JDN 2025

Report of Contributions

Contribution ID: **3** Type: **Oral**

On De Gennes Narrowing of Fluids Confined in Nanoporous Materials

Monday, 2 June 2025 15:45 (15 minutes)

Beyond well-documented confinement and surface effects arising from the large internal surface and severely confining porosity of nanoporous hosts, the transport of nanoconfined fluids remains puzzling by many aspects. With striking examples such as memory, i.e. non-viscous, effects, intermittent dynamics and surface barriers, the dynamics of fluids in nanoconfinement challenges classical formalisms (e.g. random walk, viscous/advective transport) – especially for molecular pore sizes. In this context, while molecular frameworks such as intermittent brownian motion, free volume theory and surface diffusion are available to describe the self-diffusion of a molecularly confined fluid, a microscopic theory for the collective diffusion (i.e. permeability) – which characterizes the flow induced by a thermodynamic gradient – is lacking.

Here, to fill this knowledge gap, we invoke the concept of "De Gennes narrowing" which relates the wavevector-dependent collective diffusivity D0(q) to the fluid structure factor S(q) [Kellouai et al. J. Chem. Phys. 160, 024113 (2024)]. First, using molecular simulation for a simple yet representative fluid confined in a prototypical solid (zeolite), we unravel an essential coupling between the wavevector-dependent collective diffusivity and the structural ordering imposed on the fluid by the crystalline nanoporous host. Second, despite this complex interplay with marked Bragg peaks in the fluid structure, the fluid collective dynamics is shown to be accurately described through De Gennes narrowing. Moreover, in contrast to the bulk fluid, departure from De Gennes narrowing for the confined fluid in the macroscopic limit remains small as the fluid/solid interactions in severe confinement screen collective effects and, hence, weaken the wavevector dependence of collective transport.

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Session Classification: Contributed talks

Contribution ID: **4** Type: **Oral**

Bond-dependent interactions and ill-ordered state in the honeycomb cobaltate BaCo2(AsO4)2

Monday, 2 June 2025 16:00 (15 minutes)

Following the proposed materialization of Kitaev-bond-dependent spin liquid physics in honeycomb lattices of heavy transition metals with 4d or 5d electrons [1], it has been proposed that this can be extended to 3d transition metals, in particular Co2+ [2]. A first step in validating the prospect of finding a quantum spin liquid is to demonstrate the presence of these anisotropic bond-dependent interactions in such materials. These could promote new types of behavior or provide insight into certain materials not elucidated to date. This is the case of BaCo2(AsO4)2, a honeycomb cobaltate whose ground state and Hamiltonian have been debated for decades [3]. We have investigated the magnetic properties of a BaCo2(AsO4)2 single-crystal through neutron diffraction and inelastic scattering, as well as by very-low temperature magnetization and AC susceptibility measurements. The latter measurements, which reveal slow dynamics and non-equilibrium responses, are consistent with an original ill-ordered magnetic compound with intrinsic defects as proposed previously [4]: collinear zig-zag ferromagnetic chains in a up-up-down-down arrangement interspersed with additional chains to agree with the propagation vector of 0.27 imposed by competing interactions. To interpret these results, we propose an exchange model with bond-dependent anisotropic interactions on the first neighbors and Heisenberg interactions up to the fourth neighbors. Monte Carlo calculations show that our model successfully reproduces key experimental observations, namely spin-wave dispersions (figure), magnetization curves with a 1/3 magnetization plateau, and the faulty collinear spin configuration, leading to a coherent picture that had not been achieved to date [5]. This highlights the potential of including these new ingredients (anisotropic Kitaev and off-diagonal interactions) in understanding long-standing puzzling behaviors and discovering exotic physics.

