flexibility in the SUNDIALS Suite of Nonlinear and Differential/Algebraic Equation Solvers", ACM Trans. Math. Softw. 48, 1557-7295, (2022).

(2) I. Maliyov, et al, "Dynamic mode decomposition of nonequilibrium electron-phonon dynamics", Nature Partner Journal Comput. Mater., 10, 123, (2024).
(3) J.-J. Zhou, et al, "Perturbo: a software package for ab initio electron-phonon interactions", *Comput. Phys. Commun.* 264, 107970, (2021).

*Speaker

UNDERSTANDING THE MANY-BODY ELECTRONIC STRUCTURE OF THE NITROGEN-VACANCY CENTER IN DIAMOND

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Understanding the behavior of the ground and excited states of the negatively charged nitrogen vacancy center (NV-) in diamond under pressure is of fundamental interest to determine the pressure range in which superconductivity can be probed with NV centers in the diamond anvil cells. The nature of the ground (3A2 triplet) state and of photoluminescence signals were first identified using optically detected magnetic resonance, however the symmetry and position of the singlet energies with respect to the ground state are still under debate. In the present work, we combine first-principle generalized DFT calculations with an in-house extended Hubbard model to describe the defect many-body energy states. Using DFT-HSE06 and the ΔSCF method, we performed calculations of the ground state and of some excited states total energies, which we used to parameterize our Hubbard model. Inclusion of spin interactions beyond the intrasite and intersite correlation terms, as well as the electron-lattice interaction, turns out to be necessary to properly describe the correlated singlet-singlet transitions under pressure.
Calculations have been done using the Quantum ESPRESSO package. Computer time has been granted by the EU PRACE Project No. 2019204962 and French GENCI. Funding by DIM SIRTEQ and ANR (SADAPTH project) is gratefully acknowledged.

Keywords: Point Defects, Hubbard model, DFT, Nitrogen, Vacancy Center

*Speaker

Thermodynamic and optical properties of point defects in wurtzite boron nitride

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The wurtzite polymorph of boron nitride (wBN) plays the role of intermediary in the hexagonal (hBN) to cubic (cBN) phase transition, with the hexagonal to wurtzite phase transformation occurring at around 13 GPa (1). Millimetre-sized samples of wBN have been successfully prepared and been shown to be stable at ambient pressure (2). The wide band gaps of hBN, cBN and wBN make these materials interesting as potential defect hosts, providing a wide range of energies available for defect-induced levels. In this seminar we present the study of the thermodynamics for some simple point defects in wBN (vacancies and carbon substitutionals) using hybrid functional DFT and the supercell method. In particular the formation energies and charge transition levels (CTLs) (3) have been derived using a correction scheme (4) to account for the electrostatic interaction between the defect periodic images.

We investigate the optical properties of defected wBN by solving the Bethe-Salpeter equation for such systems. Since evaluating the screening for the supercell may be computationally prohibitive we circumvent this practical obstacle by using the one of the pristine unit cell. We then present our results when the Bethe-Salpeter equation is solved including the remapped screening in the kernel. This cheap approach also allows us to easily use the Franck-Condon model to estimate the zero phonon line and study the multiphonon emission for such defects.

Keywords: Optical properties, Boron Nitride, Defects

*Speaker

Processing Multilayer graphenes: what information is hidden in Raman spectra

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Richness and complexity of Raman spectra related to graphene materials is established from years to decades, with, among others: the well-known G, D, 2D,... bands plus a plethora of weaker bands related to disorder behavior, doping, stress, crystal orientation or stacking information (1). Herein, we report on how to detect crumpling effects in Raman spectra, using a large variety of few and multilayer graphene (2). The main finding is that these crumples enhance the G band intensity like it does with twisted bi layer graphene. We updated the D over G band intensity ratio versus G band width plot, which is generally used to disentangle point and linear defects origin, by reporting surface defects created by crumples, introducing '2D defects'. Moreover, we report for the first time on the existence 23 resonant additional bands. These bands are only observed at 633 nm, with a resonance mechanism. Twelve of these twenty-three bands are observed in the range 600-1600 cm-1. The eleven other bands are observed at higher wavenumber, and are interpreted as second harmonic or a combination of the twelve wavenumbers cited previously. Their attribution will be discussed in light of recent GERS (Graphene Ehanced Raman Spectroscopy) literature. We use Raman plots (2D bands versus G band positions and widths) to gain qualitative information about the way layers are stacked (3). For some samples, we also report on the Raman behavior of low frequency shear and layer breathing modes. We will also present results related to hexagonal/rhombohedral transition for multilayer graphene.

(1) A. Merlen, et al. *Coatings 2017, 7,* 153

(2) D. Nikolaievskyi, et al. *Carbon* 2023, 203, 650

(3) C. Pardanaud, et al., *J. Phys. Chem. Lett.* 2019, 10, 3571

Keywords: graphene, raman, AFM, mechanical exfoliation, CVD, stacking

*Speaker

Ab initio modeling of electronic and magnetic properties of small Wigner crystals

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In this presentation, I will show my numerical and theoretical studies aimed at investigating the properties of small Wigner crystals (1) made of spinless electrons in a one-dimensional (1D) system at zero temperature. The theoretical study of these electronic crystals is motivated by the recent observation of their charge distribution in experiments (2,3,4). In particular, we look at their groundstate energy and the electronic density profile, from which we observe the electronic localization, that is the signature of Wigner crystallization. Since the former two quantities are obtained after solving the related eigenvalue problem, the number of basis elements (Slater determinants) necessary to get numerically converged results increases as soon as we increase the number of particles in the system and the strength of interactions. For this reason, we need a criterion to reduce the number of basis elements in order to get numerically convergence in the spectrum and in the electronic density distribution. I will show a method I developed that selects a priori the most relevant Slater determinants that contribute to the groundstate wavefunction. With this method, we can group basis elements in sets, ordered in terms of relevance in the groundstate wavefunction, such that, as soon as we include new ones, the eigenvalues' relative change monotonically decreases. In the low-density limit, I will also present an analytical approximation we developed for benchmarking our numerical results. The latter is built starting from the original interacting Hamiltonian, from which we can obtain also analytical expressions for the groundstate density and energy.

(1) Giuliani, G. and Vignale, G. Quantum theory of the electron liquid, Cambridge University Press (2005)

(2) I. Shapir et al. Science **364**, 870 (2019)

(3) T. Smolenski et al. Nature **595**, 53 (2021)
(4) Y. Zhou et al. Nature **595**, 48 (2021)

Keywords: carbon nanotubes, Wigner crystals, ab initio methods

*Speaker

2DMS5 - Ultrafast dynamics in 2D and quantum materials

Ultrafast photostriction in the multiferroic material BiFeO3: pump-probe X-ray diffraction study

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Multiferroics are functional materials exhibiting both ferroelectricity and magnetic ordering, pivotal for key applications such as electromechanical sensors, as well as electronic, spintronic and advanced photonic devices. Achieving light-control of these materials on (ultra)fast timescales is a rather recent

*Speaker

problematic, driven by the increasing demand for high-rate data processing. In multiferroics, both the ferroelectric polarization and magnetic orders are intrinsically coupled to the lattice strain through piezoelectric and magnetoelastic effects, respectively. A full knowledge of the unit-cell distortions induced by ultrashort laser pulses is thus required for understanding the ferroic responses to such stimuli.
It is well established that a laser pulse impinging on a sample yields a depth-dependent elastic stress and, in turn, a strain wave that propagates from its surface towards its interior. We used time-resolved X-ray diffraction to quantitatively determine the laser-pulse-induced strain in the prototypical multiferroic material BiFeO3. Our samples exhibit a polarization vector with non-null components parallel to their surfaces. Following laser excitation, both longitudinal and shear strains are thus expected to develop, owing to the pre-existing symmetry breaking at samples' surfaces. To date, most diffraction experiments have focused on the determination of the longitudinal strain. We developed a methodology to retrieve also the amplitude of the shear strain, which has been challenging in terms of diffraction geometry and sensitivity required. Simultaneous measurements of the longitudinal and shear strains revealed interesting elastic behaviors, such as the retarded development of shear strain in a bulk crystal of BiFeO3 (1) or the oscillation of the direction of ferroelectric polarization in a single-domain BiFeO3 thin-film (2). Overall, our results pave the way for manipulating ferroelectric polarization on the picosecond timescale, one of the important steps for future THz technologies.

(1) V. Juvé *et al.*, PRB **102** 220303(R) (2020)
(2) R. Gu *et al.*, Sci. Adv. **9** eadi1160 (2023)

Keywords: multiferroics, bismuth ferrite, pump, probe diffraction, ultrafast dynamics, coherent acoustic phonons, photostriction

ULTRAFAST PHOTO-INDUCED DYNAMICS TRIGGERED BY ELECTRON TRANSFER IN 1D VAN DER WAALS HETEROSTRUCTURE

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Recent studies have shown that layered-materials that are atomic-thick exhibit new properties. The static properties of these structures, such as electrical conduction, have been widely studied. However, their dynamic properties, such as photo-induced electron transfer and the subsequent structural dynamics have been explored to a lesser extent.
In this study, we have unveiled a new phenomenon where, upon light excitation, a nested structure of carbon nanotubes enveloped in boron nitride nanotubes allows for a peculiar electronic channel resulting in interlayer charge transfer. We synthesize nested cylindrical structures by wrapping carbon nanotubes (CNTs) in boron nitride nanotubes (BNNTs), refer to as 1D van der Waals heterostructure, and monitor the motion of electrons and atoms induced by ultrashort UV light excitation. On the one hand, the electronic dynamics are observed using broadband ultrafast optical spectroscopy measurements, which can capture the instantaneous changes in molecular and electronic structures. On the other hand, the structural dynamics are captured using ultrafast time-resolved electron diffraction with a time resolution of about one picosecond.
The experimental results, supported by theory, demonstrate that that free electrons generated by UV light (3 eV) in the CNTs part can be transferred to the BNNTs wide bandgap (6 eV) part through an electronic channel resulting from the interlayer interactions in these 1D materials. In addition, the energy of these excited electrons is rapidly converted into thermal energy within the BNNTs, resulting in a faster radial expansion in this 1D heterostructure compared to bare CNTs.

Keywords: ultrasfast, photo, induced, Van Der Waals, optical spectroscopy

*Speaker

SLIDING CHARGE DENSITY WAVE SYSTEMS AND EFFECT OF DIMENSIONALITY STUDIED BY MHz XFEL BEAM

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A Charge Density Wave (CDW) is a modulation of electronic density depending on the Fermi surface's nesting property and a periodic distortion of the atomic lattice. An incommensurate CDW can slide under an external current, leading to an additional current and non-Ohmic behavior above a threshold current, with Narrow Band Noise (NBN) reflecting the pulsed character of the extra current. While the type of charge carriers and propagation mode in CDW materials are not entirely understood, charge transport through CDW compounds is evident through resistivity measurements and X-ray diffraction. The sliding phenomenon is linked to deformations of periodic lattice distortion, observable by monitoring satellite reflections versus current. In recent experiments, our group imaged the CDW wave-front curvature under current in the quasi-1D system (2) using X-ray micro-diffraction. This demonstrated the effect of surface pinning and marked the first observation of CDW wave-front curvature under an external current.
Quasi-2D materials exhibit also sliding phenomenon similar to quasi-1D materials with a similar non-Ohmic behavior and NBN. However, the deformation of the CDW structure associated to the excess of current is not known.
To investigate these phenomena and their dynamics, we conducted experiments at the European XFEL facility, where the beam's repetition rate aligns with the expected CDW dynamics, i.e. in the Mhz range. These experiments aimed to observe how the diffraction pattern evolves and changes with varying external currents. Our preliminary results will be presented, illustrating the effects of different applied currents on the diffraction patterns and contributing to a deeper understanding of CDW behavior under external currents in different CDW systems.
1) R.M. Fleming and C.C Grimes, Physical review Letters 42 (1979) 1423 (2) E. Bellec et al.,Phys. Rev. B 101, 125122 (2020)

Keywords: charge density wave, XFEL, sliding, 2D material, diffraction

*Speaker

Phonons and phase transitions in 1T-TaS2

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This works concerns the 1T-TaS2 material which exhibits charge density waves (CDW) behavior with a rich phase diagram. In particular we explore how coherent phonon dynamics probe structural changes within the hysteresis loop between the commensurate (C) and nearly commensurate (NC) phases. Additionally, a unique feature of the phonon dynamics reveals a photo-induced phase transition to a hidden (H) phase.

Coherent phonon spectroscopy was performed using time-resolved reflectivity measurements with infrared ultrafast spectroscopy in a pump-probe setup. The pump pulse had a frequency of 1.55 eV (0.8 μm) with a 35 fs duration, while the probe, using an optical parametric amplifier (OPA), was set to an outgoing photon energy of 0.6 eV (2.1 μm). The sample was mounted in a helium cryostat, allowing measurements from 7K to 300K.

Experimental results show two phonon modes centered at 2.05 and 2.3 THz, respectively. The amplitude of both modes significantly increases during the C-to-NC phase transition, compared to the NC-to-C phase transition, indicating a strong interplay between the charge degree of freedom and these coherent phonon modes. Moreover, continuous wavelet transformations of the signal allow us to follow the frequency changes of the phonon modes versus time delay. Specifically, the phonon mode at 2.05 THz undergoes a frequency jump between 5 and 8 ps after the pump pulse, consistent with the previously reported phase transition into the hidden phase. This frequency jump is well-described by combining acoustic quantum confinement of the phonon wave-functions and a flickering domains model.

Keywords: Ultrafast dynamics, phase transition, phonon, hidden phase

*Speaker

Phonon dynamics in hybrid nano-acoustic resonators

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Semiconductor nano-acoustic cavities, consisting of nanometer-thick multilayer structures with contrasting elastic properties, have opened new avenues for engineering acoustic phonons at the nanoscale (1). Our research advances this frontier by investigating hybrid nanostructures that integrate materials with potentially tunable elastic properties into Distributed Bragg Reflector (DBR) based resonators (2). Specifically, we focus on open resonators featuring YBCO/STO DBRs and Nickel resonating layers (3). We present the design and simulation of this hybrid nanostructure, along with experimental methodologies and results obtained using pump-probe transient reflectivity techniques. The experiments, conducted with a femtosecond laser, explore phonon dynamics within the proposed nanostructures at a frequency of _˜120 GHz. An ultrashort laser pulse induces thermal stress, launching acoustic phonons that are subsequently detected via time-delayed probe pulses. Preliminary results reveal promising dynamics within the hybrid resonators, with transient reflectivity signals demonstrating distinct oscillatory behavior of the resonant frequency modes for different thicknesses of Ni resonators. Our study highlights the potential of hybrid DBR-based nanostructures in creating responsive nanoacoustic devices, paving the way for future innovations in phonon engineering and high-frequency applications.

(1) Priya, E. R. Cardozo de Oliveira, and N. D. Lanzillotti-Kimura, *Perspectives on High-Frequency Nanomechanics, Nanoacoustics, and Nanophononics*, Applied Physics Letters **122**, 140501 (2023).

(2) E. R. Cardozo de Oliveira, C. Xiang, M. Esmann, N. Lopez Abdala, M. C. Fuertes, A. Bruchhausen, H. Pastoriza, B. Perrin, G. J. A. A. Soler-Illia, and N. D. Lanzillotti-Kimura, *Probing Gigahertz Coherent Acoustic Phonons in TiO2 Mesoporous Thin Films*, Photoacoustics **30**, 100472 (2023).
(3) S. Sandeep et al., *Phonon Dynamics in Novel Materials and Hybrid Structures*, in *Advances in Ultrafast Condensed Phase Physics IV*, Vol. 12992 (SPIE, 2024), pp. 10–13.

Keywords: Nanophononics, Coherent Acoustic Phonons, Ultrafast pump, probe technique, Reconfigurable Acoustic Resonators

*Speaker

NN2 - Mechanics at the nano-scale : in-situ measurements and simulation under extreme conditions

Operando synchrotron X-ray diffraction to study dislocation structure evolution during additive manufacturing

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Dislocation structures are ubiquitous in any additively manufactured alloy. Until recently, there were two main hypotheses on their origin in these alloys. One hypothesis is that they form in inter-dendritic regions during rapid solidification and do not significantly evolve, if at all, during subsequent solid-state thermal cycling (SSTC) due to addition of layers. The opposing hypothesis is that thermo-mechanical forces occurring during SSTC result in significant changes in the dislocation structures formed during rapid solidification. Both hypotheses were based on studies performed on as-built samples; yet, it is impossible to univocally separate the role of SSTC from that of solidification on dislocation structure and internal stress formation and evolution during AM by solely analyzing as-built samples. A clear insight can only be gained by tracking their evolution during AM.
To that end, we have conducted an *operando* synchrotron X-ray diffraction experiment to track the evolution of the 2D diffraction pattern (the radial direction and an azimuthal direction) generated from a single grain during AM of a single-phase material. Furthermore, high resolution reciprocal space mapping (HRRSM) is also performed on the same grain before and after adding layers above the layer containing that grain, in order to generate 3D reciprocal space maps. This experiment provides an insight on the impact of SSTC on the dislocation structure and internal strain evolution during AM.

This study reinforces the conclusions of the HRRSM study conducted in (1) and they together pave the way for performing simulations using the recently developed dislocation thermomechanics theory (2) and its numerical implementation (3, 4).

References

(1) Gaudez et al., *Addit. Manuf.*, 71 (2023) 103602. DOI: 10.1016/j.addma.2023.103602

(2) Upadhyay, *JMPS*, 145 (2020) 104150. DOI: 10.1016/j.jmps.2020.104150.

(3) Upadhyay, Bleyer, *Special Issue: "Emerging Leaders 2021" MSMSE*, 30 (2022) 034002. DOI: 10.1088/1361-651X/ac44a7.
(4) Lima-Chaves, Upadhyay, CMAME 421 (2024) 116763. DOI: 10.1016/j.cma.2024.116763.

Keywords: XRD, dislocation, 3D printing, in situ, microstructure

*Speaker

Elementary deformation mechanisms in single-crystal MAX phase Cr2AlC: analyses by micromechanical testing and transmission electron microscopy

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MAX phases are a family of materials with a nano-lamellar structure that advantageously combines the properties of metals and ceramics. Although these materials have interesting properties, their deformation mechanisms remain not well understood. MAX phases have a hexagonal crystallographic structure and their plastic behaviour is mainly governed by basal slip. However, such a mechanism is not sufficient for accommodating a given plastic deformation. Recently, deformation twinning has been reported and characterized in Ti2AlN and Cr2AlC MAX phases. This was new since twinning had been ruled out in the early papers about MAX phases. This leads to a complete re-examination of the mechanical properties and elementary deformation mechanisms of these materials. In this study, we aim to determine the elementary plastic deformation in MAX phases, particularly twinning and its interaction mechanisms with basal plane dislocations. The objective is to examine the deformation structure induced by nanoindentation and micropillar compression tests on samples oriented in configurations where basal slip is the least favourable. This will lead to a more varied deformation structure, highlighting these interactions more prominently. To achieve this, the use of different experimental techniques is necessary, combining surface characterization techniques such as atomic force microscopy (AFM), scanning electron microscopy (SEM), and electron backscatter diffraction (EBSD) with volume characterization techniques such as transmission electron microscopy (TEM) and automated crystal orientation mapping (ACOM-ASTAR). TEM thin foils and micropillars are prepared using focused ion beam (FIB), ensuring the area of interest is precisely targeted. This will lead to a more comprehensive view of the structure under analysis and a better understanding of the development of deformation twinning and its interactions with basal slip.

Keywords: Max Phases, Twinning, Dislocations, Nanoindentation, AFM, TEM

*Speaker

Electrically induced viscous flow in oxide glasses at room temperature: electrical-nanoindentation tests vs e-beam effect

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Over the past decade, several studies have demonstrated the possibility of inducing strong creep/relaxation phenomena in amorphous silica at room temperature during mechanical testing under TEM/SEM electron beam irradiation. Depending on the e-beam parameters, the viscous flow can be so pronounced that silica exhibits ductile behavior, described as superplastic by the authors, allowing it to be shaped at room temperature. These intriguing observations raise several questions. What electrical magnitude drives the mechanical processes? Does the phenomenon also occur in other oxide glasses? Is this solely an effect of electron irradiation, or can it be replicated with a DC current? The present work aims to address these questions by performing electrical-nanoindentation tests on amorphous thin films, deposited on silicon substrates, of a dense Al2O3 model material and a nanoporous SiOCH material used in microelectronic applications. The tests involve biasing the substrate and measuring the current flowing through the tip during mechanical loading. Significant viscous flow was observed in both materials, indicating that this is indeed a purely electrically-assisted phenomenon and appears to be generic to oxide glasses. Furthermore, electrical-nanoindentation tests have also shed light on the relevant electrical magnitude, which was previously challenging to determine in e-beam irradiation experiments that involve multiple less well controlled parameters: acceleration voltage, probe current, magnification, irradiation time, irradiated volume, etc. Finally, micropillar compression tests of amorphous silica under e-beam irradiation were conducted to quantify the mechanical response of the oxide glass in relation to the electrical quantity of interest.

Keywords: Electrical nanoindentation tests, Oxides glasses, Viscous flow, Micropillar compression

*Speaker

Dynamical and structural evolution of high aspect ratio nanowires under high temperature gradients

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High aspect ratio nano-cantilevers have recently become one of the gold standard for ultra-sensitive nanomechanical sensing. The principle is to access an external driving phenomenon via its effect on the deformation of the cantilever, which is to be further readout using suitable techniques. The force to motion conversion factor is essentially set by the inverse of the spring constant, which reaches extremely high values for ultra-low mass, low-frequency nanomechanical cantilevers, and which explains their current unanimous acclaim.
Sensitive nanomechanical readout is generally achieved by monitoring the fluctuations of a high energy probe mode, coupled to the motion of the cantilever. Ideally, such coupling is aimed at being dispersive, with the absorption of the probe power being negligible. However, at these scales and due to their peculiar geometry, nanocantilevers display very high thermal resistances and are therefore prone to very high thermal gradients, even at very low levels of residual absorption. While this represents a pivotal challenge to both the development and operation of nanomechanical sensing technologies, a systematic and quantitative approach of the consequences of these thermal effects either on their structure or dynamics remains missing.

Here, we report early studies on the impact of strong thermal gradients on InAs nanowires' structure and mechanical behavior. These nanowires exhibit unique nanomechanical transduction and high thermal resistance, increasing with temperature. They are mounted in a FESEM electron microscope, operating with parameters (3 keV, _˜1 nm beam size) enabling simultaneous heating and detection of nanomechanical vibrations.
Our approach analyzes vibrational behavior based on e-beam excitation and nanowire geometry. We address challenges in mechanical and thermal properties, showing e-beam heating dominates over charging. We introduce methods to decouple structural and dynamical effects, enabling precise measurement of thermal conductivity under gradients exceeding 1000 K. We conclude with challenges and future plans.

*Speaker

Visco-elasto-plastic behaviour of Zr50Cu50 metallic glass using the molecular dynamics wave packet method

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We study acoustic attenuation and visco-elasto-plastic response of Cu50Zr50 metallic glass using molecular dynamics simulations. The dynamic response of the material is studied through its vibrational properties using the wave packet method. For a wide range of wave frequencies and amplitudes, wˆ(2.7–3.1) dependencies of attenuation were observed for a longitudinal polarisation. For sufficiently large amplitudes, a frequency-dependant transition to anharmonic behaviour is revealed, associated with non-linear acoustic modes. Transverse polarisation is also studied, with greater attenuation and wˆ(2.1–2.4) dependencies of attenuation. These dependencies are compared to the predictions given by the theories of wave scattering, in the low scattering and in the stochastic regimes, and are also compared to the same simulations performed in silica samples. The irreversibility is also studied by extracting the residual plastic strain. A transition from sparse plastic deformation to local shear banding is observed, and compared to short laser pulse experiments performed in silica samples.

Keywords: metallic glass, molecular dynamics simulations, wave packet method, acoustic attenuation, non linear, irreversibility

*Speaker

In-situ nano-mechanical studies of single ZnO nanowires

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Piezoelectric semiconductor nanowires (NWs) have been researched as building blocks for various energy transducing applications including mechanical energy harvesting, sensors and piezotronic devices. The electromechanical interaction, also known as piezoelectricity, couples the mechanical and the electrical state in crystalline materials with no inversion symmetry, *i.e.*, the application of mechanical strain results in the generation of electrical charge and vice versa. The effective piezoelectric coefficient was suggested to increase with decreasing NW diameter due to finite size effects, thus increasing the conversion efficiency of mechanical into electrical energy and back making NWs promising candidates for future mechanical energy transducers. In addition, nanostructures such as NWs were demonstrated to exhibit yield strengths reaching the ultimate limit of the respective material. Such increased elasticity limit may increase the elastic strain that can eventually be converted into electricity by electro-mechanical coupling. Furthermore, while many semiconductors are brittle at room temperature, it was further shown that they may become ductile at ambient conditions below a critical size. Here, we report on *in-situ* Laue microdiffraction studies of the mechanical response of individual suspended ZnO NWs loaded in a three-point bending configuration using a custom-built atomic force microscope During the mechanical testing of the ZnO NWs, Laue peaks are displaced on the detector. The diffraction patterns were indexed using the LaueTools software providing access to the orientation of the crystals as a function of the applied load. The rotation of the three orthogonal lattice planes demonstrates a bending as well as torsion of the NW. The applied load was increased until NW failure occurred representing the maximum mechanical strain that could be converted into electrical energy by piezoelectricity. Additionally, the microstructural defects generated by these deformations, notably "Plasticity", were analysed by transmission electron microscopy.

Keywords: Nanomechanics, ZnO, Synchrotron, Laue microdiffraction, elasticity, plasticity, SEM, TEM, AFM

*Speaker

Transformation-induced plasticity in zirconia: combining micropillar compressions and atomic-scale simulations

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Like steels, zirconia ceramics exhibit transformation-induced plasticity (TRIP) due to a transformation between a tetragonal (t) and a monoclinic (m) phase. This unique feature gives zirconia ceramics substantial plastic deformation, reaching up to a remarkable 7% plastic strain. However, this effect is far from fully understood, hindering the development of ceramics with macroscopic deformability in excess of 1%. Moreover, the absence of interatomic potentials capable of describing polymorphism and phase transformations in zirconia makes fundamental understanding of the TRIP effect at the atomic scale difficult.

In this work, we combine experimental characterizations by in-situ Laue diffraction on micropillars and atomic-scale simulations to obtain microscopic information on transformation conditions, in particular the effect of compression direction on the ease of inducing transformation. The simulations required the development of a neural network-based interatomic potential to take account of zirconia's polymorphism. We characterize both experimentally and numerically the deformation processes, critical stress-strain states and phase transformations for a large number of compression directions covering the entire standard triangle. Our results challenge the prevalent idea that the TRIP effect in zirconia is governed by a limited number of variants, as all potential variants are observed as a function of compression direction. Furthermore, we observe through simulations a complex interplay between competing stable and metastable, orthorhombic and monoclinic phases, some as yet experimentally unknown. Our work thus provides new insights into the microscopic processes behind zirconia's unique plasticity.

*Speaker

Complexity of plastic flow in a mesoscopic-scale range: wave-intermittence duality

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Recent observations of a serrated character of plastic flow of micro sized crystals, as well as statistical investigations of acoustic emission during deformation of samples of various size, proved a self-organized intermittent nature of the dislocation dynamics at nano/micro scales. On the macroscopic scale, the deformation curves of bulk samples become either approximately smooth, conforming to the continuous approach to plasticity, or, in the case of plastic instability, macroscopically serrated, corresponding to an outmost self-organization of the dislocations. The transition between these scales attracts a strong theoretical interest but is little known experimentally. The aim of the talk is to present recent experimental investigations of plastic flow at intermediate scales in different materials, based on the evaluation of the local strain-rate field with the aid of digital image correlation and supported by the acoustic-emission measurements. Examples will be provided for distinct cases including both smooth and serrated plastic flow. These examples show that the manifestations of the dislocations self-organization can depend on the scale of observation. Whereas power-law statistics of the acoustic emission confirmed its intermittent character, the local strain-rate bursts may present different statistics depending on the experimental resolution. Moreover, the local strain-rate maps reveal a spatiotemporal organization of strain bursts in hierarchical wave patterns, which confirm the recent conjecture of a wave-intermittence duality in the collective dynamics of dislocations.

Keywords: Plastic deformation, Dislocation self organization, Digital image correlation, Acoustic emission

*Speaker

Understanding dislocation - grain boundary interactions by quasi in-situ nanoindentation and electron channeling imaging at the example of a tensile twin boundary in MgY.

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Solute-defect interactions have been proven essential to grain boundary engineering employed in the development of novel high-performance Magnesium alloys. We aim at unraveling the influence of solutes on the mechanical response of grain boundaries by investigating a tensile twin boundary decorated with Y atoms compared to the counterpart boundary in pure Mg. Quasi in situ-nanoindentation, electron channeling contrast imaging (ECCI), a non-destructive SEM method based on the detection of back scatter electrons, and EBSD were employed to first induce localized deformation in the vicinity of a twin boundary and subsequently analyze the corresponding mechanical grain boundary response. Interactions between emitted dislocations and the twin boundary were investigated according to the indents distance from the boundary, the presence of solutes and the dislocation type. The presented combined approach of quasi in-situ nanoindentation and ECCI observations is an effective and non-destructive method for the investigation of nanomechanical phenomena advancing the current knowledge of solute effects on mechanical grain boundary properties. Corresponding molecular dynamics simulations are currently in progress to complement and deepen the understanding of the complex interplay between solutes, dislocations and grain boundaries.

Keywords: grain boundary, defect interaction, solute effects, in, situ nano, indentation, ECCI, EBSD

*Speaker

Update of the HTSI method: application to mechanical characterization of CaF2 up to 800∘C

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The recent development of the High-Temperature Scanning Indentation (HTSI) method (1) allows for the characterization of material mechanical properties quasi-continuously over a large temperature range in 1-day experiments. However, such a technique employs a nanoindentation cycle with a constant maximum load applied regardless of the temperature. Thus, for materials exhibiting an Indentation Size Effect (ISE), the variations in hardness with temperature can stem from both temperature and ISE. It becomes more challenging to differentiate between these two effects and analyze their impact on the mechanical properties.
To address this issue, a new 1-second indentation cycle has been implemented. A 0.5-second half-sine function is utilized during loading, followed by a 0.1 to 1-second creep segment and the 3-step unloading function used previously. To control the maximum achieved depth across temperatures, the maximum applied load is adjusted experimentally between each indentation, using previous indentation tests and results. This approach allows for the determination of hardness, Young's modulus, and creep properties of a material at a given maximum depth over a wide temperature range.

