

**JDN
2024**

**JOURNÉES DE LA DIFFUSION
NEUTRONIQUE**
Multidisciplinary science
with neutrons

Book of abstracts



Ile de Porquerolles
Sept. 30 - Oct. 3



Welcome to the **Journées de la Diffusion Neutronique 2024**, a multidisciplinary science conference gathering of experts, researchers and young scientists in the field of neutron scattering. This year, we are pleased to host this conference on beautiful island of Porquerolles, a perfect place for inspiring scientific discussions and initiating new collaborations.

Neutron scattering continues to be an indispensable tool in probing the structure and dynamics of matter, driving progress across a wide range of fundamental and applied research. Various topics will be covered in the thematic sessions organized in the respective fields of **Biology, Condensed Matter, Instrumentation, Soft Matter** and **Magnetism**.

Each of this session will start with an invited plenary talk (40 min) and a keynote talk (30 min). It will be followed by several oral communications.

This year's program is enriched by a **special session on "Neutrons Beyond Scattering,"** that will explore cutting-edge applications of neutrons in areas beyond traditional scattering methods.

At last, sessions will be dedicated to **Neutron Scattering Associations** (SFN and ENSA), **News from the facilities and the French Federation of Neutrons** (ESS, ILL, LLB and 2FDN) and the **SFN PhD award Ceremony**.

The organising committee wish you a pleasant conference and very fruitful scientific discussions



Vanessa Coulet, MADIREL
Carine Chassigneux, MADIREL
Sandrine Bernardini, IM2NP/MADIREL
Daniel Ferry, CINaM
Vasile Heresanu, CINaM
Peter Fouquet, ILL
Lucile Mangin-Thro, ILL
Frédéric Ott, LLB

PROGRAM

Monday, September 30

15:00-15:50	Registration and coffee	
15:50-16:00	Opening	
16:00-17:10	BIOLOGY p 7 Chair: Giovanna Fragneto	
16:00-16:40	Plenary: Fabienne Testard <i>Nanostructured nanoparticles made of self-assembled bioconjugates: formation and interaction with proteins</i>	
16:40 - 17.15	Keynote: Francesca Natali <i>Probing biology with neutrons, from environment to health</i>	
17:15-18:00	BIOLOGY p 9 Chair: Sylvain Prevost	CONDENSED MATTER p 13 Chair: Diane Rebiscoul
17:15-17:30	Christian Beck <i>Following the Dynamics during Crystallization with Time-Resolved Scattering</i>	Marc de Boissieu <i>Phasons modes in the incommensurately modulated Rb₂ZnCl₄ phase</i>
17:30-17:45	Luca Genovese <i>First-principles characterization of protein-protein and protein-ligand interactions</i>	Max Warburton When water meets solids: unexpected liquid-solid THz dynamic coupling
17:45 - 18:00		Michael M. Koza <i>Systematic study of silver chalcogenides for wearable thermoelectrics</i>
18:10-19:30	NEUTRON SCATTERING ASSOCIATIONS European Neutron Scattering Association (ENSA) General Assembly of the French neutron Scattering association (SFN) – Pascale Launois Annual report and financial statement. Election of the new board members	
20:00	Dinner	

Tuesday, October 1 (Morning)

9:00-10:10	CONDENSED MATTER p 11 Chair: Denis Morineau	
9:00- 9:40	Plenary: Stéphane Rols <i>The perfect match! Neutron Spectroscopy reveals the fine structure of quantum excitations in endofullerenes</i>	
9:40-10:10	Keynote: Valentina Giordano <i>The microscopic origin of a glass-like thermal transport: the role of disorder</i>	
10:15 - 11:00	CONDENSED MATTER p 16 Chair: Pascale Launois	MAGNETISM p 47 Chair: Francoise Damay
10:15-10:30	Thomas Marescot <i>Intrusion, extrusion and phase transitions of water in hydrophobic nanopores</i>	Frédéric Bourdarot <i>TbB4 under high magnetic field</i>
10:30-10:45	Diane Rebiscoul <i>How cations - silica surface interactions affect water dynamics in nanoconfined electrolyte solutions</i>	Romain Sibille <i>Neutron scattering signatures of quantum spin ice in cerium pyrochlores</i>
10:45-11:00	Nadim Kamar <i>Deep Eutectic Solvents: Properties Induced by Nanometric Confinement</i>	William Liege <i>Search for loop currents in the kagome superconductors CsV3Sb5.</i>
11:00-11:30	Coffee	
11:30-12:20	INSTRUMENTATION p 23 Chair: Robert Cubitt	
11:30-12:00	Invited: Florence Porcher <i>The DREAM multipurpose diffractometer at ESS</i>	
11:55 - 12:20	Invited: Nicolas Pichoff <i>ICONE project Presentation</i>	
12:30-14:00	Lunch	

Tuesday, October 1 (Afternoon)

14:00-14:25	INSTRUMENTATION p 25 Chair: M. Koza	
14:00-14:25	Invited: Nicolas Martin <i>SAM: the new LLB small-angle neutron scattering instrument at the ILL</i>	
14:30-15:30	INSTRUMENTATION p 26 Chair : Alexis Chennevière	CONDENSED MATTER p 19 Chair : Peter Fouquet
14:30-14:45	Stanislav Savvin <i>XtremeD: pushing the limits of research under extreme conditions at ILL</i>	Robert Cubitt <i>Going to Extraordinary Lengths with SANS</i>
14:45-15:00	Martin Boehm <i>Bent Silicon Revolution in Inelastic Neutron Scattering</i>	Bettina Schwaighofer <i>Oxide Ion Dynamics in Bi2O3-based Solid Electrolytes: Combining Quasielastic Neutron Scattering with Ab Initio Molecular Dynamics</i>
15:00-15:15	Giuliana Manzin <i>Boosting the ILL instruments suite: the H15 guide and instruments project</i>	Lucas Fine <i>Local structure and vibrational dynamics in the nitride-hydride Ca3CrN3H7</i>
15:15-15:30	Elhoucine Hadden <i>Innovative holographic structures for efficient manipulation of slow neutron beams</i>	Abdelmajid. Elmahjoubi <i>Percolation scenario for hexagonal semiconductor alloys: A test case by applying inelastic neutron scattering and ab initio calculations to wurtzite-Zn1-xMgxS (x ≤ 0.33)</i>
15:30-16:00	Coffee	
16:00-18:00	NEUTRONS BEYOND SCATTERING p 31 Chair: Arno Hiess	
16:00-16:40	Ulli Koester <i>Dead neutrons keep patients alive</i>	
16:40-17:10	Hartmut Lemmel <i>Interferometry for understanding quantum physics</i>	
17:10-17:50	Tobias Jenke <i>Ultracold neutrons test gravity at short distances and cosmological models</i>	
18:00-19:30	NEWS From FACILITIES and 2FDN European Spallation Source – Giovanna Fragnetto Institut Laue Langevin – Jacques Jestin Laboratoire Léon Brillouin – Arnaud Desmedt Fédération Française de la Neutronique – Marie Plazanet	
20:00	Dinner	

Wednesday, October 2

9:00-10:10	SOFT MATTER p 35 Chair: Marie Plazanet	
9:00- 9:40	Plenary: Sandrine Dourdain <i>Neutrons for Solvent Extraction</i>	
9:40-10:10	Keynote: Marion Grzelka <i>Probing friction mechanisms at solid/liquid interface with optical microscopy and neutron scattering</i>	
10:15-11:00	SOFT MATTER p 37 Chair: Isabelle Morfin	MAGNETISM p 50 Chair: Elisa Rebolini
10:15-10:30	Armin Mozhdhehi <i>Proton Conductivity in Hydrated Sulfonated Porous Aromatic Framework</i>	Antoine Roll <i>Nature of the low energy quadrupolar dynamics in Tb₂Ti₂O₇ under temperature</i>
10:30-10:45	Firoz Malayil <i>Surfactant-free microemulsions: how molecular dynamic reflects nano-structuration</i>	Ketty Beauvois <i>Interplay between structural and magnetic chiralities in NiCo₂TeO₆</i>
10:45-11:00	Apostolos Vagias <i>Soft matter thin films under pressure: A morphological investigation under Grazing Incidence Neutron Scattering</i>	Sylvain Petit <i>Spin ice and high entropy materials</i>
11:00-11:30	Coffee	
11:30-12:20	SFN PhD Award Ceremony p 43	
11:30-11:55	Laurent Michot, President of Jury <i>Swelling clay/water interactions at various spatial scales: insights from neutron-based techniques</i>	
11:55-12:20	Laureate – To be annouced	
12:30-14:00	Lunch	
14:00-15:30	Poster Session p 57	
15:00-15:30	Coffee	
15:30-20:00	FREE TIME	
20:00	Conference dinner	

Thursday, October 3

9:00-10:10	MAGNETISM p 45 Chair: Philippe Bourges	
9:00-9:40	Plenary: Nikolaos Biniskos <i>Topological magnons in the centrosymmetric ferromagnet Mn_5Ge_3</i>	
9:40-10:10	Keynote: Dalila Bounoua <i>Hidden Magnetic Texture in the Pseudogap Phase of the High-Tc Superconducting $YBa_2Cu_3O_{6+x}$</i>	
10:15-11:00	MAGNETISM p 53 Chair : Quentin Faure	SOFT MATTER p 40 Chair : Christiane Alba-Simoniesco
10:15-10:30	Yassine Oubaid <i>Structural and magnetic properties of the iron-based superconductor $BaFe_2S_3$</i>	Daniel Dudzinsky <i>Mixing green fatty acids to tunes surfactant self-assemblies structure and properties</i>
10:30-10:45	Elisa Rebolini <i>Ab-initio calculations of magnetic excitations in strongly-correlated materials</i>	Benedetta Rosi <i>Structural and dynamical properties of PS-PNIPAM block copolymer micelles in concentrated samples</i>
10:45-11:00	Olivier Demortier <i>Thermal conductivity in terbium-based compound : KTb_3F_{10}</i>	Bastien Lebreux <i>Small Angle Neutron Scattering measurement of Aqueous Biphasic System</i>
11:00-11:30	Coffee	
11:30-12:30	ROUND TABLE Future of neutrons	
12:30-14:00	Lunch	

Nanostructured nanoparticles made of self-assembled bioconjugates: formation and interaction with proteins

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Over the last 20 years, synthetic internally self-assembled nanoparticles (ISASOMES) have gained significant interest for their applications in catalysis, drug delivery, solubilisation, food and cosmetic materials,...[1]. The specific internal nanostructuring of these nanoparticles offers new properties by combining a high specific surface area, encapsulation properties, mechanical properties, surface activity and controlled release of encapsulated compounds. Recently, nanoparticles that combine pharmaceutical activity with nanoscale formulation (often referred to as nanodrugs) have demonstrated several advantages in the field of nanomedicine, such as reduced toxicity, improved targeting, and optimized pharmacokinetics, among others. The advantages are further increased when nanoparticles are formulated through nanoprecipitation from bioconjugates, where the drug is linked to an hydrophobic and biocompatible moiety [2]. Among the different materials, the squalene have proven to be highly efficient and versatile for formulating a wide range of nanodrugs, offering the significant advantage of not requiring additional surfactants for stabilization [3, 4]. On this particular example of squalene-based nanoparticles developed by the Institut Galien Paris Saclay, we developed in CEA/LIONS a methodology to analyze their physico-chemical properties and their interaction with model protein. In this talk, I will present 1) how SANS can be used for the dimensional characterization of formulated nanodrugs ISASOMES at their final stages or during the different steps of their formation and 2) how SANS is a powerful tool to study the interactions between nanodrugs and model protein such as BSA [5, 9].

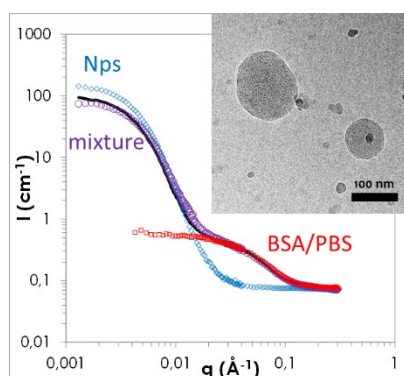


Figure 1 : SANS diagram of squalene-Adenosine (SqAd) NPs in D_2O or in BSA/PBS. Black line is a linear combination of SqAd NPs and BSA. Inset shows a cryoTEM image of SqAd NPs in D_2O .

[1] Glatter, O., & Salentinig, S. Inverting structures: from micelles via emulsions to internally self-assembled water and oil continuous nanocarriers. *Current opinion in colloid & interface science*, (2020) 49, 82-93.

[2] Li, G., Sun, B., Li, Y., Luo, C., He, Z., & Sun, J. Small-molecule prodrug nanoassemblies: an emerging nanoplatform for anticancer drug delivery. *Small*, (2021) 17(52), 2101460.

[3] Desmaële, D., Gref, R., & Couvreur, P.. Squalenoylation: a generic platform for nanoparticulate drug delivery. *Journal of controlled release*, (2012) 161(2), 609-618.

[4] Feng, J., Lepetre-Mouelhi, S., & Couvreur, P.. Design, preparation and characterization of modular squalene-based nanosystems for controlled drug release. *Current Topics in Medicinal Chemistry*, (2017) 17(25), 2849-2865.

[5] Saha, D., Testard, F., Grillo, I., Zouhiri, F., Desmaële, D., Radulescu, A., ... & Spalla, O. The role of solvent swelling in the self-assembly of squalene based nanomedicines. *Soft matter*, (2015) 11(21), 4173-4179.

[6] Rouquette, M., Ser-Le Roux, K., Polrot, M., Bourgaux, C., Michel, J. P., Testard, F., ... & Lepetre-Mouelhi, S.. Towards a clinical application of freeze-dried squalene-based nanomedicines. *Journal of drug targeting*, (2019) 27(5-6), 699-708.

[7] Gobeaux, F., Bizeau, J., Samson, F., Marichal, L., Grillo, I., Wien, F., ... & Testard, F. Albumin-driven disassembly of lipidic nanoparticles: the specific case of the squalene-adenosine nanodrug. *Nanoscale*, (2020) 12(4), 2793-2809.

[8] Caillaud, M., Gobeaux, F., Hémedi, M., Boutary, S., Guenoun, P., Desmaële, D., ... & Massaad-Massade, L. Supramolecular organization and biological interaction of squalenoyl siRNA nanoparticles. *International Journal of Pharmaceutics*, (2021) 609, 121117.

[9] Lepetre-Mouelhi, S., Gobeaux, F., Da Silva, A., Prades, L., Feng, J., Wien, F., ... & Testard, F. Leu-Enkephalin Lipid Prodrug Nanoparticles: Relationship between Nanoparticles' Structure, Interaction with Bovine Serum Albumin, and Analgesic Activity. *Chemistry of Materials*, (2024) 36(2), 694-707.

Probing biology with neutrons, from environment to health

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Neutrons scattering spectroscopy provides information on atomic molecular dynamics on the ps-ns time scale, which is essential to biological function.

To date, the domain of biological scientific fields studied with neutrons spans from the single amino acid (the smaller component of the protein primary sequence), to in vivo cells and brain tissue. I will present examples of key results recently obtained on relevant biological samples with impact on different scientific fields and applications, from Environment to Health. Particular attention will be also focused on the investigation of the physics piloting water diffusion in brain tissue at the micrometer-to-atomic scale, through combined diffusion magnetic resonance imaging and neutron scattering experiments on bovine brain tissue, allowing to probe diffusion distances up to macromolecular separation. This will include healthy tissue as well as tissue affected by brain pathologies. Significant interregional asymmetries (lateralization) in bovine brain hemispheres, observed in the myelin arrangement and water dynamics, will also be reported and results interpreted in terms of hemisphere-dependent cellular composition (number of neurons, cell distribution, etc.) as well as specificity of neurological functions (such as preferential networking).

Following the Dynamics during Crystallization with Time-Resolved Scattering

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Crystals of macromolecules, notably proteins, are of great interest for the three-dimensional structure determination at an atomic level in structural biology by X-ray crystallography, and for drug formulations in pharmacological applications. The interest here is in high quality single crystals, which are often difficult to obtain. One important bottleneck consists in the crystallization pathway which can include several different intermediate steps, starting from a homogeneous solution, and ending in a solution containing macroscopic crystals. In the past we have shown that different crystallization pathways and morphologies can be triggered by adding multivalent salts to the protein solution [1,2].

By changing the crystallization inducing salt concentration, we are able to change the crystallization pathways, the crystal morphology and tune the crystal lattice spacing of the crystals, which can be probed by investigating the position of the Bragg peaks in diffraction experiments.

As a model system, we investigate the crystallization of human serum albumin (HSA) in the presence of LaCl_3 in D_2O . At constant protein concentration (75mg/ml), we identified a salt concentration where the resulting crystal are featured by Bragg peaks which differ significantly from the Bragg peak positions of the adjacent conditions tested. To understand the origin of this difference, we investigated the diffusive and structural properties of the crystal growth on a wide range of time and length scales using time-resolved neutron spectroscopy, namely neutron backscattering at IN16b (ILL) and neutron spin echo spectroscopy at WASP (ILL), small angle scattering (D22 at ILL), light scattering and microscopy. Employing previously established analysis frameworks [3-5], we have been able to disentangle the different contributions to the scattering signal and observe new insights in the salt induced crystallization pathways.

The results are compared with previous studies on different protein salt combinations to obtain a comprehensive picture.