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Session Classification: Contributed talks

Contribution ID: **5** Type: **Poster**

Water Intrusion in Nanoporous Materials: Implications for Energy Storage

Monday, 2 June 2025 19:00 (15 minutes)

Nanoporous materials, such as mesoporous silicas (e.g., MCM-41 and SBA-15) and metal-organic frameworks (MOFs), exhibit unique properties that make them essential for various applications, including catalysis, separation, and energy storage. A key aspect of energy storage in these materials is the intrusion of water into their pores, a process that converts mechanical energy into interfacial energy. This phenomenon depends on the pore size but essentially on the chemical nature of the material surface, ranging from hydrophilic to hydrophobic, and requires the application of external pressure, as governed by the Laplace law. The intrusion/extrusion processes and their implications for energy storage are studied thanks to the combination of homemade high-pressure calorimeter and high-pressure neutron diffraction experiments performed on the instruments G6.1 and G4.4 at the LLB and D16 at the ILL, with materials synthetized and characterized at the LLB. These experiments enable the investigation of material properties on one side, and, on the other side, the phase transitions of the confined fluid at various P and T, under various compression modes, such as liquid or gas compression. Understanding the influence of confinement on the thermodynamic properties of fluids is crucial, as confinement leads to significant modifications in these properties and the resulting heat exchanges. Different phase diagrams of confined water are found affecting their potential applications, by not only optimizing the conditions of use of these materials for energy storage, but also giving access to unexpected properties of water, opening up new perspectives in biology and geology.

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3. Osta-Rangel, Oriana. « Water Confined in Hydrophobic Nanopores : Towards a New Phase Diagram », s. d.
4. Karbowiak, Thomas, Guy Weber, et Jean-Pierre Bellat. « Confinement of Water in Hydrophobic Nanopores: Effect of the Geometry on the Energy of Intrusion ». Langmuir 30, no 1 (14 janvier 2014): 213 19.

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Presenter: MARESCOT, Thomas (LLB)

Session Classification: Posters

Contribution ID: **6** Type: **Oral**

Enhanced dynamics in disordered non-Kramers spin ice Ho2(Ti1–x-Hfx)2O7 : toward the Coulomb quantum spin liquid state

Monday, 2 June 2025 16:30 (15 minutes)

Dy2Ti2O7 and Ho2Ti2O7 classical spin ice compounds have been extensively studied over the past 30 years. Their excitations, described as emergent magnetic monopoles, exhibit very slow dynamics at low temperature, which manifests by a freezing and a strong irreversibility in Zero Field Cooled - Field Cooled (ZFC-FC) magnetization measurements. It has been proposed that in spin ices made of non-Kramers magnetic ions, i.e. where J is an integer so that the ground-state crystal electric field (CEF) is a non-protected doublet, such as Ho2Ti2O7, non-magnetic disorder induces quantum fluctuations that can push the system toward a Quantum Spin Liquid phase (QSL). This phase is characterized, inter alia, by a much faster dynamics.
We present a study performed on Ho2Ti2O7 where non magnetic disorder is introduced through a controlled substitution of Ti4+ ions by Hf4+ ions, with substitution rate from 0 to 40%. X-ray and neutron diffraction (HRPT - SINQ) show that the crystal structure and the spin ice correlations are preserved up to at least 30% and that the introduction of disorder results in an oxygen depletion of the Ho3+ coordination shells, so-called Frenkel pair defects, that locally break the CEF symmetry. As a result, a broadening of the CEF levels is observed in inelastic neutron scattering (EIGER - SINQ). Nevertheless, DC magnetic measurements indicate that the Ising nature of the single-ion ground state remains. Interestingly, AC susceptibility and Neutron Spin Echo (WASP - ILL) reveal a faster dynamics below 30 K as the substitution rate grows. In addition, ZFC-FC measurements show that the freezing temperature is lowered. This speeding up of the dynamics strongly suggests that disorder indeed enables quantum fluctuations in the system. This opens the way to the stabilization of a Coulomb QSL phase at lower temperature.

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Session Classification: Contributed talks

Contribution ID: **7** Type: **Oral**

Diffraction data processing for DREAM at the European Spallation Source

Monday, 2 June 2025 16:45 (15 minutes)

The European Spallation Source (ESS) will operate a suite of diffractometers. One of the first operational instruments will be DREAM [1], a diffractometer developed and built for ESS by the consortium Forschungszentrum Jülich (Germany) and Laboratoire Léon Brillouin (France).
To ensure smooth operation even for the first-time users, the ESS Data Management and Software Centre is developing an integrated data pipeline linking all the steps from data acquisition and live visualisation to data analysis. To test this pipeline during the construction phase of ESS and of its instruments, we use instrument simulations with McStas [2] combined with GEANT4 [3] due to the complex three-dimensional geometry of new 10B detectors of the ESS diffractometers. Here we report on preliminary implementations of the data processing pipeline for diffraction data from raw NeXus [4] event files to data archiving.