This methodology has been applied to CaF2 single-crystal from room temperature (RT) to 800∘C. The implemented cycle enables the characterization of this material at 1000nm depth over the entire temperature range. Comparison with tests performed using the previous indentation cycle highlighted the impact of the ISE in temperature. The obtained results were compared to conventional indentation results.
(1) Tiphéne *et al.*, *J. Mater. Res.*, 36, 12, 2383-2396, 2021

Keywords: Nanoindentation, High Temperature, Mechanical Characterization, CaF2, Single, Crystal, Indentation Size Effect

*Speaker

Deformation mechanisms of DSA-sensitive C-Mn steel welds: New insights from in-situ TEM nanomechanical testing

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C-Mn steel welds for the secondary circuit of nuclear power plants might be sensitive to Dynamic Strain Ageing (DSA). DSA is based on interactions between interstitial atoms and dislocations, leading to a change in mechanical properties. Indeed, macroscopic tensile tests on these welds show an increase in tensile strength at 300∘C, associated with a rise in work-hardening rate. Kocks-Mecking analyses suggest that dynamic recovery is hindered during high temperature tensile tests due to interstitial atoms segregation to dislocations. In-situ TEM tensile tests were therefore performed at room temperature and 300∘C to explore this hypothetical decrease in dynamic recovery.
Room temperature in-situ TEM tensile tests suggest that dislocations are pinned by interstitial atoms, prior to plastic deformation, thus increasing the stress required to activate dislocations glide. We observe that the stress decreases as plastic deformation occurs, probably due to dislocations being unpinned from the segregated atoms. In-situ TEM tensile tests at 300∘C show a different deformation mechanism to those at room temperature. No individual movement of dislocations is observed. Rather, plastic deformation occurs by dislocation bursts, so-called "dislocation avalanches", a mechanism characteristic of dynamic strain-ageing. The deformation by dislocation avalanches and the decrease in dynamic recovery seem caused by the segregation of interstitial atoms to dislocations, which restrict their movements, in accordance with the macroscopic Kocks-Mecking model.
Thus, it appears that the change in mechanical properties at the macroscopic scale caused by DSA could be explained by a change in the deformation mechanism at the microscopic scale, as evidenced by in-situ TEM tensile tests at different temperatures. These in-situ tensile tests at the microscopic scale allow for a better understanding of complex industrial problems.

Keywords: Steel, Welds, Dynamic strain aging, tensile tests, TEM

*Speaker

NN5 - Properties of metal clusters and nanoparticles

Equilibrium and Kinetic models for Ag-Pt nanoalloys

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Nanoalloys are commonly nanoparticles of alloys whose both size and composition influence their structures and properties. The chemical arrangement at their surface plays a major role in catalysis, whereas optical and magnetic effects are sensible to the overall chemical configuration. It is important to characterize these structures at equilibrium but also out of equilibrium, depending on their elaboration conditions.

Ag-Pt nanoparticles present very interesting (electro)-catalytic properties and experimental studies have been performed to characterize their morphology and chemical configuration (1) to better understand and improve their reactivity.

The question we address, in this theoretical study, is how the chemical configuration evolves with time starting from an out of equilibrium configuration, either a random disordered one, a core/shell or even Janus configuration.
Ag-Pt nanoparticles are modelled using a new energetic model on rigid lattice to reproduce both the L11 ordered phase at equiconcentration, the order/demixion transition around 1000 K and the demixion/disorder transition around 1400 K. This model depends on the effective pair interaction energies, and a concentration- and temperature-dependent size effect to account for the change in lattice structure.

Monte Carlo at equilibrium and kinetic Monte Carlo are performed using multi-cell algorithm to characterize the atomic configurations of nanoparticles of a few nanometres in size. The results at equilibrium are compared to other theoretical studies performed with or without atomic relaxations (2,3) and to experimental results (1). Kinetic Monte Carlo simulations describe how the nanoalloys recover (or not) their equilibrium configuration starting from a core-shell, disordered or Janus structures.
(1)) J. Pirart, A. Front, D. Rapetti, C. Andreazza-Vignolle, P. Andreazza, C. Mottet, R. Ferrando, Nature Communications 10 (2019) 1982
(2) A. Hizi, A. Front, M. Said, F. Berthier, G. Treglia, C. Mottet, Surf. Sci. 700 121626 (2020)
(3) A. Front, C. Mottet, Phys. Chem. Chem. Phys. 25 (2023) 8386.

Keywords: Nanoalloys, thermodynamics, kinetics

*Speaker

Convolutional neural networks for cluster structure classification

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A general method to obtain a representation of the structural landscape of nanoparticles in terms of a limited number of variables is proposed (1). The method is applied to gold clusters of 90 and to gold, silver and copper clusters of 147 atoms,
The method employs convolutional neural networks to learn the radial distribution functions of the nanoclusters in order to derive a set of few collective variables that are sufficient to describe the energy landscape with a very good resolution of structural motifs. The presented approach offers a general, low-dimensional set of differentiable variables that has the potential to be used for exploration and enhanced sampling purposes.

(1) Emanuele Telari, Antonio Tinti, Manoj Settem, Luca Maragliano, Riccardo Ferrando, and Alberto Giacomello, ACS Nano 2023, 17, 21287–21296

Keywords: Metal clusters, neural networks

*Speaker

Modelization of the structure and chemical ordering of AgCuNi nanoalloys

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Metallic nanoparticles of alloys called "nanoalloys" have a great impact on industry, medicine, and environment because of their extended properties in catalysis, optics or magnetism. These properties depend on the size, morphology, atomic structure and chemical arrangement of the chemical species in the nanoparticle.
With the recent breakthrough of high entropy alloys (HEA) in metallurgy, which are systems essentially composed of several chemical elements in comparable concentrations, we extended our study of bimetallic nanoalloys to ternary systems.

Using Monte Carlo simulations and interatomic potentials fitted on binary alloys, we studied the atomic structure and chemical arrangement of ternary AgCuNi alloys nanoparticles. This system is a prototype of system with demixing tendency since made of three binary systems AgCu, AgNi, CuNi with phase separation in bulk, and surface segregation at infinite surfaces. We considered nanoparticules of some hundreds to some thousands of atoms for which the core can be compared to the bulk alloy, and the surface made of (100) or (111) facets to the infinite surfaces of equivalent orientation, where surface segregation takes place.

Whereas infinite surfaces and nanoparticles of CuAg and NiAg have been widely studied in the past, both experimentally and theoretically (see (1-3) for examples), ternary systems are much less studied and present interesting synergetic properties and possible morphological instabilities due to strain because of lattice misfit between the three components.

(1) M. Briki, PhD thesis, Université Paris-Sud (2014)
(2) D. Bochicchio, R. Ferrando, Phys. Rev. B 87, 165435 (2013)
(3) L. Delfour, J. Creuze, B. Legrand, Phys. Rev. Lett. 103, 205701 (2009)

Keywords: nanoparticles, alloys, Monte Carlo simulations, phase diagram, surface segregation, interatomic potentials

*Speaker

Surface dynamics of Cobalt nanoparticles: a machine learning approach

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Accurately characterizing the dynamic behavior of nanoparticles is crucial for understanding and improving their catalytic properties. We present a machine learning method to analyze the surface dynamics of cobalt nanoparticles at finite temperature. Using unsupervised clustering with gaussian mixture models, we capture subtle changes in atomic environment, providing insights into melting processes and reactivity. This approach highlights the potential of advanced simulations in revealing the complex behaviors essential for catalysis.
The training set consists of a trajectory where a nanoparticle is heated to a temperature where there is no surface diffusion. The trajectories were generated using a machine-learned potential specifically trained for bulk, surface, and nanoparticles of cobalt. Atomic environments are encoded in BSO4 descriptors and classified among different classes (such as facets, edges and vertices) that are learned from the data, without human supervision. Then, atomic environments from higher temperature trajectories are classified, and a statistical distance (distortion score) is used to extract outliers.

The evolution of the initial classes' population gives access to kinetic information about the melting process, such as the temperature at which atoms become mobile, which varies significantly across different facets, as well as the melting rate and temperature of the different facets. The method efficiently annotates atoms and allows to fully exploit the atomic resolution of MD, rather than mere averaged-out quantities.
Outliers' atoms offer valuable insights for catalysis since they include all surface patterns that appear when the nanoparticle is heated. Low-coordinated atoms, such as ad atoms, are extremely reactive and thus highly important for catalysis. Classifying the outliers provides useful information concerning the nanoparticle's reactivity, such as the onset temperature of adatom diffusion, but also their quantity as a function of temperature.

Keywords: cobalt, nanoparticles, machine, learning, surface, ad atoms, melting

*Speaker

The packing of icosahedral shells as a design principle for multi-metallic clusters

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Multimetallic clusters are being intensively researched for their applications in catalysis, optics and magnetism. Because of the complexity of these systems, a general method for designing stable structures is currently lacking. Here we propose a general theory for constructing multimetallic icosahedral clusters by assembling concentric shells of different chiral and achiral types, consisting of atoms of different sizes (1). Our method is based on mapping the sequences of icosahedral shells into paths in the hexagonal lattice and allows us to establish simple and general rules for the construction of a wide variety of new magic icosahedral clusters. In addition, we evaluate the optimal size-mismatch between particles of different shells, which is a key factor in the construction of stable structures. Our method has been applied to different binary and ternary systems, such as NaK, NaRb, NaKRb, NaKCs, AgCu, AgNi, AgCo, and AgPdNi. Molecular dynamics simulations have been used to study the growth of these systems (2), confirming the predictivity of our design strategy.

References

(1) N. Canestrari, D. Nelli and R. Ferrando, arXiv:2406.07137

(2) D. Nelli, C.Roncaglia, R. Ferrando, Z. Kataya, Y. Garreau, A. Coati, C. Andreazza-Vignolle and P. Andreazza, Nanoscale 2023, 15, 18891

Keywords: multi, metallic, clusters, material design

*Speaker

Growth of gold-palladium nanoalloys by oblique angle deposition: Exploration of their structure and optical properties

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Multimetallic nanoparticles are currently attracting a great deal of interest in scientific research because of their unique physical and chemical properties, which can be applied in many fields such as optics, catalysis and biosensors. These properties are highly dependent on nanoparticle characteristics, including size, shape, composition, structure and environment. For example, the use of gold and palladium enables the amalgamation of distinct characteristics inherent to each component, such as the plasmonic attributes of gold and the reactivity properties of palladium. These combined characteristics make these bimetallic nanoparticles particularly attractive for many applications such as sensing applications, most notably hydrogen detection.
In this study, we investigate AuxPd1-x nanoparticles synthesized by electron beam evaporation and the influence of deposition parameters on their optical properties and structure. The nanoparticles have been produced in a unique device that enables monometallic and multimetallic nanoparticles (up to 5 different metals) to be synthesized, while controlling a wide range of deposition conditions and monitoring their optical response in real time by in situ transmittance measurements. For example, we will demonstrate the evolution of the optical response of gold with the addition of different levels of palladium. In addition, it is possible to create nanoripples patterns on the surface by ion beam sputtering at oblique incidence, which influences the organization and orientation of the nanoparticles, as well as their polarization-dependent plasmonic properties.

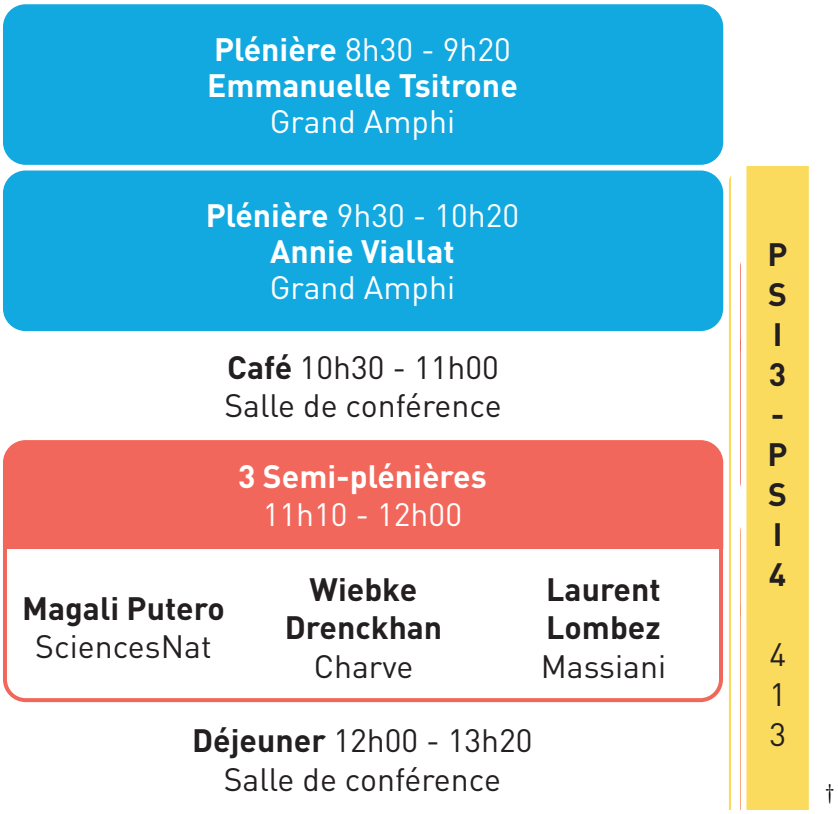
Real-time studies are complemented by ex situ characterizations by transmission electron microscopy, which confirm that the optical response of nanoparticles strongly depend of their structural characteristics.

In conclusion, this research opens the way to understanding alloying mechanisms for the development of more efficient and selective materials for a wide range of applications.
The authors acknowledge financial support from the French Government programs "Invertissements d'Avenir" EUR INTREE (reference ANR-18-EURE-0010), LABEX INTERACTIFS (reference ANR-11-LABX-0017-01), and ExcellencES UP-SQUARED.

Keywords: nanoparticles, gold, palladium, optical properties, plasmonic response

*Speaker

31 October 2024, morning



‡All rooms with a number are located in building 15

Plenary

Emmanuelle Tsitrone

IIRFM-CEA, Cadarache France

Plasma Facing Materials in fusion devices : when the 4 states of matter get together

Developping nuclear fusion is one of the possible option for providing a carbon-free baseload energy source. Significant progress has been achieved over the last decades, and the international ITER project, presently under construction in Cadarache (France), is targeted at demonstrating the scientific and technical feasibility of fusion as an energy source.

The most efficient fusion reaction for energy production has been identified as the reaction between deuterium (D) and tritium (T), yielding a helium (He) nucleus and a neutron. In order to reach the extreme temperatures required for an efficient DT fusion reaction ($\sim$150 millions ^{o}C), the DT fuel is heated up to form a plasma – often referred to as the fourth state of matter. The most advanced configuration for containing this hot plasma is called a tokamak, in which magnetic fields are used to confine the charged plasma particles. The plasma facing materials are exposed to harsh conditions in fusion devices, both in terms of heat and particle loads stemming from interactions with the plasma. The boundary of fusion devices is a place where the solid plasma facing materials, using liquid based active cooling to handle heat loads, meet the fusion plasma as well as the gas resulting from plasma recycling on the walls, hence a place where the 4 states of matter get together. Taming the interactions between the solid walls of a fusion device and the plasma is a key issue for operating future fusion reactors.

This contribution will review the challenges for plasma exhaust in fusion devices, outlining how the plasma facing material evolves under plasma exposure. In particular, it will describe how to select adequate plasma facing materials, as well as how to design and operate plasma facing components (PFC) in a tokamak environment.

After a short introduction showing how fusion works and what the constrains on plasma facing components are, the focus of this presentation will be on describing the mechanisms involved in plasma wall interactions. This includes processes such as erosion of the wall material by the plasma (D/T/He and impurities) and subsequent wall material transport by the plasma, surface microstructural changes under plasma exposure, fuel trapping in the plasma facing material or dust production after erosion / deposition of the wall material. Both experimental and modelling aspects will be discussed.

The rationale for selecting a suitable plasma facing material will be presented. Due to its good thermomechanical properties and low activation behaviour under neutron irradiation, tungsten is presently identified as one of the most promising plasma facing material for future fusion reactors. ITER will operate with tungsten plasma facing components, both for the main chamber walls and the divertor, which is the most heavily loaded component in a fusion device. In order to prepare for a safe and reliable divertor operation in ITER, the WEST tokamak, run by the Institute of Research on Magnetic Fusion from CEA in Cadarache (France), has been recently equiped with an ITER grade divertor. The main findings from WEST in terms of material behaviour under plasma exposure in tokamak conditions will be presented. Finally, additional issues to consider for plasma material interactions in a future fusion plant will be discussed.

Plenary

Annie Viallat

CINaM, Marseille

Function, robustness and optimization: transport on ciliated epithelium, blood microcirculation

Some physiological functions rely on very specific physical processes and structural and dynamic organizations of living matter. Examples include the protection of airways by the circulation of a protective layer of mucus on their surface, the protection of the skin of fragile organisms by vigorous washing, the filtration of rigid aging red blood cells from the bloodstream, the vigilance against respiratory infections by a specific circulation of leukocytes in the pulmonary bed.

In these examples, we may ask whether the physical processes and organization of living matter are optimized to best fulfill the physiological function, or whether the important thing is the robustness of the function, which must be maintained even when systems are degraded by the many life hazards, old age or disease. Using these examples, I'll show and discuss the power of simple physics concepts, but how we must sometimes be wary of physicists' intuitive approaches, generally based on optimization.

Semi plenary

Magali Putero

Aix Marseille Univ, CNRS, IM2NP, Marseille, France

Phase change materials: from emerging memories to switchable optics and active metasurfaces

Phase change materials (PCMs) are a class of materials, primarily composed of chalcogenide glasses, that attract significant attention due to their unique properties. PCMs can be reversibly and rapidly (in a few ns) switched between a high-resistivity amorphous state (generally low-reflectivity) and a low-resistivity crystalline state (generally high-reflectivity) through thermal annealing[1,2]. This characteristic has been exploited in nonvolatile optical memories such as CD-RW, DVD-RW, and Blu-ray discs, taking advantage of the substantial reflectivity difference between the two states. Besides, PCM properties are exploited in Phase Change Random Access Memory (PCRAM) applications. PCRAM is the most mature and promising technology among emerging memory concepts due to its scaling potential, overcoming the limitations of conventional flash-based approaches[3].

The two most studied and prototypical materials for PCRAM applications are GeTe and $Ge_2Sb_2Te_5$ alloys. However, many compositions within the Ge-Sb-Te ternary phase diagram (GST) have been studied, including Ge-rich GST alloys for automotive applications. Such alloys, whether doped with other elements like N, C, or As, exhibit key material properties (crystallization temperatures, mode and kinetics, electrical and optical contrast) that are composition-dependent and drive the final devices properties (reliability, scalability, cyclability, power consumption). Material studies are thus essential for technological development and can be advanced by combining several *in situ* experiments, such as x-ray diffraction, x-ray reflectivity and sheet resistance measurement, to simultaneously monitor both structural and electrical properties upon crystallization[4,5].

A more recent application for PCMs concerns nanophotonics, where managing the propagation of light and its properties with greater control and efficiency has become a major challenge. This can be achieved with large arrays of sub-wavelength metallic or dielectric nanostructures known as metasurfaces. Typically, these are static, "fixed-by-design", meaning their design determines their optical properties. The next major milestone in the development of metasurfaces is to incorporate tuning capability into their design by implementation of PCMs such as $Ge_xSb_yTe_z$ or Sb_2S_3 alloys. Since PCM alloys can be reversibly switched between their amorphous and crystalline states with a unique contrast in both optical and electronic properties, they are ideal candidates to pair with dielectrics metasurfaces. This aims to develop tunable photonic devices[6] (e.g. waveguides, phase shifters...) with the ability to change the displayed information in real time. However, the integration of PCM in photonic devices often relies on typical top-down microfabrication technologies (e.g. standard lithography, lift-off, etching) that are high-cost, cumbersome, difficult to implement on chalcogenides, and lead to small active surface areas. In this talk, I will first introduce what a phase change material is, how it can be reversibly switched, which compound can be used for volatile or non-volatile applications, and the link between material properties and device performances. The second part of the talk will be dedicated to examples

of combined in situ PCM studies. Finally, the last part of the talk will focus on the current progresses, main achievements and perspectives of exploring the use of the soft Nano Imprint Lithography (soft-NIL) methods[7,8] to elaborate PCM active metasurfaces with various features, dimensions and pitches, aiming to beak classical fabrication methods to achieve low-cost and wide panels of active surface dimensions and substrates.

[1] M. Wuttig and N. Yamada, Nat. Mater., 2007, 6, 824?32.
[2] M. Wuttig et al., Adv. Mater., 2018, 30, 1803777.
[3] P. Noé et al., Semicond. Sci. Technol., 2018, 33, 13002.
[4] M. Putero et al., APL Mater., 2013, 1, 062101.
[5] J. Remondina et al., Sci. Rep., 2024, 14, 14677.
[6] P. Hosseini et al., Nature, 2014, 511, 206.
[7] S. Checcucci et a., Adv. Opt. Mater., 2019, 7, 1801406.
[8] M. Modaresialam et al., Chem. Mater., 2021, 33, 5464.

Semi plenary

Wiebke Drenckhan

CNRS Institut Charles Sadron / Université de Strasbourg

From bubbles to balloons: mechanical self-assembly of soft objects with interface-controlled interactions

The mechanical assembly of bubbles or drops in a liquid generates foams or high internal phase emulsions. With increasing packing density, their morphology ranges from neatly packed spherical objects at jamming to space-filling polyhedra. The structural features of these assemblies are entirely dictated by the minimisation of interfacial area (i.e. by capillarity) and obey fairly strict rules which start to be well understood. In order to access a wider variety of morphologies, it is important to find methods to interfere with the mechanical equilibrium of the packing in a controlled manner. This can be done by explicitly tuning the interactions between the bubbles (or drops) away from pure capillarity by adding friction, adhesion and/or interfacial elasticity. I will provide a short state-of-the-art of the subject, showing different methods to tune and characterise the interactions between bubbles (or drops) and how they impact the overall foam (emulsion) morphology in the final equilibrium. Advancing our fundamental understanding of these complex mechanical assemblies will not only help in the description of foams (emulsions) with complex interactions, but also inspire the creation of original, mechanically self-assembled, architected materials and tissues.

Semi plenary

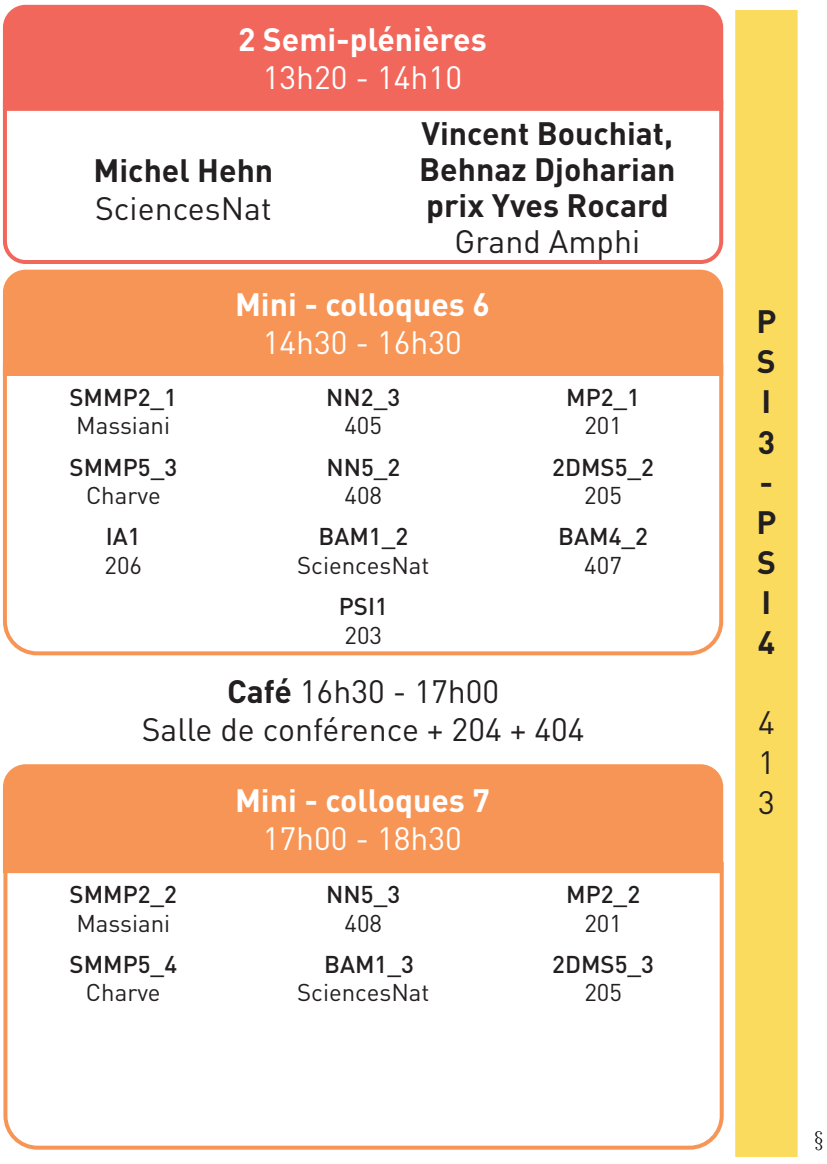
Laurent Lombez

LPCNO, Toulouse

Towards the control of excitonic transport in two-dimensional semiconductor materials

Similar to the excitement generated by graphene, the scientific community is now interested in the properties of new 2D semiconductor materials that exhibit extraordinary optical and electronic properties, paving the way for numerous optoelectronic devices. In particular, transition metal dichalcogenide (TMD) monolayers, where electron-hole pairs (excitons) remain strongly bound even at room temperature. It is thus important to measure the transport properties of these particles and their spin transport properties to develop an optoelectronic and/or spintronic device. To achieve this, I will demonstrate how optical methods, such as luminescence imaging, are ideal for probing both transport and recombination properties. I will present results on WSe_2 monolayers as well as on coplanar 2D heterostructures. I will also discuss how it is possible to control the excitonic flow.

31 October 2024, afternoon



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Semi plenary

Michel Hehn

Institut Jean Lamour, Université de Lorraine, Nancy

A single laser pulse to reverse magnetisation without any applied magnetic field

The development of new strategies for changing the magnetic state of nanostructures on ultra-short time scales meets an ever-growing demand from the information storage industry using magnetic memory points (hard disk, MRAM magnetic random access memory). Historically, magnetic media were written by using a magnetic field. However, this method proved limiting when the size of the bits was reduced to a scale of less than a hundred nanometres and the writing speed was increased beyond GHz. Alternative solutions have emerged, using spin-polarised currents in nanometer-sized magnetic structures, such as spin-transfer torque switching or, more recently, spin-orbit torque switching. However, these technologies are limited by the sharp increase in current density required when the pulse duration is reduced, which rules out their use on time scales of less than 100 picoseconds.

In 1996, Beaurepaire and colleagues demonstrated that excitation of a thin Ni film by a femtosecond laser pulse led to its demagnetisation in a fraction of a picosecond [1]. This major discovery launched the field of femtomagnetism. Nearly fifteen years later, all-optical switching (AOS) of the magnetisation of ferrimagnetic GdFeCo alloys was demonstrated using a single laser pulse [2], with magnetisation reversal achieved in 1 picosecond. The effect is explained by an ultra-fast heating process linked to the distinct dynamics of rare-earth and transition metal elements and related to the high transient temperature of electrons in disequilibrium with the lattice. The observation of AOS has long been limited to materials containing Gd.

In this presentation, we will describe the evolution of this field of research over the last ten years. We will show that this reversal is not restricted to the use of materials containing Gd [3,4,5], that it is a fairly general phenomenon, that these materials can be integrated into commercial MRAM-type devices [6] and that it is even possible to do away with ferrimagnetic alloys by using exclusively ferromagnetic materials already used in commercial devices [7].

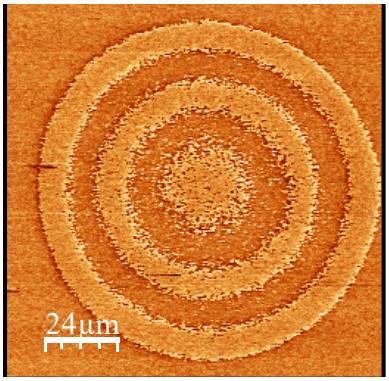

Figure: Domain structure stabilised after a single laser pulse of 5 ps. Image obtained by magnetic force microscopy. The orange (respectively brown) areas correspond to domains pointing upwards (respectively downwards) perpendicular to the plane of the sheet/screen.

[1] E. Beaurepaire, J.-C. Merle, A. Daunois, J.-Y. Bigot, Ultrafast spin dynamics in ferromagnetic nickel. Phys. Rev. Lett. 76, 4250 (1996).
[2] I. Radu, K. Vahaplar, C. Stamm, T. Kachel, N. Pontius, H. A. Durr, H. T. A. Ostler, J. Barker, R. F. L. Evans, R. W. Chantrell, A. Tsukamoto, A. Itoh, A. Kirilyuk, T. Rasing, A. V. Kimel, Transient ferromagnetic-like state mediating ultrafast reversal of antiferromagnetically coupled spins. Nature 472, 205-209 (2011).
[3] Y. Peng, G. Malinowski, J. Gorchon, J. Hohlfeld, D. Salomoni, L. D. Buda-Prejbeanu, R. C. Sousa, I. L. Prejbeanu, D. Lacour, S. Mangin and M. Hehn, Observation of Single-shot Helicity-independent all-optical switching in Co/Ho multilayers, Phys. Rev. Appl. 20, 014068
[4] Y. Peng, D. Salomoni, G. Malinowski, W. Zhang, J. Hohlfeld, L. D. Buda-Prejbeanu, J. Gorchon, M. Verg J. X. Lin, R.C. Sousa, I. L. Prejbeanu, S. Mangin and M. Hehn, In plane reorientation induced single laser pulse magnetization reversal, Nature Communication (2023). https://doi.org/10.1038/s41467-023-40721-z
[5] B. Kunyangyuen, G. Malinowski, D. Lacour, J.-X. Lin, Y. Le Guen, J. Gorchon, S. Mangin, J. Hohlfeld and M. Hehn, Single- shot all-optical magnetization switching in ferrimagnetic Co-RE alloys single layers, submitted.
[6] D. Salomoni, Y. Peng, L. Farcis, S. Auffret, M. Hehn, G. Malinowski, S. Mangin; B. Dieny, L. D. Buda-Prejbeanu, R.C. Sousa, and I. L. Prejbeanu, Field-free all-optical switching and electrical read-out of Tb/Co-based magnetic tunnel junctions, Phys. Rev. Appl. 20, 034070 (2023).
[7] J. Igarashi, W. Zhang, Q. Remy, E. D, J. X. Lin, J. Hohlfeld, M. Hehn, S. Mangin, J. Gorchon, and G. Malinowski, Optically induced ultrafast magnetization switching in ferromagnetic spin valves. Nature Materials (2023); https://doi.org/10.1038/s41563-023-01499-z

Semi plenary

Vincent Bouchiat and Behnaz Djoharian

Grapheal SAS, Grenoble

A single laser pulse to reverse magnetisation without any applied magnetic field

Grapheal presents a technology based on two chemical vapor deposition processes for the production of perfectly continuous, monolayer graphene films deposited on polymer. This technology combines biocompatibility (1,2), mechanical flexibility, optical transparency and high electron mobility in a single film, enabling ion-sensitive field-effect detection (3). At Grapheal, we have explored the use of graphene on polymer to enable biosensing, tissue engineering (4) and the integration of an RFID component for direct connectivity with a smartphone in a single device.