[1] Sauter, A., Roosen-Runge, F., Zhang, F., Lotze, G., Feoktystov, A., Jacobs, R. & F. Schreiber., *Faraday Discuss.* 179 (2015) 41

[2] Banks, H., Surfaro, F., Pastryk, K., Buchholz, C., Zaluzhnyy, I., Gerlach, A. & Schreiber, F. *Colloids and Surfaces B: Biointerfaces*, 241 (2024) 114063

[3] Beck, C., Roosen-Runge, F., Grimaldo, M., Zeller, D., Peters, J., Schreiber, F. & Seydel, T. (2024). *J. Appl. Cryst.* 57.

[4] Beck, C., Grimaldo, M., Roosen-Runge, F., Maier, R., Matsarskaia, O., Braun, M., Sohmen, B., Czakkel, O., Schweins, R., Zhang, F., Seydel, T. & Schreiber, F., *Cryst. Growth Des.* 2019, 19, 12, 7036–7045

[5] Maier, R., Sohmen, B., Da Vela, S., Matsarskaia, O., Beck, C., Schweins, R., Seydel, T., Zhang, F., & Schreiber, F., *Cryst. Growth Des.* 2021, 21, 12, 6971–6980

First-principles characterization of protein-protein and protein-ligand interactions

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The BigDFT project was started in 2005 with the aim of testing the advantages of a computational approach with optimal features of flexibility, performance, and precision of the results. In particular, the employed formalism has enabled the implementation of an algorithm able to tackle full Quantum Mechanical (DFT) calculations of large systems, up to many thousands of atoms, with a computational effort that scales linearly with the number of atoms. We have been applying these investigation techniques to systems ranging from solid-state physics to macromolecules of interest in biology.

Our topic of collaboration with the Large Scale Structure group at ILL is based on first-principles structural studies of protein-protein and protein-ligand assemblies, and their connections with techniques like SANS and Neutron crystallography. We are presently employing the DFT techniques mentioned above to characterize the interactions of some of these systems in order to employ binding descriptors extracted from first-principles, in the context of topics like drug-design/resistance and affinity optimization. Such data can complement the array of investigation techniques at the atomistic level that is usually employed in these fields.

The technique employs first principles to identify the receptor/ligand residues that determine the chemical bonds and network of inter- and intra- protein interactions through the identification, on the basis of Quantum Mechanical chemical affinity, of the Binding Motif between a receptor and a ligand. With such a technique, it is possible, *in silico*, to compare hypothetical and observed configurations differing for single- point mutations and construct the corresponding BMs determined by the specific mutations.

The novelty of this approach consists of its non-arbitrariness, and it can, by extension, be applied to any atomic system for which a 3D crystal structure is available. Such a technique has been applied in various papers in the context of bioremediation [1] and for systems of interest in the SARS-CoV-2 binding mechanisms. [2,3]

We think this modelization approach could inform efforts in protein design by granting access to variables otherwise impervious to observation. In this contribution we will present, for a non-specialized audience, the salient points of our approach and their potential usefulness in understanding biological mechanisms.

[1] Experimental–theoretical study of laccase as a detoxifier of aflatoxins. Marco Zaccaria, William Dawson, Darius Russel Kish, Massimo Reverberi, Maria Carmela Bonaccorsi di Patti, Marek Domin, Viviana Cristiglio, Bun Chan, Luca Dellaflora, Frank Gabel, Takahito Nakajima, Luigi Genovese & Babak Momeni *Scientific Reports* volume 13, Article number: 860 (2023)

[2] Marco Zaccaria, Luigi Genovese, William Dawson, Viviana Cristiglio, Takahito Nakajima, Welkin Johnson, Michael Farzan, Babak Momeni, Probing the mutational landscape of the SARS-CoV-2 spike protein via quantum mechanical modeling of crystallographic structures, *PNAS Nexus*, /10.1093/pnasnexus/pgac180.

[3] Luigi Genovese, William Dawson, Takahito Nakajima, Viviana Cristiglio, Valérie Vallet, Michel Masella; Protein–ligand interactions from a quantum fragmentation perspective: The case of the SARS-CoV-2 main protease interacting with α -ketoamide inhibitors. *J. Chem. Phys.* 7 June 2023.

The perfect match! Neutron Spectroscopy reveals the fine structure of quantum excitations in endofullerenes

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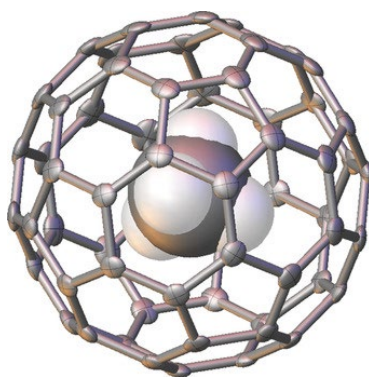
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Endofullerenes $A@C_n$ ($A = H_2, H_2O, Ne, He, CH_4, CH_2O, \text{etc.}\dots; n = 60, 70$) are a class of molecules composed of atoms or small molecules confined into carbon cages. They have gained significant attention due to their unique quantum properties resulting from the strong confinement of the encapsulated species. Neutron spectroscopy provides unique insights into low lying roto-translational quantum states of these materials, some being of purely rotational or translational character, other revealing rotation-translational coupling. Studies using high resolution inelastic neutron scattering under high pressure have shown that the behavior of the encapsulated species is highly influenced by the symmetry and potential of the fullerene cage, leading to new quantum phenomena that are not observed in free space.

In this talk, I will present a review of some of the most illustrative endofullerenes studied using a large set of neutron spectroscopy.



The microscopic origin of a glass-like thermal transport: the role of disorder

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The low and weakly temperature dependent thermal conductivity has long been thought to be a unique characteristic of glasses, and has been ascribed to a strong scattering from disorder of the main heat carriers, the atomic vibrations (phonons). Reproducing such thermal transport in crystalline materials with tailored functional properties represent today one of the main objectives in many applications, among which thermal management and energy harvesting. In fact, a similar behavior can be naturally found in many other systems, from complex crystals, such as clathrates and skutterudites to simple disordered crystals, to nanostructured materials.

If in glasses the thermal transport is today quite well understood, the underlying mechanisms in such crystalline materials are not. Identifying them carries the promise of an advanced thermal transport engineering. In the last 10 years, we have tackled this problem, using the most advanced inelastic neutron and x ray scattering techniques to investigate the phonon dynamics of several systems, focusing our efforts in the understanding of the role of disorder and complexity [1-10]. In this talk I will first briefly remind the peculiarities in the phonon dynamics of glasses leading to a low and weakly temperature dependent thermal conductivity, then I will show that, the phonon dynamics of complex and disordered crystals share some similarities with glasses, leading to the same thermal behavior, although the microscopic mechanisms are different.

[1] S. Pailhès et al., Phys. Rev. Lett. 113, (2014) 025506

[2] P.-F. Lory et al., Nat. Comm. 8, (2017) 491

[3] S. Pailhès et al. (Pan Stanford, CRC Press/Taylor & Francis Group) (2017)

[4] H. Euchner et al. Phys. Rev. B 97, (2018) 014304

[5] S. Misra et al., Physical Review Research, 2, (2020) 043371

[6] S. R. Turner et al., Physical Review Research, vol. 3, (2021) 013021

[7] S. R. Turner et al., Nat. Comm., 13, (2022) 7509

[8] S. Pailhès et al., Results in Physics, 49(4), (2023) 106487

[9] S. R. Turner et al., Phys. Rev. Mat.7, (2023) 115401

[10] R. Cravero et al., Small (2024) 2310209

Phasons modes in the incommensurately modulated Rb_2ZnCl_4 phase

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Aperiodic crystals are long range ordered structures without periodicity at least in one direction. Phason modes are one of the characteristics of the dynamics of aperiodic crystals. For all aperiodic crystals, the hydrodynamic theory predicts the occurrence of long wavelength phason modes, that are diffusive like excitations with a purely imaginary ‘dispersion’ relationship [1]. They have been observed in incommensurately displacive modulated structure, where propagating damped harmonic excitations are observed in a short wavelength regime, becoming overdamped excitations in the long-wavelength limit. They have also been observed in quasicrystal and in this case diffusive excitations have been observed at all wavelength [2,3]. This difference between the excitation spectrum of the two systems is intimately related to the microscopic realisation of phason modes: in one case phason modes results in small shift of atoms from their ideal position, whereas in the second case phason modes lead to atomic jumps.

We present an experimental study of the lattice dynamics of the Rb_2ZnCl_4 phase which displays a crystal structure where the orientations of its ZnCl_4 tetrahedrons plays a crucial role. Whereas in the orthorhombic high temperature phase the tetrahedra occupy randomly two equivalent positions, from $T_i=303$ K they order incommensurately along the c^* axis. The transition is related to the tetrahedron orientation and is mainly of the order/disorder type. One thus expects phason modes to be diffusive at all wavelength, as predicted by the theory [2,3]. At $T_c=195$ K the modulation gets locked-in with a $1/3$ ratio of the periodicity at high temperature, resulting in a periodic approximant, where phason modes should not be present anymore.

We have investigated the dynamics of this phase, as a function of temperature between 140 and 350 K, using inelastic and quasielastic neutron scattering measurement on a large single crystal.

In the incommensurate phase, a strong quasielastic signal is observed only around satellites reflection. It presents a q dependence with a width that increases as q increases in agreement with the hydrodynamic theory of phason modes. We also observe broad and dispersive phonon like excitations in a restricted momentum-energy space. On the other hand, around the main reflexions only ‘regular acoustic modes’ are observed. In the lock-in phase at 150 K the quasielastic signal around the satellite reflexions has vanished and only acoustic phonon modes are observed. This demonstrates in a very clear way that phason modes are indeed a characteristic excitations of the incommensurately modulated Rb_2ZnCl_4 phase.

Acknowledgements: This work is part of the ANR-DFG Aperiodic project.

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When water meets solids: unexpected liquid-solid THz dynamic coupling

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When a viscous liquid wets a solid surface, we generally expect the liquid dynamics to be modified [1] and do not expect the phonon dynamics of a hard solid to be impacted. However, recent experimental results have shown an unexpected temperature gradient in a quiescent water bath at the vicinity of the solid wall [2] which might suggest a thermodynamic interdependence between liquid and solid. This interdependence is now confirmed by the observation of a deep change of the vibrational state affecting both transverse and longitudinal acoustic phonons of the solid in contact with liquid water. These key results have been obtained using both X-Ray (IXS) and neutron inelastic measurements (INS), on Alumina monocrystals at room temperature (Fig.1b) [3]. The wetting induced effects on solid are reproducible and reversible. The effects are extended deep in the crystal ($> 150\mu\text{m}$ probed with IXS and $250\mu\text{m}$ probed with INS) excluding a confined nanosurface effect [4].

These new results suggest that a solid wall can no more be considered as only a simple means to confine and limit the propagation of a fluid, but that it is in turn also a "deformable" media via a complex phononic long range coupling whose impact only begins to be identified.

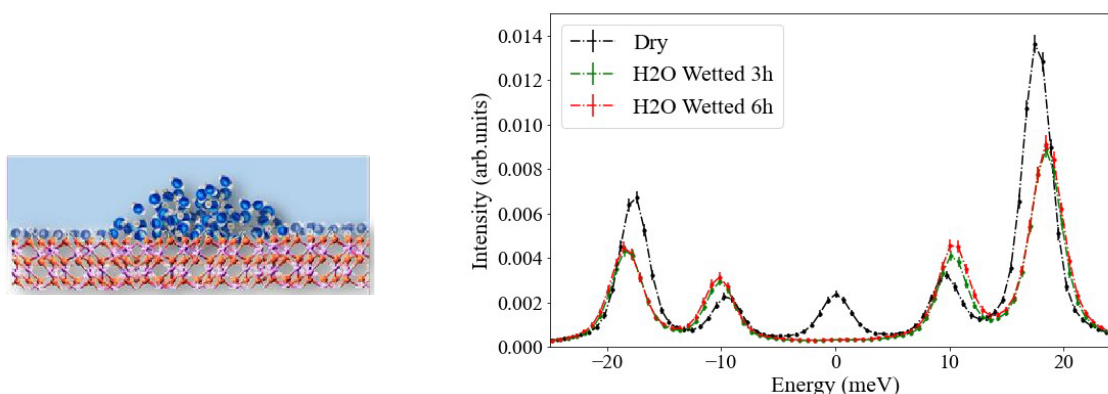


Fig.1.a) Water molecules spreading on the surface of an Alumina mono crystal (high energy surface) change the vibrational state of the solid substrate [2]. b) Inelastic scattering corresponding to: - the dry $\alpha\text{-Al}_2\text{O}_3$ (black points), - H₂O wetted after 3 hr (blue), 6 hr (red) and 9 hr (orange) at $Q = (-1\ 13.5)$. The incident beam penetration depth of roughly $150\ \mu\text{m}$. A clear change is observed for the acoustic phonon with inelastic peaks shifting to higher energies; i.e. hardening. Measurements carried out on ID28 (ESRF) at room temperature with a resolution of 3 meV (FWHM) from [3].

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Systematic study of silver chalcogenides for wearable thermoelectrics

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Wearable thermoelectric (TE) modules that generate a few watts of power are becoming a viable alternative to batteries for applications in portable electronic devices, such as for permanent medical diagnostics [1]. In addition to a good TE performance a sufficiently high ductility is a prerequisite for the materials to conform to the shape of the human body. Some $\text{Ag}_2\text{S}_x\text{Se}_y\text{Te}_z$ compounds (with $x+y+z=1$) fulfill both conditions, namely exceptional plastic deformability and high TE performance with a maximum figure of merit $ZT \sim 0.5$ at human body temperatures. In this study, we investigate ternary and quaternary $\text{Ag}_2\text{S}_x\text{Se}_y\text{Te}_z$ solid solutions with highest Se and Te doping levels of $y+z=0.5$, i.e. closer to the binary Ag_2S end.

Ag_2S lightly doped with Se and/or Te crystallizes in a monoclinic α structure (P21/c) which transforms to a cubic (Im-3m) β modification at around 450 K [2,3]. These β - Ag_2S based alloys display high cationic conductivities marking them superionic solids. The enhanced Ag^+ mobility is due to a high structural disorder in the Ag sublattice. Interestingly, the α to β transition temperature decreases with increasing doping Se/Te levels, such that the β phase can be stabilized down to base T at a sufficiently high Te content. Thus the glassy nature of the Ag sublattice can be frozen from dynamic to static disorder upon cooling.

These structurally and dynamically highly tunable $\text{Ag}_z\text{S}_x\text{Se}_y\text{Te}_z$ compounds offer some interesting prospects for macroscopic TE applications and raise some fundamental questions about their microscopic properties. What are the best (x,y,z) compositions for TE applications at human body temperatures? Does the monoclinic α or the cubic β phase favor higher ZT values? How does the high Ag^+ mobility affect the TE properties? Is dynamic or static disorder favorable for reduced thermal transport in the β phase?

We present a study of $\text{Ag}_z\text{S}_x\text{Se}_y\text{Te}_z$ compounds with high S content prepared by a rapid casting method. We discuss their TE performance based on results from temperature-dependent experiments of electrical conductivity, Seebeck coefficient and thermal properties. The macroscopic data are complemented by results of microscopic dynamics from inelastic neutron scattering and diffraction experiments. The response of phonons to temperature and the characteristics of the translational dynamics of Ag^+ in the superionic and glassy states down to base T are outlined.

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Intrusion, extrusion and phase transitions of water in hydrophobic nanopores

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We focus on the filling processes and structural properties of water confined in solid and regular materials with tunable pore sizes (from 1.5 to 8nm) and surface interactions (from hydrophilic to weakly or highly hydrophobic) (ref 1). In the case hydrophilic pores, the filling process is imbibition where penetration starts as soon as the material is in contact with a liquid droplet, while in the hydrophobic case, the process called intrusion requires an external pressure to force the liquid to enter, a pressure value obeying the Laplace law. This pressure can be measured by various methods, typically volumetric and/or calorimetric. Two categories of materials conforming to the Laplace law have been identified: those with a large slope, comprising cylindrical nanopores with amorphous silica walls and post-grafted surfaces (MCM-41, SBA type) and those with a much smaller slope, consisting of MOFs and zeolites (ref 2,3,4, Fig. 1). In this presentation, we will compare the intrusion/extrusion mechanisms in various systems of the two categories, even include the case of the hydrophilic counterpart and question the role of the compressibility of the confined fluid by Neutron Diffraction experiments (G6.1-LLB and D16- ILL). Surprisingly, when the systems are further cooled after compression, we observed that the stacking-disordered ice no longer is formed but rather Ice II and Ice III (ref 1). So exploring the phase diagram of confined water requires to be able to play with - the pore size, at least in the range where some crystallization occurs, - the amount of water trapped, - the fluid wall interactions, all with a good control of the materials characterization.

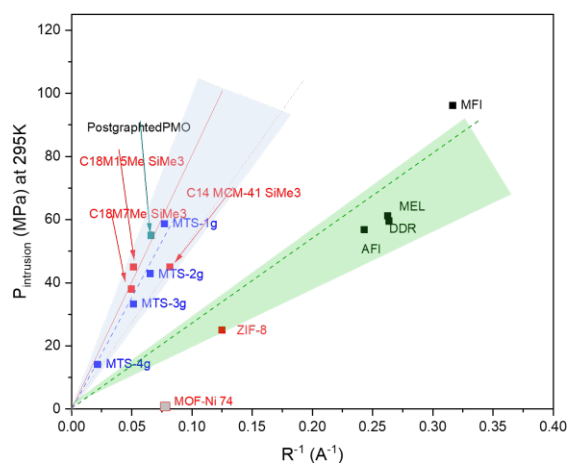


Figure 1: Water intrusion Pressure at room temperature as a function of the pore radius. The two domains and averaged lines correspond to the Laplace equation inversely proportional to the radius: - the largest slope for grafted hydrophobic mesopores with a cylindrical geometry; - the smallest slope, for zeolite frameworks with interconnected pores and MOF. In red, data from this work. The other data are from ref 2,3,4.