I will demonstrate various applications based on the functionalization of the graphene surface to implement sensitive and selective biosensors. Finally, I will show the prospects for consumer applications that unlock new use cases (5) for wearable diagnostics enabling field analysis for health and the environment.

(1) A. Bourrier et al. Adv. Health. Mat. 8 , 1801331, (2019) doi : 10.1002/adhm.201801331
(2) F. Veliev, et al., Biomaterials, Elsevier, 86, pp.33?41 (2016).
(3) F. Veliev et al. Doi : 10.3389/fnins.2017.00466 (2017).
(4) Le Gall et al. doi: 10.1101/2021.05.16.444337 (2021).
(5) https://www.grapheal.com

PSI3 – Plasma materials for nuclear fusion

Contribution of laser techniques for the study of fission and fusion materials at high temperature

Laurent Gallais * [1], Marco Minissale [2], Marianne Richou [3], Guillaume Kermouche [4], Thomas Doualle [5], Yves Pontillon [5]

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The knowledge of material properties and their evolution at high temperatures is critically important in both nuclear fission (fuels) and fusion (plasma-facing components). This includes thermophysical, mechanical, and optical properties, as well as the heat flux resistance of components subjected to high thermal loads in stationary or transient conditions. For such studies, laser techniques are particularly suitable since they can easily drive materials to extreme temperatures with a very high degree of precision and control. They can be combined with contactless instruments (pyrometry, spectrometry, thermal imaging) to derive the properties of interest of the materials. In this talk, we will discuss our recent contributions in this field with studies conducted on uranium dioxide (measurement of thermophysical properties up to 2000 K, generation of complex thermal gradients to study fuel behavior in off-normal conditions) and tungsten (studies of recrystallization kinetics at high temperatures). We will also discuss perspectives on a laser-based approach to study liquid materials for fission and fusion applications.

Keywords: combustibles nucléaires, composants face aux plasmas de fusion, laser, optique

*Speaker

Restauration de l'état de surface du tungstène par laser après des expérimentations en tokamak

Diogo Dias Aleixo * , Marianne Richou [1], Mehdi Firdaouss , Mathilde Diez [2], Sylvain Rodrigues , Jonathan Gérardin , Mateo Lelièvre , Louis Gaugoin

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Dans les tokamaks comme WEST (CEA/Cadarache), le plasma interagit notamment avec des composants constitués de tungstène, appelé PFU (Plasma Facing Unit). Ces PFUs représentent approximativement 10% de la surface en contact avec le plasma. Le tungstène s'érode dans les zones à fort flux de particules et s'accumule dans les zones à faible flux sous forme de couches adhérentes. Ces couches piègent des particules hydrogénées, et les dépôts moins adhérents peuvent se détacher, provoquant des disruptions et l'arrêt des opérations plasma de WEST. Pour limiter ce phénomène, une méthode industrielle utilisant des impulsions laser a été développée pour permettre d'enlever les dépôts en surface sans induire d'endommagement (érosion, fissuration, adoucissement) du tungstène. Des essais préliminaires à différentes puissances ont été réalisés sur un PFU neuf, afin de confirmer l'absence d'endommagement du tungstène par des analyses précises de la topographie de surface. Le paramétrage optimal a été appliqué sur des PFUs ayant subi des campagnes WEST (avec présence de dépôt), avec une vitesse de nettoyage estimée à 2 h/m^2. Les analyses de thermographie infrarouge en temps réel ont révélé des températures inférieures à 100 ∘C sur les zones ablatées. Une aspiration a été réalisée en simultané pour éviter la dispersion des poussières créées. Les analyses post-laser, incluant la microscopie optique, la microscopie confocale, l'analyseur à fluorescence X, la métallographie et la rugosité, ont confirmé que les dépôts épais de quelques dizaines de μm ont été ablatés sans altérer la surface des composants, et que la rugosité après ablation est identique à celle des composants neufs. Ceci démontre la conservation de l'état de surface initial. En vue de tester l'efficacité du procédé en conditions réelles, il est prévu d'enlever les dépôts sur un nombre significatif de PFUs pour la camapgne expérimentale de fin d'année.

Keywords: Fusion nucléaire, Traitement de surface, Nettoyage, Laser, Tungstène

*Speaker

Damage to tungsten under repeated cyclic thermal loading in magnetic melting machines

Marianne Richou * [1], Maxime Lemetais [2], Alan Durif [3], Anthony Flament [1], Guillaume Kermouche [4], Laurent Gallais [5]

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Le tungstène est considéré actuellement comme le matériau au face plasma idéal des machines de fusion magnétique. Il présente en effet l'avantage d'avoir un haut point de fusion (3400∘C) et une forte résistance à l'érosion. Cependant, lorsque celui-ci est mis en forme pour constituer un composant face au plasma, on constate que sous certaines sollicitations représentatives des chargements des machines de fusion magnétique, ce matériau face au plasma s'endommage. En effet, on constate notamment la présence de fissures suite aux chargements thermiques cycliques répétés. Ce matériau s'adoucissant lorsque sa microstructure évolue sous l'effet de la température, cet endommagement est induit par l'accumulation de déformation plastique dans le tungstène. Les deux phénomènes physiques en jeu sont la recristallisation et la restauration. A la vue de la présence de fissures qui peuvent rendre un composant impropre à son utilisation, il est apparu important de pouvoir estimer si une fissure à des risques d'apparaître au regard du chargement thermique (flux, temps de chargement) (1). Il est également apparu comme indispensable de proposer des modèles permettant d'évaluer l'état de l'évolution de la microstructure du tungstène, en fonction des chargements thermiques subis (température, temps de maintien) (2)(3) et de la microstructure du tungstène après fabrication (densité de dislocation, taille de grains) (4). Cette étude présente l'état des avancées sur ces deux sujets et intègre la description des dispositifs expérimentaux qui ont été mis en place pour aboutir à la caractérisation de l'évolution de la microstructure du tungstène (5).

(1) A. Durif et al. , 2022, doi: 10.1016/j.jnucmat.2022.153906.
(2) M. Richou et al.,2020, doi: 10.1016/j.jnucmat.2020.152418.
(3) A. Durif et al., 2022, doi: 10.1007/s10853-022-07123-w.
(4) M. Lemetais et al. 2022, doi: 10.1016/j.fusengdes.2023.113708.
(5) M. Lemetais et al., 2023, doi: 10.1016/j.fusengdes.2023.113785.

Keywords: Tungstène, endommagement, recristallisation

*Speaker

Structural and chemical characterization of helium nano-bubbles formed in irradiated tungsten by Transmission Electron Microscopy.

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In the future ITER reactor the lowest part of the torus, called the divertor, will be subjected to extremely high heat and ions loads. Tungsten is the material chosen for this component because of its thermomechanical properties and high melting point. However, plasma-wall interactions and temperature cycling modify these intrinsic properties, and their evolution under irradiation is a major issue for both reactor operation and safety. Helium implantation, in particular, has been proven to significantly affect the sub-surface microstructure of tungsten and to induce the formation of nano-bubbles. A better understanding of the fundamental mechanisms behind the formation of these pressurised nano-bubbles requires characterization of their morphology and of the density of the helium they contain. The high spatially resolved STEM-EELS method is one of the only techniques capable of probing individual bubbles on a nanometric scale. Measurements for single bubbles are essential to achieve our goal of inventorying the total helium trapped in tungsten, as the size distribution of the bubbles is generally fairly dispersed, and the He density strongly depends on bubble size. We aim to develop a methodology to quantify the atomic density of helium inside individual bubbles in order to study the density's dependence on implantation parameters and bubble sizes. Results for a single crystalline (110) tungsten sample, implanted at 2keV at the ESRF in the INS2 set up of the BM32 beamline are presented. The applied He flux was 1.9 1017 He.m-2.s-1 and the reach fluence was 1.0 1022 He.m-2. The sample temperature was maintained at 1273 K during He bombardment. The evolution of helium density and peak position with the bubble size that we measured in tungsten will be discussed and compared with those obtained previously for He nano-bubbles probed in others materials.

Keywords: nuclear fusion, plasma, wall interactions, helium nanobubbles, tungsten, TEM

*Speaker

Evidence of nanocavity diffusion in irradiated tungsten by combining experiments and multiscale modelling

Charlotte Becquart * , Andrée Debacker *

, Christophe Domain [1], Abdelkader Souidi , Marie-France Barthe [2], Etienne Hodille [3], Emmanuel Autissier , Cécile Genevois [4], Addad Farah , Antonin Della Noce

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In irradiated metals, the impinging particles create two types of defect in the crystal lattice, interstitial atoms and vacancies. The microstructure evolution results from an interference of processes leading to the defect recombination, clustering or trapping. Temperature also plays a crucial role as many process are thermally activated. Our modeling approach is multiscale and, for this work, based on an Object Kinetic Monte Carlo model (where each defect cluster is an object which can diffuse, dissociate and react following predefined properties). We put in evidence the diffusion of nanocavities by combining (i) a systematic experiment with samples irradiated, annealed up to 1800 K and analysed byTransmission Electron Microscopy; (ii) an Object Kinetic Monte Carlo numerical model of the microstructure evolution based on several thousands of atomistic data; (iii) a multi-objective optimization method in which the nanocavity diffusion, input of our model, is adjusted to reproduce the experimental data. The results draw two curves in the space of parameters delimitating the set of non-dominated solutions, i.e. the equally good solutions, also named the Pareto front. These two curves corresponding to the optimum of the size and density objectives enlightening that our model cannot reproduce simultaneously both objectives. A posteriori, we studied the sensitivity of our model to other main parameters, i.e. the source term, choosing between several sets of displacement cascades calculated with different empirical potentials and the sub-model for the dissociation properties. Hence we determine the nanocavity diffusion and its uncertainty. Our results can offer an estimate on the nanocavity diffusion coefficient in the size range where no data existed to our knowledge. Furthermore, the comparison with classical surface diffusion theory, valid for large nanocavities, provides the activation energy of the surface diffusion coefficient.

Keywords: microstructure, modeling, OKMC, tungsten, vacancy clusters

*Speaker

Formation of He bubbles on plasma exposed tungsten via in-situ spectroscopic ellipsometry

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In fusion reactors such as ITER, tungsten (W) will be used for plasma-facing components (PFCs). It is expected to withstand ion fluxes of the order of 1e24 D/m2s, coming from the fuel plasma (deuterium, D, and tritium) and the reaction products (helium, neutrons), together with heat fluxes up to 20 MW/m2. The interaction of charged particles with W can induce modifications in the material (lattice defects, surface blistering) and this can lead to a change in W optical properties. An accurate knowledge of the evolution of W optical properties is fundamental for thermography measurements of PFCs, which will be realized through optical diagnostics (pyrometers, IR cameras). In this work, we investigate the evolution of W morphology and optical properties during He plasma via *in-situ* spectroscopic ellipsometry. Such technique uses a polychromatic source of polarized light (400-1000 nm) and measures the change in its polarization upon reflection from the surface. The experimental setup is composed by a RF plasma chamber onto which are installed the ellipsometry source and detector units. In such set-up, it is possible to expose W samples to RF He plasma generated by a planar coil antenna, and to reproduce the experimental conditions of (expected) He bubbles formation: ion flux and fluence are respectively 3x1019 m-2s-1 and 8x1023 m-2, ions energy around 80 eV. We perform different plasma exposures varying multiple parameters such as temperature, ion flux and previous surface state of W samples. We aim to use ellipsometry to follow *in-situ* and in real time the formation and evolution of He bubbles on W during plasma exposure. We couple the in-situ, fitted with an appropriate effective-medium model that takes into account the volume fraction of He bubbles in W sub-surface layer, to ex-situ measurements of the surface morphology, perfomed before and after the plasma exposure (SEM).

*Speaker

Erosion and transport of lithium from a liquid metal wall facing a fusion plasma

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In current nuclear fusion reactor designs, heat and impurities are generally recovered thanks to divertors. Presently, the plasma-facing surfaces of these divertors are made of actively water-cooled tungsten monoblocks. The choice of tungsten relies essentially on its refractory properties and its low-hydrogen retention. However, due to the high heat flux presents in nuclear fusion devices, these plasma-facing components (PFC) are still concerned by erosion, due to physical sputtering, and other degradation mechanisms, leading to periodic maintenances and ejection of heavy impurities in the core Recently, a variety of new concepts of plasma-facing components based on the use of molten metals, such as capillary porous system, vapour-box divertor or lithium-metal infused trenches have emerged to solve problems associated to current PFCs by improving heat removal, impurity extraction and reducing maintenance by protecting the vessel. Among these designs, liquid lithium seems to be an interesting choice of liquid metal because of its large working range, its low number of charges and its low neutron activation. However, the presence of liquid lithium in fusion devices leads to high erosion rates essentially induced by evaporation at high temperature.Evaporated lithium atoms can be ionized near the wall and redeposit onto the liquid surface due to electromagnetic field, or eventually migrate towards the plasma core and dilute detrimentally the fusion fuel.
It is then important to assess the plasma pollution due to lithium evaporation taking into account the redeposition phenomenon and the transport through the magnetic surfaces. We will present a 1D3V Particle-in-Cell model which allows the calculation of the lithium density in the plasma column with respect to both the incoming flux and the redeposition rate. Then the net transport of lithium to the core is estimated by using Gysela (Gyrokinetics Semi-Lagrangian code) and assuming both turbulent and neoclassical transports.

Keywords: fusion par confinement magnétique, simulations particulaires, simulations gyrocinétiques, interaction plasma surface, métal liquide

*Speaker

Post-mortem analysis of the deposit layers on the lower divertor of WEST

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Understanding the material migration and subsequent deposited layers in a metallic environment is one of the key issue for next step fusion devices as ITER. During its second phase of operation, the lower divertor of WEST was fully equipped with water-cooled ITER grade plasma facing units (PFUs) made of beveled W monoblocks (MBs). The 2022-2023 campaigns mainly focused on the deposition of high particle fluence on the divertor by repeating a large number of long discharges. A visual inspection of the divertor after plasma campaigns shows a similar erosion/deposition pattern to the one of the first phase (1) with a deposition-dominated area observed on the inner side of the divertor.
We present a physico-chemical analysis of the deposits resulting from both conditioning and plasma-wall interactions during the WEST campaigns. Deposits were collected in 2023 in the inner area (MB1-13) on two ITER grade PFUs located each at the maximal heat load area in the outer and inner side due to the ripple modulation. Deposited layers were collected " in situ " using a tape sampling procedure (2), enabling their properties (composition, thickness, morphology, adhesion) to be analyzed using various techniques (scanning electron microscopy, energy-dispersive X-ray and Raman spectroscopy).
The plasma wall interactions responsible for deposit formation, the tungsten sources feeding the deposits and the issues of retention, thermal behavior and plasma instabilities due to deposits will be introduced. The effect of high fluence plasma exposure and boronisations on the properties of the deposits will be discussed.
(1) M. Diez et al., "Overview of plasma-tungsten surfaces interactions on the divertor test sector in WEST during the C3 and C4 campaigns" Nuclear Materials and Energy (2023)
(2) M. Martin et al., "First post-mortem analysis of deposits collected on ITER-like components in WEST after the C3 and C4 campaigns" Physica Scripta (2021)

Keywords: WEST, tokamak, erosion, deposition, tungsten, boron, ITER, plasma, fusion

*Speaker

Coalescence of He bubbles diffusing in a W matrix

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Thermonuclear fusion of the hydrogen isotopes is a promising way of producing low-carbon, abundant and safe energy. The fusion plasma in a nuclear reactor is confined by strong magnetic fields, but the divertor, where open magnetic fields lines intercept, is subject to extremely high heat and ion fluxes. He atoms produced in fusion reactions can deeply penetrate in the tungsten divertor. He atoms can form clusters by displacing W atoms and eventually generate nano-bubbles (K. D. Hammond, Materials Research Express 4, 104002 (2017)). The presence of He nano-bubbles in the metal matrix modifies the thermomechanical properties of W and represents a major safety issue. At high temperature, the He bubbles grow in size. The elongated shape of large He bubbles suggests that the growth takes place by diffusion and coalescence of small bubbles (L. Corso et al., Nuclear Materials and Energy 37, 101533 (2023)). The behavior of bubbles can be approximated with that of voids.
Nichols (Journal of nuclear materials 30, 143 (1969)), and Willertz and Shewmon (Metallurgical transactions 1, 2217 (1970)) have investigated the diffusional motion of pores in solids from a continuum/analytical perspective and have found some general scaling laws. However, nano-sized voids could behave differently from the established scaling laws.
We have carried out kinetic Monte Carlo simulations to investigate the kinetics of diffusion and coalescence of nano-voids in a bcc matrix. We have found that the diffusivity of small voids as a function of their size increases, reaches a plateau before decreasing. We explain this behavior by introducing a curvature-dependent energy barrier for mass transport. The void diffusivity trend also affects the coalescence, as single vacancies displace slower than small voids, and some voids with a critical size (not too large nor too small) move and collect vacancies from the matrix.

Keywords: He bubbles, tungsten, kinetic Monte Carlo, growth, coalescence

*Speaker

Simulating plasma-surface interactions with ion and molecular beams experiments: application to ITER materials

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ITER is an international experiment under construction in France, where a plasma of hydrogen isotopes (deuterium and tritium, the fusion fuel) is heated to millions of Kelvin to produce energetic helium and power exhaust occurs on tungsten (W) plasma facing materials (PFM). A detailed understanding of W interaction with fusion fuel is needed, because tritium is scarce and radioactive. An overview of experimental studies on ITER materials realized at the PIIM laboratory and supported by models developed at the IRFM is proposed.
Our prime focus was on fuel trapping in PFM. Generally, hydrogen trapping can trap at bulk structural defects (vacancies, grain boundaries...) as well as at the PFM surface, the latter being often neglected. In a joint experimental-modeling study, we showed that both grain boundaries and near-surface native oxide trapping explain hydrogen degassing of W materials at room temperature. Using ion beam and surface science techniques, we demonstrated that hydrogen trapping at W native oxide is different than at clean W surfaces contaminated with oxygen atoms. This should have implications on fuel recycling at PFM surfaces and could impact fusion plasma control.

Besides, it was shown that He trapping in W affects hydrogen trapping. He being not soluble in metals, it was predicted 40 years ago that He clusters could nucleate homogeneously and self-trap in the W lattice. Using He ion beams with tunable kinetic energy and flux, we demonstrated that He self-trapping occurs, indeed.
Finally, 10% of ITER's PFM are made of 316L stainless steel. We demonstrated that 316L emits ammonia because of its natural nitrogen content. To understand how this could influence the nuclear safety of ITER, we performed supersonic molecular beam experiments to measure the sticking of ammonia on W and SS316L and built a kinetic model to help estimating the tritium inventory related to ammonia.

Keywords: tungsten hydrogen plasma materials

*Speaker

Multi-scale modelling of H interactions on W surfaces and W/Cu interlayers

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In this contribution, we overview our approach to modeling the interaction of hydrogen isotopes (HIs) with fusion-relevant materials developed over the past few years. This method allows us to model materials from the plasma-exposed surface to the coolant boundary using a multiscale (MS) approach. Our modeling integrates density functional theory (DFT), molecular dynamics (MD), and kinetic/thermodynamic theories. DFT describes material structure at a scale of hundreds of atoms, MD simulates larger systems, and kinetic/thermodynamic theories convert atomic data into macro-scale physical quantities. We applied this MS approach to tungsten and copper, considering perfect structures, point defects, and 2D defects like interfaces. In tungsten, we identified conditions making surface processes the rate-limiting step for HIs transport, leading to a kinetic model incorporated into the MHIMS code. These results illustrate our MS approach. We then present our latest work extending to the coolant side of divertor plasma-facing components. We developed two W/Cu interface models to determine HIs solution and diffusion properties, using DFT for interstitial sites, and thermodynamic/kinetic models for solubility. MD investigated the impact of the mismatch on copper structure near the W/Cu interface, revealing defect formation and propagation.

(1) Y. Silva-Solis et al, NME 37 (2023) 101516
(2) E. A. Hodille et al, NF 57 (2017) 056002
(3) J. Denis et al, NME 19 (2019) 550-557

Keywords: nuclear fusion, multi scale modelling, DFT, statistical thermodynamics, rate equation modelling, molecular dynamics

*Speaker

Deuterium absorption and desorption on the tungsten trioxide

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Understanding how tungsten interacts with fusion fuel (deuterium and tritium) is crucial for nuclear safety and plasma detachment due to tritium radioactivity and potential impurity effects on recycling. Therefore, models' development of fusion fuel interaction with tungsten materials is of importance and requires experimental data. The present work contributes to understanding how tungsten oxides' thickness affects deuterium retention and release.
Two tungsten trioxide samples (WO3) with thicknesses of, respectively, _˜25 and _˜50 nm were grown on polycrystalline tungsten substrates whose surfaces had been previously polished and annealed. We exposed the two WO3 samples to a beam of deuterium ions with 250 eV/D at room temperature and evaluated deuterium retention using temperature-programmed desorption (TPD). The TPD spectra were measured for various deuterium-containing molecules (HD, D2, HDO, D2O) with a line-of-sight geometry allowing a quantitative evaluation of deuterium retention in WO3 samples. Because the oxides were grown at 1073 K and the TPD measurements were realised up to 800 K, ensuring that the WO3 layers are thermally stable, systematic implantation/TPD cycles could be repeated on each sample. The data was compared to previous experiments on a 150 nm WO3 layer.
For each WO3 sample, deuterium retention and release were studied for different deuterium ion fluences and storage durations at room temperature in a vacuum. Results showed that the oxide layer evolves in the process: initially, the retention is relatively low and decays exponentially over time. With accumulated implantation/TPD cycles the deuterium retention increases and becomes stable at room temperature. Heavy water desorption during TPD and various surface characterising techniques (XPS, FIB, SEM, RBS) show that the evolution is linked to an oxygen depletion mechanism, possibly thickness-dependent. Additionally, experiments with relatively high incident fluences have shown a lower desorption-to-fluence ratio, making desorption-fluence dependence non-linear and indicating trap saturation.

Keywords: fusion, tungsten, impurity, fusion fuel recycle

*Speaker

Adsorption, absorption and release of deuterium on W(110) covered with ultra-thin oxygen layer

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In future tokamak reactors, plasma facing components (PFC) will be under both high thermal (1500 K) and particle fluxes (10^24 m-2.s-1) leading to energy density up to 10 MW.m-2 in nominal operation. The currently prefered PFC material is tungsten (W) as it has been chosen for the ITER international experiment. Tungsten is known to retain little fuel (deuterium, D) at its surface and in its bulk with a relatively low temperature of D release (below 600 K for pristine W materials). This high fuel recycling property should allow to maintain an efficient reaction rate in the reactor core. However, it has been shown that the surface state of W will modify those retention/release characteristics (1). Thus, it is of interest to study in details the D/W interactions in order to build predictive models for the behaviour of reactor's PFC in operation. In this abstract, we report on the techniques used to clean and to grow ultra-thin layers of natural impurties found in tokamaks (such as oxygen) in the submonolayer regime. Then, we present retention/release results obtained after various molecular and/or ionic D2 exposure time on different W(110) surfaces either clean or covered with ultra-thin layers of oxygen. It appears that oxygen layers modify both the surface and the bulk retention/release of D on/in W, sometime in a drastic manner which may influence locally the recycling property of W PFC.

(1) Dunand et al., Nuclear Fusion 62 (2022) 054002

*Speaker

Helium bubbles growth in tungsten by in-operando GISAXS

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In the next fusion reactor ITER, tungsten (W) has been chosen as the material facing the plasma and it must resist to harsh conditions such as intense helium (He) bombardment and high temperatures. He irradiation generates nano-sized bubbles modifying the W microstructure and its physical properties. A major concern is the increase of the radioactive tritium retention, which presents a risk for the nuclear safety. Thus, understanding the He bubbles formation is crucial for nuclear fusion exploitation.
In that perspective we have characterized in real time during He bombardment, the growth of He bubbles by *in-operando* Grazing Incidence Small Angle X-ray Scattering (GISAXS) using the INS2 setup (1) (ESRF-BM32 beamline). W single crystals have been implanted with 400 eV or 2 keV ions to address the effect of implantation damage on bubbles formation. In addition, the temperature dependence has been investigated between RT and 1200∘C during implantation and up to 1500∘C by post-implantation annealing. Below 1000∘C bubbles appear rounded, while for higher temperatures, bubbles are facetted and show {100} and {110} facets (2) forming a truncated rhombic dodecahedron. The facetted shape has been implemented in the IsGISAXS software (3) to fit the experimental data and simulate the bubbles growth. We show that the bubbles size increases by Brownian migration and coalescence of bubbles (4). The limiting step for the migration process is attributed to the nucleation of a new ledge on the bubble facets (5). These results are supported by post-mortem transmission electron microscopy analysis.

(1) G. Renaud, R. Lazzari, and F. Leroy, Surf. Sci. Rep. **64**, 255 (2009).
(2) L. Corso *et al.*, Nucl. Mater. Energy **37**, 101533 (2023).
(3) R. Lazzari, J. Appl. Crystallogr. **35**, 406 (2002).
(4) L. Corso *et al.*, In preparation.
(5) S. Curiotto *et al.*, Appl. Phys. Lett. **123**, 241603 (2023).

Keywords: fusion, tunsgten, helium bubbles, GISAXS

*Speaker

PSI4 – Quels défis et enjeux des matéraux pour les générations actuelles et futures des réacteurs nucléaires à fission ?

Accident Tolerant Fuel : A short of overview of the concepts, their benefits & the challenges from the safety point view

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The impact of the Fukushima Daichi accident renewed the nuclear industries drive to improve fuel technology, through the development of the so-called ATF concepts, to enhance again the reactor safety. Much of the motivation of these new designs is to slow down the increase of the fuel temperature in accident conditions and increase the delay of fuel melting as well as to improve the fission product gas retention to lower the radiological consequences of a potential accident. The introduction of a new fuel type requires extensive testing and evaluation. For that reason, ATF concepts under development are categorized as near term or longer term, based on their anticipated timeline to full-core deployment. A short description of the ATF technologies limited to the most-promising claddings and fuels will be given. Then the safety benefits to be understood as margin gains with respect to the current fuel rods performances (in Zr-based alloys with UO2 or MOX fuel pellets) will be discussed. In a second step, the safety challenges which remain to be addressed will be presented as well as the current experimental programs aiming to answer to these challenges . In France, the solution of a chromium coating onto M5® cladding makes this concept the preferred choice for reactor implementation soon. It aims to reduce the cladding oxidation and ballooning in LOCA conditions. In addition, ongoing research has been also conducted to enhance the retention of fission gases in the fuel itself. These efforts involve the addition of dopants (chromia) into UO2 ceramic fuel pellets. The presentation describes the experimental and analytical activities that have recently been launched at IRSN to investigate some key issues that may arise in a future assessment of the effects of ATF use in accident conditions.

Keywords: Accident Tolerant Fuels, Safety

*Speaker

ENJEUX MATERIAUX POUR LES ACCIDENTS TOLERANT FUELS

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Suite à l'accident de Fukushima-Daïchi le 11 mars 2011, la communauté internationale s'est mobilisée pour développer des combustibles de Réacteur à Eau Pressurisée (REP) offrant une résistance accrue aux situations accidentelles, notamment les Accidents de Perte de Réfrigérant Primaire (APRP). Ces combustibles, développés sous le label " Accident Tolerant Fuel (ATF) ", avaient pour premier objectif le déploiement industriel de solutions de première génération à échéance de 2025, avec des ambitions d'amélioration à plus long terme.
Le développement des ATF fait l'objet d'une veille scientifique active au sein de l'Institut tripartite (I3P) CEA-EdF-Framatome, depuis 2013, avec l'analyse d'une cinquantaine de communications (articles, brevet, conférences, rapports et thèses) par mois, qui témoignent de la vitalité de cette thématique. Les solutions étudiées reposent notamment (mais pas exclusivement) sur des options de matériaux avancés répondant aux cahier des charges des ATF.

L'exposé présentera l'historique des recherches sur les ATF, leur cahier des charges, une revue des solutions étudiées (dont les premières arrivent d'ores et déjà à maturité, avec les résultats acquis par l'irradiation de Lead Test Assemblies (LTA) aux Etats-Unis, et prochainement en France), et un état des lieux des perspectives.

Keywords: fission nucléaire, sécurité, accident tolerant fuels, matériaux avancés

*Speaker

LES PROGRAMMES R&D DU CEA EN LIEN AVEC LES MATERIAUX DES REACTEURS RNR NA ET MSR

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Le CEA et la filière nucléaire Française s'inscrivent dans la perspective long terme de la fermeture du cycle du combustible impliquant le déploiement d'un parc de réacteurs à neutrons rapides. L'objectif est que la filière nucléaire puisse disposer, le moment venu, d'outils performants pour la conception, la démonstration de sûreté et l'extrapolation industrielle.
La technologie des RNR-Na a le potentiel pour devenir une solution industrielle de référence. Pour autant, le retour d'expérience montre qu'il convient d'accroitre la maîtrise, d'augmenter les performances et de réduire les coûts préalablement au déploiement industriel. Les grands enjeux sont les suivants :

(i) développer et valider les outils de calcul scientifique de nouvelle génération, le code de construction et les données pour la conception de ces réacteurs ; réduire les conservatismes ;

(ii) explorer des solutions techniques innovantes;

(iii) prendre part au **développement de certaines briques technologiques comme le combustible, les composants**, l'instrumentation, les dispositifs de sûreté ; accompagner ces développements par des expérimentations et fournir les preuves de concepts ; transférer ces technologies vers les industriels. Ainsi, par exemple, le CEA accélère ses recherches sur la durabilité des matériaux de structure de manière à répondre aux exigences de sureté et d'exploitation sur un temps long.

Toujours dans la perspective de fermeture du cycle, la technologie des réacteurs à neutrons rapides utilisant des sels fondus chlorure (MSR) est perçue comme un complément au RNR-Na. Elle présente théoriquement des avantages pour la transmutation des actinides mineurs. Au CEA, un champ de R&D en lien avec l'écosystème industriel a été ouvert afin d'étudier la faisabilité et les performances d'un tel réacteur et à crédibiliser les MSR dans une perspective industrielle. Pour ces réacteurs MSR**, les briques " sels " et " matériaux " sont intimement liées et constituent les premiers verrous à lever pour établir la faisabilité du concept**.

Keywords: Fission nucléaire, fermeture du cycle du combustible, réacteurs à neutrons rapide, matériaux avancés

*Speaker

Réacteurs Nucléaires eau pressurisée-Défis et enjeux. Matériaux pour les générations actuelles et futures

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Les scénarios énergétiques économiquement soutenables montrent l'importance de maintenir dans le mix énergétique bas carbone national une production nucléaire significative. Ce contexte, amplifié par l'urgence climatique et la crise énergétique, challenge les conditions d'exploitation des réacteurs actuels d'EDF (Réacteurs à Eau Pressurisée) et futurs (REP EPR, SMR,...) et pousse à l'optimisation de nouveaux matériaux. Pour les composants non ou difficilement remplaçables, la mise au point de nouvelles " technologies " pour réduire leurs vieillissements (thermique, sous irradiation ...) sont également des défis à relever dans le cadre de la prolongation des réacteurs actuels. . A titre d'exemple, nous pouvons citer l'étude d'opportunité en cours au sein d'EDF pour la mise en place de grappes d'hafnium en périphérie de cœur, afin de réduire le vieillissement sous irradiation de certains de ces composants. Ce contexte industriel toujours plus compétitif et exigeant appelle, de nouvelles techniques de fabrication (WAAM, Cold Spray...) et de réparation, de nouveaux moyens d'essais expérimentaux et de caractérisations, et de nouvelles méthodes numériques et outils de simulations performants et à l'état de l'art, permettant notamment d'orienter les choix visant à satisfaire à la fois les critères de coût et de sûreté, et ce d'autant plus s'agissant de composants nucléaires. Ces composants mettant eux-mêmes en jeu une variabilité de matériaux (aciers , alliages de zirconium, ...) de différentes microstructures et compositions chimiques, et soumis à des conditions d'utilisations très sollicitantes (neutronique, ...) au cours de leur vie en réacteur. Ces conditions de sollicitations induisent, elles- mêmes, des phénomènes à différentes échelles de ces composants, et pouvant, selon les cas, conduire à une réduction de leur durée de vie. Dans ce contexte, l'objectif de cette présentation est d'exposer les défis et enjeux matériaux associés aux différents composants majeurs des Réacteurs à Eau Pressurisée d'EDF.

Keywords: Durée de vie des centrales nucléaires, nouveaux matériaux pour les centrales actuelles et futures

*Speaker

Les études engagées au CEA sur les matériaux métalliques pour répondre aux enjeux et défis des réacteurs actuels et du futur. Quelques illustrations mettant en avant les effets d'environnement, irradiation et corrosion.

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La recherche menée au CEA sur les métaux des réacteurs nucléaires employés pour les éléments de structure ou gainage du combustible, est diverse : alliages base Fe, Ni, Zr, Al..., et complexe : structures multiphasées, nanostructurées, et hétérogènes. Cette R&D multi-échelle et multi-physique vise à comprendre les évolutions microstructurales en condition de fonctionnement mais aussi en conditions accidentelles avec leurs impacts sur les propriétés physique-mécaniques..., mais ambitionne également de développer des nouveaux matériaux à très hautes propriétés. Pour cela, l'approche combinant expérimentation et modélisation est incontournable.
L'actuel sujet du Long Term Operation (LTO) avec la prolongation incontournable de certains composants non remplaçables du parc (la cuve) est un excellent exemple de la démarche faisant appel à une approche amont : calculs atomistiques et matériaux modèles irradiés aux ions.

Autre développement récent, la gaine de zirconium revêtu chrome : concept évolutif de combustibles plus tolérants aux accidents. De nombreuses études " multi-propriétés " et " multi-échelles " sont menées, reliant les procédés et conditions de dépôt des différents revêtements aux microstructures et propriétés résultantes en s'appuyant sur la modélisation et l'expérimentation aux échelles les plus fines.

Les réacteurs du futur sont également abordés avec de nombreuses innovations pour répondre au défi des Advanced Modular Reactor (AMR). Des verrous majeurs apparaissent pour ces concepts (SFR, MSR, LFR...) notamment du point de vue des effets d'irradiation couplés aux effets d'un milieu très corrosif.

Ici aussi les travaux couplant expériences et modèles sont nécessaires pour appréhender les mécanismes physiques responsables de la détérioration des matériaux. Ces mêmes outils sont employés pour concevoir de nouveaux matériaux, via des approches d'IA, et proposer des alliages à haute entropie - concentrés (HEA-CCA), voir des matériaux à gradients obtenus par fabrication additive.

Cette présentation illustrera la démarche menée par le CEA avec ses partenaires industriels et académiques.

Keywords: Irradiation, corrosion, simulation, expériences, microstructure, défauts

*Speaker

PSI1 - Matériaux et Patrimoine bâti

Salt weathering on tuffeau stones: example with the case study on the Chapel of Maurepas, Chambord, France

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Salt weathering is one of the most damaging deterioration for building stones. Porous stones are very sensitive to decay induced by salt crystallisation. Tuffeau is porous and soft limestone, widely used in the Loire Valley in France. This building stone have many technical and aesthetic advantages, allowing the construction of many historical monuments like the famous castle of Chambord. The study, presented here, is part of the health diagnosis of the chapel of Maurepas, a small medieval building located in the heart of the National Estate of Chambord. Built on lake limestone foundations, the elevations of the chapel are made of tuffeau rubble covered with lime coating, with corner quoins in tuffeau stonework. These quoins are subjected to severe powdering. Powdering is granular disintegration of finely grained stones, and tuffeau is very sensitive to powdering which can cause a high matter loss. A 3D survey was performed by laser scanner to quantify the loss of matter. Samples were also collected at different heights and different depth by drilling for chemical analysis. X-ray diffraction analyses proved the significant presence of sodium chloride NaCl whereas ion chromatography could quantify its amount. Salt content is proportional to the loss of matter by sanding. Hence, the most damaged stone course presents up to 10%wt NaCl content. For the south wall of the chapel, all stones and mortars are polluted by salt in the inner side and in the outer side of the wall. The diagnosis made it possible to set hypotheses for the salt transport, so as to propose remediation solutions. The replacement of damaged stone blocks is useless because of the great pollution of the masonry and the presence of salt in the whole masonry. Only a treatment by desalination could be useful to extract pollutant from the porosity of materials.

Keywords: powdering, sodium chloride, salt, limestone, tuffeau, porosity

*Speaker

Crystallization damage in composite layered artworks

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Tangible cultural heritage, including historical sites, artifacts, and outdoor artworks, is subject to many physical and chemical changes, each of which can have grave effects. Among various degradation factors, salt rising followed by crystallization is recognized as one of the major causes of degradation of porous materials like masonry, sculptures, and frescoes. Most of these artworks are made of an assembly of layered materials with different physicochemical properties. Salt crystallization in composite layered porous materials such as wall paintings, frescoes, tiles, and ceramics can lead to cracks or delamination of the upper layers (paintings and glaze). During the European JPICH project CRYSTINART, we gathered a complementary team of experts which allowed us to combine various high-end complementary techniques such as X-ray microtomography, Nuclear magnetic resonance, Multispectral imaging, and analytical methods like mass spectrometry and Raman spectroscopy to assess the condition of layered artworks and bring valuable insights into the materials dynamics, fluid flow in the porous structure, and the overall condition of artworks. Our findings show how open surface areas induce the asymmetrical flow of liquid and ions from the heart of the material toward the delaminated evaporative region. In parallel, using micro-macro finite-element numerical modeling, we have proposed predictive tools based on our experimental data for the deterioration process that describe the macroscopic material behavior. Our results bring new insight on why with ageing and the progress of delamination areas, the risk of accelerating the deterioration of the artworks will also increase.

Keywords: milieux poreux, sel, cristallisation, materiaux composites, heritage culturel

*Speaker

Thermo-rheological behavior of a limestone submitted to standard fire

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The behavior of built heritage materials under fire conditions is a significant concern today, especially following the fires that have occurred in recent years: Notre-Dame Cathedral in Paris (2019), Nantes Cathedral (2020), Hôtel Seignelay (2022), and Copenhagen's historic stock exchange (2024). The development of extreme thermal gradients can be responsible for important damage in the structures. Understanding material behaviors is essential for assessing post-fire damage, aiding restoration, and developing active and passive protection strategies. Most often in heritage monuments, limestones have been used as structural materials and are thus the studied material. Previous works allowed us to identify the thermal, hydric, chemical, and mechanical (THCM) behaviors kinetics of a selected limestone from ambient temperature to 1000∘C at the mesoscale. The obtained results are partially linked to the thermochemical changes modeled at the microscale, but thermochemical damages do not explain the early mechanical damages at relatively low temperatures. This work aims to better understand the thermo-rheological behavior of the limestone at the mesoscale through non-isothermal loading. Prismatic samples (4x4x16mm) are uniformly heated at 1∘C/min under fixed compressive stress. A Netzsch thermomechanical analyzer (TMA) is used to carry out the tests. Sample sizes were adjusted to avoid thermal gradients. The thermomechanical model deduced from those experiments is compared to the existing results in the literature and is then combined with an already established thermochemical model. This will allow us to model the THCM behavior of a limestone slab subjected to mechanical load under fire conditions at the macro scale and compare with experimental results obtained by subjecting a limestone slab (0.55x0.55m) to a standard ISO 834 fire on one side. This will lead to a better understanding of the fire damage kinetics in the studied limestone.

Keywords: Limestone, Mechanical damage, Fire, Thermorheology

*Speaker

Development of a thermo-mechanical digital twin of the structure of Notre-Dame Cathedral in Paris

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Until the 19th century, masonry was the preferred method of construction for long-term use. Today, there are few answers to questions about the suitability of old buildings for public use after a fire. The renovation of Notre-Dame Cathedral in Paris after the fire in 2019 makes this a topical issue. The work presented here, as part of the ANR DEMMEFI project, proposes a method for developing a thermomechanical digital twin of burnt masonry structures. This method is divided into several stages, including experimental measurement campaigns and numerical modelling. It includes (i) a phase of characterisation and modelling of the stones and mortars in-situ, at the material scale. Then (ii) a phase of calibration and validation of a numerical law for the homogeneous thermo-mechanical behaviour of masonry, using a new numerical approach for the structural analysis of masonry. This approach, developed previously in the DEMMEFI project, combines the finite element method (Cast3M code) and discrete elements (LMGC90 code) in a hybrid FEM/DEM code. Finally, (iii) a phase involving the construction of a digital twin of the structure, representing its residual structural condition after the fire. The digital twin can be used for diagnostic purposes (assessment of damage and post-fire stability of the structure) or prognostic purposes (assessment of future stability and reinforcement).

Keywords: maçonnerie, incendie, caractérisation thermomécanique, homogénéisation, modélisation

*Speaker

Study of the role of water induced swelling in the spalling degradation of tuffeau stone

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1

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The main historic monuments of the Loire Valley in France, like the famous castle of Chambord, are built with tuffeau. This porous and soft limestone presents many technical and aesthetic advantages justifying its wide use. However, the properties of tuffeau are also responsible for its vulnerability to many forms of degradations, and spalling is the main degradation affecting tuffeau stones. Spalling is the progressive development of a crack parallel to the surface exposed to the environment, generating a 1cm thick plate of superficial layer which falls, leaving a powdery surface. Several studies concerning the spalling of tuffeau were published and they highlight the presence of gypsum in the cracking zone. But among the hypotheses proposed to explain this phenomenon are the differential deformations caused by the partial humidification of the stone due to rain. Previous research has shown the interest in local deformation measurement using strain gauges while highlighting the uncertainty induced by the heterogeneity of the materials. The study presented here concerns the characterization of tuffeau from a stone block of the castle of Chambord. Samples were characterized by complementary physical and chemical techniques, including XRD, ion chromatography, SEM-EDS. The study of swelling behavior of tuffeau was conducted with the digital image correlation method used in the strain monitoring of the stone. Several factors related to the geometry of the material and the settings of the method were studied. Compared to strain gages measurements, more complex variables are involved in this method, where the deformation order to measure varies from 1 to 100 micrometers with a detectable color change. The results of this campaign showed the development of a significant shear deformation band between the dry and saturated zones. However, this type of measurement requires extensive uncertainty calculations to define and validate the measurements.

Keywords: Limestone, digital image correlation, spalling, degradation, imbibition

*Speaker

Formulation of a coating mortar based on tuffeau powder and lime for restauration purpose

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To reduce the overexploitation of granular resources, minimize the environmental impact of fine mortars, and limit the heritage impact during the rehabilitation of old tuffeaustone buildings in the Loire Valley in France, a new coating mortar was developed. Composed of aerial lime and tuffeaupowder from sawn stone blocks, this mortar promotes the reuse of mineral waste. The coating mortar must ensure high workability, sufficient mechanical performance for its application, and a visual appearance that mimics tuffeau stone as closely as possible in order to be used for restoration works. The formulation has determined the amount of water needed for the desired workability and the proportion of lime respecting aesthetic requirements and normative criteria for mechanical strength. The high water demand of the material leads to problems such as low workability, poor adhesion, and significant drying shrinkage, causing notable cracking when the coating adheres to its substrate. Various additives were used to optimize the material's performance, including a superplasticizer (SP), shrinkage-reducing agent (SRA), air-entraining agent (AEA), and rheology modifier (RM). Due to its application as a finish coat on external insulation, it requires high workability to accurately replicate the original stone aesthetic appearance of the restored building. The fresh state behavior of the material was evaluated using a methodology that combines flow table and fall cone tests, providing enhanced information for assessing consistency and determining appropriate workability in slow-hardening mortars. The shrinkage measurement was carried out under different conditions (temperature, humidity) in order to test the effect of additives on the reduction of drying shrinkage for the optimized formulation. The hardened state behavior of the mortar was evaluated by porosity measurements, mechanical measurements, as well as by measurements of adhesion on different supports.

Keywords: Mortar, Lime, Stone powder, Rehabilitation

*Speaker

Effectiveness, compatibility, and durability of consolidation treatments applied on thermally decayed Carrara marbles

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Cultural objects made in marble are highly sensitive to environmental alteration processes. Specifically, thermal variations induce a microstructural decohesion phenomenon potentially leading to bowing, sugaring, or granular disintegration of exposed marble surfaces. The conservation of such decayed objects may be improved using consolidation treatments aiming at restoring the structural integrity by bridging the cracks to a sufficient depth. However, a wide variety of products are available and their applicability on marble is often questioned. In this experimental study, three types of consolidation treatments (ethyl silicate, diammonium phosphate, and biomineralization) were applied on thermally decayed Carrara marble samples and compared in terms of effectiveness, compatibility, and durability. The mechanical strengthening provided by each treatment was first evaluated by Ultrasonic Pulse Velocity (UPV) and Nonlinear Resonant Ultrasonic Spectroscopy (NRUS). In the meantime, their penetration depth as well as their impact on the microstructure were characterized by scanning electron microscopy (SEM). The changes in aesthetic features and petrophysical properties were then respectively assessed by spectrocolorimetry and capillary absorption. Last, the consolidation ability of each treatment was followed through artificial cycles of thermos-hygric conditions. Overall, significant cohesive gains ($> 50\%$) are sensed on the consolidated samples pleading for a good effectiveness of all the considered treatments. The compatibility of some was however less satisfactory. But, far and foremost, the definition of the nonlinear parameter α from NRUS allowed to point the contrasting capacity of these treatments to bridge microcracks. The results of this study thus highlight the importance of combining classical techniques with non-linear (non-classical) ones to decouple macroscopic cohesive gains from mesoscopic microcracks bridging. In this respect, consolidation treatments must satisfy both criteria to meet the requirements of durability expected for the preservation of marbles.

Keywords: Marble, Consolidation, Microcracks, Nonlinear Resonant Ultrasound, Nondestructive testing

*Speaker

SMMP2 - Physics of divided matter

Fractures in cohesive granular materials

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Cohesive granular materials can fracture on a large scale, a process in which new surfaces are created, unlike dry frictional granular materials. This observation is obvious in the case of a granular medium partially saturated with liquid, where capillary bridges provide cohesion. Less commonly, however, transient ruptures are also observed in dense Newtonian suspensions. The rupture of such media can drastically modify their mechanical strength or permeability properties, and it is essential to understand this phenomenon in order to account for it in models.
We study the mechanisms of fracture formation during impact on partially saturated granular materials, like wet sand, and dense granular suspensions. Surface imaging coupled with surface profilometry measurements allow us to elucidate the mechanisms by which these fractures occur. As the granular medium dilates under impact, radial cracks develop around the impactor. In the case of a partially saturated material, this occurs regardless of the initial density, and the cracks formed survive the impact. In the case of a granular suspension, cracks form as soon as the initial density of the suspension exceeds the critical density above which shear-induced dilatancy is observed (1). These cracks are transient, healing after a few 100ms as the surrounding liquid migrates. We explain that such a different phenomenology between cracks observed in the partially saturated medium and in the suspension are due to differences in their inherent rheology (2,3).

(1) Reynolds, O. On the Dilatancy of Media Composed of Rigid Particles in Contact. *Philos. Mag. (Ser. 5)* **20**, 469 (1885).

(2) Mandal, S., Nicolas, M. & Pouliquen, O. Insights into the rheology of cohesive granular media. *PNAS* **117**, 8366-8373 (2020).
(3) Jerome, J. J. S., Vandenberghe, N. & Forterre, Y. Unifying Impacts in Granular Matter from Quicksand to Cornstarch. *Phys. Rev. Lett.* **117**, 098003 (2016).

Keywords: newtonian suspension, cracks, rheology, cohesive granular materials

*Speaker

Cracks in cohesive granular material

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Wet granular media often exhibit curious behaviors. For example, under certain loadings, cracks can develop, like in solids. This property can lead to catastrophic events, avalanches and landslides are good examples. It is still unclear how the cohesive force, coming from capillary effects between grains, combines with friction and other granular medium properties. We offer a solid mechanics perspective on the issue, focusing on the study of crack propagation within this type of matter to build a model able to predict fracture advancement. The cracks are generated by the quasi-static intrusion of solid objects into the granular material.
We use spherical glass beads with a radial distance of about a hundred microns mixed with silicone oil. To reduce the natural heterogeneity of wet grains and to control the compaction ratio, the material is vertically vibrated at a low frequency, allowing us to conduct reproducible experiments.
Using X-ray tomography, we show that for dense enough material, the overall compaction is homogeneous in our medium. We demonstrate that our preparation method reduces both large and small pores in the wet grains, thereby increases homogeneity of the media. We measure the force as a function of penetration depth and show a dependency on the compaction ratio. For very loose packing, cracks are imperceptible to the human eye. Above a critical compaction ratio, we can characterize the crack pattern. The number of cracks remains constant for a given indentation radius and is independent of the bead size and compaction ratio.

Keywords: Grains, crack propagation, cohesion, indentation, experimental study

*Speaker

Rheology of coated grains

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In many powder technology processes, coating is applied to fine particles to control their properties or fonctionalize them. In this study, we investigate the role of a polymer coating made of PBS on silica particles. This material has been originally designed as a model cohesive granular material, whose cohesion can be finely controlled by the thickness of the coating (Gans et al., 2020). However, we show that the coating not only introduces adhesion but also modifies the friction between the grains. Due to the viscoelastic properties of the coated layer, the friction coefficient between two particles is observed to increase with the load and decrease with the velocity. By means of numerical DEM simulations, we show that this complex tribology induces a pressure-thickening and velocity weakening for the bulk rheology and eventually leading to shear thickening and shear-banding. Those observations can be successfully rationalized by a mean field theoretical approach. Gans, A., Pouliquen, O., & Nicolas, M. (2020). Cohesion-controlled granular material. Physical Review E, 101(3), 032904.

Keywords: Granular, cohesion, lubrication

*Speaker

Fracture initiation in a cohesive granular layer

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Among different types of avalanches, the "slab avalanches" initiate by a long crack perpendicular to the slope, and rapidly propagate downhill during the flow. Modeling these avalanches presents challenges, including predicting the threshold for crack initiation in such a cohesive granular material, and understanding the impact of snow properties on fracture propagation. To address these questions, we conducted experiments using a cohesion-controlled granular material encompassing a wide range of cohesion. We established an experimental setup specifically designed to explore the formation of fractures in a quasi static regime. In our setup, a layer of the cohesion-controlled material undergoes flexural deformation. Upon reaching a threshold in tensile stress, cracks emerge with a distinct wavelength that increases with cohesion. We compare these measurements to phase-field model used in damage mechanics.

Keywords: granular media, fractures

*Speaker

Quasi-2D magnetic hourglass - Slowing down the sands of time

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Since the pioneering work of Hagen in 1852, we know that the discharge rate of grains through an aperture is constant, regardless the remaining particles in the upper chamber. This is the reason why hourglasses are filled with sand rather than water. Beverloo's law (1961) describes empirically the impact of the grain and aperture size on the discharge rate. However, the underlying microscopic mechanism still challenges our fundamental understanding, preventing a clear explanation of the phenomenon.
Therefore, we propose here to revisit such a classic, by studying experimentally the discharge of a quasi-2D silo, a Hele-Shaw cell (600 μm gap), filled with a monolayer of ferromagnetic grains (500 μm diameter steel beads). Applying an external magnetic field B perpendicular to the cell plane allows to control the amplitude of the induced repulsive magnetic pair interactions. We furthermore investigate the impact of the aperture size as well as, the hourglass geometry with either a flat bottom or a 45◦ funnel separating the two chambers.

We observe a constant granular flow rate during the discharge (in agreement with Beverloo's law) which decreases systematically with the amplitude of the external magnetic field applied, either linearly for 45◦ funnel aperture, or as the square of the magnetic field amplitude for a flat-bottom one, until the emergence of jamming arches. The effect of the repulsive magnetic interactions can be modeled and interpreted as an additional effective tunable friction with the walls of the cell.
Interestingly, while the outlet flow rate remains constant during the discharge, we also reveal very large spatio-temporal fluctuations of the granular packing density and velocity fields within the upper chamber of the cell, particularly evident for magnetic field of high amplitudes, suggesting the emergence of density waves.

Keywords: Discharge, 2D silo, Magnetic interactions, Friction

*Speaker

Revisiting the role of friction in transient granular flows through non-smooth simulations and experiments

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In this work (Rousseau et al. 2023), we confront experiments of granular column collapses with the corresponding 3D continuum-based numerical simulations to carefully investigate the role of friction in transient granular flows. The collapses are carried out with different bed slopes, ranging from 0○ to 20○, different channel widths, and different materials, and the impact of frictional dissipation within the material or with its enclosing walls is analysed by comparing experimental data to numerical simulations performed with different friction coefficients and models.

Our simulation method leverages the non-smooth MPM-based continuum framework introduced in (Daviet et al. 2016) to accurately resolve the plastic Drucker-Prager threshold without regularisation, and carefully accounts for all the experimental setup, including friction with the lateral walls and the lifting gate. We notably compare simulations obtained with the fully plastic Drucker-Prager and the viscopastic μ(I) (Jop et al. 2006) rheologies, and compare both the resulting transient and final states with experimental measurements of the free-surface profiles and material velocities measured at the side wall.

While our results confirm the weak impact of the viscous effects introduced by the μ(I) rheology in this regime, as previously suggested in (Lagrée et al. 2011, Ionescu et al. 2015), they also stress the importance of setting the – constant – plastic bulk friction coefficient to the value extracted from the avalanche angle in order to accurately predict collapse rest states, instead of the stop angle measured from the steady flow experimental protocols (Pouliquen 1999), as is usually done.

We finally discuss the role of hysteretic effects at the rest-to-flow transition, and highlight the need for further exploration of the frictional effects in the low inertial number regime.

Keywords: transient granular flows, non, smooth, friction

*Speaker

Structural evolution of a two-dimensional granular fault

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A granular ensemble of about 4000 bidisperse disks is confined in a cylindrical cell. The grains are compressed at a constant pressure from the top and continuously and very slowly sheared from the bottom of the cell. Mechanical energy is stored in the granular structure and liberated by sudden reorganization events, associated with acoustic emissions. Both mechanical and acoustic energies follow power law distributions (1). By merging 24 synchronized images, panoramas of the whole granular ensemble are obtained. The centers and the inter-grains contacts are detected and, thanks to the photoelasticity of the disks, the whole force network is also computed. Each panorama is simplified by mapping it into a graph where *nodes* correspond to the centers of the disks and *links* to the inter-grain contacts, weighted by the value of the local force.
The evolution of the graphs is analyzed and correlated with the mechanical and acoustic signals, particularly around large events. By computing the changes in the force network and in the inclination of the force chains, it is possible to explain the results that we get in the mechanical measurements, corresponding to different kind of events: sudden contraction (or dilation) of the structure and sudden release (or accumulation) of mechanical energy (2). Currently we explore with structural patterns are linked to the generation of very large events.

(1) S. Lherminier, R. Planet, V. Levy dit Vehel, G. Simon, K. J. Måløy, L. Vanel and O. Ramos,Continuously sheared granular matter reproduces in detail seismicity laws, Phys. Rev. Lett. 122, 218501 (2019).
(2) V. Levy dit Vehel, T. Hatano, L. Vanel, K. J. Måløy,and O. Ramos, Dilation as a precursor in a continuous granular fault, EPJ Web of Conferences 249, 15006 (2021).

Keywords: Fracture, Scale, invariant, Earthquakes, Granular Media, Image Analysis

*Speaker

Laboratory granular landslides

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Study of landslides is a pressing issue as these hazards imply a huge cost in lives, economy and ecology. To predict the properties of these enormous mass movements, and especially how far they would travel is a major objective of landslide research. A well-known feature of all landslides first reported by Albert Heim in 1932 (1) is the positive correlation between landslide volume and landslide runout, so that larger landslides can travel many times further than one can naively predict using the energy balance between initial potential energy and frictional dissipation. Different mechanisms have been suggested suchsuch as friction weakening due to self-induced oscillations; or simply volumetric spreading. An obstacle for these explanations is that it is difficult to test them by a systematic and independent study of the parameters for naturally occurring landslides.
Here we performed miniature granular landslides in laboratory using a simplified geometry (Fig 1.). Focusing on the maximum travel distance, we were able to reproduce at the laboratory scale the positive correlation between landslide volume and its runout. The versatility of the set-up enables us to study the motion of the mass. In particular, we found non-trivial relations between the flow thickness, the speed of the landslide front and the landslide size that might be useful to test the validity of proposed mechanisms for the increase in mobility.

Finally by analysing the laboratory data and a variety of data from large-scale landslides (2) we found that correctly accounting for the fall height and the granularity quantitatively unites experiments and field data, bringing together many kinds of mass movements that are often treated differently.

1. A.Heim, *Bergsturz und Menschenleben*, 20 (1932).
2. R. T. Cerbus *et al.* *A grunular scaling approach to landslide runout.* Accepted.

Keywords: Granular flows, Landslides, Experiments

*Speaker

Collapse dynamics of a cylindrical granular column applied to tsunami generation

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The collapse of cliffs, glaciers or volcanoes into water can generate tsunami waves as recently shown by the collapse of the Anak-Krakatau volcano in Indonesia. To better understand this complex phenomenon, a fruitful approach is to model and study the collapse dynamics of a granular column in water (1). Radial spreading dynamics of the grains are crucial to understanding the wave shape and amplitude (2-4). We carried out collapse experiments on cylindrical columns of different aspect ratios made of monodisperse glass beads on a rough horizontal bottom, initially without water. Using image processing and analysis, we tracked the vertical dynamics of the top of the column and the horizontal spreading dynamics of the grain front at the bottom. Analysis of these dynamics shows an initial phase of acceleration and highlights a characteristic time that depends on the column's aspect ratio, i.e. the ratio of its initial height to its initial radius. This dependence is different in the geometry of cylindrical columns compared with rectangular columns (5).

(1) M. Robbe-Saule & al., Tsunamis generated by granular landslides: From the lab to real events, Scientific Reports 11, 18437 (2021)

(2) M. Robbe-Saule, & al., Experimental investigation of tsunami waves generated by granular collapse into water, Journal of Fluid Mechanics 896, A8 (2021)

(3) W. Sarlin & al. Nonlinear regimes of tsunami waves generated by a granular collapse, Journal of Fluid Mechanics 919, R6 (2021)

(4) W. Sarlin & al., From granular collapses to shallow water waves: A predictive model for tsunami generation, Physical Review Fluids 7, 094801 (2022)
(5) W. Sarlin & al., Collapse dynamics of dry granular columns : From free-fall to quasistatic flow, Physical Review E 104, 064904 (2021)

Keywords: Milieu granulaire, Effondrement granulaire, Tsunamis, Écoulement gravitaire, Granular medium, Granular collapse

*Speaker

Influence of interfaces for fluid migration in sedimentary layers

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Sedimentary basins are very large areas located at the bottom of oceans, where various particles accumulate due to the transport and deposition of eroded grains and pelagic rain, including organic matter. Due to bio-physico-chemical reactions, these pluri-kilometer-thick layers are generating large quantities of gases and liquids. These fluids then migrate through the sedimentary layers, up to the seafloor. These structures can jeopardise anthropogenic activities, particularly transoceanic optical fibers for telecommunication or offshore resources. Despite the advances in seismic imaging over the last decades, the most recent techniques are unable to capture the dynamics of such structures. Laboratory experiments make possible to model and characterize fluid migration through an immersed multilayer granular medium. Liquid is injected locally at the base of immersed grains, confined in a Hele-Shaw cell. We consider either a monolayer or a bilayer and vary the granulometry and injection flow-rate. In a given range of experimental parameters surprising instabilities can be observed, such as the emergence of a periodic fluidisation pattern.

Keywords: multiphase flows, granular matter, instabilities, geophysical applications

*Speaker

Emptying a bottle filled with a suspension

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Emptying a bottle filled with a suspension is an ideal setup to study multiphase flows. Recent reviews show that the draining of a vertical bottle is an alternation between the formation of liquid jets and the rising of air bubbles. The understanding of such an interaction between groups of bubbles and particles is one of the main challenges in fluid mechanics. Indeed, a fundamental knowledge of the physical mechanisms at play during bubble-particle interactions is crucial in geophysics or for the optimization of many industrial processes.

We investigate this question by means of a simplified experimental set-up. We use a cylindrical tank, which we fill with different isodense suspensions: hydrogel beads in a water/UCON mixture, polyamide beads or polystyrene beads in salt water. A force sensor is used as a scale below the experiment to assess the flow rate. A pressure sensor at the top of the bottle quantifies the pressure variations above the suspension. Finally, two cameras capture the evolution of the suspension free surface and the jet dynamics at the reservoir exit. The draining behaviour is explored depending on the particle-to-hole ratio and the beads packing fraction.