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How cations - silica surface interactions affect water dynamics in nanoconfined electrolyte solutions

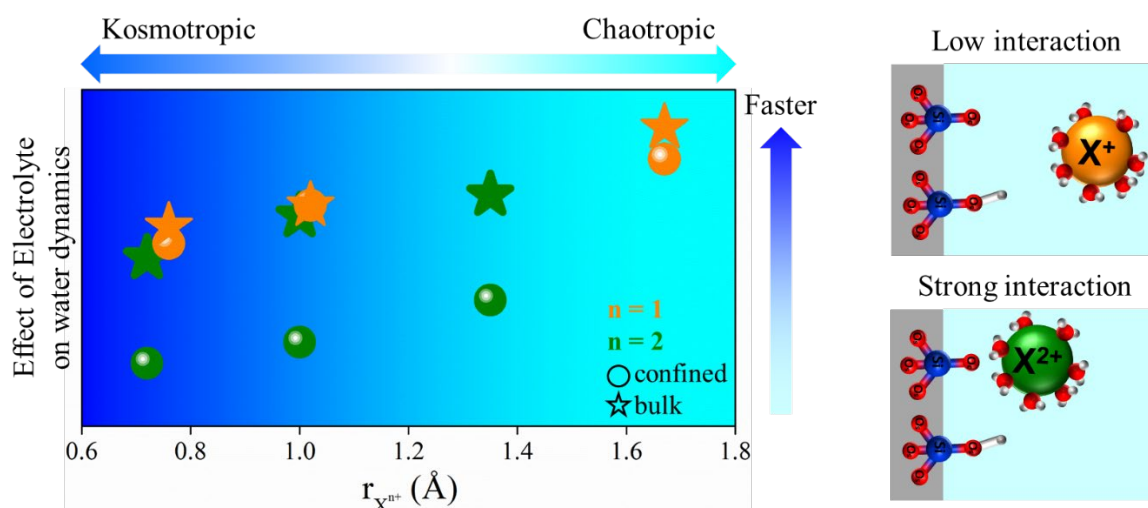
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Probing electrolytes behavior at the atomic level provides valuable insights into understanding the reactive transport of electrolyte solutions in nanoconfinement and help explaining and predicting the macroscopic behavior of industrial or natural nanoporous materials. In this study, we focused on water and ion behaviors in silica nanocylinders of 2.6 nm filled with electrolyte solutions, XCl at 1M with X = Li, Na and Cs, monovalent cations presenting various kosmotropic/chaotropic properties. Using a combination of experiments and theoretical modeling, we analyzed the water dynamics at a picosecond timescale by Quasi-Elastic Neutron Scattering (IN5 time-of-flight spectrometer, Institut Laue-Langevin, Grenoble, 4.8 Å, 86 μeV 7 ps) based on three primary effects: the confinement, the electrolyte, and the interfacial ion-porous material surface interaction. Comparing the water dynamics obtained with divalent cations previously studied by Baum et al. [1], we highlight that monovalent cations present weaker interactions with silica surfaces than divalent cations. This latter significantly impacts the water dynamics in addition to the confinement and electrolyte effects. This study pinpoints the importance of ion behavior within the interfacial layer and its impact on water transport in nanoconfinement. These results are significant for explaining various industrial or natural processes such as membrane filtration or glass alteration [2].



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Deep Eutectic Solvents: Properties Induced by Nanometric Confinement

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Over the past decade, Deep Eutectic Solvents (DESs) have garnered significant attention within the scientific community due to their remarkable functional properties, positioning them as promising alternatives to conventional solvents in green chemistry initiatives [1,2]. Notably, DESs exhibit unconventional behavior stemming from the formation of nanoscopic domains and dynamic heterogeneity across nanometers scale, attributed to the intricate interplay of ionic and hydrogen bonding interactions among their molecular constituents [3,4]. Consequently, unravelling the physicochemical intricacies of DESs at the mesoscopic level has emerged as a pivotal pursuit. The interrogation of DES behavior under mesoporous confinement stands as a particularly pertinent endeavour, given the pivotal role of interfaces and nanopores in numerous targeted applications of these solvents. Hence, a pressing question arises regarding the impact of mesoporous confinement on the dynamic (diffusion, rotation and relaxation) heterogeneities inherent within DES systems [5,6].

We have investigated the dynamics of Ethaline (DES composed of choline chloride and ethylene glycol) confined in mesostructured porous silicas (SBA-15 & MCM-41) by incoherent Quasielastic neutron scattering experiments. An extended dynamical range was achieved by combining time-of-flight (IN5) and backscattering (IN16B) Quasielastic neutron spectrometers providing complementary energy resolutions. This study provides a comprehensive microscopic view on the dynamics of Ethaline confined in mesopores in terms of non-mobile/mobile fraction, jump-diffusion coefficient, residence time, relaxation time, and their temperature dependence [7-10].

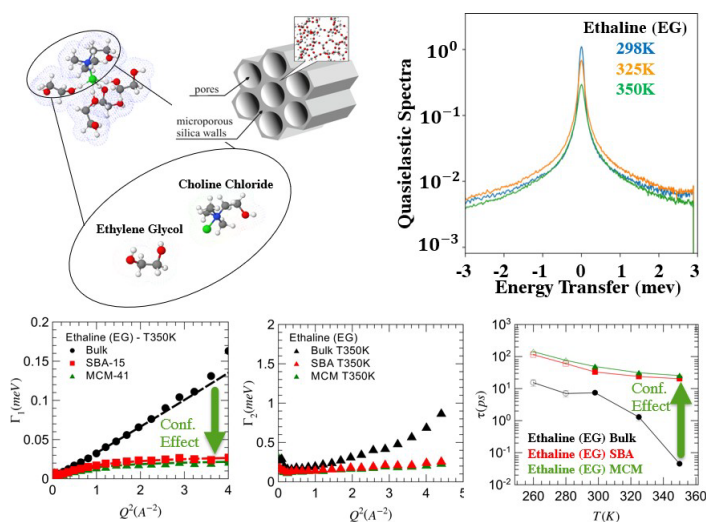


Figure: (upper panel) Sketch of studied systems and their dynamic structure factor. (lower panel) Confinement effect on the Quasielastic broadening of the slow (jump-diffusion) and fast (rotation) processes, and temperature dependence of the residence time

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Going to Extraordinary Lengths with SANS

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The largest accessible length scale in conventional small angle neutron scattering is determined by the combination of the longest available neutron wavelength and the smallest resolvable scattering angle. Conventionally this allows the very longest small angle instruments to access a few μm [1]. We present a method that circumvents this limitation and is able to extract much larger length scales from the low- q power-law scattering using a modification of the well-known Porod law connecting the scattered intensity of randomly distributed objects to their specific surface area [2]. We show that in the special case of a highly aligned domain structure the specific surface area determined from the modified Porod law can be used to determine the mean length scale of the domain structure. The analysis method is applied to study the magnetic field dependent micrometer-sized domain structure found in the intermediate mixed state of the superconductor Niobium. Figure 1 shows the extracted domain length scale over the entire field range of the intermediate mixed state that fits well with Landau's theory of domains in superconductors [3] and previous efforts to extract this length scale using ultra small angle neutron scattering methods [4]. The analysis approach allows to extend the range of accessible length scales from 1 μm to values of up to 40 μm using a conventional small angle neutron scattering setup and should be applicable to any such aligned system.

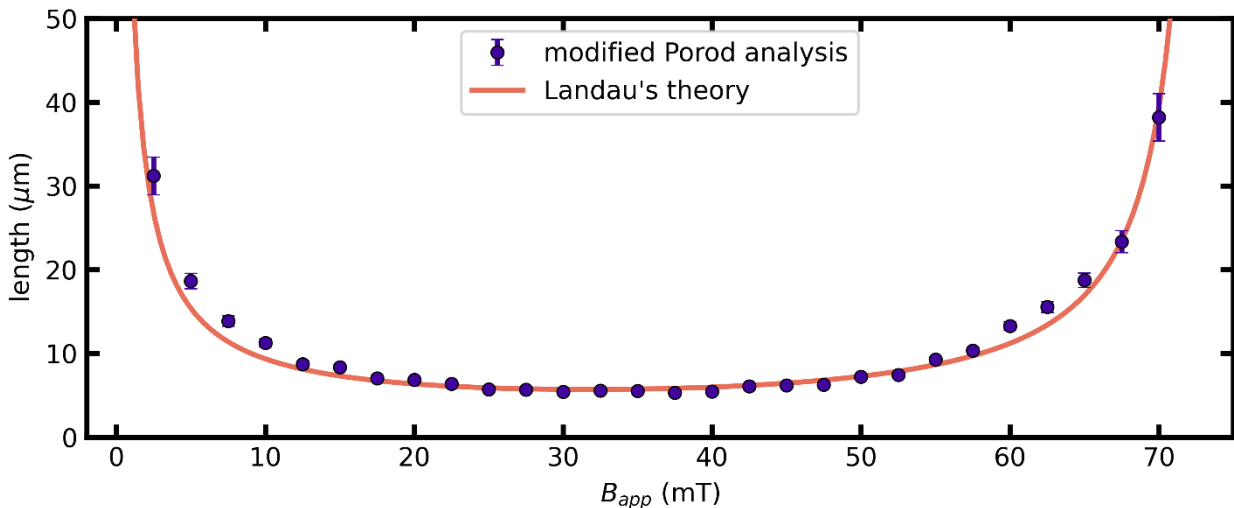


Figure 2: The variation of the total length scale of the domains in Niobium as a function of applied field derived from the modified Porod analysis and the fit to Landau's theory of domains in superconductors.

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Oxide Ion Dynamics in Bi₂O₃-based Solid Electrolytes: Combining Quasielastic Neutron Scattering with Ab Initio Molecular Dynamics

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Solid oxide ion conductors are important materials in applications like oxygen-permeable membranes and solid oxide fuel cells (SOFC). In the latter, they are used as solid electrolytes. Current SOFC electrolyte materials, however, require high temperatures to achieve a sufficiently high oxide ion conductivity for device applications. Developing materials with excellent ionic conductivity at intermediate temperatures (400–600 °C) is a crucial step in making SOFC more widely applied. Understanding the relationship between structural properties and high ionic conductivity is therefore an important part of current research on energy materials. Quasielastic neutron scattering is an excellent method for studying solid state diffusion and allows the observation of oxygen dynamics on a microscopic timescale. Combined with ab initio molecular dynamics simulations, it can provide a comprehensive insight into diffusion processes on the atomic scale. We used this combined approach to investigate and compare the different oxide ion dynamics in two isostructural materials: Bi_{0.852}V_{0.148}O_{1.648} and Bi_{0.852}P_{0.148}O_{1.648}, and account for the superior performance of the vanadate. Using the backscattering spectrometer IN16b and the time-of-flight spectrometer IN5 at the ILL allowed direct observation of dynamics on the nanosecond and picosecond timescales, and analysis in conjunction with molecular dynamics simulations allowed us to elucidate the structural characteristics important for oxide ion conduction in these doped bismuth oxides.

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Local structure and vibrational dynamics in the nitride-hydride $\text{Ca}_3\text{CrN}_3\text{H}$

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Hydride-ion (H^-) conductors attract more and more interest for their potential application as solid electrolytes in, e.g., batteries, fuel cells, and for catalysis. A particularly promising class of hydride-ion conductors are nitride-hydrides, which accommodate both nitride ions and hydride ions in the same crystal structure. Recently, the new nitride-hydride $\text{Ca}_3\text{CrN}_3\text{H}$ was discovered and shown to be promising to be used as a catalyst for ammonia synthesis [1,2]. For the rational development of $\text{Ca}_3\text{CrN}_3\text{H}$, or related materials, towards such an application, a fundamental understanding of its hydride-ion dynamics is crucial.

In this work, we report results from variable temperature inelastic neutron scattering (INS) experiments, harmonic phonon calculations, and ab-initio molecular dynamics (AIMD) calculations of the vibrational spectra of $\text{Ca}_3\text{CrN}_3\text{H}$. Combined analyses of the experimental and theoretical data show that the vibrational spectra of the hydride-ions are characterized by an intense band at around 95 meV, which is assigned to vibrational dynamics polarized in the crystallographic ab plane, and a broad band ranging from 80 to 130 meV, which is assigned to a strongly dispersive mode polarized along the crystallographic c axis. Its dispersive character is a consequence of significant hydrogen-hydrogen interactions between in the material and it is found that all hydride-ions are surrounded by at least one another hydride-ion. Furthermore, it is shown that the vibrational dynamics of the hydride-ions are anharmonic in nature at elevated temperatures, which may be a signature of diffusional dynamics of the hydride-ions.

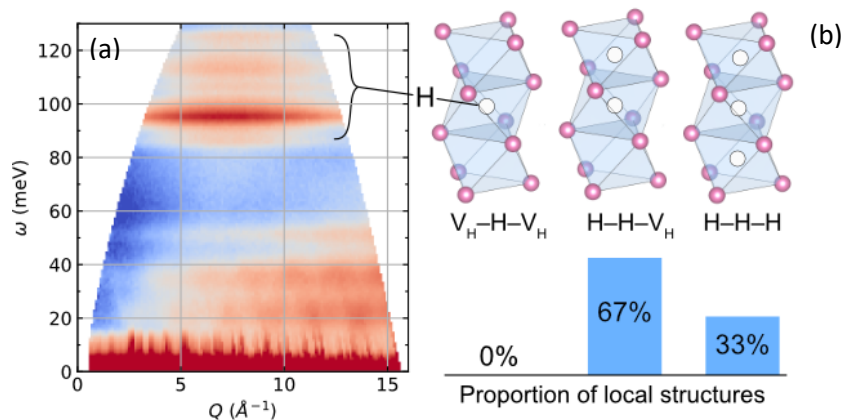


Figure 1. (a) INS spectrum of $\text{Ca}_3\text{CrN}_3\text{H}$ measured on 4SEASONS at J-PARC. (b) Illustration of three local coordination environments around hydride-ions, together with their respective proportion found in the sample.

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Percolation scenario for hexagonal semiconductor alloys: A test case by applying inelastic neutron scattering and *ab initio* calculations to wurtzite-Zn_{1-x}Mg_xS (x ≤ 0.33)

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The A_{1-x}B_xC semiconductor alloys are like geometrical objects and thus ideal to study experimentally the A↔B substitution, which relates to the percolation theory. For doing so one needs a local probe, such as the bond force constant (k) addressed by vibrational spectroscopies. Our pioneering studies of the phonon dispersion of cubic-Zn_{1-x}Be_xSe combining inelastic neutron (INS) and Raman scattering [1] revealed a sensitivity of k to the local (A- or B-like) environment across the Brillouin zone. This sensitivity has been formalized through the percolation model (1-bond → 2-mode scheme) recently developed by our group [2], deviating from the historical MREI (modified random-element-isodisplacement) model (1-bond → 1-mode scheme) proposed by Chang and Mitra (1968) [3], which is inherently blind to the local environment. Our aim in the present work is to test how the percolation model transfers to a less-symmetrical system based on an exhaustive study of its phonon dispersion curves by INS, using hexagonal-Zn_{1-x}Mg_xS (x≤0.33) as a case study. The discussion is supported by *ab initio* calculations within the framework of density functional theory.

INS experiments were conducted on two large wurtzite (*P6₃mc* space group) single crystals of (low-alloying) Zn_{0.94}Mg_{0.06}S (6x8 mm² size in length and diameter, respectively) and (high alloying) Zn_{0.67}Mg_{0.33}S (15x8 mm² size in length and diameter, respectively), at the IN8 thermal neutron triple-axis spectrometer in a high flux reactor of the Institut Laue-Langevin in Grenoble. The INS spectra were measured in \vec{c}^*/\vec{a}^* scattering plane at 12 K along the two main crystallographic directions \vec{c}^* and \vec{a}^* in the constant final momentum mode ($k_f=2.67\text{\AA}^{-1}$). *Ab initio* phonon calculations for wurtzite Zn_{0.67}Mg_{0.33}S were performed using Siesta code on two large 360-atoms supercells extended along the [001]($||\vec{c}^*$) and [100]($||\vec{a}^*$) directions with quasirandom Zn↔Mg substitution.

The ZnS-like A₁(TO), E₁(TO), E₂^H and B₁^H optical phonon modes exhibited distinct percolation doublets across the Brillouin zone, consistent with *ab initio* predictions. The Zn-S percolation doublets are found to be intrinsic to random Zn↔Mg substitution and due to alloying. The microscopic mechanism of ZnS-like splitting is elucidated by *ab initio* calculations at dilute limit (x~0). The main results of this work reinforce the status of the percolation model as a robust descriptor of phonons in semiconductor alloys with highly symmetrical cubic structure as well as with less symmetrical hexagonal structure.

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The DREAM multipurpose diffractometer at ESS



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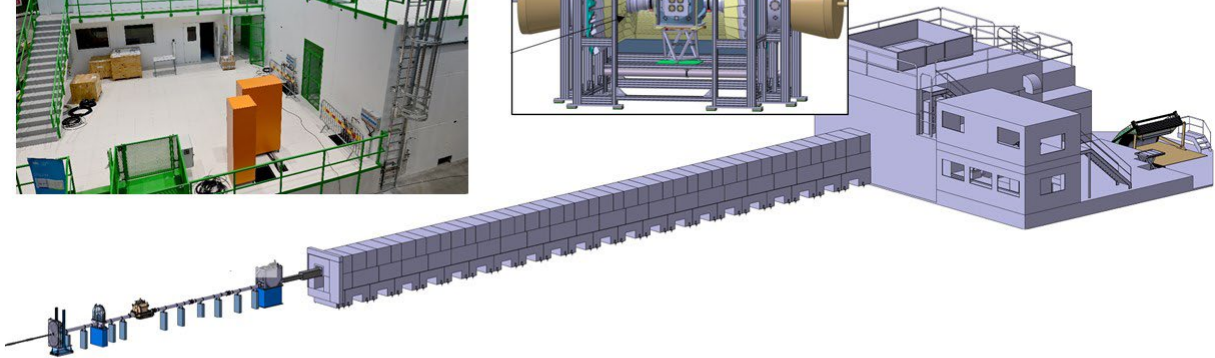
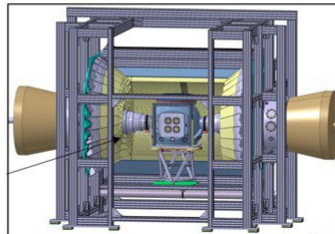
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The European Spallation Source (ESS) under construction in Lund in Sweden should see its first neutrons in 2025 and welcome its first users in early 2027. One of the first operational instruments will be DREAM, a diffractometer developed and built for ESS by the consortium (Forschungszentrum Jülich (Germany) / Laboratoire Léon Brillouin (France)) DREAM will be a time-of-flight diffractometer mainly dedicated to diffraction on powders, with additional capability for single crystal neutron diffraction. Its scientific field will be particularly vast - nuclear and magnetic structural studies, complex materials with large lattice parameters, *in situ* measurements, extreme conditions of temperatures, pressure, magnetic fields, etc., small samples... - with the ambition of responding to the ever-growing needs of the various scientific communities. This versatility will be enabled by the unique design of this spectrometer which will combine thermal and cold neutrons ($0.5\text{Å} < \lambda < 4.4\text{Å}$ typically) in the same measurement, while the set of choppers will allow the resolution/intensity of the neutron beam on sample to be adjusted as desired. This wide bandwidth will cover a Q range from 0.01 to 25Å^{-1} in a single acquisition, which is ideal for multi-scale studies combining several scattering techniques: Small Angle Neutron Scattering (SANS), powder diffraction and pair distribution function (PDF) measurements. The polarized cold neutrons will be available to the users from day one. I will present the design of DREAM, its current construction at ESS and its expected performance. After an overview of the differences between time-of-flight diffraction measurements and the monochromatic measurements that are today the norm on reactors, I will give insights into the specific data reduction flow that is being designed for DREAM.



ICONE project Presentation



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Neutrons are a powerful tool to explore the matter (life or inert). Since the shutdown of ORPHEE in 2019, neutron beamtime available to the French scientific community has significantly decreased. To address this situation, CEA and CNRS propose to construct a national neutron facility, ICONE, based on an innovative High Intensity Compact Accelerator (HICANS). ICONE will be a perfect complement to the existing and upcoming neutron sources in Europe (ILL, ESS, ...).

In 2024, the project entered a two-year Technical Design Phase (APD) aiming to define the scientific needs and requirements for a national neutron facility as well as presenting its design and development plan. In this presentation, we present the expected performances of ICONE facility, the project organisation, and the preliminary status of the ongoing APD studies.

SAM: the new LLB small-angle neutron scattering instrument at the ILL

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Small-angle neutron scattering (SANS) is a ubiquitous technique in condensed-matter physics with applications spanning a great number of scientific areas (soft-matter, biophysics, material science, magnetism & superconductivity). With such a large user base, the technique requires maintaining an access to efficient beamlines. SAM is the fourth small-angle neutron scattering (SANS) instrument put in operation at the Institut Laue Langevin (ILL, Grenoble) [1]. The instrument has been designed and built through a collaboration between the Laboratoire Léon Brillouin (LLB) and the ILL. Its construction has begun in June 2023 and was completed by the end of February 2024. First neutrons were subsequently detected on March 4th, marking the "true birth" of the instrument and the beginning of its "hot commissioning" phase.

We will present SAM's main features and discuss the outcome of the characterizations performed during its first two cycles of operation. The latter revealed very good performances, notably in terms of neutron brightness and beam polarization. A quick survey of the experiments performed at SAM in the frame of the "friendly user" program shall also be given. Finally, we will sketch our plans for future upgrades.



Left – Top view of the SAM instrument as installed in the ILL guide hall. **Right** – Part of the SAM team at the end of the installation phase (F. Dohou, C. Boix, I. Calsina-Estañan and P. Lavie).

[1] <https://www.ill.eu/users/instruments/instruments-list/sam/description/instrument-layout>

XtremeD: pushing the limits of research under extreme conditions at ILL

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 Structural studies under extreme conditions of temperature, pressure and magnetic field are progressively gaining importance for both fundamental research and development of new functional materials. Quite often, external stimuli dramatically alter atomic interactions and coordination environments in condensed matter leading to groundbreaking discoveries. Near-room temperature superconductors [1], high-pressure synthesis of superhard materials [2], metastable off-stoichiometric compounds [3] and field-induced bosonic condensation in spin-nematic phases akin to superconductivity [4] are just a few examples of such outstanding findings. Therefore, tools enabling the studies of materials structure under extreme conditions open up unprecedented possibilities to pinpoint structure-property relationships in conventional and more exotic materials. In this context, neutron diffraction provides unparalleled opportunities and complements X-ray scattering especially when it comes to locating light elements in the crystal structure, studying magnetic ordering, telling apart elements with close atomic number, etc.

XtremeD (Fig. 1) is a new powder and single-crystal diffractometer recently commissioned at the Institut Laue-Langevin (ILL). The instrument is operated by the Aragon Nanoscience and Materials Institute and Spanish National Research Council (CSIC) in the format of a Collaborating Research Group (CRG) accepting the beam time requests both through the ILL and Spanish National CRG proposal calls (via spins.unizar.es). The instrument has been conceived to get the most out of relatively small sample gauge volumes in bulky sample environments such as high-pressure cells and magnets through maximizing the neutron flux on the sample and detector solid angle. A wide range of incident wavelengths (from 0.9Å to 4Å) is available thanks to two different focussing monochromators (Si and HOPG) with variable take-off angle.

The latest instrument updates will be discussed and illustrated by results of recently performed official experiments.

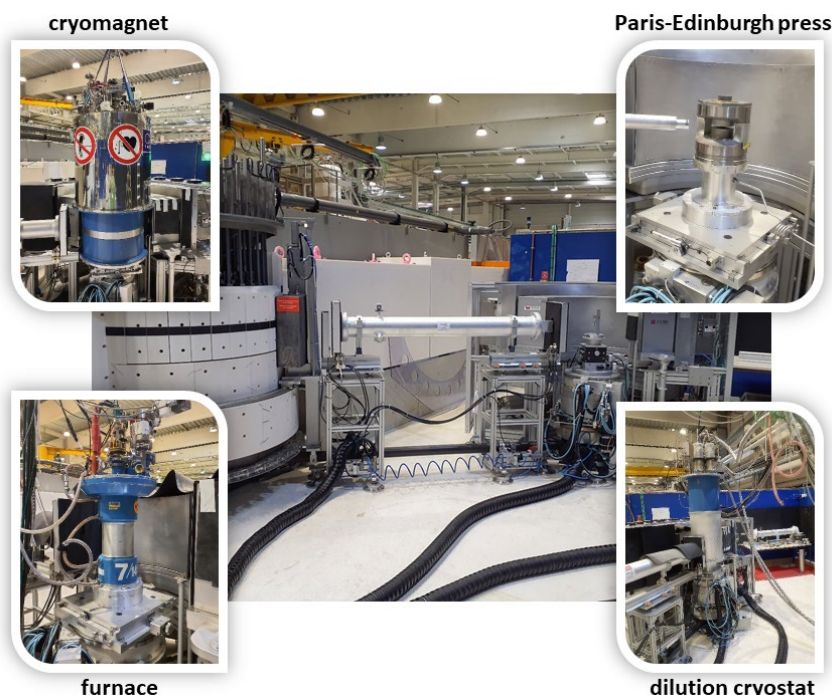


Fig. 1. XtremeD and its sample environment equipment

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 [1] A.P. Drozdov et al., Nature, 569 (2019) 528.
 [2] Y. Wang et al., Sci. Rep., 2 (2012) 520.
 [3] W.L. Mao et al., Science, 302 (2003) 425.
 [4] E. Fogh et al., Nat. Commun., 15 (2024) 442.

Bent Silicon Revolution in Inelastic Neutron Scattering

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Recent advancements in neutron optics have introduced a novel bent silicon (Si) crystal technology, poised to become a crucial alternative to pyrolytic graphite (PG002) crystals, particularly in light of potential supply shortages in Europe. This new technology, based on a thermal protocol developed at the Institut Laue-Langevin (ILL), allows silicon wafers to maintain a predefined curvature without the need for any mechanical bending device. This breakthrough offers significant flexibility in the design and construction of new monochromators and analysing systems for neutron scattering. Two possible applications of this technology are demonstrated : the MARMOT project on the triple-axis spectrometer ThALES (ILL) and a new analysing system for IN8 (ILL) :

The MARMOT analyser system represents a significant evolution in the analyzing of neutron energies for multiplexed neutron spectrometers, that began with earlier innovations such as the Flatcone analyser at the Institut Laue-Langevin (ILL) [ref.] and the CAMEA spectrometer at the Paul Scherrer Institute (PSI) in Switzerland [ref.]. It builds on a particular focusing geometry with a large set of bent Si 111 analysing blades, that allows analyzing a quasi-continuous range of final energies transfer (about 3.5 to 7 meV) simultaneously and over a wide range of scattering angles (about 70 degrees).

Similar to the existing IN1-Lagrange secondary spectrometer with a massive array of pyrolytic graphite analyser crystals collecting scattered neutrons in the huge solid angle of about 2.5 steradian [ref], we propose to build a new fixed energy focusing analyser with bent silicon crystals to use on the thermal neutron spectrometer IN8. This analyser should provide similar solid angle for the scattered neutron beam to that of Lagrange, with substantially smaller sizes and better energy resolution in the thermal energy range. To this end we are going to use the technology for bending of silicon crystals with controlled fixed curvature developed at ILL. We consider that such evolution will extend complement the capacities for vibrational spectroscopy at ILL in the thermal and lower energy range for the user experiments.

These advancements are set to redefine neutron scattering methodologies, ensuring continued progress in the field.

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[1] Kempa M. et al., Physica B **385-386** (2006), 1080-1082.

[2] Lass J. et al., Rev. Sci. Instrum. **49** (2023), 023302.

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Boosting the ILL instruments suite: the H15 guide and instruments project

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Progress in neutrons guide's fabrication allows these days to implement ambitious neutron delivery paths showing improved transport efficiency thanks to the ability to build elaborate guides' geometries with high m values. The new H15 cold- guide at the ILL has a rather complex design, starting with an opposing-curved expanding section, informally known as 'the trumpet'. It allows to spatially expand the guide permitting the creation of multiple individual branches and dedicated end-of-guide beam positions. Moreover, the opposing curve leaves a characteristic correlation between the divergence profile and spatial position at the end of the trumpet, allowing guide branches to be more widely separated in angle. This, again, create space for substantially more instruments down-stream [1].

Thanks to this design, on the new H15 it has been possible to install or refurbish 4 instruments and one R&D station, each profiting of an end of guide position.

The four H15 instruments (D007, D11+, SAM and SHARPER) have been built benefitting of the latest technologies in terms of neutrons transport, optics, polarization and detection. The results after the first phase of their commissioning show that better science and new science will be possible.

SHARPER and D007 profit from an increase in count rate of more than an order of magnitude. The increased flux made possible to equip D007 with a spectroscopy option on top of the original diffuse scattering diffraction mode to entangle coherent and incoherent inelastic scattering [2]; the relocation of D11+ favored the design of a reliable and optically clean collimation and a better detector positioning system. SHARPER now benefits of a brand new primary spectrometer that, thanks to the increased flux, enables measurements on small samples under extreme conditions, like high magnetic fields, high temperature and levitation. SAM, a new SANS CRG instrument with MEIZE option, has been the first ready for neutrons, and is now in operation showing a flux as high as predicted by simulations.

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Innovative holographic structures for efficient manipulation of slow neutron beams

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The push to establish high flux neutron sources must be complemented by the development of efficient optics to ensure effective neutron beam manipulation, particularly in the cold and very-cold wavelength range. Experiments utilizing neutrons in this spectrum face challenges due to the inherently low flux of slow neutron beams and the lack of efficient optics. Significant advancements have been achieved over the past decade in creating cold and very cold neutron optical devices, where perfect crystals are replaced by artificial holographic structures. We will briefly present recent findings using nanoparticle-polymer composite holographic gratings with record scattering length density modulation amplitudes. Additionally, we will highlight the versatility of commercially available Covestro Bayfol® HX200 photopolymer gratings, both as single and multi-layered foils. These holographic gratings offer excellent performance in slow-neutron beam control, pivotal for advancing research with long-wavelength neutrons.

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Dead neutrons keep patients alive

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In neutron scattering applications the neutrons act as *messenger*. After interaction with a sample, they “stay alive” and carry information on the microscopic properties of the sample via their change of direction and, sometimes, also their change of energy.

However, neutrons can also act as *artisans* by changing the properties of a sample. Neutrons that are captured by a nucleus will “disappear”, but secondary particles are emitted and one or more product nuclei remain, that are usually different from the initial nucleus. Often these product nuclei are radioactive and they can serve for a variety of diagnostic and therapeutic applications in the field of nuclear medicine.

So-called *molecular imaging* enables non-invasive studies of functional processes in the human body that may indicate abnormal functions of organs or various types of diseases. The distribution of radionuclides injected into patients in form of specific molecules is made visible with Gamma cameras or Single Photon Computed Emission Tomography (SPECT). A prominent example is the radionuclide technetium-99m that is produced in large quantities in research reactors and used in about 30 million imaging procedures worldwide every year.

Radioactive nuclides also serve for therapeutic applications in so-called *targeted radionuclide therapy*. Specific biomolecules, e.g. peptides, that are capable of targeting certain types of cancer cells are used to transport radionuclides close to or into the cancer cells. Upon decay of the radionuclides the emitted short-range radiation such as electrons (β^- , conversion or Auger electrons) or α particles will deposit their radiation energy very locally, capable of destroying cancer cells, while leaving normal tissue at larger distances unharmed. Since many decades, the radionuclide iodine-131 is being used to treat thyroid cancer. Today, the radionuclide lutetium-177 is in high demand to treat neuroendocrine tumors or metastasized prostate cancer. Other radionuclides with specific nuclear and chemical properties that are promising for medical applications are being studied in preclinical and clinical research.

High-flux reactors and in particular that operated by ILL play a crucial role in the worldwide production network of lutetium-177 and of novel radionuclides that are not yet commercially available. The EU project PRISMAP makes novel radionuclides available for medical research projects [1].

[1] PRISMAP – the European medical radionuclide programme. <https://www.prismap.eu>

Interferometry for understanding quantum physics

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Neutron interferometry based on perfect silicon crystals was established 50 years ago and is still a very versatile tool [1]. It is used in various fields of physics, from scattering length measurements to cosmology and quantum physics. I will explain how it works and present some typical experiments. In the second part, I will go into the details of a new version of the classical double-slit experiment [2] and present the concept of “weak values” in quantum mechanics.

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Ultracold neutrons test gravity at short distances and cosmological models

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In recent years, gravity experiments have been experiencing a renaissance for several reasons: Modern astronomical observations point to the existence of dark energy and dark matter. However, their true nature and content remain a mystery. Furthermore, prominent candidates for formulating a consistent quantum theory of gravitation require extra spatial dimensions.

Slow neutrons are excellent probes to test gravity at short distances, as they are electrically neutral, only hardly polarizable, and offer large observation times. A very competitive approach is the precision study of bound quantum states of ultracold neutrons in the Earth's gravity field, as it allows to combine gravity experiments at short distances with powerful resonance spectroscopy techniques.

In the last years, the qBounce collaboration has been setting up a dedicated spectrometer at the ultracold neutron facility PF2 of the Institut Laue–Langevin to precisely study quantum transitions between gravitational levels by applying Ramsey's method of separated oscillating fields. The main run of the experimental campaign has led to a 42-fold improvement of the statistical precision so far.

In my talk, I will review the experiments, explain key technologies and summarize the results obtained.

Neutrons for Solvent Extraction



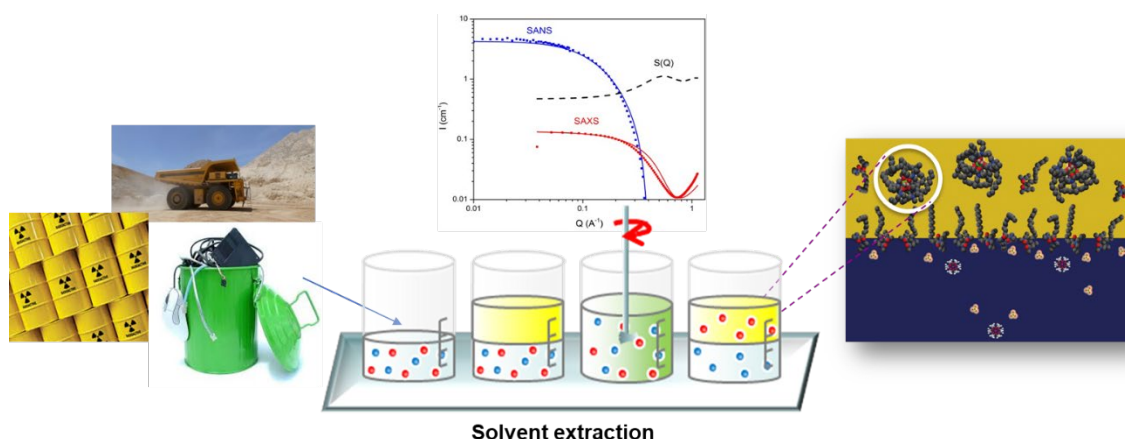
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Metal extraction plays a key role in applications such as ore mining, waste recycling, or water decontamination. Among the hydrometallurgical processes, solvent extraction is used as a separation/purification technique where metals are transferred from an aqueous to an immiscible organic phase. While effective, solvent extraction faces many challenges, requiring to better understand its mechanisms.