For small packing bead fractions, emptying the bottle results in a constant flow rate and the suspension behaves as an effective fluid. For packing fractions above 30-40%, an additional regime appears after a given time. Particles accumulate far from the hole and the liquid free surface velocity switches to a larger value. One of the peculiar observations is that the suspension flow rate remains constant in both regimes during the whole draining.

Keywords: Multiphase flows, bubbles, suspension, clogging

*Speaker

Delayed glass transition in a dense suspension of core-shell particles

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Soft glasses are dense suspensions of jammed particles that flow like liquids under external shear and recover solid-like properties almost instantly upon flow cessation. Here, we examine the case of a dense suspension composed of latex particles dispersed in water. These particles exhibit attractive interactions due to their hydrophobic nature while being stabilized by a shell of short polymers grafted at their surface. Such a polymer corona leads to effective repulsive interactions that delay the recovery of the viscoelastic properties upon flow cessation and allow us to record viscoelastic spectra across the liquid-to-attractive glass transition using time-resolved mechanical spectroscopy. These spectra can be rescaled onto a master curve, showing that the present glass transition obeys a time-connectivity superposition principle. Moreover, the rescaling parameters display a stair-step shape as a function of time that points to a critical time tc associated with the liquid-to-glass transition. Experiments at various temperatures confirm the robustness of our findings and show that tc vanishes at a finite temperature, beyond which attractive hydrophobic interactions between latex particles permanently overcome the steric repulsion of the polymer brush. Finally, the yielding behavior of the attractive glass probed by large amplitude oscillations at different ages shows a ductile-to-brittle transition, in agreement with the increasing cohesion from the linear measurements. Our work offers a detailed rheological account of the increasingly cohesive behavior of a hairy colloidal attractive glass, and contributes to a better understanding of this system commonly used in industrial applications such as paints, coatings and the construction sector.

Keywords: core shell particles, attractive glass

*Speaker

Self-assembly of vibrated granular mixtures: from quasi-crystalline order to non-equilibrium phase coexistence

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Granular materials provide an accessible and diverse playground for nonequilibrium physics. When subjected to mechanical vibrations, they undergo so-called vibrofluidisation, reaching a nonequilibrium steady state through the balance between dissipation and external forcing.

It has been known for more than two decades that monodisperse vibrofluidised granular materials undergo a liquid-solid-like phase transition to a hexagonal periodic structure similar to that of hard-sphere thermal systems. In my talk, I will present experimental and numerical results showing how this analogy extends to the case of granular binary mixtures, which form much more complex structures.

First, I will report the experimental observation of quasi-crystalline self-assembly at the millimetre scale (1), obtained by vibrating spherical grains of two sizes on a substrate. The particles initially arrange into three types of tiles, which eventually align to form a structure with eightfold long-range orientational order, representing the first instance of a spontaneously assembled quasi-crystal at the macroscopic scale, where thermal motion does not play a role. I will then focus on the self-assembly of a periodic square binary crystal, obtained in the same setup for a different composition of the two particle species. Using a combination of experiments and simulations, we have studied the transition from a disordered granular fluid to the square crystal by increasing the overall packing fraction of the system. Remarkably, at intermediate packing fractions we observed a stable regime where the two phases coexist at different granular temperatures. Finally, we investigated the effect of the non-equilibrium properties of the system (i.e. driving and dissipation) on the phase diagram.

The results discussed provide a suitable testing ground for a better understanding of the physical mechanisms underlying ordering phenomena in athermal systems.

(1): A. Plati, R. Maire, E. Fayen, F. Boulogne, F. Restagno, F. Smallenburg, and G. Foffi, Nature Physics 20, 465–471 (2024)

Keywords: Granular materials, Nonequilibrium phenomena, Self assembly, Quasicrystals

*Speaker

Elasto-granular coupling : how a granular heap deforms a soft substrate ?

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Many problems involve an interplay between granular matter and elastic structures, including food packaging (e.g. coffee beads in plastic bags), cell membrane deformations in plants, or soil-root interactions. Here, we explore this coupling in a simplified system, investigating how an elastic structure deforms under the weight of grains. We set up a two-dimensional experiment consisting of an extensible ribbon, placed between two walls, onto which grains are deposited to form a heap. We show that the ribbon, as it deforms, acts as a reservoir of grains, altering the shape of the grain pile, including the spreading of the heap, depending on the initial tension and rigidity of the ribbon. By increasing then significantly the volume of grains, the ribbon deflection and the spreading of the heap eventually saturate above a threshold related to the nonlinear behavior of the ribbon.

Keywords: Elasto, granular coupling, Granular media, Granular heap, Soft ribbon, Experiments

*Speaker

SMMP5 - Surface tension, soft solids and fluid-structure interactions

Studies on the circular hydraulic jump

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When a liquid jet impinges a plate, as in a kitchen sink, at some distance from the jet the height of the liquid suddenly rises to a higher value an hydraulic jump appears. It's surprising that such a simple and common phenomena, which hides intriguing and a rich dynamics (1, 2, 3), remain still not well understood. From experimental point of view we are using new technical tools to measure the profile of the fluid and investigate the presence of capillary waves experimentally (first depicted in (4)). These measures are challenged with our model (5) to predict the thickness profile.

(1) J. B. Belanger. Notes sur l'hydraulique. Ecole Royale des Ponts et Chaussees, Paris, France, session, 1842 :223, 1841.

(2) T. Bohr, V. Putkaradze, and S. Watanabe. Averaging theory for the structure of hydraulic jumps and separation in laminar free-surface flows. Physical review letters, 79(6) :1038, 1997.

(3) J. W. M. Bush, J. M. Aristoff, and A. E. Hosoi. An experimental investigation of the stability of the circular hydraulic jump. J. Fluid Mech., 558 :33–52, 2006.

(4) E. Rolley, C. Guthmann, and M. S. Pettersen. The hydraulic jump and ripples in liquid helium. Physica B : Condensed Matter, 394(1) :46–55, 2007.

(5) N. Rojas, M. Argentina, E. Cerda, and E. Tirapegui. Inertial lubrication theory. Phys- ical review letters, 104(18) :187801, 2010.

Keywords: HYDRAULIC JUMP, CAPILLARY WAVES, SURFACE TENSION

*Speaker

Parametric coupling between waves on a rivulet

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When injecting a liquid in an air-filled vertical Hele-Shaw cell, it forms a rivulet in which the fluid flows downwards in between two meniscii forming a liquid bridge between the plates. The dynamics of the interface strongly depends on the fluid flow inside the rivulet, which itself is imposed by the geometry of the free surface. The resulting movement of the rivulet is the result of a competition between capillarity, inertia and viscous dissipation near the contact line. This makes the system exhibit complex behaviour even when using simple, totally wetting fluids.
When imposing an homogeneous, additive forcing, the response of the system creates a parametric coupling between longitudinal and transverse waves along the rivulet. Because of this, even in regimes where both of these perturbations should be linearly damped they can amplify one another, resulting in a previously unreported instability.
We describe and characterize this phenomenon, explaining the physical origin of the nontrivial coupling at play. We present a model for this instability and confirm its relevance using experimental evidence.

Keywords: instability, nonlinearity, rivulet, free surface flow, capillarity, inertia, moving contact line

*Speaker

Fingering instability in adhesion fronts

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The adhesion of two surfaces relies on the propagation of an adhesion front. What are the dynamics of the front when both surfaces are coated with a thin layer of viscous liquid? Standard criteria from fingering instabilities would predict a stable front since viscous fluid pushes away air of low viscosity. Surprisingly, the front propagation may be unstable and generally leads to longitudinal growing fingers. We first demonstrate with model experiments where the two adhering surfaces are slightly tilted, that the origin of this interfacial instability relies on feeding the front from the surrounding thin film. We show experimentally that the typical wavelength of the instability is mainly dictated by the thickness of the oil layers.
In this wedge geometry, the front propagates with a square root of time dependence and saturates at a distance from the apex set by the ration of the films thickness with the wedge angle.
In most practical applications, only one surface is adhesive, which involves contact line dynamics. Our experiment conducted with a dry plate brought in contact with an adhesive substrate curiously lead to transverse fingers growing upon successive nucleation events.
As in practice surfaces may be rough, we finally conducted experiments with model surfaces presenting regular grooves. These experiments confirm the crucial role of the thin film in the instability mechanism.

Keywords: instabilities, interfaces, adhesion

*Speaker

Fluids, mechanics and fluid mechanics problems in the making of glass wool

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Although glass wool is one of the best performing insulation materials, and as such a key material for the environmental transition, the general public knows very little about the technical and scientific challenges behind its industrial manufacturing.
In this talk, I will explain the process to make glass wool and show how the current requirements to make these products with increased thermal and acoustical performance while decreasing their environmental footprint has forced Saint-Gobain Isover to tackle complex scientific problems so far untouched despite decades of industrial exploitation.

The glass wool manufacturing process involves producing glass filaments at ca. 1000∘C, spraying the newly created fibres with a chemical solution, organising them in a layered mat before curing the insulating material to polymerize the binder and to obtain a glass wool mat. All these steps involve interactions between fluids and solids, with additional thermal and chemical phenomena.
Whereas most of them have received little interest from physicists, I will show how rich they are and how much they could be a source of inspiration for scientists.

Keywords: glass wool, spraying, filtering, curing, manufacturing, turbulent jet, fibre, porous

*Speaker

Mechanisms of Instability and Pattern Formation in Confined Viscoelastic Flows

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Pressure-sensitive adhesives (PSAs) are viscoelastic liquids composed of slightly crosslinked entangled polymer chains. They exhibit a rubbery plateau modulus G ranging from 10ˆ5 to 10ˆ6 Pa and a relaxation time spectrum between 10ˆ{-4}to10ˆ{-1}seconds. PSAs are commonly used in medical plasters. The tack test is an industry-standard method to measure the work of adhesion in PSAs, which ranges from 10ˆ2 to 10ˆ4J/m^2, typically 10 to 100 times their interfacial energy with most solid substrates. This test involves measuring the force required to debond a thin cylindrical PSA layer at a defined speed.

During the initial phase of the tack test, the elastic response of the PSA generates a force that depends on the material's modulus and the geometry of the PSA layer. Specifically, the force scales with the modulus, the square of the layer's radius, and the square of the vertical extension, while being influenced by the aspect ratio of the layer. In the final phase of the test, the extension of fibrils within the PSA layer plays a major role. Here, the force required to continue the debonding process is related to the viscosity of the PSA, the rate at which the layer is extended, and the surface fraction of fibrils. Between these initial and final stages, energy is dissipated through several mechanisms: the formation and growth of cavities within the PSA layer, the movement of the cavities's contact lines, and their merging. These complex processes contribute to the overall force required for debonding and not fully understood.

Our experimental investigation focuses on these dissipation mechanisms by varying the velocity, aspect ratio, and temperature to control their respective characteristic times. This approach aims to elucidate the coupling between these mechanisms and potentially enable control over the resulting adhesion patterns.

Keywords: Viscoelasticity, Instabilities, Adhesives, Rheo, Optics.

*Speaker

Fragment size statistics and dynamics in a laboratory model of fragmentation of a 2D floating membrane by surface waves.

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When particles of a few tens of microns are spread on the surface of water, they aggregate under the action of capillary forces and form a thin floating membrane, a particle raft. In a tank with a raft made of graphite powder,we generate gravity surface waves, whose wavelength about 17 cm is very large compared to the thickness of the raft of order 10 μm . For a sufficiently strong wave amplitude, the raft breaks up progressively by developing
cracks and producing fragments whose sizes decrease on a time scale long compared to the period of the wave 1. We investigate here the area distribution of the fragments produced during the fragmentation process. The visual appearance of the size-distributed fragments surrounded by open water resembles the floes produced by the fracturing of sea ice by waves. The fragmentation concepts and morphological tools developed for sea ice floes can be applied to our macroscopic analog. Although the fracture mechanisms and physical properties of the two materials differ, our experiment provides a model laboratory system for studying the fragmentation of floating 2D materials ; a subject of prime importance for understanding sea ice dynamics.

Keywords: Particle raft, Surface waves, Fragmentation, Capillarity

*Speaker

Reconfiguration of drag of a Flexible Ribbon sedimenting in a viscous Fluid

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The motion of a deformable elastic structure in a viscous fluid is of fundamental importance, from flagellar propulsion of microorganisms and small flying insects, to biopolymer (e.g., DNA or actin microfilaments) or polymer science. The interaction between internal elastic forces and hydrodynamic forces results in deformations of the object that govern its velocity.
Inspired by previous studies on the settling of elastic cylindrical fibers or rigid slender ribbons, we investigate the dynamics of the deformation, the drag, and the settling velocity of elastic ribbons, at low Reynolds number combining experiments and a simple bead-spring modeling of the ribbon.

We show that the deformation of the ribbons is governed by the competition between the torque applied by gravity to the ribbons and the typical elastic resisting torque, captured by a nondimensional number B.

Depending on the value of B, i.e., the relative magnitude of these two effects, we observe three regimes of deformation, characterized by the length and the thickness of the ribbon, and independent of its width. These regimes can be classified as low and high deformation regimes, characterized by a drag proportional to the settling velocity, and an intermediate regime, which exhibits a non-linear drag-velocity relationship.

Keywords: Drag reconfiguration, fluid, structure, low Reynolds, deformable objects

*Speaker

Drying of flexible fibers suspensions

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Nonwovens fibre-based materials such as paper are widely used for a variety of applications and could be largely developed as a sustainable alternative for fossil-based plastics. The first limitation of their widespread use is their response to moisture and more generally to liquids. Indeed, when wetted or dried, those materials exhibit irreversible deformations, structural changes and failure. The final mechanical properties of paper products highly depend on the initial fibre suspension and fabrication process. In particular, the removal of water from the suspension is a complex and crucial step which permanently affects the web structure and its subsequent inter- actions with liquids. To gain a deeper understanding of the dewatering of fibrous networks, we investigate the drying of a model suspension composed of long and flexible hydrogel fibres. We show how the drying dynamics and the network pattern are influenced by the drying conditions and the fibres characteristics : length, diameter and flexibility.

Keywords: Elastocapillarity, fiber suspension

*Speaker

Dew formation on soft substrates

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Vapor molecules can nucleate on cool substrates, provided the surrounding humidity is high enough. Dew formation has been investigated on both rigid (and rough!) solids as well as on liquids. However, how substrate elasticity affects the condensation process remains elusive. In this talk, I will present how water condenses on soft, elastic gels that are smooth at the nanometer scale. We prepare PDMS gels whose softness varies between that of a rigid substrate and an un-crosslinked polymeric liquid.
Although elasticity should be marginal at the nanometric scale at which drops form, we report that the nuclei density is highly sensitive to the substrate softness. In this talk, I will delve into the intricate dynamics of condensation and try to explain some of the intriguing characteristics we have observed. Among these are the influence of softness on nucleation; the sub-diffusive growth of droplets; and the absence of secondary nucleation events (unlike what is classically observed in heterogeneous nucleation). Later, when neighboring drops get closer, they attract each other due to interactions mediated by substrate deformations. Drops then gather into clusters that seem reluctant to coalesce. This ultimately results in the formation of a persistent, ordered, honeycomb-patterned liquid film.

Keywords: Soft gels, elastocapillarity, phase change

*Speaker

Soft textured sheets mimic the hummingbird's tongue for efficient fluid capture

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Passive and effective fluid capture and transport at small scale is crucial for industrial and medical applications, but also for the feeding of small nectarivores. Among them, hummingbirds have developed a highly specialised tongue made of two soft open grooves that efficiently trap nectar by elastocapillary effects. Inspired by this observation, we design a fast and efficient fluid capture device at the capillary scale. The device consisting in soft grooves stacked together on a flat sheet exhibits a sequential capillary rise when dipped in a liquid bath. Combining elasticity, capillarity and viscous flow, we rationalize the speed of the liquid fronts as well as the deformation of the structure. This device captures more liquid that its rigid flat counterpart and captures a given amount of liquid much faster than its rigid closed counterpart. Such structures may open the way for the design of optimal devices for fluid capture, aliquoting and transport in microfluidics.

Keywords: elastocapilality, fluid structure interaction

*Speaker

Sticking without contact: elastohydrodynamic adhesion

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When pulling apart two solid surfaces immersed in viscous liquid, an adhesive force arises from a negative suction pressure. A variety of animals exploits this mechanism to catch prey like chameleons or frogs. Here we investigate viscous adhesion between soft bodies using a sphere-plane model system. We perform numerical simulations and theoretical analysis based on lubrication theory. The negative pressure inside the thin viscous film between the solids generates significant elastic deformations. The combine effects of lubrication flow and elastic deformations leads to an off-center stagnation point of the flow. Hence, the liquid film within the apparent contact radius is stable such that the two bodies stick without contact, reminiscent of the JKR contact theory. Using self-similar solutions we analyse (i) the initial increase of elastic stresses and (ii) the dynamical snap-off once the contact radius is sufficiently small.

Keywords: Elastohydrodynamic, adhesion, lubrication flows

*Speaker

Fibroblast persistent migration on soft hydrogel: how surface tension affects cell direction of motion

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As matrix stiffness has become a key factor in a wide range of biophysical and biomedical applications (migration, differentiation, organoid development, implants, regenerative medicine, cancer metastasis...), soft polymer-based substrates have been now widely employed to tackle mechano-transduction processes. Previous works have revealed the impact of substrate stiffness on 2D and 3D cell adhesion and migration (spreading area, speed, focal adhesion size, directionality) with different gels and elastomers(1,2). However, in most of these studies, it was not possible to control separately substrate stiffness and adhesion molecules density (ECM proteins, RGD peptides). Moreover, the elasto-capillarity properties of such soft solids are largely ignored, especially when surface tension becomes predominant than the elastic bulk modulus at water/solid interface(3).
Thus, we proposed a parametric study based on the use of fibronectin coated soft hydrogel of well controllable stiffness and surface tension, to study the impact of its mechanical properties on 2D fibroblast migration. These hydrogels are prepared via a cross-linking between poly(L-lysine) dendrigrafts (DGL) and PEG-NHS molecules. The mechanical properties of our hydrogel were characterized using optical tweezers with micro-beads through (i) active bulk microrheology (ii) surface micro-indentation. Two different subsets – normal fibroblasts (WPMY-1) and activated fibroblasts (exp-CAF2) – were studied on different hydrogels of varying DGL concentrations to adjust the surface tension. The behavior of these cells was analyzed through single cell tracking with combined epi-fluorescence and phase contrast imaging. Direction and speed autocorrelations were computed and analyzed(4) with the relevant "stick-slip" model proposed by H. Flyvbjerg(5), well suited to interpret double-exponential decay of the velocity autocorrelation functions. Finally, we clearly demonstrated that fibroblasts adopt a directional persistence motion when the surface tension increases, highlighted by an increase of the time associated to the direction changes and decrease of the corresponding angles.
References:(1).D.Missirlis,Biomacromolecules.**15**,195-205(2014).(2).A.Nousi,Biochem.Biophys.Rep.**28**,101120(2021.(3).
118(2017).(4).R.Gorelik,Nat.Protoc.**9,**1931-1943(2014)(5).D.Selmeczi,Eur.Phys.J.Spec.Top.**157**,1-15(2008).

Keywords: surface tension, persistent migration, hydrogel, fibroblasts

*Speaker

Solid Marangoni Stresses

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Despite its importance in any adhesion and wetting phenomena, there is a fundamental property that is not yet understood in soft solids: surface elasticity. Also called the Shuttleworth effect, surface elasticity is intimately linked to the solid physico-chemistry and can be boiled down to one question. Does stretching the surface of a soft solid change its surface tension? In 2021, we demonstrated that the mechanical response of a textured silicone gel could only be explained by an elastic surface (1). It is, however, still unclear whether the measured surface elasticity is a true material property or a mere consequence of the surface preparation. This presentation will focus on a novel experimental setup that exploits Marangoni stresses to characterize the surface mechanics of pristine surfaces. (1) Nicolas Bain, Anand Jagota, Katrina Smith-Mannschott, Stefanie Heyden, Robert W. Style, and Eric R. Dufresne Phys. Rev. Lett. 127, 208001 – Published 8 November 2021.

Keywords: Surface tension, soft solids, gels

*Speaker

BAM1 - Dynamics of biological and bio-inspired systems, from single particles to suspensions

Scale-free active turbulence in bacterial suspensions

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Dense suspensions of motile bacteria display at low Reynolds number fascinating collective motion with swirls and jets, reminiscent of inertial fluid turbulence. Recently, an intense endeavor aimed at understanding the fundamental concepts behind the spontaneous emergence of collective motion displayed by biological objects of many different kinds and sizes, such as cells, insects, birds, fishes or mammal populations. Macroscopic theories, mostly based on phenomenological symmetry arguments, categorize such dynamical structures featuring a preferred mesoscopic length scale that expresses the interplay between microscopic activity and the fluid constitutive properties. Here we show that contrarily to those generic predictions, motile E.coli suspensions rather displays scale-free turbulence reaching at least 400 times a single cell size. The maximal extend of the turbulent vortices scales proportionally to the externally imposed confinement height. We also reveal the existence of a long transient state featuring an extremely large vortex (ELV) which coherence over time and space defies so far any theoretical prediction. This work provides novel indications that the conceptual picture of momentum-conserving active bacteria suspensions is still largely incomplete. The understanding of an ELV state as well as the establishment of macroscopic hydrodynamic equation for such a "critical" fluid conceptually remains a challenging task.

Keywords: Active turbulence, Collective motion, Fluid dynamics, Chaos, Bacteria suspensions

*Speaker

Microfluidic "niche on a chip" controls the emergence of micro-aerotactic bands

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MSR-1 (magnetospirillum gryphiswaldense) are magnetotactic bacteria that can be grown in the lab. They display two essential features also present in the wild: micro-aerotaxis and magnetotaxis, both properties intimately related to the MSR-1 ecological niche taking place at low O2 concentration. This condition is optimal for the synthesis of organelles (the magnetosomes) which are responsible for a biased motility in the presence of a magnetic field. The interplay between microaerotaxis and magnetotaxis remains a subtle and still unraveled issue that needs to be fully modeled. To clarify this question, we built a microfluidic chip where the environment in terms of oxygen level, oxygen gradients and magnetic field can be fully controlled around the niche concentration. This device allows to study the collective organization of MSR-1 populations in various conditions. In parallel, we designed and solved a simple theoretical model suited to reproduce the aerotactic responses switch around the niche level (low O2 concentration).
We present a direct comparisons between the theoretical model and experiments where O2 concentrations at the channel edges are systematically varied, hence fixing oxygen levels and mean gradients.
We also designed a method to measure in-situ oxygen concentration fields using an encapsulated ruthenium fluorescence probe. Quantitative agreement between the model and the experiments allows to extract the characteristic features of the MSR1 aerotactic response and the oxygen consumption. The spatial stability of these structures is probed by adding a magnetic field as well changing the magnetotactic polarity of the bacteria.

Keywords: Magnetotactic bacteria, micro, aerotactic behaviour

*Speaker

confinement driven flows in bioconvection

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A dense solution of Chlamydomonas Reinhardtii (CR) spontaneously destabilises to form plumes. Surprisingly, currents generated in these convection cells are up to 10 times faster than the swimming speed of a single microalgae itself. The wavelength that naturally appears in this pattern is proportional to the depth of the solution, and the plumes are statistically steady. But, what happens when the thickness of the solution is not constant?
We study how spatial confinement affects symmetry breaking of these active fluids, coupling experimental and numerical tools, both developed in our group. A continuum approach (Pedley & Kessler 1990) is implemented within NekStab (Frantz et al. 2023), providing 3D measurements and global modes, key to identify the underlying physics. We show how this asymmetric confinement gives rise not only to a geometrical, but also to a temporal symmetry breaking of this out-of-equilibrium biological system.

Keywords: bioconvection, transition, micro, algae

*Speaker

Roll formation in a bio-active fluid

Anaelle Givaudan * [1]

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The unicellular alga *Chlamydomonas* has two flagella whose beating enables it to swim in a breast stroke. *Chlamydomonas* is bottom heavy, which reorients its spontaneous swimming to the top (gravitaxis). Moreover, like plants, algae get energy from photosynthesis and to assure this behavior, they swim towards light. This natural bioconvection favours the accumulation of a layer of denser cells at the free surface, with subsequently destabilizes into sinking plumes.
In order to study the plume migration, we use light to impose a specific direction of swim to *Chlamydomonas.* In addition to the plume 's travelling, we observe the emergence of a periodic structure all along the illuminated wall. This behavior highlights the formation of a new destabilization inside the bio-active fluid. But, what drives this symmetry breaking ? Where do these structures come from ? We assume that they follow the rise of a roll at the wall driven by gravitaxis and phototactic swimming of the algae.

The experimental set-up allows us to record the top view of the solution in order to follow the pattern evolution formed by algae. We study the caracteristic length between the structures by varying the light intensity, solution depth and *Chlamydomonas* concentration. The wavelength dependance with the light intensity reminds us the Taylor-Couette instability and based on the classical hydrodynamic instabilities, we develop a model adapted to this active fluid.

Keywords: chlamydomonas, microswimmer, instability, hydrodynamic, phototaxis, active, fluid, algae

*Speaker

Kinetic model of the static and dynamic patterning in the system of self-propelled agents.

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The self-propelled agents (SPP) are often used as a workhorse model of the collective motion of such bio-systems as bacterial colonies, fish schools, bird flocks, to name a few. The reported work looks into the formation of steady non-equilibrium states of the SPP undergoing the competitive processes of the Turing patterning, rotational relaxation and rotational diffusion of the SPP self-propulsion velocities. The developed kinetic model predicts several non-trivial steady (moving and resting) states of the SPP system. The transitions between these states are caused by the intricate interplay among the involved effects of the pattern formation, orientational order, and coupling between the SPP density and orientation fields. In its non-equilibrium steady state, the patterns of SPP are shown to exhibit collective motion with the constant velocity predicted by the model. As a main result of the reported study, the transition between the resting and moving non-equilibrium steady states of the SPP system are quantitatively explained by rationalizing the primary and secondary instabilities experienced by this SPP system. The obtained analytical results show excellent agreement with the performed rigorous numerical simulations.

Keywords: active matter, self, propelled particles, kinetic model, patterning, stability.

*Speaker

The Countoscope: Quantifying Particle Dynamics by Counting Particles in Boxes

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Quantifying the ensemble dynamics in particle suspensions is a widespread interest in soft matter. For instance, probing the motion of cells or larger organisms can help us understand biological behavior. When multiple particles interact, they perform collective dynamics, which visually translates into a zoology of effects, including dynamic aggregation to ensemble and directed motion. Yet, accurately labeling particles is difficult in dense and heterogeneous systems, challenging trajectory reconstruction, commonly used to quantify dynamics. In addition, particles inescapably leave the field of view, making the tracking of groups of particles to measure collective dynamics cumbersome.

Here, we shift this paradigm by introducing a broadly applicable technique that probes dynamics simply by counting particles in finite observation boxes of an image. Through colloidal experiments, simulations, and theory, we demonstrate the practical benefits of analyzing fluctuating counts: we can determine individual motion properties, such as self-propulsion or self-diffusion coefficients, including in dense states, while overcoming the challenges of trajectory reconstruction. Moreover, by increasing the observation box size, we can naturally probe collective dynamics. We explore our framework on various suspensions, from ions to active and biological particles such as bacteria. The "Countoscope" offers the unique possibility of systematically linking individual and collective behavior, opening up broad perspectives in soft and statistical physics.

Keywords: Diffusion, Motility, Dynamics, Microscopy

*Speaker

Understanding margination of white blood cells in blood flow, from vessels to vascular network.

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White blood cells (WBCs) margination corresponds to a key step for efficient body response to infection in which WBCs migrate to the blood vessel walls. This process enhances WBC rolling for example. In physics, margination seems similar to a segregation of WBCs according to RBCs which flow at the center of a vessel. Such a segregation also appears in flowing granular media with different sizes of particles. However, cells and vessel walls are soft and so experience hydrodynamic interactions of a different kind. An open question is the nature of margination in a microvasculature network. Indeed at each bifurcation, the pattern of margination is broken and must be re-established. By means of microfluidic experiments, we investigate the process of WBCs margination in a network of arterioles and venules, and we also evaluate the effect of the vessel cross section on the margination.

Keywords: Margination, Blood flow, vascular network, white blood cells

*Speaker

Phyllotactic structures in reactive spatial symmetry-breaking systems

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Phyllotactic patterns, i.e. regular arrangements of leaves or flowers around a plant stem, are beautiful and fascinating examples of complex structures encountered in Nature. In botany, their peculiar symmetries develop when a new primordium periodically grows in the largest gap left between the previous primordium and the apex. Experiments using ferrofluids droplets have also shown that phyllotactic patterns spontaneously form when identical elements repulsing each other are periodically released at a given distance from an injection center and are advected radially at a constant speed. More recently, we did observe analogous spiralling patterns in the context of carbonate precipitation experiments obtained by radial injection in a confined geometry. Inspired by those experiments, we show here that classical models of phase separation and Turing patterns do also produce spiralling patterns when coupled to a radial injection dynamic. Our results suggest that these models are part of a larger family of self-organised phyllotactic structures, which originate when a spatial symmetry-breaking system giving spotted structures with an intrinsic wavelength is coupled to radial growth.

Keywords: Self Organisation, symmetry breaking, instabilities, phyllotaxis, growth, Hele Shaw cell, reactive fronts

*Speaker

Characterizing the dynamics of the Cellular Potts Model

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Characterizing the dynamics of the Cellular Potts model :

The cellular Potts model (CPM) is one of the most widely accepted models of a multicellular system. It is widely used for simulating cellular systems in various fields of physics and biology, such as coarsening and mechanics of foams, tissue morphogenesis, or cell sorting. The CPM is a lattice-based model in which each cell in the system is given a different label (cell ID). A given cell is then represented by the subset of lattice sites that share the same cell ID.

Cell shapes and positions are updated using a Monte Carlo algorithm and the dynamics are governed by an energy function rather than forces. As a result, properties of cells, such as their diffusion coefficient or motility, are outcomes of the simulation, and their dependence with control parameters such as simulation temperature or cell size is not controlled. Furthermore, Monte Carlo algorithms were originally invented to efficiently sample from equilibrium distributions, and their extension to out-of-equilibrium systems such as active moving cells is questionable.

I try to obtain analytical expressions for the diffusion coefficient and the motility of cells corresponding to the CPM dynamics in the continuous limit, starting with the simplest case of a single, one-dimensional cell in an infinite medium.

I will try to explain the principles of the cellular Potts model and the methods that I use to study its dynamics.

Thank you for your attention,

Nino Despeignes

Keywords: Cellular Potts Model, out of equilibrium statistical physics, stochastic processes

*Speaker

Instability of the interface of two cellular tissues with cellular division and cellular apoptosis

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Stability of the boundary between epithelial tissues is key to preserve their integrity and thus their biological functioning. We numerically investigate the stability of the frontier between two confluent cell monolayers that divide at constant rates. We show that even when the two tissues have the same mechanical properties, the same cell division rate and the same homeostatic pressure, the interface is unstable: the interface location is subject to fluctuations that are of the same order of magnitude of the system size, leading eventually to the disappearance of one or the other tissue. When these parameters differ, a constant drift superimposes on this random dynamics of the boundary location. Our results reveal that a regulation mechanism on cell division must exist to guarantee the stability of the tissue boundaries.