Since the pioneering work of Osseo Azare et al, it is recognized that the structure of the organic phase plays a crucial role in influencing both the metal transfer and the occurrence of demixion problems such as the third phase. Typically, it is often considered that the extractant molecules self-assemble into reverse micelle-like aggregates, which interact attractively and collapse, ultimately leading to the macroscopic demixing.[1]



Considering this hypothesis, X-ray and neutron scattering techniques have significantly contributed to understanding various challenges in solvent extraction, even leading to some process optimization pathways. In this presentation, several case studies will be discussed to illustrate the powerful role of Small-Angle X-ray Scattering (SAXS) and Small-Angle Neutron Scattering (SANS) in investigating solvent extraction mechanisms. It will be shown how scattering techniques revealed the structural organization of extractants into reverse micellar aggregates, providing insights that helped interpret and resolve issues related to organic phase demixing. Additionally, in a recent and innovative study where the organic phase is replaced by a porous liquid, we will show how neutron scattering was employed to characterize the permeability of the functional nanocavities.



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Probing friction mechanisms at solid/liquid interface with optical microscopy and neutron scattering

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When a fluid flows on a solid surface, it usually sticks to the surface leading to the classical no-slip boundary condition. In some cases, the adhesion is not strong enough and the fluid slips on the surface leading to an interfacial friction. Identifying the transition from adhesion to slip at solid-liquid interfaces is a critical question in rheology and extrusion processes. It is also of fundamental importance, as it offers unique insights into the dynamics of different liquid constituents (such as polymer chains, micelles, particles) near the interface. In this presentation, we will demonstrate how optical microscopy and neutron scattering can be used to investigate friction mechanisms at solid-liquid interfaces, focusing on two different types of liquids: polymer solutions and wormlike micelles.

Regarding polymer liquids, slip mechanisms of polymer melts are now well understood due to recent experiments based on direct slip length measurements [1]. The case of polymer solution is more complex since it involves a priori a competition between the frictions of the solvent and the polymer at the interface. The friction mechanism on smooth surfaces can be potentially affected by the existence of a depletion layer or can be described in terms of the friction of the polymer chains on the solid surfaces. We will explain how we understood the molecular mechanisms involved in the friction of liquid polymers, using a multi-scale approach. Using a velocimetry technique based on photobleaching, we measured the dependence of slip length as a function of polymer concentration [2]. Then, using neutron reflectivity, we studied the nanoscale structure of the interface at the nanoscale, both at rest and under flow conditions [3]. We showed that for the studied system, at rest, polymer chains are globally depleted from the solid surface. Contrary to common assumptions, some chains do adsorb onto the wall. Under flow conditions, we experimentally demonstrate that the depletion layer remains stable, a finding that has been hypothesized but rarely measured in the literature.

We will then present preliminary results obtained for another well-studied system: wormlike micelles (WLMs), which are elongated and semi-flexible aggregates formed by the self-assembly of surfactant molecules in aqueous solutions. Due to thermodynamic equilibrium, WLMs are constantly breaking and recombining, leading to complex non-linear rheological behavior. In particular, when flowing in a channel over specific conditions, a heterogeneous structural ordering, called shear-banding, occurs. The impact of wall slip on the origin of shear-banding is still an open question. Using a homemade flow cell easily rotatable under the neutron beam, we compared the near-wall alignment of the micelles at rest and under flow with different shears. We probed the in-plane structure of WLMs near the wall parallel and perpendicular to the flow direction, by applying depth-resolved grazing incidence time of flight neutron scattering (ToF- GISANS).

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Proton Conductivity in Hydrated Sulfonated Porous Aromatic Framework

¶
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Polymer electrolyte membrane fuel cells (PEMFCs) convert chemical energy into electricity efficiently. Nafion®, a branched fluorinated copolymer with sulfonic acid groups, is the leading material for proton conductive membranes due to its high ion exchange capacity and proton conductivity. However, it has limitations such as a narrow operating temperature range, high synthesis costs, and environmentally harmful degradation products. To overcome these issues, new inorganic, organic, and hybrid materials have been developed, offering high proton conductivities and improved water retention. Recently, some of us synthesized and investigated sulfonated porous aromatic framework (SPAF) aqueous electrolyte-host systems, which demonstrate high proton conductivities, excellent chemical and mechanical stability, and efficient water management [1,2].

This study investigates the water dynamics and proton conduction in SPAF with sulfonation degrees of 50% and 80% at 93% relative humidity, across three temperatures. To do so, quasielastic neutron scattering (QENS) measurements, which are highly sensitive to hydrogen atom motion, were utilized to analyze the diffusional, rotational, and jump processes of water molecules at the nanometer scale. In this way, the IN5B disk chopper time-of-flight spectrometer at ILL, known for its high flux and resolution (i.e., energy resolution of 100 μeV for the wavelength 5 Å), was employed to accurately measure and distinguish the contributions from various motion types and hydrogen subensembles.

According to measured spectra, molecular dynamics are consistently characterized by the combination of two independent motions: fast local motion around the average molecular position and confined translational jump diffusion of the molecule's center of mass. All molecules exhibited local relaxations, while the translational motion of some molecules was immobilized on the timescale of the instrument. Our findings provide a microscopic perspective on the dynamics of water within SPAFs with varying degrees of sulfonation, focusing on the self-diffusion coefficient, residence time, and their temperature dependence. It is demonstrated that the degree of sulfonation in SPAFs regulates the translational diffusion of water molecules, which plays a critical role in manufacturing fuel cells.

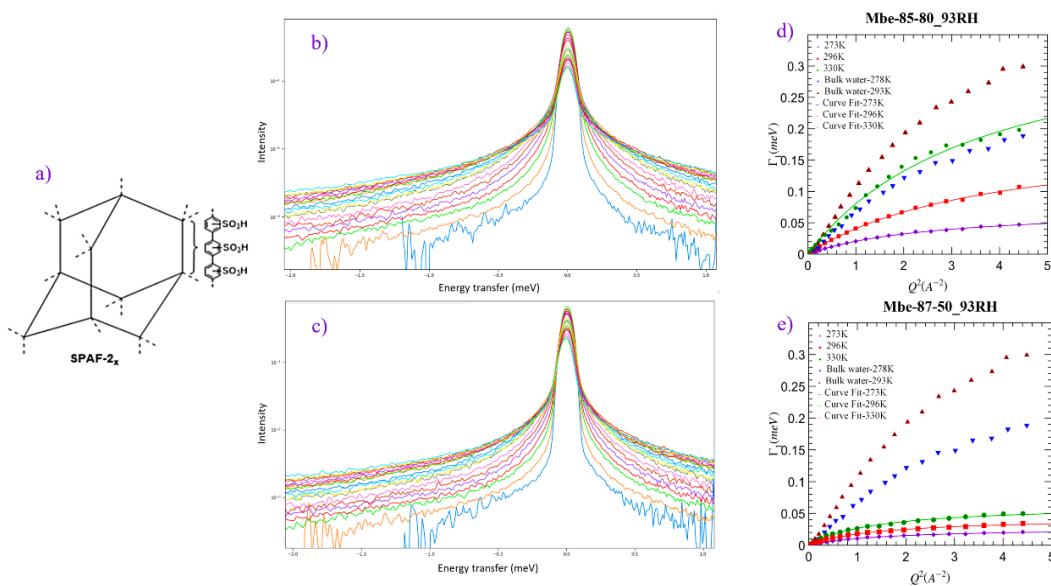


Fig.1. a) Schematic representation of SPAF-2 molecular structure. QENS spectra of b) SPAF 80% and c) SPAF 50% at different transfer of momentum (Q). Evolutions of the half width at half-maximum of the sharp Lorentzian as a function of Q^2 obtained from the fitting of QENS spectra measured in d) SPAF 80% and e) SPAF 50%.

Soft Matter

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Surfactant-free microemulsions: how molecular dynamic reflects nano-structuration

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Mixtures of simple molecules can lead to complex systems with fascinating properties, as observed in aqueous solutions of alcohol and oil, commonly found in products like cosmetics or solvents for liquid-liquid extraction. One interesting example is the mix of water, ethanol, and octanol. In the region of low octanol content, structuring occurs across various scales. Long-lasting emulsions emerge rapidly when water is introduced into the biphasic region, a phenomenon known as the Ouzo effect. Preceding this, a stable area exists above the binodal and around the critical point, where mesoscale organization occurs, described as pre-Ouzo droplets. The structuring involves aggregates reminiscent of micro-emulsions, enveloped by an ethanol excess in a water- ethanol solution with minimal octanol. Our objective is to explore the boundaries of this region.

Initially, by employing Neutron Spin Echo, QENS and NMR, we investigated the interplay between organization and dynamics, enabling us to measure droplet lifetimes and delve into the timescale within the phase diagram. Subsequently, using small-angle X-ray scattering, we mapped the phase diagram and characterized the liquid's organization from the octanol-rich area to pre-Ouzo droplet formation, determining the boundaries of the pre- Ouzo region indicated by the Lifshitz line.

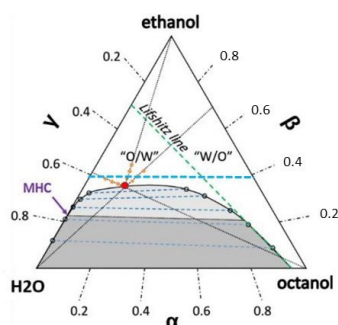


Figure 1: phase diagram (wt.%) of the ternary mixture octanol/ethanol/water. The critical point (red dot), binary region (grey), Lifshitz line (delimitates the onset of structural organisation), Minimum Hydrotropic concentration (MHC): indicates the minimum quantity of ethanol required to form a monophasic solution when octanol is added to water; the dynamics was investigated along the blue dotted line.

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Soft matter thin films under pressure: A morphological investigation under Grazing Incidence Neutron Scattering

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Using a custom-designed pressure cell [1], we tune hydrostatic pressure and combine Grazing Incidence Small Angle Neutron Scattering (GISANS) with specular and off-specular reflectivity under pressure (P) to probe morphologies of soft matter layers immersed in heavy water at P = 1 bar and P = 800 bar. Our results [2] reveal chemical composition dependencies concerning nanostructural rearrangements upon P-increase for (Fig. 1) weakly incompatible (poly((2,2,3,3,4,4,5,5-octafluoro)pentyl methacrylate)) POFPMA/ poly(2-(dimethylamino)ethyl methacrylate) PMMA homopolymer brush mixtures vs. (Fig. 2) strongly incompatible POFPMA/PDMAEMA homopolymer brush mixtures anchored on Si substrate.

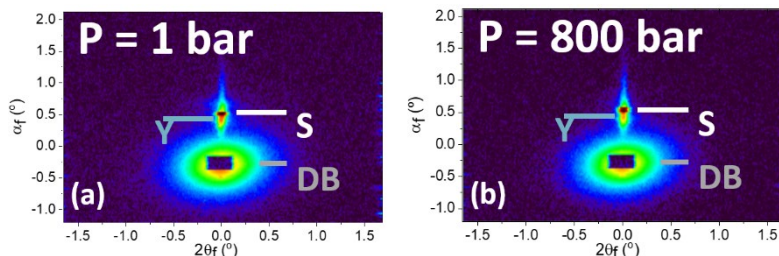


Figure 1: 2D GISANS patterns for weakly incompatible POFPMA/PMMA polymer brush mixture at T = 45 °C for (a) P = 1 bar and (b) P = 800 bar. Specular (S), Yoneda peak (Y) and direct beam (DB) regions are indicated.

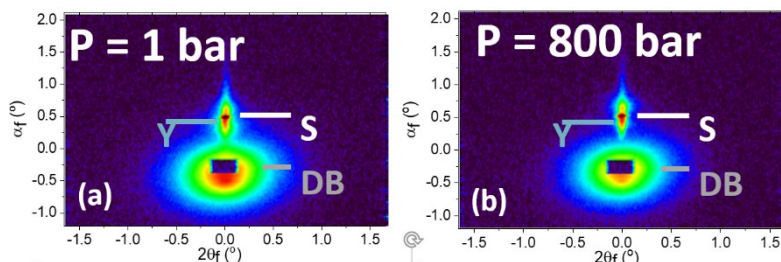


Figure 2: 2D GISANS patterns for the strongly incompatible POFPMA/PDMAEMA polymer brush mixture at T = 45 °C for (a) P = 1 bar and (b) P = 800 bar. Specular (S), Yoneda (Y) and direct beam (DB) regions are indicated.

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Mixing green fatty acids to tunes surfactant self-assemblies structure and properties

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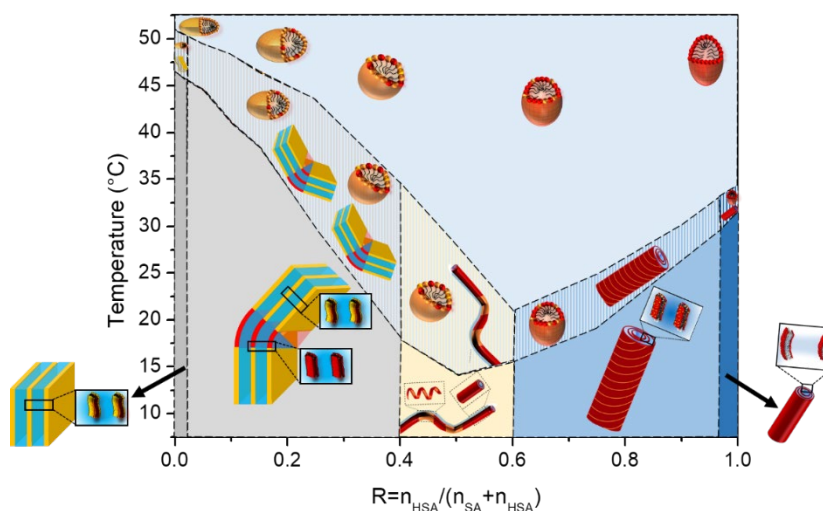
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This presentation focus on the study of aqueous mixtures of stearic acid (SA) and its hydroxylated counterpart 12-HydroxyStearic Acid (12-HSA) as a function of the 12-HSA/SA ratio (R) and the temperature. The solubilisation of the fatty acids at a constant total concentration of 2%wt is achieved through the use of a counterion – ethanolamine – added in excess so that the carboxyl heads are negatively charged.

At room temperature, the morphologies of the self-assembled aggregates are obtained through a multi-structural approach that combines small angle neutron scattering (SANS) and wide-angle X-ray scattering (WAXS) measurements with confocal and cryo-TEM microscopies, coupled with rheology measurements[1]. For all R, the self-assembled structures are locally lamellar, with bilayers composed of crystallized and strongly interdigitated fatty acids. For pure HSA these lamellae assemble into multi-lamellar tubes which dimensions can be tuned through the substitution with low amount of SA. On the other hand for pure SA sample the lamellae form planar objects which start to bend consecutively to the doping with HSA. This bending phenomenon is associated with some partitioning occurring within the aggregates up to intermediates R and eventually leads to the formation of hybrid ribbon-like structures. The rheology of the solutions follows accordingly with the evolution of the structures from a viscous behaviour for the mainly planar object to gel-like behaviour as soon as some entanglements may occur.

Such systems are also thermo-responsive [2] and exhibit a morphological transition from the multi-lamellar self assemblies to small ellipsoidal micelles above a different given threshold temperature for each R. The micelles transit from oblate to prolate, with an ellipticity that is tuned by R, as shown by SANS. These transitions are also associated with a change in rheological properties of the solutions, namely a significant drop of their complex shear moduli. The precise determination of the threshold temperature, using DSC and transmittance measurements, allows for the construction of the whole phase diagram of the system as a function of R.



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Structural and dynamical properties of PS-PNIPAM block copolymer micelles in concentrated samples

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¶
Concentrated solutions and gels of block copolymer micelles demonstrate both the cohesive strength of solids and the diffusive transport characteristics of liquids, and are subject of theoretical and technological interest [1]. Special attention is devoted to polymers containing a stimuli-responsive "switching" block that imparts the system the ability to undergo sharp, reversible changes in response to variation of external control parameters (e.g. temperature). Among them, poly-N-isopropyl acrylamide (PNIPAM) is attractive due to thermoresponsive behaviour, with a lower critical solution temperature (LCST) in water close to physiological range (LCST $\approx 32^\circ\text{C}$). Current applications of PNIPAM-based block copolymer micelles include targeted drug carriers, engineered tissues, and "switching" membranes [2]. We recently synthesised block copolymers containing thermoresponsive PNIPAM and persistently hydrophobic polystyrene (PS) blocks. In diluted aqueous solution, PS-PNIPAM diblock and PS-PNIPAM-PS triblocks form respectively starlike and flower-like micelles [3]. In the latter case, both the PS end blocks are sticking in the same micellar core as the PNIPAM block folds in a loop. However, such a configuration is entropically unfavourable and one of the two PS blocks might stick out of the original core, eventually forming a network of interconnected micelles at high concentration. The existence of bridges is thought responsible for the formation of physical gels in concentrated PS-PNIPAM-PS samples, although the relative contribution of loops and bridges is debated, as well as the influence of structural parameters such as block length and composition. Additional information on the microscopic structure of these systems is therefore desired. Moreover, there are surprisingly few studies on the dynamical properties on such microscopic scales. Connecting mechanical stability to local mobility is important e.g. to quantify transport properties within the gel. Here we use rheology to investigate the mechanical properties of concentrated PS-PNIPAM diblock and PS-PNIPAM-PS triblock copolymers in water, and we connect them to structural and dynamical information on the microscopic level, obtained by combining small-angle neutron scattering with neutron spin echo and neutron backscattering spectroscopy. We found that the presence of bridging triblocks has a striking influence on the mechanical response of our systems. The chain mobility is largely decoupled from the mesoscopic network, but it is still reminiscent of confining effects due to the micellar architecture. The systems undergo significant changes in structure and dynamics upon increasing temperature but the micellar structure is preserved, and the transition is reversible.