Keywords: Cellular tissues, Interface of two tissues, Instability, Population dynamics model, Biophysics

*Speaker

Recovering the dynamics of hidden variables in stochastic living systems

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Studying the dynamics of biological systems most frequently requires dealing with incomplete data: we can only keep track of a limited number of degrees of freedom necessary to fully characterize a system, while possibly many others go unobserved. The description of phenomena in such scenarios remains an open question, given we cannot measure every quantity we may wish for. However, we can expect that if some unobserved variables have their dynamics tightly correlated to that of observed ones, it may be possible to start from an incomplete dataset and recover a mathematical model describing the dynamics of both observed and hidden variables. The recovered model would allow the reconstruction of unobserved trajectories using the observed ones, opening new paths for investigating complex biological systems.
In this presentation, I will discuss preliminary results on inferring models from incomplete data and using these inferred models to recover the dynamics of hidden variables, with applications to simple systems, from active Brownian particles to small ecological communities.
Our methods rely on working with stochastic differential equations through the state-space filtering/smoothing formalism, which allows the precise definition of dynamical and measurement models, separating observed and latent variables. We use the same formalism to derive the likelihood of incomplete datasets, used for model inference through Markov chain Monte Carlo or approximations such as variational inference.

Keywords: Stochastic Processes, Hidden Variables, State, Space Filtering, Variational Inference

*Speaker

Dynamics of pedestrians, regarded as biomechanical entities endowed with decisional capabilities

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Pedestrians routinely display remarkable navigation and coordination abilities. But suboptimal routing choices, collisions, or even in the most tragic cases stampedes are indeed also prominent features of crowd dynamics.

Models capable of describing these complex entities and their interactions within crowds would be highly beneficial for practical purposes, when it comes to designing new pedestrian facilities (such as a stadium, a railway station, etc.), but also from a more fundamental perspective.

To capture these features, we have put forward a continuous agent-based model (dubbed ANDA) hinging on a transparent delineation of a decision-making process, wherein a desired velocity is selected as the optimum of a perceived cost, and a mechanical layer that handles contacts and collisions. The proposed model departs from the assumption that pedestrians behave like mere particles in interaction or robots, and instead brings together elements pertaining to different fields, from game-theory, used for the decision-making layer, to the contact mechanics used to describe the effect of physical contacts.

The versatility of ANDA is demonstrated by numerical simulations that successfully replicate empirical observations in a very wide range of scenarios. These scenarios vary from collision avoidance involving one, two, or more agents, to collective flow properties in unidirectional and bidirectional settings, and to the dynamics of evacuation through a bottleneck, where contact forces are directly accessible. Remarkably, the model is able to replicate the enhanced chaoticity of the flow observed experimentally in 'smartphone-walking' pedestrians, by reducing the frequency of decisional updates, replicating the digital distraction effect.

Finally, we will show that not all ingredients of the model matter in all situations. Dimensionless numbers will be introduced for crowd dynamics, as in Fluid Mechanics, whose values indicate which processes critically need to be included, and which ones can be overlooked depending on the scenario.

Keywords: pedestrian dynamics, crowds, biomechanical cost

*Speaker

Exploring space under confinement: a quantitative view on bacteria spreading

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In natural environments, physiological ducts, gastro-intestinal tracts or in soils, bacterial motion alternates between three-dimensional (3D) swimming in the bulk and a quite distinct two-dimensional (2D) kinematics at surfaces. Large-scale transport or contamination processes depend crucially on this interplay, which remains, theoretically and experimentally, poorly understood. Boundless exploration of peritrichous bacteria such as E. coli is often assumed to follow a memory-less run-and tumble (R-&-T) kinematics stemming from Poisson-distributed sequences of R-&-T times. However, it was shown recently that the internal molecular machinery rather leads to a non-Markovian stochastic exploration inducing memory and large run-times distribution. Considering a prototypical set-up, we address this fundamental problem both experimentally and theoretically and show how the spreading dynamics is influenced by confinement, internal memory and detailed kinematics at surfaces. We propose an approximated analytical expression for the diffusivity that depends on the average bulk and surfaces residence times. Our results provide crucial and more general insights into how bacteria explore complex environments where the micro-swimmers are bound to alternate between 2D and 3D motion.

Keywords: bacteria microswimmer exploration confinement

*Speaker

Periodic Behavior of an Anisotropic Trumbbell Settling Under Gravity

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We will present a study of a V-shaped rigid conglomerate of three spherical particles of the same radii (trumbbell), which settles under gravity in a viscous fluid. The side spheres have equal masses, but the middle sphere has a different mass and touches the other ones. The configuration of the trumbbell is parametrized by the apex angle α (generally, the side spheres do not touch each other).
Previous studies (1) shows that a trumbbell with equal masses orients itself towards a stable stationary configuration. However, recent results regarding natural sediment flocs(2) as well as the settling process of a rigid U-shaped disk (3) under gravity show that an anisotropic mass distribution might lead to quasi-periodic evolution of the system.

In our case, translational $\mathbf{U}$ and rotational Ω velocities of the rigid conglomerate are linear functions of the total force $\mathbf{F}$ acting on the conglomerate:
$\mathbf{U} = \underline{\mu}\hat{}\{tt\} \cdot \mathbf{F}$, $\Omega = \underline{\mu}\hat{}\{rt\} \cdot \mathbf{F}$
where $\mathbf{U}$ is the velocity of the conglomerate center-of-mass, and the mobility tensors $\underline{\mu}\hat{}\{tt\}$ and $\underline{\mu}\hat{}\{rt\}$ are calculated in the CMS frame of reference in which torque vanishes. For
theta $= \phi = \psi = 0$, $\underline{\mu}\hat{}\{tt\}$ is the diagonal 3×3 matrix and only non-zero components of $\underline{\mu}\hat{}\{rt\}$ are $\mu\hat{}\{rt\}\_\{yx\} = -\ \mu\_a$ as well as $\mu\hat{}\{rt\}\_\{xy\} = \mu\_b$. The hydrodynamic interactions are essential in this problem, and we find the components of the mobility tensor using precise HYDROMULTIPOLE codes for the multipole expansion (4) with the truncation at L=8.

We find that trumbbells with the anisotropic mass distribution show qualitatively different long-time dynamics than those with equal masses. When $\mu\_a \cdot \mu\_b < 0$, the system shows instability towards the long-time periodic motion.

(1) M. L. Ekiel-Jeżewska & E. Wajnryb; *J. Phys.: Condens. Matter* **21**, 204102 (2009)
(2) K. Spencer et al., *Water Research* **222**, 118835 (2022)
(3) T. Miara et al., *Commun. Phys.* **7**, 47 (2024)
(4) B. Cichocki, et al., *J. Chem. Phys.* 111}, 3265 (1999)

Keywords: sedimentation, Stokes flows, multipole expansion, periodic motion

*Speaker

BAM4 - Physics of plants

Biophysical study of plant morphogenic movements

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Peculiar movements have been observed in growing leaves such as *Persea americana* (avocados tree), citrus, or oak, which can only be explained by a synchronisation of the growth of the midribs and the blades. Our working hypothesis is that this growth synchronisation is due to mechano-sensitivity: the shape taken by the leaf at each time point is the results of the elastic equilibrium state of the local growth. However, while the elastic equilibrium state minimises the global elastic energy, some residuals stresses are still present locally, and can affect the growth process in a mechanical feedback loop.
For this, we choose a kinematic approach in studying growing leaf using time lapses to record the z(x,y) of a growing avocado leaf and to tack the texture embedded in 3D. From there, we track artificial markers in time and using it to obtain the 3D+t evolution of those markers in Lagrangian coordinates and to measure the local growth inhomogeneity in time. The goal is to link the spatiotemporal dynamics of the growth pattern to the motions.

Keywords: kinematics, plants, mechano, sensitivity, biophysics

*Speaker

A very expressive plant: Spathiphyllum reactions to water stress

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During a period of drought, the content of water in plants decreases, leading to a decrease in turgor pressure. If the effects are not easily visible with trees and other lignified trees, it is not the case with Spathiphyllum, a popular interior plant.

After two weeks without watering, the plant seems to desperately cry for help, showing leaves completely falling on the ground. Fortunately, such a state is reversible, and the plant soon recovers its shape after watering. What is so specific about this plant?

Anatomically, sections in thin slices of the stems show that the plant contains a water-fillled core with large cells. The soft core shrinks under drought.

Mechanical tests show that the bending rigidity of the stems decreases, but not enough to explain this dramatic change in shape. A good answer could be found at the base of the plant: if the stems are round in cross section, their attachement to the base assumes the shape of thin U-shaped sheet.

We observe that the U-shaped sheet of the base bends when the plant is very dry; this is analogous to the buckling of the metal measuring tape, except that the transition we observe here is likely supercritical.

We then introduce a biomimetic hollow beam model: assuming the elasticity is dominated by their external stiff layer, inflatable hollow beams under internal turgor pressure are good candidates for a description of the behaviour of this plant.

Keywords: turgor pressure, mechanical instability

*Speaker

Embolism at negative pressure in biomimetic veins

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Embolism is the phenomenon of bubble nucleation and expansion within the venation network of ascending sap. It poses a significant threat to plant life and is becoming an even more concerning issue with the progression of global warming. The ascent of sap depends on the creation of negative pressure (tension), but this makes the sap highly susceptible to embolisms in arid conditions. The compartmentalization of the plant's venation bundles into vessel elements (interconnected channels) limits the spread of embolism, resulting in a complex "stop and go" dynamics at various time and spatial scales. This is particularly evident in the filming of embolism propagation in leaves.
I will first present original high speed movies revealing fast embolism propagation in real leaves occuring at negative pressure. Then I will focus on our approach of this problem using a bottom-up method. I micro-fabricate biomimetic leaves with vessel-like channels in water-swelling hydrogels that are notably stiff and capable of withstanding high negative pressures. I then submit these devices to hydric stresses to simulate water conditions in ascending sap. I observe the system's multiscale response, which includes slow poroelastic water transport and rapid cavitation bubble growth where inertia and acoustics play a role. These observations pave the way for identifying the physical parameters governing embolism in veins under negative pressure in water-swelling materials. I will discuss the meaning of these results for the understanding of fast embolism dynamics in real plants.

Keywords: cavitation, osmosis, hydrogel, fast camera, negative pressure, plant embolism

*Speaker

Timelapse of the dehydration of a plant: some insights on the loss of rigidity

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Drought is a life-threatening stress for plants. Nature brings different responses to drought: an apple tree loses its leaves to prevent transpiration, a cherry tree changes leaf orientation to limit sun exposure... but a basil plant is almost ressourceless and dries quickly. Actually before dying the basil plant wiltens : leaves and twigs have lost rigidity.
We address the origin of plant rigidity loss during the wilting process. This loss of rigidity is surprising for plants: a well watered tulip is able to self-support its weight; after a weak dehydration, the tulip wiltens and is unable to support self-weight and if dehydration is complete, the dried tulip is again able to support self weight.

Actually, drying not only changes the rigidity but also the density of the plant tissue. We observe the drying of a basil plant over several days and discuss the physical origin of the loss of rigidity of its soft organs. An automated set-up measuring independently petiole radius and bending rigidity is presented. We show that the loss of bending rigidity, EI, is non trivial: When cells deflate, the young modulus E increases but the second moment of area I decreases. We show that this "first order" linear effect is unable to account for the total decrease of rigidity of the plant and that non linear cell wall elasticity is necessary to account for pressure-induced rigidity of plants.

Keywords: plant biomechanics, pressurized cellular solid, Elasticity

*Speaker

Observation of the water imbibition into cellulose fibre stack

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Water transport is crucial for natural materials such as plants and wood, made of cellular hygroscopic structure that contains water with different dynamics including free water in the cavities and in the cell walls. Considering that up to 30% of the dry mass of plants can be adsorbed as bound water in the amorphous regions between the microfibrils of cellulosic fibers, it is significant to understand its potential role in the complex transport phenomenon within these materials. To this end, the present work investigates the spontaneous penetration (imbibition) of water into a model plant or wood sample, i.e., a porous cellulose fiber stack, which can absorb free water in its pores and bound water inside the fibers. To get an insight into the resulting complex process, we simultaneously follow the advancement of the wet region (i.e., the liquid rise), the sample swelling (essentially along its longitudinal axis), and the total mass of adsorbed liquid. Two distinct stages were identified in the standard vertical imbibition experiments. In stage , the liquid rise, sample swelling, and the mass of adsorbed liquid are proportional to the square root of time. With the wet cellulose/dry cellulose surface and the wet cellulose/water surface, the water accessible volume within the wet region of the sample and thus the corresponding saturation mass is estimated. We find that the measured mass of adsorbed liquid is 10-30% lower than the saturation value evidencing that cellulose is partially saturated in this stage. When the liquid front reaches the other end of the sample (i.e., no dry area left) or the water bath is removed, stage commences where the sample swelling retains the power law with the constant shift from 0.5 to _˜0.15. All this information reveals the significant coupling effects of bound water adsorption and standard capillary imbibition.

Keywords: Cellulose fibre stack, Spontaneous penetration, Bound water adsorbtion

*Speaker

Bound water transport by diffusion in wood revealed by Nuclear Magnetic Resonance

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During the lifespan of a plant, various types of water transfer can occur, including sap, drying, imbibition. However, the process is often complex due to the intricate internal structure of plants. Additionally, the presence of bound water, which can constitute up to 30% of the dry mass, adds more complexity as its transport might be coupled with free water flow.
In this study, we aim to elucidate the hydrodynamics of free water and the transport properties of bound water. For this purpose, we investigate the imbibition of liquid in hardwood samples through NMR measurement. This technique allows us to obtain the probability density function of water transverse relaxation time, enabling us to separately see the global evolution of different types of water in the material.

This investigation revealed that the invasion dynamics of bound water is the fastest, i.e., it rapidly invades the cell walls of the whole sample. In parallel but at a lower rate the water invades the fibers, and then the vessels. To understand the potential coupling between the invasion of different pore types, we examined the specific diffusion properties of bound water by determining its diffusion coefficient in the absence of free water. This was achieved by filling the sample with oil, which essentially fills the vessels, and when in contact with water, only a negligible amount of water can penetrate the fibers. Finally, the invasion of the cell walls by bound water was followed by NMR, and the corresponding diffusion coefficient was determined.
We further examined this diffusion process using MRI experiments, employing two different sequences to distinguish between signals of oil and bound water. Finally, we compare the diffusion coefficient in the absence of free water to the value observed in the presence of free water to appreciate the coupling between the two processes.

Keywords: wood, bound water, diffusion coefficient, NMR, MRI

*Speaker

Microfluidic models of osmotic sap transport in phloem using hydrogel-membranes

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Vascular plants passively exploit the gradients of water chemical potential in two coupled vascular " microfluidic " systems, *xylem* and *phloem* (transverse dimensions 10-100 μm) to make the different organs communicate with each other. More specifically, evapotranspiration moves water contained in the soil up to its vapor phase in the atmosphere, through the xylem connecting the roots to the leaves, to maintain plant hydration. At the same time, sugars photosynthesized in the mesophyll cells of the mature leaves are transported through the phloem by **forward osmosis** to the sink sites (flowers, roots, etc.) for plant growth and storage. Despite the relatively well established qualitative understanding of these processes, many fundamental questions remain open, particularly relative to the phloem. A complementary strategy to *in planta* measurements consists in mimicking sap transport in vascular plants using microfluidic models. In this work, we have developed microfluidic chips integrating pressure-resistant hydrogel membranes to mimic flows and sugar thansport similar to those occuring in the phloem. In particular, we showed that our membranes (width 30 μm) are able of withstanding hydrostatic pressures up to 0.5 MPa and have hydraulic permeabilities close to the membrane permeability of phloem tubes (Lp=7 10E-13 m/(Pa s)). Using sucrose and dextran (9KDa) solutions, these hydrogel membranes can generate osmotically-driven flows with osmotic pressures up to 1 MPa. Interestingly, these flows are transient for sucrose as its molar mass (Ms=342 g/mol) is lower than the molecular weight cutoff of the membrane. In this specific case, our microfluidic experiments lead to simultaneous meaurements of the reflection coefficient of the membrane and sucrose diffusivity in the hydrogel. As these membranes are leaky, they are possibly suitable candidates for mimicking on-chip loading (unloading) of sugar in (from) the phloem.

Keywords: microfluidics, transport, membrane, osmosis

*Speaker

MP2 – Functional materials for spintronics

GeTe Ferroelectric Rashba semiconductor: from growth to spintronic

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Among ferroelectrics, a new class of materials for spintronics has recently been introduced: The Ferroelectric Rashba semiconductors (1). The main results, obtained on GeTe thin films, have demonstrated that reversal of the ferroelectric polarization leads to a change in the spin chirality of the band structure (2,3). A spin-to-charge conversion has also been demonstrated at room temperature using ferromagnetic-GeTe stacks (4). In the perspective of addressing the spin-dependent electronic properties of GeTe thin films, the polarization state must be controlled. Quasi single crystalline GeTe thin films have been grown on Si(111) by molecular beam epitaxy, by first depositing an atomic monolayer of Sb (5-7). Ferroelectric domain volume fraction and domain size were measured by X-ray diffraction and low energy electron microscopy over a wide range of film thicknesses (1-1800 nm). Second harmonic generation microscopy combined with polarimetric analysis reveal the local symmetry of these domains. The reversible appearance/disappearance of ferroelectric domains by thermal cycling is attributed to thermal stresses induced by the thermal expansion differential between GeTe and Si (8). Concerning the electronic properties we demonstrate a giant Rashba effect in GeTe thin films by ARPES for film thickness down to 1 nm and we put an evidence THz emission through spin-to-charge conversion in a Fe/GeTe/Si(111) stack.
(1) D. Di Sante et al., Adv. Mater. 2013, 25, 509
(2) C. Rinaldi et al., Nano Lett., 2018, 18, 2751
(3) J. Krempasky et al., Phys. Rev. X, 2018 8, 021067
(4) S. Varotto et al., Nature Electronics, 2021, 4, 740
(5) B. Croes et al., Phys. Rev. Materials, 2021, 5, 124415
(6) B. Croes et al., Phys. Rev. Materials, 2022, 6, 064407
(7) B. Croes et al., Phys. Rev. Materials, 2023, 7, 014409 (8) B. Croes et al., J. Appl. Phys., 2023, 134, 204103

Keywords: Ferroelectric Rashba semiconductors, GeTe, Growth, ARPES, THz emission

*Speaker

Spin-to-charge conversion control for THz generation

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In less than a decade, spintronic Terahertz (THz) emitters have become powerful material platforms both for THz and magnetism communities. Indeed, they open attractive perspectives for THz technology development - powerful, tunable and broadband THz generation with nm-thick emitters - as well as a unique platform to explore spin-charge interconversion mechanism in a contact-less way. These objectives however fundamentally rely on the ability to fabricate high-quality materials with targeted physical properties.

Therefore, recent development of new functionnal materials for spintronic THz emission, such as topological insulators, 2D materials and antiferromagnets - which can be grown and transfered on various substrates - paves a way for designing novel kind of emitters. These materials indeed allow to tailor spin-charge interconversion in order to reach crucial technological requirements, such as efficiency enhancement and THz emission tunability.

In this talk, emission properties - probed by THz time-domain spectroscopy with tunable photon pump energy - of spintronic THz emiters composed by various functionnal materials, as well as spin-to-charge current conversion mechanisms (i.e. Rashba Edelstein or Spin Hall effect) will be discussed. We will

*Speaker

present results obtained with topological insulators such as BiSb or Bi2Se3 as well as the impact of adding 2D materials spacer such as PtSe2. In a second part, we will discuss the contribution of ferroelectric materials such as LiNbO3 or GeTe, which should provide additional control. Finally, the ability to spectrally tune THz emission in antiferromagnetic emitters made of Pt/BiFeO3 will be developped.

Keywords: Terahertz, topological insulator, ferroelectricity, antiferromagnet, spintronic emitter

Integration of garnets with perovskites in hybrid multilayers

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Perovskites and garnets are at the cornerstone of many applications in spintronics. Their integration in multifunctional devices will open new possibilities to harness their individual and coupled properties. Despite their numerous applications, their integration into a single hybrid heterostructure remains to be a great challenge due to their highly dissimilar structural properties.
In this work we show how to growth high quality YBa2Cu3O7 (YBCO) on Y3Fe5O12 (YIG) in-situ by pulsed laser deposition (PLD), using a 10 nm-thick interlayer buffer of ZrO2.Y2O3 (YSZ). The YBCO is a high Tc-superconducting perovskite extensively used in microwave sensors and resonators while YIG is the most popular ferrimagnetic insulator, widely used in magnonics due to its low magnetic damping. Although similar approaches have been explored in the past1,2 to fabricated tunable microwave components, here we show that the heterostructure can be grown entirely in-situ by PLD and the buffer layer thickness can be thin enough to permit a large dipolar coupling between the layers. Moreover, the in-situ deposition permits to growth ultrathin films of these materials to explore strain effects.

The potential applications of these method span from low-loss tunable microwaves resonators and filters, as well as tunable magnonics crystals.

1. Jia, Q. X., Arendt, P. N., Foltyn, S. R., Holesinger, T. G. & DePaula, R. F. Superconducting YBCO films on polycrystalline yttrium-iron-garnet using IBAD-YSZ as a template. *IEEE Transactions on Applied Superconductivity* **11**, 3489–3492 (2001).

2. Silliman, S. D. *et al.* Magnetically Tunable Microwave Filters based on YBCO/YIG/GGG Heterostructures. *J Electroceram* **4**, 305–310 (2000).

Keywords: Thin films, spintronics, superconductivity

*Speaker

Spin pumping in Py/YBCO d-wave superconductor hybrids

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Spin-pumping into superconductors (SC) has recently attracted significant interest due to its relevance in the realization of efficient superconducting spintronics components, exploiting the dissipationless electron transport and quantum coherence characteristic of superconductivity (1-4). The focus has been on structures incorporating mainly s-wave superconductors.
Here, we extend the search into a d-wave superconductor, YBa2Cu3O7-d (YBCO), joined to a sputtered metallic ferromagnet (FM), Ni80Fe20 (Py). We used wideband ferromagnetic resonance (FMR) to study spin-pumping from the FM (Py) perspective, combined with transport measurements, to probe the ISHE in the SC.

We evaluated the spin conductance at the Py/YBCO interface by analyzing the magnetization dynamics in Py. Across the superconducting transition, the spin-sinking efficiency of YBCO reduced as seen by a drop in the damping, which could be explained by the opening of the superconducting gap (5), hampering the angular momentum transfer. However, and surprisingly, the ISHE signal reveals an exponential increment (a peak) at the critical temperature, which has been associated in other systems with the coherence peak of the quasiparticles' density-of-states at the FM/SC interface (6,7), but is difficult to conciliate with the observations of a drop in the magnetization damping. The different scenarios to explain these results will be discussed.

Work supported by ANR-22-EXSP-0007 PEPR SPIN "SPINMAT" and ANR "SUPERFAST".

References

(1) F. S. Bergeret *et al*, *Phys. Rev. Lett.* **86** (2001) 4096–4099.
(2) M. G. Blamire *et al*, *J. Phys.: Condens. Matter.* **26** (2014) 453201.
(3) J. Linder *et al*, *Nat. Phys.* **11** (2015) 307–315.
(4) M. Eschrig, *Rep. Prog. Phys.* **78** (2015) 104501.
(5) S. J. Carreira, *et al*, *Phys. Rev. B* **104** (2021) 144428.
(6) F. S. Bergeret *et al, Reviews of Modern Physics*, **90** (2018) 41001. (7) K.-R. Jeon *et al*, *ACS Nano* **14** (2020) 15874–15883.

Keywords: spin pumping, dwave superconductor, superconductivity, spintronics, YBCO, Py, FMR, ISHE

*Speaker

Tailoring Perpendicular Magnetic Anisotropy in (Mn3Ge / Co2FeGe) Heusler Super-Lattices

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The discovery and engineering of new materials that fully satisfy the requirements for low energy consumption devices is a continuous challenge in spintronics. Besides the need of a high spin polarization at the Fermi energy and a low Gilbert damping coefficient, obtaining perpendicular magnetic anisotropy (PMA) is one of the most important conditions to improve the efficiency of next generation devices relying on magnetization reversal by spin transfer torque (1) and spin-orbit torque switching (2).
On the one hand, ferrimagnetic tetragonal Mn3G (G=Ga, Ge) Heusler compounds have attracted much attention in the last decade due to their strong magnetocrystalline anisotropy along their c-axis and small overall magnetic moments (3). On the other hand, it has recently been demonstrated that epitaxial Co2MnZ (Z=Al, Si, Ga, Ge, Sn) Heusler compounds are half metal magnets with a spin gap in their electronic structure (4) and the lowest Gilbert damping coefficients reported for conductive layers (4). For these reasons, Super-Lattices (SL) composed of those two types of materials represent promising systems to combine small magnetic moments, full spin polarizations, reduced Gilbert damping values and PMA, thus offering a new pathway toward efficient spin torque devices.

In this presentation, we will focus on ((Mn3Ge)3nm/(Co2FeGe)t)5 SLs with t ranging from 1 to 5 nm. The growth of fully epitaxial samples will be presented together with a structural characterization study done by X-ray diffraction, demonstrating the high structural quality. The magnetic properties are investigated using X-ray magnetic circular dichroism measurements where a tuning of the magnetic anisotropy is achieved by changing the sublayers thickness.
(1) S. Mangin et al., Nat. Mater. 5, 210 (2006).(2) I. M. Miron et al., Nature 476, 189 (2011).(3) B. Balke et al., Appl. Phys. Lett. 90, 152504 (2007).(4) C. Guillemard *et al., Phys. Rev. Appl.* **11**, 064009 (2019).

Keywords: Heusler, epitaxy, spintronic, xmcd, super, lattice

*Speaker

Oriented growth of thin films of chalcogenide materials for spintronic applications

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Chalcogenide materials exhibit a wide range of unique properties making them attractive for many applications in optics/photonics, thermoelectric as well as for data storage (1). In a world of constantly increasing data generation, data processing and storage are becoming major challenges. The strong spin-orbit coupling present in certain chalcogenide materials offers the possibility of designing a completely new type of electronics with ultra-low energy consumption (2). Using the possibilities offered by spin-orbitronics, proofs of concept have been acomplished using 2D topological insulators (TIs) or ferroelectric (FE) alloys with Rashba effects deposited on small size samples by Molecular Beam Epitaxy. TIs show great potential for Spin Orbit Torque-MRAM (SOT-MRAM) devices, while ferroelectric GeTe is the material of choice for the innovative concept of Ferro-Electric Spin Orbit (FESO) devices (3). Here, we study the large-scale elaboration of high-quality ferroelectric α-GeTe(111) and of pseudo-2D Sb2Te3 thin films, TI with high spin-charge conversion efficiency. The potential use of these materials in the microelectronics industry for SOT-MRAM or FESO devices will also be discussed.
(1) P. Noé et al, Semicond. Sci. Technol. 33, 013002 (2018)
(2) S. Teresi et al., Advanced Functional Materials 33, 44, 2303878 (2023)
(3) S. Varotto et al., Nat Electron 4, 10, 740 (2021)

Keywords: growth, chalcogenides, phase change materials, ferroelectricity, spintronics

*Speaker

Epitaxial growth and magnetic properties of Mn5(SixGe1-x)3 thin films

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Manganese silicide and manganese germanide compounds have the advantage of being rare earth-free alloys. They are drawing great attention, both in the field of spintronics and magnetocaloric materials. Mn5Ge3 and Mn5Si3 exhibit strong similarities but also fascinating differences. These two intermetallic alloys have the same hexagonal D88-type structure but Mn5Ge3 exhibits ferromagnetic while Mn5Si3 is antiferromagnetic with two first-order transitions. Considering the difference in the magnetic behaviors of Mn5Ge3 and Mn5Si3, it is interesting to study the ternary alloys, denoted as Mn5(SixGe1-x)3.
Structural and magnetic properties of Mn5(SixGe1-x)3 thin films were investigated. The films were grown on Ge(111) substrates by co-deposition using molecular beam epitaxy with controlled Si concentrations ranging from 0 to 1. A combination of techniques, including reflection high-energy electron diffraction (RHEED), X-ray diffraction (XRD), atomic force microscopy (AFM), and high-resolution transmission electronic microscopy (HR-TEM) were employed to investigate the structural properties of the films. The thin films were relaxed by dislocations at the interface with the substrate. A lattice parameter variation was observed as the Si content increased. RHEED diagrams and XRD profiles showed that lattice parameters a and c are shrinking and that the surface roughness and crystallinity degrade as the Si amount increases.
Magnetometric measurements (VSM, SQUID) revealed a ferromagnetic behavior for all Si concentrations. The measured average ferromagnetic moment per manganese atom decreased from 2.33 to 0.05 μB/Mn atom. Furthermore 55Mn NMR experiments have been performed on the Mn5(SixGe1-x)3 films. The Si/Ge substitution creates a new population of manganese atoms located in the 6(g) sublattice with lower magnetic moment. The amount of new manganese environments coincides with a probability of Mn having two Si neighbors as first neighbors. The magnetic behavior is influenced by inter-atomic distances and the nature of the non-magnetic atoms.

Keywords: Epitaxial growth, Mn5(GeSi)3, Magnetic structure, Manganese germanide, Manganese silicide, Ferromagnetism, Antiferromagnetism

*Speaker

Epitaxial Topological Insulator $Bi_{1-x}Sb_x$ films on GaAs substrates for Spintronic applications

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Topological insulators (TI) are functional materials holding unique promises for future spintronic applications. An elegant strategy to design and create efficient systems relies on exploiting the metallic surface in such materials. This particular edge state exhibits a robust spin polarisation protected by time-reversal symmetry and strong spin-orbit interactions, enabling efficient charge-to-spin conversion. Bismuth antimony (BiSb) alloys outstand other TIs by their large spin-hall angle (θSH $\approx$ 52) generating a high spin-orbit field and a very low critical switching current density. The hastening quest for efficient SOT generators for future devices has led to multiple attempts to grow BiSb thin films on different substrates using various techniques. Crystallinity and defect density are crucial elements in preserving the topological properties and enabling on-top device fabrication. Our present work shows the importance of in-depth structural characterization and theoretical calculations to understand and optimize films' growth. As a result, successful integration of single-crystalline Bi(x)Sb(1-x) films on (111)-oriented GaAs substrates is achieved by Molecular beam epitaxy. The topologically protected surface state is evidenced by ex-situ ARPES measurements for films having a composition within the TI range. ($0{,}7 \leq x \leq 0{,}19$). Moreover, adjacent magnetic Co layer-based heterostructures are successfully deposited on our films. The obtained magnetic anisotropy is Co-layer thickness and spacer material-dependent providing a flexible basis for engineering efficient TI-based spintronic devices.