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Small Angle Neutron Scattering measurement of Aqueous Biphasic System

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Recycling metals, for example from batteries and electronic components, is an important challenge in our society. Most processes for metallic ion separation and recycling include a liquid-liquid extraction step. This step can be achieved using ternary Aqueous biphasic systems (ABS), which are less toxic solvents than the one classically used, hence the important effort dedicated to understanding the properties of such aqueous ternary systems. In this context, we investigate the ABS composed of water, salt (NaCl), and the tributyltetradecylphosphonium chloride [P_{4,4,4,14}]Cl ionic liquid. This mixture can undergo a phase separation depending on the concentration of each component, with a biphasic region in the phase diagram increasing with temperature, corresponding to the presence of an LCST (Lower Solution Critical Temperature).

In previous studies [1], it has been shown that the system [P_{4,4,4,14}]Cl / H₂O forms spherical micelles with a radius varying from 12 to 17 Å and an effective radius from 20 to 38 Å. We are now looking for the impact of NaCl on the micelles form and system structure by using Small Angle Neutron Scattering apparatus (line SAM from ILL, Grenoble). We are coupling those structural measurements with macroscopic rheological studies leading to the evolution of viscosity with NaCl addition. By using the Krieger-Dougherty equation, it is possible to link the viscosity to the volumic fraction of spherical micelles. The rheological measurements show a non-monotonic evolution of viscosity with salt, which first decreases until a minimum corresponding to a maximum in terms of distances between objects. The presence of this minimum corresponds to a maximum in the effective radius obtained from the structure factor of SANS, thus showing a link between the macroscopic rheological and microscopic SANS studies.

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Swelling clay/water interactions at various spatial scales: insights from neutron-based techniques.

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Swelling clay minerals are major hydrated components of soils and sedimentary rocks both on Earth and Mars where they play a key role in the control of water cycle. Their hydration behaviour impacts various geological processes and is also of prime importance in numerous industrial applications (oil industry, civil engineering, cosmetics, waste management...). These materials are multiscale by essence, and to understand their behavior, it is crucial to study their properties in various time and space windows.

At the molecular level, detailed data about the structure, dynamics and reactivity of water confined in swelling clay minerals can be obtained by combining and collating results obtained from various neutron techniques (diffraction, QENS, inelastic, spin echo...) with advanced simulation techniques. At higher spatial scale, the high penetration of neutrons presents a definite advantage, and neutron scattering experiments can provide information about the organization of clayey materials at spatial scales relevant to their application under various hydration conditions. In addition, due to its sensitivity to water, neutron imaging experiments can be particularly useful for assessing water mobility in clay samples. This talk will present a brief overview of some of the work we carried out on these various aspects emphasizing the unique set of information obtained from the use of neutron experiments.

Plenary talk by the Laureate of the SFN PhD award

To be announced during the JDN

Topological magnons in the centrosymmetric ferromagnet Mn_5Ge_3

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Recent developments in condensed matter physics have been driven and explained by the concepts of topology. Topology is ubiquitous in the physics of electrons in solids, from the integer quantum Hall to topological insulators and their quantum spin Hall effect, and to gapless systems such as Weyl semimetals, to name but a few. Topology is agnostic to whether the (quasi)particles are fermions or bosons, so magnons can also be responsible for novel topologically-nontrivial physical effects. Nowadays two main current strands of research are identified: topological magnon insulators in two-dimensional materials, such as CrI_3 and CrSiTe_3 , and gapless Dirac magnons in three-dimensional magnetic materials, such as Cu_3TeO_6 , CoTiO_3 , and elemental Gd. However, experimentally confirming the topological character of these magnons is challenging, which hampers further developments in this field.

In the first part of this talk I will present our recent study of a three-dimensional ferromagnetic material, Mn_5Ge_3 [1], whose magnonic properties were unexplored. By a synergistic combination of inelastic neutron scattering experiments and theoretical simulations, we achieved a comprehensive understanding of this material's unusual magnon band structure. Our central discovery is the existence of Dirac magnons with an energy gap. We theoretically show that this gap originates from the Dzyaloshinskii-Moriya interaction and we experimentally demonstrate how it can be closed. This both validates the gap generation mechanism and the topological nature of the magnons, thus establishing Mn_5Ge_3 as the first realization of a gapped Dirac magnon material in three dimensions. As its magnetic properties can be tuned by chemical substitution or grown in thin film heterostructures, we foresee that the features of the newly-discovered topological magnons can be engineered and subsequently integrated into novel device concepts for spintronic and magnonic applications. In the second part of my talk I will shortly present the development of a device which aims to revolutionize the co-alignment process of small single crystals through the integration of machine learning and cutting-edge technologies. The co-alignment of multiple individual single crystals is a common practice in techniques that require samples of about 1cm^3 like inelastic neutron scattering, particularly when limited by the ability to grow larger crystals. To glue small crystals as close to each other as possible and with mosaic spread below 0.3° , we have developed an online algorithm for irregular polygon stacking; a series of benchmarking tests proved, that it is the most efficient online algorithm available.

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Hidden Magnetic Texture in the Pseudogap Phase of the High-Tc Superconducting $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

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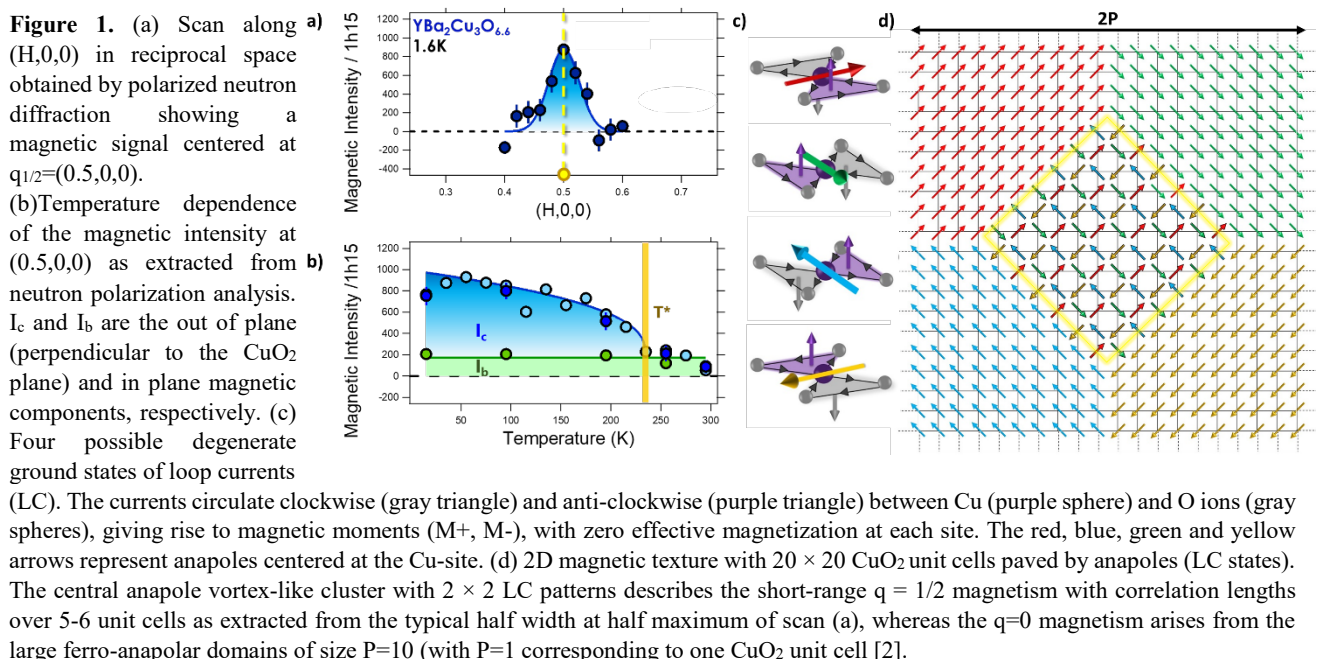
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Despite decades of intense researches, the origin of the enigmatic pseudogap phase of high-Tc superconducting cuprates remains an unsolved mystery. In the last 20 years, condensed matter physicists discovered that this mysterious phase hosts symmetry breaking states such as an intra-unit cell (or $q=0$) magnetism preserving the lattice translational (LT) symmetry and breaking the time-reversal and parity symmetries [1]. This $q=0$ magnetism gives rise to magnetic scattering on top of nuclear Bragg peaks and is interpreted in terms of loop current (LC) patterns accompanied by anapoles (or polar toroidal moments, Fig.1) [1]. It is followed, upon cooling, by an additional incipient charge density wave breaking the LT symmetry. However, none of these states can (alone) account for the partial gapping of the Fermi surface.

Our recent polarized neutron diffraction measurements in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ single crystals with different hole doping levels [2,3] reveal a novel hidden magnetism that breaks LT symmetry and that may be crucial to elucidate the pseudogap puzzle. This short-range magnetism (with typical correlations over 5-6 unit cells) is carried by the CuO_2 layers and settles in at T^* . Distinct from the $q=0$ magnetism, the related magnetic signal appears at wavevectors of the form $q=(0.5,0,0)$ and $(0,0.5,0)$, yielding a (2×2) quadrupling of the magnetic unit cell ($q=1/2$ magnetism). The associated magnetic moment is strongly anisotropic, predominantly pointing perpendicular to the CuO_2 planes, which is consistent with the picture of a LC state as the microscopic origin of the $q=1/2$ magnetic correlations (Fig.1). Finally, the $q=1/2$ magnetism vanishes in the overdoped regime, following the doping dependence of the pseudogap [3].

We discovered that the $q=0$ and $q=1/2$ magnetisms could be embedded within a single complex and highly spread-out chiral magnetic texture of LCs consisting in an anapole vortex-like pattern accounting for the $q=1/2$ magnetism binding larger ferro-anapolar domains of the $q=0$ magnetism (Fig.1). Such a magnetic texture is consistent with the recent proposal of LC supercells, breaking the LT symmetry and able to account for the pseudogap opening [4]. The existence of such broad entities reveals an unexpected aspect of the pseudogap physics that may modify our understanding of this state of matter.



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TbB₄ under high magnetic field

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TbB₄ belongs to the tetraboride family that crystallizes in the tetragonal space group *P4/mbm* and can be mapped to the Shastry-Sutherland lattice (SSL), a well-known example of a geometrically frustrated system with an exact ground state solution. The SSL consists of a square lattice with antiferromagnetic nearest-neighbor and alternating diagonal next-nearest-neighbor interactions [1]. Tetraborides have attracted much interest due to their diverse magnetic properties ranging from simple antiferromagnetic structures to more complex magnetic structures. In these compounds, particularly exciting physics arises upon application of a magnetic field that induces a cascade of magnetic phase transitions linked to fractional magnetization plateaus. In TbB₄, magnetization and magnetostriction measurements [2] performed when applying a magnetic field perpendicular to the easy magnetic plane revealed a series of successive magnetization plateau phases and a complex phase diagram (Fig.1).

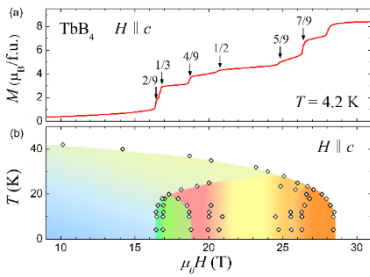


Fig.1: (a) Magnetization vs magnetic field at $T = 4.2$ K for $H//c$ axis. (b) Temperature vs magnetic field phase diagram [2-3].

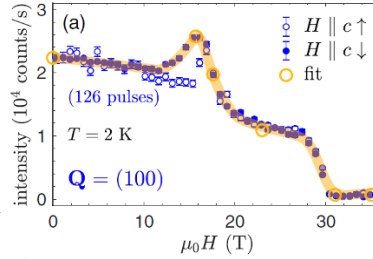


Fig.2: $Q = (100)$ peak intensities as a function of increasing/decreasing magnetic field (open/solid symbols) applied along the c axis

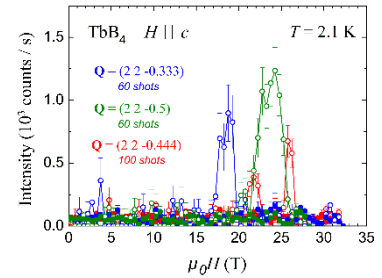


Fig.3: Intensities at $Q = (2\ 2\ -\delta)$, with $\delta = 1/3, 1/2, 4/9$ as a function of increasing/decreasing magnetic field (open/solid symbols) applied along the c axis.

In a previous experiment [3] where the dependency of the antiferromagnetic peak $Q = (1\ 0\ 0)$ was measured under a high magnetic field, it seemed that the system was only slightly hysteretic (Fig.2). In recent neutron diffraction studies at high magnetic fields, we observed a magnetic field-induced signal at position $(h\ h\ \delta)$ with $\delta = 1/3, 4/9$ and $1/2$ suggesting a stacking model along the c axis for the magnetic structure of the corresponding plateau phases. Intriguingly, for fields up to 32 T, we only observed magnetic satellites at increasing magnetic field. As no intensity could be found in the $(h\ h\ l)$ plane once the threshold field was exceeded, we suspect that magnetic superstructure reflections may be found on $(\delta\ 0\ 0)$ positions on the decreasing side of the field pulse. All these new results will be presented here.

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Neutron scattering signatures of quantum spin ice in cerium pyrochlores

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Magnetic systems with competing interactions often adopt exotic ground states, which can be relevant to study new physics in quantum matter [1]. A recurrent ingredient to stabilize such phases is frustration, like in pyrochlore oxides where rare-earth magnetic moments decorate a lattice of corner-sharing tetrahedra. In the pyrochlore $\text{Ho}_2\text{Ti}_2\text{O}_7$ for instance, a local constraint – the 2-in-2-out ‘ice rule’ acting on each tetrahedron [2,3] – leads to a manifold of degenerate ground states in which the spin correlations give rise to emergent magnetostatics [4]. Spin flips violating the ice rule generate magnetic monopole excitations [5], a mobile magnetic charge regarded as a quasiparticle carrying half of the dipole moment. A quantum analogue of the spin ice state is predicted to be a special type of quantum spin liquid formed through the coherent superposition of spin ice configurations [6,7]. Remarkably, the low-energy physics of this quantum spin ice state is predicted to be a lattice analogue of quantum electrodynamics.

We review our recent results that aim at tracking experimental signatures of such a quantum spin ice in pyrochlore oxides based on Ce^{3+} [8-9]. We discuss the importance of high-resolution neutron spectroscopy to unveil and distinguish the signatures of the different types of excitations expected in quantum spin ice materials: gapless ‘magnetic photons’ and gapped electric/magnetic monopoles that are reminiscent of spinons in one-dimensional systems. In Ce^{3+} -based pyrochlores, the magnetic degrees of freedom can be decomposed into magnetic dipolar and octupolar components. Dominant exchange interactions between some of these components can lead to form a manifold of ice states, while weaker terms in the Hamiltonian define sources of quantum fluctuations.

In $\text{Ce}_2\text{Hf}_2\text{O}_7$ using neutron low-energy time-of-flight neutron spectroscopy and thermal neutron diffraction, we show how the gapless photon and gapped monopoles translate into different spectral weights of dipolar and octupolar nature, which are challenging to measure and separate. We show how the response in this specific material can be interpreted as stemming from a hybrid ‘dipolar-octupolar’ manifold of ice states with quantum monopole excitations [8].

In $\text{Ce}_2\text{Sn}_2\text{O}_7$ using neutron backscattering spectroscopy, we show how a detailed measurement of the density of states of the gapped monopole excitations [9] can be understood considering recent theoretical studies [12-13]. The multiple peaks observed in the continuum of monopole excitations are specific signatures of the effect of the gauge field emanating from quantum spin ice correlations, providing spectroscopic evidence for fractionalization in a three-dimensional quantum spin liquid.

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Search for loop currents in the kagome superconductors CsV₃Sb₅.

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Kagome metals of the AV₃Sb₅ types with A={K,Cs,Rb} are under the spotlight recently due to their non-trivial topological Z² nature and their strongly correlated electronic phases at low temperature reminding the ones of high-T_c superconducting cuprates. For instance, CsV₃Sb₅ exhibits both a charge density wave phase below 94K with a 2x2 doubling of the unit cell and a superconducting phase below 2.5K [1]. These materials also show strong anomalous Hall effect, but no spin ordering has been found in these materials both by muon spin spectroscopy and neutron diffraction. To explain this without relying on spins, the possibility of an orbital magnetism coming from a loop current phase, emerging alongside the charge density wave, has been theoretically predicted [2,3]. This phase exhibits some similarities with the current loop phase predicted and observed in cuprates [4]. To check for the presence of this loop current phase in kagome materials, we carried out polarized neutron diffraction experiments on the IN22 (CRG-CEA) triple-axis spectrometer located at ILL. This measurement was experimentally challenging and went close to the limit in accuracy obtainable with polarised neutron diffraction in a reasonable time. Most models predict loop currents to produce magnetic intensity at M1=[1/2 0 L] or M2=[1/2 1/2 L] reciprocal space positions with L={0,1/2} [2,3]. We investigated both momentum positions. For the first one, no magnetic signal was observed ruling out the possibility of having a magnetic moment larger than 0.01 μ_B by vanadium atoms. However, measurements at M2 do not exclude the possibility of a magnetic signal, suggesting a moment of only 0.02 ± 0.01 μ_B per unit cell. This shows that current models have to be refined whether toward a lowering of the expected magnetic moment or toward a different loop current pattern giving rise to magnetic intensity at different reciprocal space positions to be compatible with our measurements. A manuscript will be soon submitted to Phys. Rev B.

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Nature of the low energy quadrupolar dynamics in $\text{Tb}_2\text{Ti}_2\text{O}_7$ under temperature

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Despite the large number of studies carried out over the last 2 decades on rare earth pyrochlore materials [1-8], the physics of terbium-based compounds, notably $\text{Tb}_2\text{Ti}_2\text{O}_7$, remains puzzling. This particular material shows no long-range order down to sub-kelvin temperature, yet exhibits static and dynamic magnetic correlations that still defy our understanding. We present here an in-depth study that sheds new light on this issue. In the first step, we considered the dispersion of the first excited crystal field doublet, located at about $\Delta = 1.5$ meV above the ground doublet. RPA simulations, based on an anisotropic bilinear exchange Hamiltonian [11] yield spectra directly comparable with the data [9], enabling us to determine a set of magnetic exchange parameters [12]. We also have studied the low energy sector by polarized inelastic neutron scattering, revealing the dispersion of a magnetic mode (0.1-0.3 meV) and completing the results reported in [9]. Our study is supported by RPA calculations of the $S(Q,E)$ scattering function, taking into account quadrupole-quadrupole interactions among the elements of the ground CEF doublet [9,10,11]. We could reproduce the dispersion of this mode and place our system on a phase diagram obtained from different multipolar order parameters (dipolar and quadrupolar ones) [13]. We finally performed a simulation analysis with respect to temperature, and found peculiar results: the M_z channel seems to be a goldstone mode associated to a ferroquadrupolar nature, and the M_y channel to a soft mode related to the dipolar magnetic interactions. Both mode disappear in temperature; we could therefore propose a new temperature phase dependence for $\text{Tb}_2\text{Ti}_2\text{O}_7$.

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Interplay between structural and magnetic chiralities in NiCo₂TeO₆

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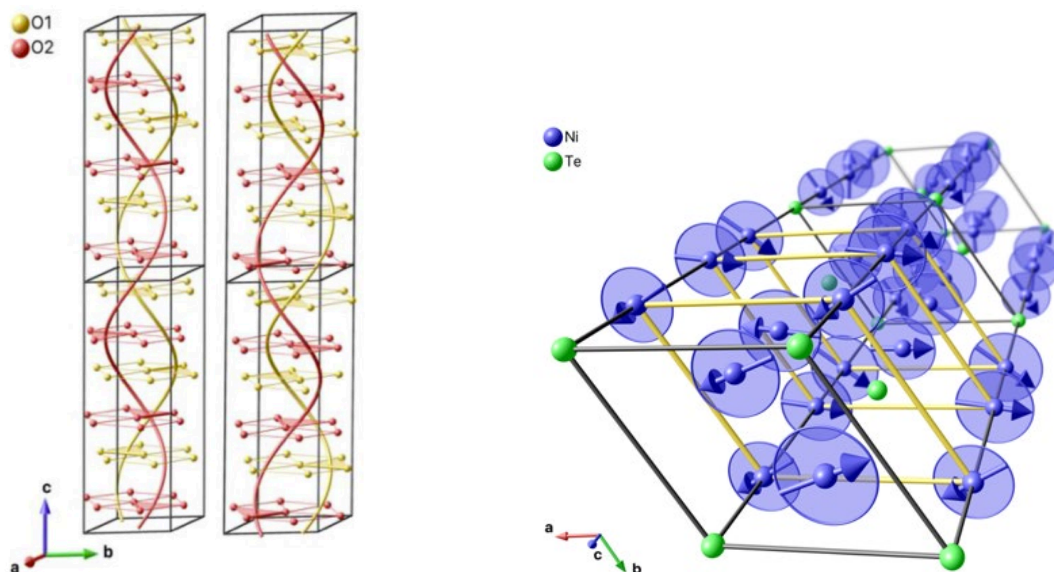
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NiCo₂TeO₆ crystallises in the R3 space group where the displacements of the O₁/O₂ oxygen atoms in the triangular plaquettes lead to left-handed and right-handed structural chiralities [1]. This compound is particularly interesting because an anomaly was observed in the dielectric susceptibility at T_N suggesting the presence of magnetoelectric behaviour [2]. A long-range magnetic order (magnetic space group R3.1'(00γ)ts) develops below 52 K consisting of ferromagnetically coupled *a-b* layers of Ni²⁺ that rotate along *c* with an incommensurate propagation vector $k = (0, 0, 0.211)$ [2]. It is not yet clear if the magnetic helix echoes the feature of two helices of opposite handedness where the globally preferred chirality emerges as a difference between the displacements or if it presents a single chirality. Therefore, we probed the structural and magnetic chiralities using polarized neutrons on the D3 diffractometer at the ILL, following the successful methodology from our previous work on a langasite compound [3]. We studied two NiCo₂TeO₆ single crystals, one of each structural chirality. Spherical neutron polarimetry and Schwinger scattering were exploited to deduce the magnetic and structural chiralities, respectively, while our complementary X-rays results yield information concerning the coupling of those two quantities. Our findings constitute an important step towards the understanding of the magnetoelectric properties of this compound.



Left: Visualization of the left- (structure to the left) and right-handed (structure to the right) structural chiralities. Right: Visualization of the magnetic structure with planes (emphasized by yellow cylinders) of Ni²⁺ spins rotating along the *c* axis.

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Spin ice and high entropy materials

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The high-entropy approach is a new and promising concept to design new materials with unprecedented properties. It offers a vast and rich playground in which, for instance, fine tuning of disorder becomes possible. Here we utilize this concept to explore the impact of disorder on the celebrated rare earth pyrochlores physics. These compounds have long been the cornerstone of frustrated magnetism, providing with their framework of corner-sharing tetrahedra the first experimental realizations of spin ice along with their quantum counterpart, described by an emergent U(1) gauge field theory. The high entropy process creates a smooth disorder on the B site of the general $A_2B_2O_7$ formula of pyrochlore compounds, different from what has been investigated so far, as it does not play with the B site charge distributions or with the presence of interstitial oxygen. In this presentation, we shall especially discuss the case of $Dy_2(TiZrHfGeSn)_2O_7$, $Tb_2(TiZrHfGeSn)_2O_7$ and $Nd_2(TiZrHfGeSn)_2O_7$. Extensive characterizations were performed using X-ray and neutron diffraction, inelastic neutron scattering, as well as magnetization and specific heat measurements, leading to a comprehensive picture of the impact of disorder on the ground state of these exotic magnets.

Structural and magnetic properties of the iron-based superconductor BaFe_2S_3

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Since the discovery of the first iron-based superconductor in LaFePO in 2006 [1]. The Iron-based compounds has become one of the top research fields in condensed matter physics. Most of them are two-dimensional superconductors based on iron pnictides or iron chalcogenides planes. Recently a spin ladder chalcogenide family, namely BaFe_2X_3 ($\text{X}=\text{Se}, \text{S}$), has been found to present superconductivity (SC) under pressure (10-17 GPa) with a T_c between 10 and 26 K [2,3] (see Fig. 1b). Its singularity lies in its quasi unidimensionality, requiring a different, somewhat simpler, theoretical framework. The crystal structure of these compounds consists of 2 Fe^{2+} ladders per unit cell, formed by edge-sharing FeS_4 tetrahedron, separated by Ba ions (see quadruple unit cell in Fig. 1c). At low temperature, a different magnetic order appears depending on $\text{X}=\text{S}$ or Se (see Fig. 1c dot $\text{X}=\text{S}$). While a comprehensive study of the member BaFe_2Se_3 has been realized in past few years, a similar investigation of the $\text{X}=\text{S}$ composition is lacking to provide a unified picture for this family's properties.

We will present a comprehensive study of the crystalline and magnetic structure combining X-ray and neutron diffraction on powder and single crystal, made possible by high quality single crystal synthesis. We have obtained several significant results marked by a series of phase transitions: a non-centrosymmetric orthorhombic structure at room temperature, a previously undetected structural transition at 120K followed by a non-collinear monoclinic magnetic structure below 100K, and a weak magneto-elastic coupling compared to the parent compound BaFe_2Se_3 . These results will be discussed in light of the literature on this compound and the parent compound BaFe_2Se_3 to present a comprehensive and coherent interpretation of the magneto-structural properties of this family.

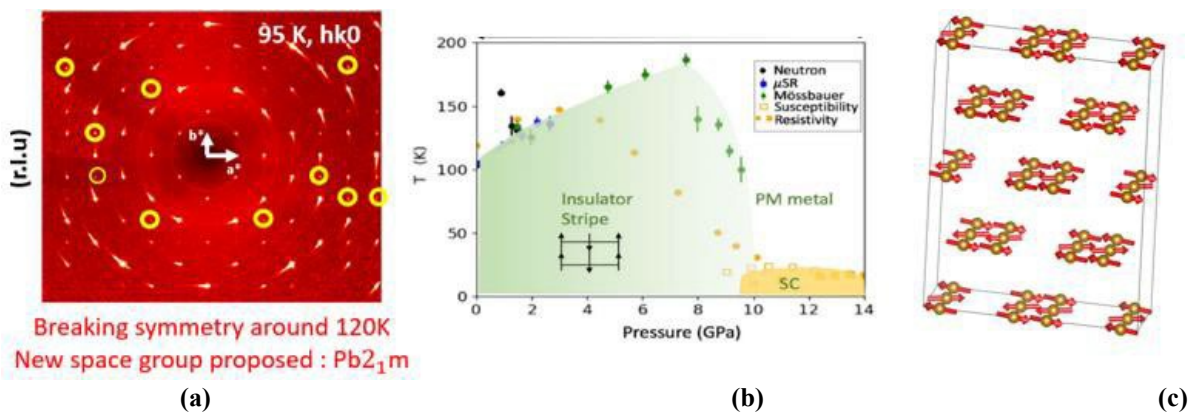


Fig 1 : (a) BaFe_2S_3 reciprocal lattice reconstruction of (0KL) plane. (Experiment done in Cristal Beam line (synchrotron Soleil)) (b) : BaFe_2S_3 (P,T) phase diagram. (c) : The magnetic structure of BaFe_2S_3 in the magnetic unit cell (4 times the atomic unit cell)

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Ab-initio calculations of magnetic excitations in strongly-correlated materials

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Inelastic neutron scattering provides among other things precious insights into the magnetic structure and excitations of the system under study. However, the analysis and fitting of such data to an effective model can be quite challenging for complex systems. The idea behind this work is to provide quantitative magnetic exchange couplings from ab initio calculations as input to these models. The ab initio calculation of magnetic excitations for strongly correlated materials is a theoretical and computational challenge due to the complexity of the physics involved and the size of the systems of interest. The Selected-Active-Space+Single method has been implemented in the RelaxSE code [1] and provides a mean to obtain these excitations. However, it is only one of the many steps of a long computational workflow where fragments have to be designed and embedded, bridging orbitals need to be localised, ground and excited magnetic states of an effective Hamiltonian need to be extracted. In this talk, I will present our methodology, some of our latest results on the pyrochlore-like NaCu_3F_7 system [2] and the challenges we are still facing.

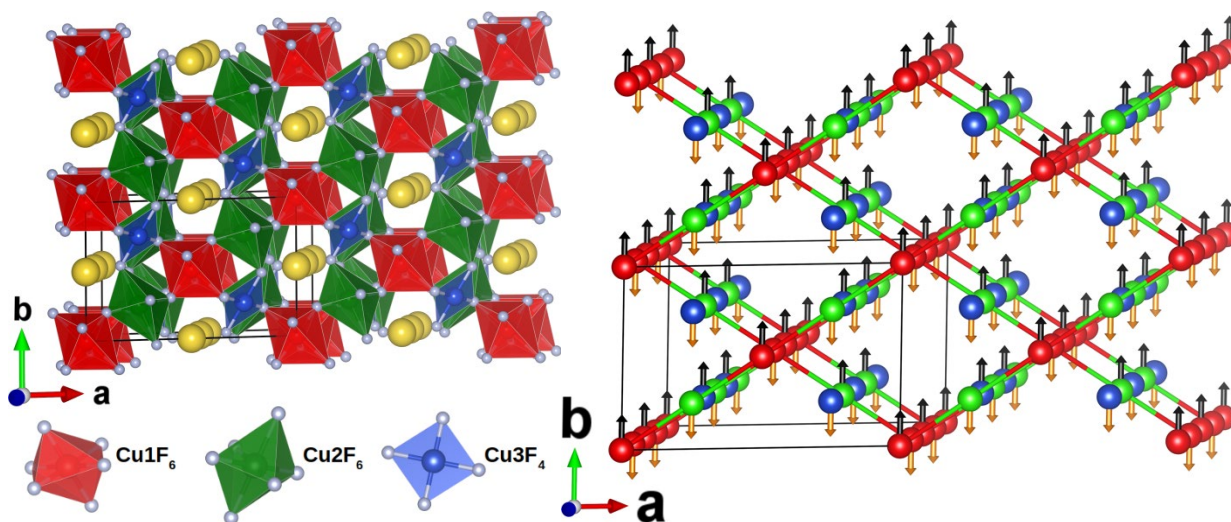


Figure: (left) Schematic representation of the NaCu_3F_7 crystal structure, The F atoms are in light gray, and the Na in yellow. The three independent Cu are pictured in different colours: Cu1 in red, Cu2 in green and Cu3 in blue. (right) Ground-state magnetic order of NaCu_3F_7 obtained from ab-initio calculations.

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Thermal conductivity in terbium-based compound : $\text{KTb}_3\text{F}_{10}$

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$\text{KTb}_3\text{F}_{10}$ is a terbium-based compound with a cubic structure ($Fm-3m$ space group), in which the magnetic Tb ions form an unusual network of corner sharing octahedra [1-4]. Tb ions sit on the 24e Wyckoff site (C_{4n} point group) and are surrounded by 8 fluorine atoms, forming a slightly distorted dodecahedra cage. Interestingly, because of the cubic three-fold symmetry, there are three possible orientations of this fluorine cage in the structure : the 4-fold axis of each cage can be parallel to either of the three cubic axes.

This compound exhibits a very low thermal conductivity at room temperature, about $2 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ which is expected in amorphous materials such as glass. More interestingly, the thermal conductivity curve at low temperatures is not proportional to T^3 as expected for a system where only phonons conduct heat but instead comprises a local extremum (Figure 1). Since this unexpected feature has been observed in other Tb based compounds, which all have low energy CEF levels, magnetic excitations are likely to play a role in this macroscopic property. Indeed, measurements have shown that the magnetic field was able to drastically affect the thermal conductivity in those terbium-based compounds, while phonons should not be affected in the approximation of an absence of CEF-Phonon coupling.

In that context, neutron diffraction and inelastic neutron scattering experiments as well as calculations were carried out to characterize the magnetic properties of $\text{KTb}_3\text{F}_{10}$ and emphasize the microscopic signature of such coupling.

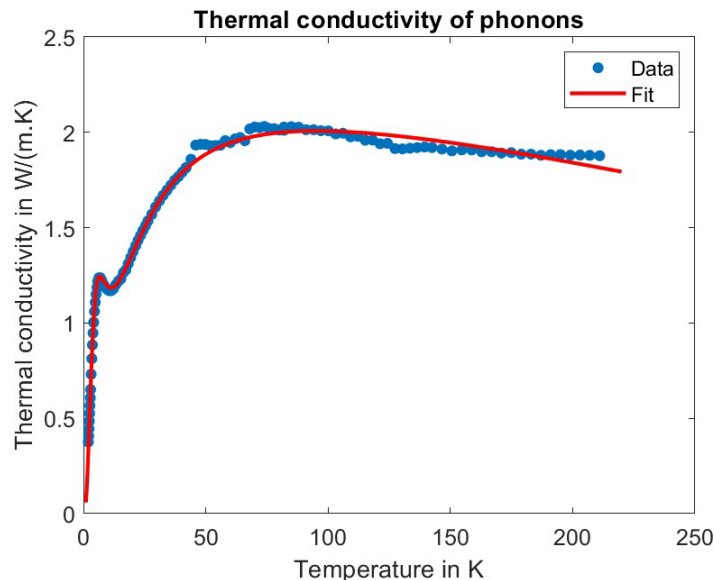


Figure 1 : Thermal conductivity of $\text{KTb}_3\text{F}_{10}$ as a function of temperature

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Neutron Backscattering at Discrete Energy Transfers: New Possibilities and Challenges of Fixed Window Scans

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Neutron backscattering offers a unique access to the total scattering function $S(q, \omega)$ and allows a quantification of diffusive processes on the nanosecond time scale. During a classical acquisition, the energy and momentum transfer are investigated simultaneously. Being a flux limited technique, the acquisition time for full QENS spectra required acquisition times of several hours and high concentrated samples [1]. On backscattering spectrometers with a doppler driven monochromator, the neutron flux can be increased by investigating discrete energy transfers instead of full QENS spectra. These so called Fixed Window Scans (FWS) therefore allow the investigation of low concentrated samples (e.g. 0.5 mg/ml) as well as the investigation of the short time diffusion during kinetic processes. Recently, we presented a new analysis framework for the FWS for colloidal suspensions [2], resulting in quantitative agreement with the analysis of QENS spectra and FWS.