Keywords: Topological insulator, $Bi_{1-x}Sb_x$, Epitaxy, ARPES, Spin, orbit, torque

*Speaker

Selective Area Epitaxy of In-Plane HgTe Nanostructures on CdTe(001) Substrate

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Topologically protected systems such as HgTe/CdTe are of great interest for the future of electronic, spintronic and quantum technologies. Nevertheless, their device integration remains challenging. Selective area growth (SAG) of in-plane nanostructures on a SiO2-masked substrate by MBE is a promising technique to address this issue and enable the realization of complex 1D networks, with accurate control of dimensions, geometry and material quality.
For the first time, we evidence the growth of several micron-long HgTe nanostructures (nanowires, rings and networks) grown on CdTe(001) along the three in-plane crystal directions ((110), (1-10) and (100)) with well-defined cross-junctions. A good selectivity is achieved with very little parasitic growth on the mask. The nanowire shape strongly depends on the slit orientation. Indeed, we found that (1-10)-oriented ridges show {111}A facets with adatoms accumulation on the edges of the top surface. We also demonstrated the morphology evolution of nanowires as function of the growth time: increasing the deposited thickness yields to a triangular cross-section with smooth {111}A facets and then lateral expansion of the nanostructure. Regarding a (110)-oriented nanowire, it shows a trapezoidal shape with {111}B facets in the center and two grains on the sides made of (001) planes but tilted of +/- 70.5◦, as the symmetry with respect to {111} planes. We also studied the influence of the growth temperature that changes the surface diffusion of adatoms on HgTe as well as the diffusion on the mask, and so, the lateral overgrowth of the nanostructures. Transmission electron microscopy images revealed the continuous epitaxial relation between the CdTe substrate and the HgTe NW that is found free of misfit dislocations, which is crucial for transport applications.
Thus, we identified the major levers for the SAG of HgTe nanostructures and their morphology can thereby be tuned before performing transport electronic measurements.

Keywords: Molecular beam epitaxy, selective area epitaxy, HgTe, topological insulator

*Speaker

IA1 - Advances in machine learning for materials modelling

Nucleation phenomena in liquid metals: what can be gained from machine learning ?

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Nucleation phenomena are commonly observed in our everyday life, manifesting in various forms such as the formation of clouds, crystallization of sugar in candy making, freezing of water into ice, and casting of steels and aluminum alloys in transportation industries. Focusing on crystal nucleation in liquid metals, the early stages where the liquid-to-solid transition occurs upon undercooling and starts on a nanometer length and sub-picosecond timescale that can still hardly be observed experimentally. To reveal their structural features, atomistic simulations have to be conducted and need at least two important features. Firstly, an accurate knowledge of interactions, which can be achieved with DFT. Secondly, MD has to be carried out on a sufficiently large scale to observe a reasonable number of nucleation events, often involving millions of atoms. Combining these two ingredients seems at first sight incompatible given the size achievable by DFT-based simulation. Recent advances in ML potentials allows us to overcome this difficulty and address crystal nucleation by means of MD simulations at DFT accuracy. A well-established high-dimensional neural network potential trained on a set of configurations generated by AIMD, containing various crystalline structures and liquid states at different pressures, including their time fluctuations over a wide range of temperatures, was shown to be relevant for solidification phenomena. Subsequently, tracking relevant structural information from a nucleation pathway produced by such large-scale MD simulations can be performed without a priori using an unsupervised learning approach founded on topological descriptors borrowed from persistent homology concepts. The translational and orientational ordering of the liquid prior to nucleation, as well as the morphology of nuclei when homogeneous nucleation starts, were studied for various monatomic metals. Results reveal the specificity of the nucleation pathways depending on the element considered, with features beyond the hypothesis of Classical Nucleation Theory.

Keywords: machine learning, molecular dynamics, density functional theory, nucleation, liquid metals

*Speaker

Insights from symmetry: Improving machine-learned models for grain boundary segregation

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Grain boundary (GB) segregation substantially alters structural properties of metallic alloys. A critical factor rooting the variability of GB segregation is the atomic structure of the boundary. In this context, we propose two efficient and user-friendly Machine-Learning (ML) framework capable of predicting the segregation of different solute atoms at GBs in the form of a segregation energy distribution (SED), from the corresponding virgin GB atomic structure. For that purpose, an extended set of descriptors encompassing smeared Steinhardt Bond orientational order (BOO) parameters is first generated. Second, two efficient learning algorithms are compared: Extra-Tree (ET) regression on the one hand, and Deep Neural Network (DNN) on the other hand were implemented, which allowed to outperform a previous study (1). We also show that ML provides a fresh and promising perspective to address the long-standing issue of GB structure-segregation property relationship.
To this, GB structural symmetry was characterized by the Kernel Principal Component (kernel PCA) analysis of the GBs features matrix for the first time, while the normalized integral of the SED served as an indicator of the degree of symmetry of GB segregation pattern. With this, we concluded that the degree of segregation symmetry increases monotonically with virgin GB structural symmetry. Part of the presented results have recently been published in (2).

(1) L. Huber & al. (2018), npj Computational Materials, 4(1), 1-8.
(2) Y. Borges & al. (2024). Computational Materials Science, 232.

Keywords: Machine Learning, Grain boundary Segregation, Kernel PCA, Structure segregation property, Extra trees, Deep Neural Network, Structural symmetry

*Speaker

Deterministic and probabilistic descriptor models in atomic simulation

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I will discuss how descriptors (high-dimensional, many-body order parameters of point clouds) can be used to coarse-grain atomic simulations of materials. These are typically used in a deterministic setting, i.e. to predict energy and forces given atomic positions. Capturing model uncertainty in this regime requires proper treatment of model misspecification which is entirely neglected when training with the expected loss, but the true generalization error can be approximately minimised(1). Deterministic models can also capture important microstructural features such as dislocation densities, correlation functions, or vibrational entropies, offering many efficiencies when deploying at scale. Descriptor timeseries extracted from simulation trajectories can be used to make probabilistic forecasts of simulation futures; in this setting, ideas from active learning are very useful to quantify and qualify prediction uncertainty(2). The opportunities provided by descriptors for data-driven analysis will be illustrated through application to nanoparticles and plastic deformation of metals.

(1) TD Swinburne and D Perez, arXiv 2402.01810 (2024)
(2) TD Swinburne, Phys. Rev. Lett. 236101 (2023)

Keywords: Molecular Dynamics, Machine Learning, Uncertainty Quantification, Coarse Graining

*Speaker

Activation entropy of dislocation glide predicted by machine learning

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In body-centered cubic metals, low-temperature plastic deformation is controlled by the thermally-activated kink-pair mechanism, where screw dislocations propagate under an applied stress tensor. The activation entropy of this process is notoriously challenging to compute, often necessitating the use of simplifying assumptions such as constant values or enthalpy-based estimates, within the harmonic approximation. Recent attempts using traditional radial interatomic potentials (IAPs) have challenged these assumptions (1-2), but doubts remain, as these IAPs have limited accuracy. We developed a new machine-learning (ML) IAP based on (3), tailored for accurate dislocations simulations in iron, which quantitatively reproduces dislocation properties computed by *ab initio* methods. We employed the Projected Average Force Integrator (PAFI) method (2) to compute the Gibbs free energy for kink-pair nucleation at scale, beyond the harmonic assumption. Our results illustrate the improved accuracy achieved by ML compared to traditional IAPs, while uncovering entropy-enthalpy relations that depart from classical phenomenological predictions (based on the Meyer-Neldel rule or temperature dependence of bulk properties). Our work demonstrates the potential of ML methods to lift long-standing limitations in molecular dynamics, accurately predicting the deformation of metals at finite temperature.
(1) Zotov & Grabowski, Model. Simul. Mater. Sci. Eng. 30, 065004 (2022).
(2) Swinburne & Marinica, Phys. Rev. Lett. 120, 135503 (2018).
(3) Goryaeva et al., Phys. Rev. Mater, 5, 103803 (2021).

Keywords: plasticity, molecular dynamics

*Speaker

Artificial intelligence algorithm development dedicated to formulation of geopolymer

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Geopolymers have shown real potential for various microwave frequency applications. This new class of ecomaterials results from the dissolution of reactive aluminosilicate under the effect of alkaline solution. The properties of geopolymers are strongly impacted by the precursors used. Our work relies on advanced deep and machine learning techniques to develop the first artificial intelligence-based geopolymer formulator. While in literature, machine learning applications focus on predicting material properties from theorical chemical formulation, we here target the inverse design problem. Specifically, our models are capable of formulating material precursors and their relative proportions from a user-defined target mechanical, dielectric and/or thermal properties. This implies that the models exclusively propose reactive mixtures that can be realized in laboratory, in order to ensure that the work of creating new materials goes beyond the theoretical stage and enables applications in industry and research. To this end, a large experimental database of different geopolymer formulations and their structural characteristics and final properties was collected and structured. This in-house database ensures a full reliability and consistency of the data used to feed the AI models. We developed deep neural networks constrained by geopolymerization laws to identify correlations between target and precursor properties, resulting in precursor mixture formulas. The model validation is based on a comparison between predictions and experimental measurements. The first results have shown a mean error of 6.7% on the formulation of precursor proportions and a relative error of 7% between target and measured property values. Work is in progress to minimize this error.

Keywords: geopolymer, neural networks, material formulation

*Speaker

Hydrogen, oxygen and lead adsorbates on Al13Co4(100) : accurate potential energy surfaces at low computational cost by machine learning and DFT-based data

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Intermetallic compounds are promising materials in numerous fields, especially those involving surface interactions, such as catalysis. A key factor to investigate their surface properties lies in adsorption energy maps, typically built using first principles approaches. However, exploring adsorption energy landscapes of intermetallic compounds can be cumbersome, usually requiring huge computational resources. In this work, we propose an efficient method to predict adsorption energies, based on a few density functional theory estimates achieved on sites selected through the Farthest Point Sampling (FPS) process, that feeds a machine learning (ML) scheme. We detail its application to the construction of adsorption energy maps on the Al13Co4(100) quasicrystalline approximant surface for several atomic adsorbates (H, O and Pb). On this specific example, our approach is shown to outperform both simple interpolation strategies and the recent ML force field MACE, especially when the number n of selected sites used for interpolations or training is small, i.e. namely between 9 and 36 sites. The ground-truth DFT adsorption energies are much more correlated with the predicted FPS-ML estimates (Pearson R-factor of 0.71, 0.73 and 0.9 for H, O and Pb, respectively, when n=36) than with the interpolation-based or MCAE-ML ones (Pearson R-factor of 0.43, 0.39 and 0.56 for H, O and Pb, in the former case and 0.22, 0.35 and 0.63 in the latter case). Overall, the unbiased root mean square error (ubRMSE) is lower for FPS-ML than for interpolation-based and MACE-ML predictions (0.15 eV, 0.17 eV and 0.17 eV, respectively, for hydrogen; 0.17 eV, 0.25 eV and 0.22 eV for lead and 0.55 eV, 0.47 eV and 0.46 eV for oxygen, with n=36). We believe that these findings and the corresponding methodology can be extended to a wide range of systems, which will motivate the discovery of novel functional materials.

Keywords: adsorption energies, surfaces, machine learning, intermetallic compounds

*Speaker

2DMS5 - Ultrafast dynamics in 2D and quantum materials

Ultrafast Control of Quantum Materials using Intense Laser Fields

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All-optical spectroscopy of matter is a well established technique to access properties of electrons and quasi-particles in matter. The description of these optical properties is usually done employing linear response methods.
Recent advances in experimental techniques have opened up the possibility to develop novel types of spectroscopies based ultrashort and intense laser pulses, allowing for instance to access non-equilibrium dynamics of condensed-matter systems, coherently control magnetization on ultrafast timescales, or to allow for exploring non-equilibrium phase diagram of correlated materials.

The strong-field electronic dynamics in solids have received a lot of attention, in particular due to the experimental observation of high-harmonic generation in solids. The dynamics associated with strong laser fields requires a non-perturbative description of the electronic dynamics. One possible way of describing this strong-field dynamics by *ab initio* methods is to use real-time time-dependent density functional theory (1).

In this talk, I will present some examples of how intense lasers can be use to coherently control materials' properties, in particular correlation(2), magnetic properties(3), or topology(4), but also how we can use high-harmonic generation as a spectroscopical tool in condensed matter(5).

(1) . N. Tancogne-Dejean, et al., Phys. Rev. Lett. 118, 087403 (2017)

(2) . N. Tancogne-Dejean, et al., Phys. Rev. Lett. 121, 07402 (2018)

(3) . O. Neufeld, N. Tancogne-Dejean, et al., npj Comp. Mat. 9, 39 (2023)

(4) . O. Neufeld, N. Tancogne-Dejean, et al., Phys. Rev. X 13, 031011 (2023)

(5) . A. Mondal, et al., Nature Phys. 19,1813 (2023)

*Speaker

Real-time electron dynamics: from non-linear response to pump and probe spectroscopy

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Pump-probe spectroscopy uses two laser pulses to extract dynamical information from the sample of interest.
The pump initiates the optical process by exciting part of the sample from the electronic ground state to an accessible electronic excited state, an exciton. The probe then interacts with the already excited sample. The change in absorbance after pumping provides information about the transitions between the excited states and their dynamics. In this talk I will present a real-time approach to study these phenomena in solids and nanostructures. First, I will discuss some applications with a single laser source related to the nonlinear optical response, and then we will move on to pump and probe spectroscopy. The results are then analysed using a Fermi-Golden rule approach formulated in the excitonic basis set and in terms of the symmetries of the excitonic states. Using bulk LiF and 2D hBN as two prototype materials, we discuss the selection rules for transitions involving strongly bound excitons for which the hydrogen model cannot be used.

References:
(1)D. Sangalli, M. D'Alessandro, C. Attaccalite, Phys. Rev. B, **107**, 205203 (2023)
(2)C. Attaccalite, M. Grüning, Phys. Rev. B, **88**, 235113 (2013)
(3)C. Attaccalite, M. Grüning, H. Amara, S. Latil, F. Ducastelle, Phys. Rev. B, **98**, 165126 (2018)

Keywords: pump and probe, real, time dynamics, ab, initio simulation, theory

*Speaker

Floquet Valleytronics in $2H - WSe_2$

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Driving quantum materials out of equilibrium allows the generation of states of matter that are not accessible using standard equilibrium tuning methods. Upon periodic coherent driving of electrons using electromagnetic fields, Floquet–Bloch states emerge and enable the creation of exotic quantum phases. In transition metal dichalcogenides (TMDCs), broken inversion symmetry within each monolayer results in a non-zero Berry curvature at the K and K' valley extrema, leading to chiroptical selection rules, which are at the heart of valleytronics. Here, we bridge the gap between Floquet engineering and valleytronics. Using time- and polarization-resolved extreme ultraviolet momentum microscopy, we demonstrate the formation of valley-polarized Floquet-Bloch states in 2H-WSe$_2$ upon below-bandgap coherent driving of electrons using chiral light pulses. We investigate quantum path interference between Floquet-Bloch and Volkov states, which is shown to be valley- and light-helicity-dependent. We performed advanced characterization of valley-polarized Floquet-Bloch states through circular dichroism in photoelectron angular distributions (CDAD). Our results shed light on the emergence of a novel type of engineered out-of-equilibrium phase upon breaking time-reversal symmetry by coherent dressing of winding Bloch electrons with chiral light.

Keywords: 2D materials, Floquet, engineering, Ultrafast, TMDC, Valleytronics

*Speaker

Attosecond Spectroscopy of the Correlated Insulator Nickel Oxide

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Strongly correlated materials present peculiar behavior of both technological and fundamental interest, due to repulsive electron-electron interactions. Nickel oxide (NiO) was the first material in which strong correlations were evidenced, as they change its behavior from metallic to insulating. Despite decades of research, its response to light excitation remains unclear. The challenge is that purely electronic dynamics typically occur in a few femtosecond or less, requiring attosecond temporal resolution. At these time scales, do correlations cause a strong sub-optical-cycle response to an external laser field? Or instead, do they screen the field, hampering the ultrafast response?
To address this question, we used attosecond transient reflectivity in the extreme ultraviolet (XUV) range with time resolution below the optical cycle of light. We first benchmarked with magnesium oxide, a band insulator showing oscillations at twice the pump laser frequency, a signature of the well-studied dynamical Franz Keldysh effect by which the field coherently distorts the bands of the solid. This shows both the expected behavior of a non-correlated insulator and that our experimental setup resolves sub-optical-cycle dynamics.

Strikingly, NiO does not show any sub-optical-cycle dynamics. Instead, it presents a much slower response taking the form of a redshift emerging in 20 femtoseconds. To explain this, we conduct state-of the-art calculations in the framework of time-dependent density-functional plus self-consistent U theory, which describes ultrafast dynamics in strongly correlated systems. Our results, in good agreement with the experiment, explain this behavior as a light-induced renormalization of the correlation parameter U in the Hubbard model, emphasizing the key role of correlations.
Our study uncovers a new dynamic specific to correlated insulators as opposed to the known dynamical Franz Keldysh effect in band gap insulators. It shows that correlated materials respond intrinsically differently to light fields at ultrashort times, potentially impacting their behavior at all timescales.

Keywords: Attosecond, Correlated materials, Ultrafast dynamics, Hubbard model

*Speaker

Ultrafast THz generation in Bismuth ferrite

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Ultrafast light excitation is expected to trigger new states in solids, which are not accessible by varying the pressure, temperature, or doping in standard thermodynamic equilibrium conditions. The understanding of the lattice dynamics in ferroic compounds driven by an ultrashort light pulse is an exciting research direction due to the exceptional non-linear properties (optical, elastic, electric and magnetic) of ferroic and multiferroic materials. Multiferroics materials possess multiple ferroic orders, possibly coupled together, that opens new perspectives for many applications.
Here we investigate the ultrafast response to a short light pulse of the prototypical ferroelectric Bismuth ferrite (BiFeO3). BiFeO3 is the most famous multiferroic material, exhibiting both a large ferroelectric polarization and a non-collinear antiferromagnetic order at room temperature. The ultrafast transient response in BiFeO3 is monitored *via* terahertz (THz) emission spectroscopy technique. This technique allows to directly address carriers and lattice dynamics at picosecond timescale.
The BiFeO3 sample studied is a 180 nm-thick film featuring single ferroelectric domain. Above band gap excitation with femtosecond laser pulses at 400nm was used and the subsequent THz radiation was then characterized by an electro-optic sampling technique. From the THz transient we disentangle the carriers' dynamics (ultrafast current generation) from the lattice dynamics. The evolution of these two distinct dynamics is then tracked as a function of the light's polarization angle and the orientation of the ferroelectric polarization, to gain insight into the physical mechanisms at play in BiFeO3.

Keywords: terahertz THz ultrafast ferroic multiferroic

*Speaker

Non-equilibrium carrier dynamics in HgTe quantum dots revealed by mid-infrared pump-THz probe spectroscopy

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Colloidal semiconductor nanocrystals (NCs) exhibit unique optical and electronic properties induced by the quantum confinement effects, making them ideal candidates for a wide range of applications from visible to mid-infrared spectral range. Mercury telluride (HgTe) nanocrystals are emerging as promising active quantum materials for THz applications. Indeed, we demonstrated a broad absorption resonance centered at ≈4.5 THz resulting from multiple intraband transitions of single carriers between quantized states (1,2). Also, a coherent THz emission from large HgTe NCs excited by femtosecond optical pulses via second-order nonlinear effects has been recently demonstrated (3). The peak emission frequency is tunable from 0.4 to 0.8THz and induced by transient photocurrents arising from both photogalvanic and photon drag effects.

Here we probe the non-equilibrium carrier dynamics at low energy in large HgTe NCs using mid-infrared pump-THz probe experiment. We report on carrier lifetime as long as > 10 ps. Our study evidences that Auger recombination is irrelevant in this system. We attribute the main carrier recombination process to direct energy transfer from the electronic transition to the ligand vibrational modes and to nonradiative recombination assisted by surface traps. The dependance of the hot carrier dynamics with the lattice temperature highlights the role of the electron-phonon interaction. Also, our study shows a broad photoinduced absorption reaching up to 30 %, with spectrally resolved features. Our study opens interesting perspectives for the use of large HgTe NCs for the development of easily integrable THz optoelectronic devices such as emitters and detectors, and for quantum THz devices.

References
(1) N. Goubet, et al., J. Am. Chem. Soc., 140, 5033 (2018).
(2) T. Apretna, et al. Nanophotonics, 10, 2753 (2021).
(3) T. Apretna; et al. Appl. Phys. Lett. 121, 251101 (2022).

Keywords: Quantum dots, Nanocrystals, TeraHertz, Pump, Probe, Mid, Infrared

*Speaker

Ultrasmall and tunable TeraHertz surface plasmon cavities at the ultimate plasmonic limit

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Terahertz (THz) frequencies are particularly interesting due to the diversity of excitations that occur in this low-energy range. Their interaction with light can result in hybrid light-matter states, opening new ways to manipulate the properties of quantum materials (1). At these micrometric wavelengths, achieving strong localization of light within sub-wavelength structures is crucial to reach the ultra-strong light-matter coupling. So far, surface plasmons has been widely used for this purpose. But the usual cavity architectures are based on noble metals which inherently limit light confinement.
In this work, by relying on localized surface plasmon modes of the semiconductor indium antimonide (InSb), we achieved light confinement into unprecedentedly small THz cavity footprints. Remarkably, we find that these cavities can operate until the emergence of nonlocality and Landau damping, which together form the ultimate plasmonic limit. We demonstrate nonlocal plasmonic phenomena at exceptionally low frequencies and large spatial scales. Additionally, compared to conventional THz cavities, we achieve large frequency tunability with temperature (2). Thanks to the plasmonic tunability of semiconductor, our work opens new pathways for exploring sub-wavelength THz cavities with functional properties (3).
(1) F. Schlawin et al. Applied Physics Reviews, vol. 9, p. 011312, 2022
(2) I. Aupiais et al. Nat. Comm. 14, 7645 (2023) (3) I. Aupiais et al. arXiv :2404,15270 (2024)

Keywords: Terahertz, cavity, plasmonic, surface plasmon

*Speaker

Defects induce phase transition from dynamic to static rippling in graphene

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Many of graphene's remarkable properties are intrinsically linked to its inherent ripples. Defects, whether naturally present or artificially introduced, are known to have a strong impact on the rippling of graphene. However, how defects alter ripple dynamics in two-dimensional (2D) materials in general, and graphene in particular, remains largely unexplored. Here, using machine learning-driven molecular dynamics simulations, we reveal a fundamental connection between defect concentration and ripple dynamics in freestanding graphene sheets. Specifically, we find that at a critical concentration of approximately 0.1%, dynamic rippling undergoes a transition from freely propagating to static ripples. This is in quantitative alignment with the experimentally observed turning point in the non-monotonic scaling of the Young's modulus and emphasises the critical interplay between defects and material dynamics. Our work not only unveils the significant impact of defects on rippling dynamics in graphene but also paves the way to design two-dimensional devices with tailored properties.

Keywords: Graphene, rippling dynamics, numerical simulations, atomic defects

*Speaker

Tr-ARPES: Unveiling ultrafast dynamics and complex quantum phases in 2D materials

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Two-dimensional (2D) materials are one of the main topics of modern research in condensed matter, ever since the past decade that saw groundbreaking results on graphene. In these systems, a rich landscape of quantum phases can be found, across, many of which remain unexplored. Topological features, often inherent in these materials, can coexist with other quantum phases such as magnetism and correlations. hence, the ultrafast dynamics of these materials presents several features that are specific to their even richer non-equilibrium behavior.
We present here time-resolved ARPES (tr-ARPES) results on 2D materials showing a strong interplay between topological properties and correlation effects, in particular for excitonic effects in monolayer WTe_2, as well as between magnetism and topology, in layered compounds like MnSb2TeE4 . We discuss how analyzing the ultrafast response of the ARPES signal following optical excitation on can get the insight into the peculiar properties of these systems.

Keywords: tr, ARPES, topology, correlations, ultrafast dynamics

*Speaker

Unveiling the Electronic Properties of α-SnTe: From Ferroelectric Distortion to Unexpected Topological Surface State

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α-SnTe offers a combination of semiconducting and ferroelectric properties, further enriched by a non-trivial topological behavior. At room temperature, SnTe has a rocksalt atomic structure with a mirror symmetry that protects a metallic topological surface state. However, when the temperature drops below a critical point, a spontaneous structural distortion occurs that not only suppresses the topological surface state but also leads to a macroscopic electric polarization, resulting in a significant Rashba splitting in the valence band. Firstly, we track with angle-resolved photoemission spectroscopy (ARPES) the evolution of the Rashba splitting as an indicator of the structural distortion to provide insights into the ferroelectric transition, suggesting an order-disorder phase transition. Moving to the second part, we present recent data obtained through time-resolved ARPES. At odds with the expectation that ferroelectric SnTe(111) should behave as a trivial insulator, we demonstrate how photoinduced processes can trigger a topological transition, even while the atomic structure remains distorted. Thanks to a careful fluence and wavelength dependent study, we conclude by proposing a scenario based on Floquet physics.

Keywords: SnTe, TR, ARPES, Floquet, Ferroelectricity, Topology

*Speaker

Tracking the mid-infrared fine structure of quasi-1D excitons controlled by magnetic order

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We use phase-locked few-cycle mid-infrared pulses to probe internal Rydberg-like transitions of quasi-one-dimensional excitons in the magnetic semiconductor CrSBr (1). The experimentally observed fine structure encompasses a lifted degeneracy of the 2p states induced by the anisotropic optoelectronic properties of the crystal. Furthermore, the Coulomb correlations are effectively controlled via the magnetic structure.
By inducing a phase transition from antiferromagnetic to paramagnetic states either thermally or by applying an external magnetic field, we can switch excitons from strongly bound and monolayer-localized to weakly bound and interlayer-delocalized species (2). A state-of-the-art many-body theory fully captures these findings and identifies the spin restrictions of interlayer tunneling. In the paramagnetic phase, the reduced quantum confinement lowers the binding energy and increases the phase space for scattering. This in situ control of Coulomb correlations opens a path to shape phase transitions on demand.

(1) N. P. Wilson et al., "Interlayer electronic coupling on demand in a 2D magnetic semiconductor," Nat. Mater. 20, 1657–1662 (2021)
(2) M. Liebich, N. Nilforoushan et al., "Controlling Coulomb correlations and fine structure of quasi-1D excitons by magnetic order," under review (2024)

Keywords: van der Waals magnets, anisotropic excitons, ultrafast dynamics, mid, infrared spectroscopy, fine structure

*Speaker

Stochastic and deterministic approches for modelling laser induced ultrafast demagnetization of Nickel

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In this study, we delve into the ultrafast demagnetization procedure of pure Ni specimens by employing atomistic spin dynamics (ASD) and femtosecond laser heating. This method involves the numerical resolution of the stochastic Landau-Lifshitz-Gilbert (sLLG) and the dynamical Landau-Lifshitz-Bloch (dLLB) equations for each spin within a multi-spin system (1-3). The Curie temperature TC of Ni is first determined by sLLG and dLLB equations, which both eectively replicated the experimental values. However, upon analyzing the magnetization as a function of thermostat temperature, we reveal that these methods are less successful in capturing the shape and the behavior of the magnetization at lower temperatures. These inconsistencies are recognized challenges for classical spin models, and numerous research studies have endeavored to tackle this issue by employing a diverse range of correction techniques (4-5). We consider an alternative route by obtaining relevant informations from the magnon band structure, which can either be experimentally measured (6) or computationally determined for Ni systems, that better captures the energy transfers from the thermal reservoirs to the spins. Subsequently, we simulate the ultrafast demagnetization curves of Ni samples using femtosecond laser heating with both sLLG and dLLB methods hence correctly connected to the thermostats, and find that the results align with experimental data. We then establish that the dLLB equation can serve as an ecient substitute to model any all optical switching mechanism, by eliminating the need of multiple statistical realizations inherent to the sLLG approach.

(1) O.Eriksson, A.Bergman, L.Bergqvist, and J.Hellsvik, Atomistic spin dynamics: founda-tions and applications (Oxford university press, 2017)
(2) P.Thibaudeau, J.Tranchida, and S.Nicolis, IEEE Trans.Mag. 52, 1 (2016)
(3) J.Tranchida, P.Thibaudeau, and S.Nicolis, Phy.Rev.E 98, 042101 (2018)
(4) R.F.L.Evans, U.Atxitia, and R.W.Chantrell, Phys.Rev.B 91, 144425 (2015)
(5) M. Kuzmin, Phys.Rev.Lett.94, 107204 (2005)
(6) E. Thompson and J. Myers, Phys.Rev.153, 574 (1967). (7) E.Beaurepaire, et al. Phys.Rev.Lett. 76, 4250 (1996)

Keywords: Ultrafast demagnetization, Atomistique spin dynamics, Thermal fluctuations

*Speaker

NN2 - Mechanics at the nano-scale : in-situ measurements and simulation under extreme conditions

Atomic scale simulations of plasticity in Ag/Cu nanolayers

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In the last decades, modern synthesis methods, such as severe plastic deformation, were developed and applied to metallic lamellar composites to reduce the width of their layers to less than 100 nm. These nanostructured materials offer outstanding mechanical properties which are partly attributed to the increasing role played by interfaces in their plastic behavior. This role is crucial in the nanolamellar bi-metallic Cu/Ag composite. Indeed, experiments show that such composites can contain different kinds of interfaces, whose interaction with extended defects such as dislocations and mechanical twins is very different. In particular, the "heterotwin" interface is a strong obstacle for the transmission of twins, while they are easily transmitted across the "cube on cube" interface.
Atomistic simulations, and mainly molecular dynamics, are well-suited atomic scale tools to figure out the elementary mechanisms involved and study the specific plastic behavior of these nanostructured materials.
During severe plastic deformation, the material is submitted to a complex stress field. In this context, we performed molecular dynamics simulations of Cu/Ag nanolayers to investigate the plastic behavior of systems under different stress fields. The effect of the stress orientation, as well as that of interface defects, provoking the nucleation and slip of either Shockley partial dislocations or extended perfect dislocations, is then analyzed and discussed in this presentation.

Keywords: Cu/Ag nanolayers, interface, plasticity, molecular dynamics

*Speaker

ENRICHING NANOINDENTATION WITH IN SITU ELECTRICAL MEASUREMENTS AND SEM OBSERVATIONS

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A nanoindentation set-up coupled to electrical measurements and integrated into an SEM will be presented. Its application to the understanding of the interplay between mechanical and electrical behaviors of materials will then be discussed.