In a first part, we employ the framework to dilute protein solutions, show its applicability and separate the internal dynamics from the center-of-mass motion. The diffusion coefficients are later compared to the translational long-time diffusion coefficient determined from DLS.

We also applied the same acquisition mode to follow the temperature-triggered formation of protein fibers. The *in situ* observation of the process reveals the time resolved diffusion coefficient of the proteins which provides new insights into the fibril formation.

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Exploring local structure in some oxygen deficient perovskite polymorphs by Total Neutron Scattering

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Oxygen-deficient perovskite oxides have attracted significant attention over the past few decades due to their rich chemistry, structural complexity, intriguing properties and applications, such as ionic conductors, oxygen sensors, and electrocatalysts. Various structures can emerge from the basic perovskite framework, showing different oxygen vacancy orderings or structural distortions. As an example, the brownmillerite structure, with the general formula $A_2BB'O_5$, is formed by releasing one-sixth of the oxygen atoms along the [110] direction of the cubic perovskite. This structure thus consists of alternating octahedral (O) and tetrahedral (T) layers and exhibits orthorhombic symmetry due to the formation of empty one-dimensional oxygen vacancy channels along the [100] direction (Fig.1). Space group attribution can be ambiguous due to subtle structural changes, making it challenging to differentiate between various types of tetrahedral chain ordering and space group symmetries ($Pnma$, $Imma$, and $I2mb$). These structural differences are crucial for interpreting their potential for oxygen ion conductivity, as $Pnma$ and $I2mb$ result in ordered $(BO_4)_\infty$ tetrahedral chains, while $Imma$ leads to an average and potentially disordered orientation, which can be static or dynamic.

Recently, we reported on the oxygen diffusion mechanisms in a novel oxygen-deficient perovskite, Sr_2ScGaO_5 . Depending on the synthesis route, Sr_2ScGaO_5 exhibits two polymorphs: a brownmillerite and a cubic perovskite structure [1-3]. For the brownmillerite-type structure, Pair Distribution Function (PDF) analysis and Rietveld refinements of neutron diffraction data provided identical structural descriptions. However, on a local scale, a brownmillerite-type vacancy structure was observed in the oxygen-deficient cubic polymorph, indicating complex short-range ordering and a distinctive microstructure (Fig.2) [4].

In the present study, we aimed to investigate through neutron PDF the local structure of several oxygen-deficient perovskites (Ba_2InFeO_5 , Sr_2ScFeO_5 , Sr_2ScCoO_5), that exhibit a brownmillerite structure and a cubic perovskite configuration as a function of heat treatment. Data have been collected on the D4 disordered materials diffractometer at ILL. Despite the average structures being significantly different, it appears that, on a local scale, the cubic structures show a brownmillerite framework. This suggests that the retention of the brownmillerite-like structure influences the formation of short-range correlations of oxygen vacancies along with B cation ordering, indicating the presence of brownmillerite nanodomains within the cubic phase, which appears to be a persistent feature of oxygen deficient perovskites. In this context, neutron scattering has proven to be indispensable, as it allows for the detailed analysis of oxygen ordering, which is challenging to observe with X-ray diffraction.

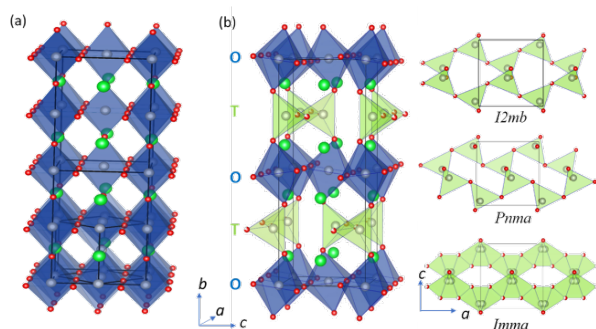


Figure 1. (a) Perovskite and (b) brownmillerite structures, showing alternating octahedral (O) and tetrahedral (T) chains. On the right, different orientations of the $(BO_4)_\infty$ -tetrahedral chains are shown, giving different possible space groups in

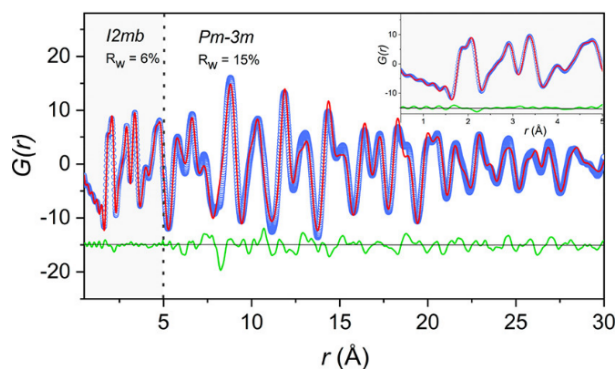


Figure 2: Long- and short-range $G(r)$ values obtained for cubic-perovskite, refined with the $I2mb$ structure in the low- r region, while in the medium- and high- ranges data are refined with the average cubic structure $Pm\bar{3}m$. D4C@ILL data ($\lambda = 0.4989\text{\AA}$, $0.35\text{\AA}^{-1} < Q < 2.25\text{\AA}^{-1}$) [4]

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Current and future experimental possibilities for investigating actinide-based materials with neutrons

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Since many decades neutron-based scattering and non-scattering techniques have significantly contributed to our understanding of actinide-based compounds. Due to the unique properties of neutrons these experimental possibilities remain invaluable to gain microscope insights and are complementary to other techniques including x-ray scattering [1]. We will recall some scientific examples with an emphasis on intermetallic quantum materials: Concerning unconventional superconductivity, inelastic neutron scattering revealed signature of superconductivity in the spin dynamics e.g. ‘Superconducting Resonance’ of U(Pd/Ni)₂Al₃ [2], UBe₁₃ [3] and UTe₂ [4]. Small Angle Neutron Scattering (SANS) was used to investigate the flux line lattice in UPt₃ [5]. Concerning exotic magnetism, neutrons revealed the NpO₂ multipolar order [6], UO₂ quadrupolar excitations [7], USb excitation above T_N [8] and URu₂Si₂ dotriacontapole order [9] and field-induced spin-density wave beyond hidden order [10]. Polarised neutrons probed PuCoGa₅ and NpCoGa₅ electronic states [11].

The instrument suite for neutron scattering experiments at the Institut Laue Langevin (ILL), Grenoble, France has significantly evolved in recent years which provides unprecedented possibilities also for research into actinide materials. We will present some recent instrumentation developments mainly related to cold neutron (direct and indirect) spectroscopy but also (polarised neutron) diffraction.

Actinide research relies heavily on the scientific support infrastructure and all proposals for ILL beamtime will be evaluated for technical feasibility and safety. A large range of sample environment is available for uranium-based compounds. For transuranium (TU) experiments a special low temperature TU insert is available with a base temperature of 5K.

The neutron eco-system is constantly evolving and the European Spallation Source (ESS) will start neutron production next year. ESS shall provide user access to some instruments from 2027 onwards. We will highlight their unique instrument suite providing new experimental possibilities. Again, a range of scientific support infrastructure will be available as required for an (initial) user programme.

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Proton dynamics at pressures up to 25 kbar measured on IN1-Lagrange

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IN1-Lagrange at ILL offers advantageous conditions for studying of relatively small samples thus favouring experiments at high pressures. Applying high pressures, that represents itself an ideal action on the material through temperature independent variation of interatomic distances, sets a challenge for neutron scattering experiments because of reduced transmission of neutron beams in the material of pressure cells and accordingly enhanced background. Optimization of neutron scattering experiments requires taking into account spectrometer geometry, in particular, in the case of large solid angle open for the scattered beam. We have designed compact high-pressure cells of a generic type “piston-cylinder” in order to make use of a special scattering geometry of the neutron spectrometer IN1-Lagrange at ILL. The most optimal cell shape comprises a rounded tail without additional neutron absorbing hard-metal inserts. We used Ni-Cr-Al alloy for the main cell body with the belt-shape support of titanium metal in the reinforced variants. The cell sizes are chosen through calculation of the optimal signal-to-background ratio. The engineered and fabricated cells have been used in several tests as well as in regular user experiments at ILL. We present some of the collected data on cell background and attenuation together with examples of measurements of the temperature dependent proton dynamics in different hydrogen-based materials in the energy range up to several hundred millielectronvolts and quasi-hydrostatic pressures up to 25 kbar.

Search of magnetic textures in high critical temperature superconducting cuprates

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Cuprates are superconducting materials characterized by high transition temperatures (above liquid nitrogen temperature >77K) at ambient pressure, which places them in the family of unconventional superconductors. At the atomic scale, these compounds feature a crystal structure dominated by the presence of CuO₂ conduction planes and reservoir blocks facilitating charge carrier transfer during doping.

Depending on the degree of doping, they present a general phase diagram divided into zones with different physical properties.

In the underdoped zone of the phase diagram delimited by what is known as T*, physicists reported a partial gap opening at some portions of the Fermi surface resulting in a loss of electronic density of states. This zone is known as the « pseudo-gap ». It could play a role in the emergence of superconductivity but its origin remains a mystery to this day.

The pseudo-gap contains a magnetic phase, which breaks the symmetries of inversion and time-reversal, interpreted as being the signature of magneto-electric quantum state of the « current loops » type [1,2]. This phase preserves the lattice translational symmetry and is qualified as “q=0 magnetism”. The recent discovery of additional magnetic correlations induced by these quantum states in the CuO₂ planes and leading to a doubling of the unit cell (q=1/2 magnetism) suggests the existence of a magnetic texture that could play a key role in the physics of the pseudo-gap [3-5].

Using the floating zone technique, we synthesize single crystals of bismuth-based cuprates with general formula Bi₂(La, Sr)₂Ca_{n-1}Cu_nO_{4+2n} and yttrium-based cuprates (YBa₂Cu₃O_{7-δ}).

In the single-layer compound (n=1) named Bi2201 of bismuth cuprates, we aim at studying the magnetism at q=0 and q=1/2 by polarized neutron diffraction on several single crystals with different hole-doping levels. In particular, strontium substitution by lanthanum allows covering the entire phase diagram (from the underdoped to the overdoped regime)

In the yttrium-based compound, we aim at studying the q=1/2 magnetism in the overdoped region of the phase diagram.

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ReMade@ARI: a hub for materials research

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As a result of the progressive depletion of natural resources, together with increasing waste, a cooperation aimed at shifting the global economy towards a circular economy is urgently needed. This change requires substantial research on materials that have high recycling potential, while exhibiting competitive functionalities.

In order to address this challenge, the most significant European analytical research infrastructures have joined forces in the ReMade@ARI Horizon Europe project, which provides a support hub for materials research while facilitating a step change to a circular economy.

ReMade@ARI offers comprehensive analytical services for research that focuses on the development of new materials for the circular economy [1]. The project offers coordinated access to over 50 research infrastructures across Europe, including neutron sources (ILL, SINQ, FRM II, ISIS, BNC), electron microscopy facilities, synchrotrons, free electron lasers, high magnetic field laboratories, and ion or positron beam facilities. Senior scientists, facility experts and young researchers contribute scientific knowledge and extensive support to provide user services [2]. Particular attention is given to the implementation of comprehensive support mechanisms for researchers and developers from industry [3].

ReMade@ARI releases calls for standard access (ReMade-TNA) twice a year. Separate calls for additional modes of access that are dedicated to industry (ReMade-SME and (ReMade-IND) are released separately. The schedule of calls for different modes of access are outlined in Fig. 1.

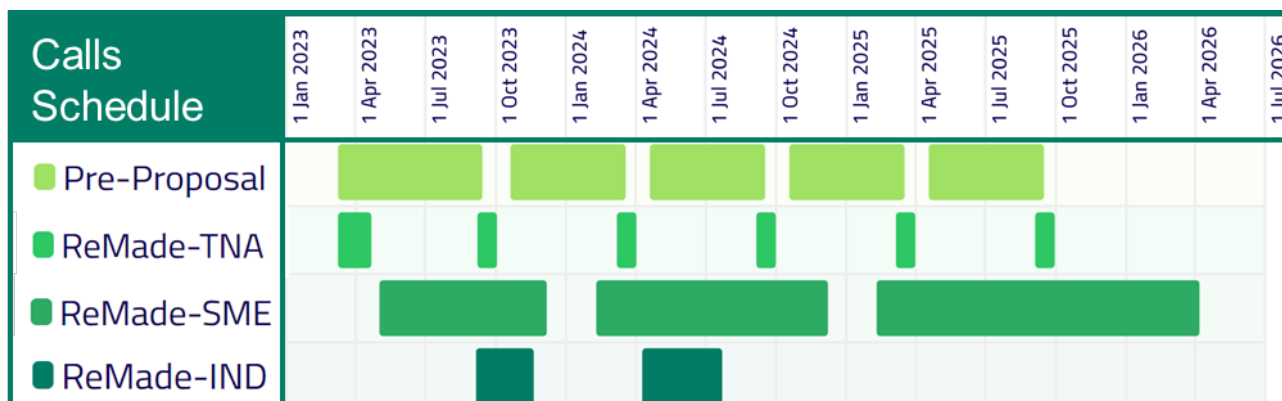
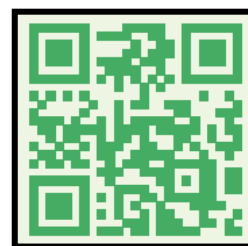


Fig. 1: Schedule of calls for access to ReMade@ARI analytical research infrastructures [4].

References:

- [1] info@remade-project.eu (for general information)
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Pr₃Ga₅O₁₂ garnet synthesis and physical properties

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Refrigeration at low temperature relies on helium cooling systems, which are becoming increasingly expensive to run, owing to He scarcity. Alternative refrigeration techniques, like magnetic refrigeration, which is based on the magnetocaloric effect, are thus becoming mandatory. Gadolinium gallium garnet has good magnetocaloric properties at high magnetic field and low temperature [1], and is already used in magnetic refrigeration devices, but new materials with enhanced properties are needed. This work aims at optimizing magnetocaloric properties in rare-earth garnets through a better understanding of the impact of chemical substitutions on their crystal structure, magnetic ground state and magnetic properties. As a part of this study, a single-crystal garnet Pr₃Ga₅O₁₂ has been synthesized by the optical floating zone technique (Figure 1) and characterized.

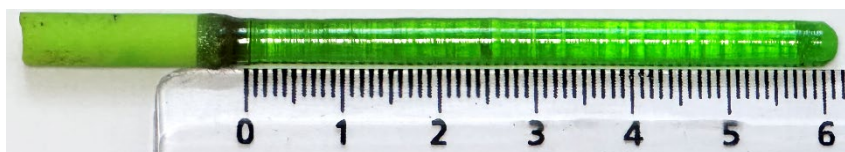


Figure 1: Pr₃Ga₅O₁₂ third crystal growth

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Mon 30 Sept. 2024		Tues 1 Oct. 2024		Wed 2 Oct. 2024		Thurs 3 Oct. 2024		
		9:00-10:10	CONDENSED MATTER	9:00-10:10	SOFT MATTER	9:00-10:10	MAGNETISM	
		9:00-9:40	Plenary: S. Rols	9:00-9:40	Plenary: S. Dourdain	9:00-9:40	Plenary: N. Biniskos	
		9:40-10:10	Keynote: V. Giordano	9:40-10:10	Keynote: M. Grzelka	9:40-10:10	Keynote: D. Bounoua	
		10:15-11:00	CONDENSED MATTER	10:15-11:00	SOFT MATTER	10:15-11:00	MAGNETISM	
		10:15-10:30	T. Marescot	10:15-10:30	A. Mozhdhehi	10:15-10:30	Y. Oubaid	
		10:30-10:45	D. Rebiscoul	10:30-10:45	F. Malayil	10:30-10:45	E. Rebolini	
		10:45-11:00	M. Kamar	10:45-11:00	A. Vagias	10:45-11:00	O. Demortier	
		11:00-11:30	Coffee	11:00-11:30	Coffee	11:00-11:30	Coffee	
		11:30-12:20	INSTRUMENTATION	11:30-12:20	SFN PhD Award Ceremony		ROUND TABLE Future of neutrons	
		11:30-12:00	Invited: F. Porcher	11:30-11:55	L. Michot, President of Jury	11:30-12:30		
		11:55-12:20	Invited: N. Pichoff	11:55-12:20	Laureate			
		12:30-14:00	Lunch	12:30-14:00	Lunch	12:30-14:00	Lunch	
		14:00-14:25	INSTRUMENTATION		Poster Session			
		14:00-14:25	Invited: N. Martin	14:00-15:00				
		14:30-15:30	INSTR.					
		14:30-14:45	S. Savvin					
		14:45-15:00	M. Boehm	15:00-				
		15:00-15:15	G. Manzin	Coffee				
		15:15-15:30	E. Hadden					
		15:30-16:00	Coffee					
		16:00-17:10	BIOLOGY	16:00-18:00	NEUTRONS BEYOND SCATTERING			
		16:00-16:40	Plenary: F. Testard	16:00-16:40	U. Koester			
		16:40-17:15	Keynote: F. Natali	16:40-17:10	H. Lemmel			
		17:15-18:00	BIOLOGY	17:10-17:50	T. Jenke			
		17:15-17:30	C. Beck					
		17:30-17:45	L. Genovese					
		17:45-18:00	M. de Boissieu					
			M. Warburton					
			M. Koza					
		18:10-19:30	ENSA and AG SFN	18:00-19:30	NEWS From FACILITIES and 2FDN			
		20:00	Dinner	20:00	Dinner	20:00	Conference dinner	