First, it will be shown how electrical measurements can be used to monitor the contact area between the indenter tip and the sample during indentation. The case of ideal materials (oxide-free surface (1)) or real materials (with a passivating surface layer (2)) will be considered. The in-situ SEM configuration is used for the precise positioning of indents on a complex system (precision ~100nm, Figure 1). The local mechanical properties will then be extracted accurately at a micrometer-scale (Figure 2).

Then, the interplay of mechanical and electrical behaviors of dielectric thin films will be addressed. First, we will show how a mechanical stress can modify the electrical conduction mechanism in a dielectric film (3). Counterintuitive observations will be fully explained numerically (by FEM analysis) by correcting the Poole-Frenkel conduction law with a strain-dependent factor. A threshold strain is identified as the keystone linking this strain-dependent conduction to the current line distribution within the dielectric. Finally, we will briefly show how an electrical stress can degrade the mechanical properties of dielectrics.

This presentation aims at demonstrating the strength of coupling electrical measurements to nanoindentation, either to process mechanical raw data or to understand the strong mechanical-electrical interplay in materials.

Keywords: Electrical, nanoindentation testing, In, situ SEM, Contact area monitoring.

*Speaker

The role of grain boundaries on plasticity in hexagonal crystals: an atomistically informed discrete dislocation dynamic study

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Hexagonal close-packed (HCP) metals and alloys exhibits specific characteristics, such as high anisotropy, high strength-to-weight ratio and limited plasticity. This make Ti or Mg base alloys, for exemple, excellent choices for applications where strength and low weight are essential, e.g. aerospace, automotive, and medical industries. However, the comprehension of plasticity mechanisms in such materials remains a major challenge, and grain boundaries play a major in this context.
In this work, we considered tilt and twist grains boundaries (GB) in Ti and Mg within the Coincidence Site Lattice (CSL) theory. We performed molecular static simulations to study their optimized atomistic configuration and determined their Nye dislocation density tensor. Based on a novel atomistic to continuum description of crystal defects with dislocation density fields, we performed discrete dislocation dynamic (DDD) simulations fed by these atomistic characterization. More specifically, we use an hybrid field dislocation mechanics (FDM) - DDD approach to capture the mechanical fields induced by dislocation-GB interaction during nanomechanics. This uniquely allow our DDD mesoscale simulation to account for the precise characteristics of low and high angle GB during the plastic deformation of a polycrystalline sample.

Keywords: FDM, DDD, Polycristall, Molecular Static, Nye Tensor, Grain Boundaries

*Speaker

Reversible Raman D-band evolution for the in situ probing of the pressure-induced collapse of carbon nanotubes

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The intrinsically vast variety of properties of carbon nanotubes can be further expanded if we take into account their effective geometrical state. When subjected to high pressure in anvil cells, nanotubes can transition from classical circular cross-section to different oval or collapsed geometries, with evolution depending on their diameter and their number of walls (1). In situ experimental probes which would allow to discriminate between circular or collapsed states, and to accurately follow the intermediate steps, are of high interest.
Here we make use of a sapphire anvil cell (instead of usual diamonds) to open the D-band Raman spectroscopic window of carbon nanotubes. We follow the appearance of a defect-free Raman D-band contribution in bundled samples which is assigned to their pressure-induced radial buckling (2), as already discussed on radially collapsed nanotubes at ambient pressure (3). On pressure release, this contribution to the D-band disappears, confirming the reversibility of the process and our interpretation. We further applied this approach to the study of isolated tubes, following the collapse transition of a 1.7 nm diameter starting at 1 GPa and ending at 2 GPa. This demonstration of a new direct spectroscopic signature opens up new roads for the detection and characterization of the shape evolution of nanotubes induced by pressure, potentially resolved at the single nanotube scale to unveil chirality and local environment effects.

(1) *Magnin et al. Carbon 178 (2021) 552–562*

(2) *Galafassi et al. Under Review*
(3) *Picheau et al, ACS Nano (2021), 15, 596–603*

Keywords: high pressure, anvil cell, nanotube, Raman spectroscopy, buckling, collapse

*Speaker

Intergranular ductile fracture in alpha brass alloys

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In-situ HRTEM tensile testing has been used to characterize the ductile fracture of Cu15%Zn and Cu30%Zn alpha brass alloys at room temperature. A decomposition of the Cu-Zn alpha (FCC) solid solution is observed in-situ during the last phase of the normally ductile fracture leading to the formation of a Cu4Zn8 Hume-Rothery alloy at the nano-scale. This strain induced phase transform in an otherwise stable solid solution occurs at extremely fast rate. This decomposition is responsible for the apparition of nanoscale Hume-Rothery Cu4Zn8 phase grains followed by the "ductile" like fracture but surprisingly with an intergranular propagation mode. At the lower zinc content, this transformation is in competition with the classical vacancy mediated void initiation, gowth and coalescence. The implications for fracture of this class of materials will be discussed.

Keywords: grain boundaries, solid solution decomposition, ductile fracture, Hume, Rothery alloys, HRTEM, in, situ

*Speaker

Elucidating the mechanics of reinforcement in graphene-based composites using large-scale molecular dynamics simulations

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Using large-scale classical molecular dynamics up to tens of millions of atoms, the mechanics of nano-reinforcement of graphene-based composites have been investigated (1). Our simulations show that significant quantities of large, defect-free, and predominantly flat graphene flakes are required for successful enhancement of materials properties in excellent agreement with experimental and proposed continuum shear-lag theories. The critical lengths for enhancement are approximately 500 nm for graphene and 300 nm and for graphene oxide (GO). The reduction of Young's modulus in GO results in a much smaller enhancement of the composite's Young's modulus. Our simulations further reveal that the flakes should be aligned and planar for optimal reinforcement. Undulations substantially, potentially caused by natural vibration modes of the flakes, degrade the enhancement of materials properties. (1) Suter, James L., Maxime Vassaux, and Peter V. Coveney. "Large-Scale Molecular Dynamics Elucidates the Mechanics of Reinforcement in Graphene-Based Composites." *Advanced Materials* 35.35 (2023): 2302237.

Keywords: nanocomposites, graphene, polymer, molecular dynamics, shear lag theory

*Speaker

Strain evolution in nanocrystals under high pressure tracked with Bragg Coherent X-ray Diffraction Imaging

Abdelrahman Zakaria * [1], Sarah Yehya , Pierre Fertey , Steven Leake [2], Bjorn Wehinger [3], Mohamed Mezouar [3], Mor Levi [4], Eugen Rabkin , Marie-Ingrid Richard [2,5], Stéphane Labat

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Tremendous novel properties (1–4) and new forms of materials (5) have been revealed exclusively under high-pressure. Measuring and understanding the internal strain changes in response to external pressure provides critical information to unveil the origin of unconventional behavior of crystalline materials in high-pressure environments.

Keywords: BCDI, Defect stability, Diamond anvil cell, phase retrieval, dislocation, Metallic core, shell nanoparticles, High pressure

*Speaker

NN5 - Properties of metal clusters and nanoparticles

Electronic and Optical Properties of Size-selected Metal Cluster Polyanions

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In contrast to atoms, molecules and clusters can bind more than a single excess electron. The extra charge gives rise to a Coulomb barrier, which modifies the electronic structure and may lead to negative electron binding energies. Details of the confining potential are extracted from the photoelectron spectra of silver clusters and compared to theory. Further, the digital trap-based electron attachment method allows to produced double magic clusters The optical response, finally, shows large detachment cross section, which can be assigned to plasmon excitations, whereas direct photoemission selects the fastest Landau fragmentation channel.

Keywords: metal clusters, polyanions, electron spectroscopy, optical spectra

*Speaker

Optical spectra of silver clusters and nanoparticles of all sizes from the TDDFT+U method

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The modeling of the Localized Surface-Plasmon Resonance (LSPR) in silver clusters and nanoparticles depends on exchange-correlation functionals (xc-functionals) within Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT). While optical absorption spectra calculated using hybrid and range-separated hybrid functionals are known to have excellent agreement with experiment (1-3), their computational cost restricts their use to smaller clusters. Simple functionals such as LDA or GGA fail to describe the 4d electrons accurately, generally placing them too close to the Fermi energy. Consequently, the inter-band transitions start at lower energies than expected, leading to too low LSPR energies and over-broadening of the LSPR peak. (RT)TDDFT+U emerges as a promising alternative (4,5), which improves the description of the 4d electrons by adding an empirical Hubbard-like effective U correction to the Kohn-Sham Hamiltonian. In our present work, we carried out (RT)TDDFT+U calculations using the same value of the effective U parameter that has been found to provide good results in bulk silver. Both the electron-hole-type discrete spectra of the smallest clusters and the broad plasmon resonances of the larger sizes (≈1000 atoms) are obtained. The good agreement with experiment for all sizes indicate that the U parameter is surprisingly transferable.

(1) Yu, C. *et al.,* Nanoscale 10, 20821 (2018).

(2) Lunskens, T. *et al.,* Phys. Chem. Chem. Phys. 17, 17541 (2015).

(3) Lecoultre, S. *et al.,* J. Chem. Phys. 134, 184504 (2011).

(4) Tancogne-Dejean, N. *et al.,* J. Chem. Phys. 152, 124119 (2020).
(5) Tancogne-Dejean, *et al.,* Phys. Rev. B 96, 245133 (2017).

Keywords: metal clusters, surface, plasmon resonance, optical properties, TDDFT, DFT+U

*Speaker

Metal clusters: efficient and accurate computational approaches for optical properties

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We report about new algorithms and computational protocols for the calculations of optical properties and able to manage large metal clusters, included in the last version of the ADF (AMS) program. The use of efficient simulation algorithms, the complex polarizability polTDDFT approach (1) and the Hybrid-Diagonal Approximation (HDA) (2,3), allows us to employ a variety of exchange-correlation (xc) functionals at an affordable computational cost. We are thus able to show, first, how the optical response of this prototypical compound, especially but not exclusively in the absorption threshold (low-energy) region, is sensitive: (1) from a methodological point of view, to the choice of the xc-functionals employed in the Kohn-Sham equations and the TDDFT kernel, and (2) from a chemical-physical point of view, to the choice of the MPC geometry. By comparing simulated spectra with experimental data, we then demonstrate how a hybrid xc-functional employed in both the Kohn-Sham equations and the diagonal TDDFT kernel at the crystallographically-determined experimental geometry is able to provide a consistent agreement between simulated and measured spectra across the entire optical region. Single-particle decomposition analysis tools finally allow us to understand the physical reason of the failure of non-hybrid approaches. Finally we will consider also the Electronic Circular Dichroism (ECD) in plasmonic chiral systems and clusters protected by ligands. The role of conformational dynamics of the ligand will be also addressed.
(1) O. Baseggio, G. Fronzoni, M. Stener, J. Chem. Phys. 143 (2016) 024106.

(2) M. Medves, L. Sementa, D. Toffoli, G. Fronzoni, A. Fortunelli, M. Stener, J. Chem. Phys. 152 (2020) 184102.
(3) Pierpaolo D'Antoni, Marco Medves, Daniele Toffoli, Alessandro Fortunelli, Mauro Stener, and Lucas Visscher, J. Phys. Chem. A 127 (2023) 9244.

Keywords: metal clusters, photoabsorption, circular dichroism, TDDFT

*Speaker

Nonlinear optical properties of silver nanoprisms covalently and noncovalently attached to graphene oxide

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[2] International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University – India

This work aims at exploring how the nonlinear optical properties of silver nanoprisms are effected by the interaction with graphene oxide sheets. For this purpose, we produce nanocomposites consisting of citrate passivated silver nanoprisms anchored both electrostatically and covalently on graphene oxide nanosheets in a cost-effective and reproducible manner. The novelty of the technique hinges on the covalent functionalization of silver nanoprisms on to graphene oxide (GO) nanosheets according to the 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride crosslinking method, using the existing carboxylic groups present both at the surfaces of the nanoclusters and the GO nanosheets. The formed hybrid nanocomposites were characterized by TEM measurements and exhibit nonlinear optical (NLO) properties, in particular a strong second harmonic scattering response as well as a multiphoton excited fluorescence spectrum characterized by a broad band in the visible range between 350 and 700 nm. In addition the NLO response is sensitive to the nature of interaction (electrostatic or covalent) and might be accounted for different charge transfer capability between covalently or electrostatically bound silver particles onto graphene oxide. Such nanocomposites are therefore promising for new applications in the areas of optoelectronics and photovoltaics.

Keywords: 2D materials, metal nanoparticles, interface, nonlinear optic properties, charge transfer, graphene oxide

*Speaker

Surface Effects For FeRh Clusters: Reaching Metallic Nanomagnets On An Oxide Substrate

Florent Tournus * [1], Sara Gonzalez [2], Ingrid Canero-Infante [2], Bertrand Vilquin [2], P. Rojo-Romeo [2], Guillermo Herrera [1], Olivier Boisron [1], Damien Le Roy [1], Véronique Dupuis [1], Matthieu Bugnet [3], A. Resta [4], A Vlad [4], A Coati [4], P. Schoeffmann [4], E. Otero [4], P. Ohresser [4]

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[4] Synchrotron SOLEIL – CNRS, CEA – France

Multiferroic composites are promising systems where the interfacial coupling between different ferroics can be driven by magnetic, voltage and strain mediation approaches to explore new technological applications (1). Bulk FeRh alloy chemically ordered in the CsCl-type B2 phase, is characterized by a remarkable magneto-structural transition close to room temperature. As in nanoscale systems, the magnetic order is very sensitive to interfaces, strain and surface terminations (2,3), we have deposited FeRh nanocrystals (NCs) on perovskite oxides substrates. Here, we focus on 3 to 7 nm FeRh NCs deposited on SrTiO3 (001), where preferential orientation effects are met (4). Concerning the metallicity of Fe atoms, which is intimately linked to the magnetic properties, we observe that unprotected FeRh particles are (partially) oxidized but can be reduced by annealing at a moderate temperature, lower than the one necessary to promote the chemical order transition from the A1 to B2 phase of FeRh. This reversible process has been established using laboratory in situ X-ray photoelectron spectroscopy investigations (XPS), and has also been observed using X-ray absorption spectroscopy (SOLEIL synchrotron), simultaneously to X-ray magnetic circular magnetic dichroism to follow the impact on the magnetic properties. In addition, the effect of in situ annealing and oxidation has been followed of the intensity of grazing incidence X-ray diffraction FeRh peaks, confirming that the oxidation is occurring at the outer surface of the metallic clusters rather that at the interface with the oxide substrate.

1. Eerenstein et al. Nature **442**, 759 (2006); Spaldin et al. Nature Mater. **18**, 203 (2019)
2. Hillion et al. **Phys. Rev. Lett. 110**, 087207 (2013) ; Herrera et al. **EPJD 97**, 32 (2022)
3. Liu et al. Euro. Phys. Lett. **116**, 27006 (2016) ; Lewis et al. J. Phys. D **49**, 323002 (2016)
4. Reyes et al. Phys. Rev. B **109**, 245410 (2024)

Keywords: Clusters, Nanomagnets, Oxidation, Surface

*Speaker

Towards Stable Nanoalloys Mixing Au or Ag With Al or In with Localized Surface Plasmon Resonances in the UV Range

Matthias Hillenkamp * [1], Emmanuel Cottancin , Elise Camus , Murilo Moreira , Michel Pellarin , Nicholas Blanchard , Olivier Boisron [2], Jean Lermé [3], Lucian Roiban [4], Pascal Andreazza [5]

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[4] MATEIS, INSA de Lyon, Bât. Blaise Pascal, 69621 Villeurbanne Cedex – Université de Lyon, Institut National des Sciences Appliquées de Lyon, Université Claude Bernard - Lyon 1, CNRS : UMR5510 – France

[5] Interfaces, Confinement, Matériaux et Nanostructures (ICMN) – Université d'Orléans, Centre National de la Recherche Scientifique, Université d'Orléans : UMR7374, Centre National de la Recherche Scientifique : UMR7374 – 1b rue de la Férollerie, CS 40059, 45071 Orléans cedex 2, France

Bimetallic nanoparticles (BNPs) are promising for fundamental research and applications, as their physicochemical properties can be tuned or enhanced with respect to the monometallic particles. In this context, the atomic and chemical structure and the optical response of AxB1-x BNPs combining gold or silver (A) with aluminium or indium (B) were investigated for various stoechiometries in order to examine if stable alloyed phases exist and show localized surface plasmon resonances (LSPR) in the UV range. The structure and morphology of matrix embedded-BNPs of a few nanometers, produced by laser vaporization, were analysed by transmission electron microscopy (TEM) and optical absorption measurements compared with Mie calculations in the dipolar approximation. The BNPs' internal structure was investigated by in situ x-ray photoelectron spectroscopy and synchrotron-based x-ray scattering techniques giving complementary information about the chemical state of the constituent elements and structural heterogeneities in the BNPs. The complementary techniques of characterization show that silica-embedded silver-based Ag-In and Ag-Al BNPs form metallic silver-rich alloyed cores surrounded by an indium or aluminium oxide shell. The initial LSPRs are in the UV range for both systems, but the difference in the kinetics of oxidation between indium and aluminium involves less blue-shifted LSPRs for Ag-Al BNPs. In the case of gold-based BNPs, we investigated the chemical structure of the gold-based BNPs in various matrices (carbon, silica, alumina) using energy-dispersive X-ray spectroscopy in a STEM and separated metallic from oxidized phases using unsupervised machine learning techniques such as principal component analysis and non-negative matrix factorization. The characterization of the metallic structures was achieved by complementary imaging in HRTEM, STEM-HAADF and SAED. Finally, by combining imaging, diffraction, and spectroscopy techniques, we show that In2Au is a good candidate to correlate plasmonic and structural properties as it shows an LSPR in the UV range and improved stability against oxidation.

Keywords: nanoalloy particles, surface plasmon

*Speaker

Dynamics of Metallic Catalysts Under Reactive Conditions

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For several decades, chemists and physicists have focused on researching increasingly efficient heterogeneous catalysts. During catalytic reactions, the catalyst, in the form of supported metallic particles (isolated atoms, clusters, and/or nanoparticles), interacts with reactants at operating temperatures. Reactants can adsorb on the particle surfaces, modifying their geometric and electronic structures, thus forming the true active phase, which can differ from the initial material introduced into the reactor. To control and optimize catalyst performance, it is essential to understand, at the atomic scale, the interactions between particles, oxide support, and reactants.
Given the computational cost of theoretical methods such as DFT, catalytic surfaces are often modeled as rigid surfaces interacting with isolated molecules. This approach ignores the structural dynamics and chemical order changes induced by the reactive environment, even though these variations play a crucial role in catalytic processes. Today, the major challenge is to predict and describe the composition and structure of catalyst surfaces and their evolution over time to correctly identify active sites and control the reaction's elementary steps.

In this presentation, I will outline the state-of-the-art methods for modeling the structural dynamics of catalysts and present results from several studies on the structural dynamics of supported nanoparticles in the presence of reactive gases. I will show surface changes and their impact on reactivity, demonstrating how this knowledge can improve catalyst design.

(1) H. Guesmi. et al. Gold Bull. **2013**, 46, 213-219

(2) Q. Wang, et al. Faraday Discuss. **2023**, 241, 375-388
(3) A. Nassereddine, et al. Small **2021**, 2104571

Keywords: Nanoparticles, metallic clusters, catalytic properties, DFT, dynamics

*Speaker

Subnanometer Clusters in Oxidative Dehydrogenation Reactions: Knobs for Controlling Activity & Selectivity

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Subnanometer Clusters in Oxidative Dehydrogenation Reactions:
Knobs for Controlling Activity & Selectivity

The presentation will focus on catalysis, performed under realistic reaction conditions of pressure and temperature, by supported monodisperse subnanometer clusters made of a handful of atoms, supported on technologically relevant oxide- and model carbon-based supports.

The performance of Co, Cu, Pd and CuPd clusters in the oxidative dehydrogenation of cyclohexene and cyclohexane will be discussed (1-4), where the atomic precision design of mono- and bimetallic clusters allows for the fine-tuning of their activity and selectivity by varying the size and composition of the clusters in an atom-by-atom fashion and by the choice of suport material and varying reaction conditions.

References:

(1) Jašík, J.; Valtera, S.; Vaidulych, M.; Bunian, M.; Lei, Y.; Halder, A.; Tarábková, H.; Jindra, M.; Kavan, L.; Frank, O.; Bartling, S.; Vajda, Š. Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer Cu4-nPdn (0≤n≤4) tetramer clusters: The effect of cluster composition and support on performance. *Faraday Discuss.* **2023,** *242*, 70-93. DOI: 10.1039/D2FD00108J, link
(2) Valtera, S.; Jašík, J.; Vaidulych, M.; Olszówka, J.E.; Zlámalová, M.; Tarábková, H.; Kavan, L.; Vajda, Š. Atom by Atom Built Subnanometer Copper Cluster Catalyst for the Highly Selective Oxidative Dehydrogenation of Cyclohexene. *J. Chem. Phys.* **2022**, *156*, 114302-114310. DOI: 10.1063/5.0065350, link
(3) Halder, A.;Ha, M.-A.;Zhai, H.;Yang, B.;Pellin, M.J.;Seifert, S.; Alexandrova, A.N.; Vajda, S. Oxidative Dehydrogenation of Cyclohexane by Cu *vs* Pd Clusters: Selectivity Control by Specific Cluster Dynamics. *ChemCatChem.* **2020**, *12*, 1307–1315. DOI: 10.1002/cctc.201901795, *front cover,* link
(4) Lee, S.; Halder, A.; Ferguson, G.A.; Seifert, S.; Winans, R.E.; Teschner, D.; Schlögl, R.; Papaefthimiou, V. ; Greeley, J.; Curtiss, L.A.; Vajda, S. Subnanometer Cobalt Oxide Clusters as Selective Low Temperature Oxidative Dehydrogenation Catalysts. *Nat. Commun.* **2019**, *10*, Article number: 954, p. 1-9. Published on line February 27, 2019, DOI: 10.1038/s41467-019-08819-5, *Communication*, link; *Editors' Highlight*

Keywords: nanocatalysis, oxidative dehydrogenation, subnanometer clusters, cyclohexane, cyclohexene

*Speaker

Reactivity of High Entropy Alloy Nanoparticles under O2 and CO Oxidation reaction studied by in-situ Transmission Electron Microscopy

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Carbon monoxide (CO) contamination has a major input in climate change. An efficient way to reduce its contribution is to oxidize CO into CO2. Therefore, many noble metal nanoparticles (NPs) has been proposed as efficient catalysis of CO oxidation reaction. However, considering the price increase of noble metals and their rarity, there is a need to come up with new catalysts that involve less of noble metals. Accordingly, High Entropy NanoAlloys (HENA) represent a new promising catalyst with tunable properties.
In this contribution, we exploit aberration-corrected in situ STEM investigations to reveal the structural and chemical evolution of single CoNiCuPtAu NPs between 100∘C and 700∘ C under O2. The HENA were synthesized using pulsed laser deposition1 and studied by in-situ gas experiments performed at atmospheric pressure combining atomic-scale STEM imaging with chemical analysis.

In comparison with our previous in-situ heating experiments of the CoNiCuPtAu NPs performed under vacuum, gas in-situ experiments show that the NP growth, that is governed by coalescence, is slowed down with the presence of O2 and that the NPs are more stable. Unlike NPs annealed under vacuum, under O2 no evaporation was observed, however structural and morphological changes of NPs were reported.

Ni-poor NPs showed facets reshaping at 100∘C (figure 1a). The NPs keep their CFC structure in the core and only the external layer will be oxidized (figure 1a) but, interestingly, at higher temperatures (up to 600∘C), the oxide layer will disappear (see figure 1b).

Conversely, Ni-rich NPs showed demixing and formation of Ni/Co oxide platelets between the NPs (see figure 2a) which remain stable even at high temperature (figure 2b).
Besides, the oxidation of HENA also causes the formation of nanovoids in NPs, phenomena known as Kirkendall effect, that we can see in figure 3.This effect will still be present at higher temperatures.

Keywords: Oxidation, in, situ microscopy, kirkendall effect

*Speaker

Polymeric matrix coatings based on multimetallic nanoparticles

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[2] Extreme Conditions and Materials: High Temperature and Irradiation – Extreme Conditions and Materials: High Temperature and Irradiation (CEMHTI),, CNRS-Université d'Orléans, UPR3079 , 1 Av. de la Recherche Scientifique, 45100 Orléans – France

Multifunctional metal/polymer nanocomposite coatings, comprising Ag and Pt dispersed within a poly (dipropylene glycol diacrylate) polymer matrix, have been developed to enhance desired properties and functionalities. Atomic vapor deposition stands out for its ability to provide a continuous flux of atoms during growth, resulting in moderate kinetic energy, low polydispersity of nanoparticle assemblies, and high throughput. This approach also offers significant potential for enhancing the performance of nanocomposites by enabling controlled growth of structural properties of thin films. To date, atomic vapor deposition methodology has been limited to monometallic (Ag,Pt) and bimetallic nanoparticles (CoAg, AgPt,CoPt, AgAl, AgIn) dispersed on silica matrices. However, strategies to produce long-term stable nanocomposites with persistent and durable structural/optical properties remain undeveloped. Polymers typically serve as matrices, facilitating ordering and anisotropic orientation on surfaces, and controlling the size, morphology, and separation distances. The substrate surface plays a crucial role, as nucleation phenomenon is primarily influenced by low-energy sites such as surface defects or impurities adsorbed on the surface, along with factors such as sticking and diffusion coefficients, and the nature and strength of substrate-adsorbate interactions. In our preliminary work, an organic component was deposited on Si/SiO2 surfaces via a photochemical process, followed by coating with a thin layer of AgPt through atomic vapor deposition to create a hybrid material with unique optical, structural, and physicochemical properties. This approach offers a novel perspective on nanocomposite synthesis, utilizing two complementary methods. Our primary objectives include minimizing polydispersity in size distribution and controlling nanoparticles' organization within the polymeric matrix.
Specifically, we conducted a parametric study to assess the influence of various experimental parameters-including deposition rate, beam atomic flux, kinetic energy, simultaneous/sequential deposition, compositions, and substrate temperature-on the structural and optical properties of nanocomposites. Complementary experimental techniques have been indispensable in unequivocally characterizing these complex metal/polymer nanostructured systems.

Keywords: bimetallic nanoparticles, alloys, fabrication, characterizations, optical and structural properties, plasmonics, atomic vapor deposition, metal/polymer nanocomposites

*Speaker

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Lundi 28 Octobre

Accueil 10h - 13h30

Ouverture 13h15-14h00
Grand Amphi

Plénière 14h00 - 14h50
Denis Bartolo
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Plénière 15h00 - 15h50
Ivan Favero, prix Ancel
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Café 16h00 - 16h40
Salle de conférence

Mini - colloques 1
16h45 - 18h45

SMMP1_1 Charve	**NN1_1** 405	**MP3_1** 201
SMMP4_1 Massiani	**BAM2_1** 407	
SMMP6_1 SciencesNat	**2DMS2_1** 205	
	2DMS4 207	

Mardi 29 Octobre

Plénière 8h30 - 9h20
Ludovic Berthier
Grand Amphi

Plénière 9h30 - 10h20
MP Besland, L Cario, B Corraze, E Janod, J Tranchant, Prix Félix Robin
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

Posters et Exposants 11h10 - 12h00
Salle de conférence

Déjeuner 12h00 -13h20
Salle de conférence

3 Semi-plénières
13h20 - 14h10

Anne Tanguy SciencesNat	**Martien Den-Hertog** Charve	**Cécile Sykes** Massiani

Mini - colloques 2
14h30 - 16h30

SMMP1_2 Charve	**NN1_2** 405	**MP3_2** 201
SMMP4_2 Massiani	**NN4** 408	**2DMS2_2** 205
SMMP6_2 SciencesNat	**BAM2_2** 407	**2DMS1_1** 207

Café 16h30 - 17h15
Salle de conférence + 204 + 404

Mini - colloques 3
17h15 - 18h45

SMMP1_3 Charve	**NN1_3** 405	**NN3** 408
SMMP4_3 Massiani	**BAM3_1** 407	**2DMS2_3** 205
SMMP6_3 SciencesNat	**BAM5** 413	

Mercredi 30 Octobre

Plénière 8h30 - 9h20
Benoît Roman
Grand Amphi

Plénière 9h30 - 10h20
Frédéric Mila, prix Charpak-Ritz
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

3 Semi-plénières
11h10 - 12h00

Thomas Cornélius SciencesNat	**Christopher Bäuerle** Charve	**Cécile Monteux** Massiani

Déjeuner 12h00 - 13h20
Salle de conférence

3 Semi-plénières
13h20 - 14h10

Amélie Juhin, prix Ancel SciencesNat	**Freek Massee** Charve	**Véronique Lazarus** Massiani

Mini - colloques 4
14h30 - 16h30

SMMP4_4 Massiani	**NN2_1** 405	**2DMS1_2** 207
SMMP5_1 Charve	**BAM3_2** 407	**2DMS3_1** 208
SMMP6_4 SciencesNat		**IA2** 206

Café 16h30 - 17h15
Salle de conférence + 204 + 404

Mini - colloques 5
17h15 - 18h45

SMMP3 Massiani	**NN2_2** 405	**MP1** 201
SMMP5_2 Charve	**NN5_1** 408	**2DMS5_1** 205
	BAM1_1 SciencesNat	**PSI2** 203
	BAM4_1 407	**2DMS3_2** 208

GALA 19h30 - 23h00

Jeudi 31 Octobre

Plénière 8h30 - 9h20
Emmanuelle Tsitrone
Grand Amphi

Plénière 9h30 - 10h20
Annie Viallat
Grand Amphi

Café 10h30 - 11h00
Salle de conférence

3 Semi-plénières
11h10 - 12h00

Magali Putero SciencesNat	**Wiebke Drenckhan** Charve	**Laurent Lombez** Massiani

Déjeuner 12h00 - 13h20
Salle de conférence

2 Semi-plénières
13h20 - 14h10

Michel Hehn SciencesNat	**Vincent Bouchiat, Behnaz Djoharian prix Yves Rocard** Grand Amphi

Mini - colloques 6
14h30 - 16h30

SMMP2_1 Massiani	**NN2_3** 405	**MP2_1** 201
SMMP5_3 Charve	**NN5_2** 408	**2DMS5_2** 205
IA1 206	**BAM1_2** SciencesNat	**BAM4_2** 407
	PSI1 203	

Café 16h30 - 17h00
Salle de conférence + 204 + 404

Mini - colloques 7
17h00 - 18h30

SMMP2_2 Massiani	**NN5_3** 408	**MP2_2** 201
SMMP5_4 Charve	**BAM1_3** SciencesNat	**2DMS5_3** 205

PSI3 - PSI4
413

*TOUTES LES SALLES AVEC UN NUMÉRO SONT LOCALISÉES DANS LE BÂTIMENT 15.