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Session Classification: Contributed talks

Contribution ID: **8** Type: **Poster**

Aqueous solubilization of hydrophobic compounds by inorganic nano-ions: An unconventional mechanism

Monday, 2 June 2025 18:45 (15 minutes)

Solubilization of hydrophobic compounds in water is commonly performed by the addition of organic solubilizers through (i) micellar or hydrotropic solubilization using amphiphilic molecules[1], (ii) co-solvency using water-soluble solvents, and (iii) host–guest complexation using macrocycles[2]. In this study, we show that the 3,3′-commo-bis[closo-1,2-dicarba-3-cobaltadodecaborane] derivatives (COSANs)—fully inorganic and non-amphiphilic ionic boron clusters with nanometric size and superchaotropic properties—efficiently solubilize model hydrophobic compounds, such as medium-chain alcohols ($0.6 < \log P < 1.5$), in water. Unlike micellar solubilization using surfactants, COSAN acts as an efficient solubilizer in its monomeric state, i.e., at concentrations well below the critical aggregation concentration. The solubilization mechanism of COSAN differs significantly from the surfactant-based solubilization. COSAN induces the bi-dimensional anisotropic growth of COSAN/alcohol co-assemblies, whereas surfactants typically induce isotropic swelling of micelles. This unconventional solubilization mechanism, based on the formation of thermodynamically stable COSANs/alcohol anisotropic co-assemblies, was revealed through spectroscopic and scattering techniques (SWAXS and SANS). We have also shown that the COSAN/2-butanol co-assemblies can be used to solubilize more hydrophobic compounds with $\log P$ values up to around 6. These findings suggest that ionic boron clusters have significant potential for solubilizing hydrophobic compounds across a broad hydrophobicity scale in various applied fields.

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Session Classification: Posters

Contribution ID: **9** Type: **Oral**

Deciphering membrane protein structures through scattering and modeling: insights into TSPO, a neuroimaging key marker

Tuesday, 3 June 2025 13:15 (15 minutes)

Membrane proteins play essential roles in cellular function and are prime therapeutic targets, yet their structural characterization remains a major challenge. Despite advances in artificial intelligence, including AlphaFold, accurately predicting their structures is still difficult. These proteins make up 30% of the proteome and 60% of drug targets, yet they are vastly underrepresented in the PDB, with only 3% of resolved structures. This is largely due to the challenge of maintaining their native state in amphiphilic environments, limiting the applicability of classical structural techniques such as X-ray crystallography, NMR, and cryo-EM.

To overcome these limitations, we combine small-angle X-ray and neutron scattering (SAXS/SANS) with ab initio modeling, offering a powerful approach to study membrane proteins under near-physiological conditions. We apply this methodology to TSPO (Translocator Protein), a highly conserved transmembrane protein with strong pharmacological relevance, particularly in neuroimaging.

Our study explores the solution structures of mouse TSPO (mTSPO) in various amphiphilic environments to unravel its structure/function relationships: (i) SDS, the detergent used for its solubilization from E. coli inclusion bodies, where mTSPO is stable and monodisperse but nonfunctional ; (ii) DPC, the detergent used to determine its NMR structure, where a stabilizing ligand enhances rigidity and induces µM affinity ; (iii) membrane-mimetic environments (DPC/DMPC bicelles), where optimized refolding restores nM affinity, approaching its native functional state.

By deciphering the structural behavior of mTSPO across these conditions, our work provides valuable insights into its function, paving the way for the development of new pharmacological molecules for diagnostics and therapeutics.

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Session Classification: Contributed talks

Contribution ID: **10** Type: **Oral**

SAM: a new SANS instrument at the ILL

Tuesday, 3 June 2025 13:30 (15 minutes)

Small-angle neutron scattering (SANS) is a ubiquitous technique for the study of static & dynamic properties of condensed matter at the mesoscale. The ever-increasing demand in SANS beamtime requires the development of new instruments with high scientific throughputs.
The SAM project was submitted in that spirit during the 'Endurance 2' call of the Institut Laue Langevin (ILL). The Laboratoire Léon Brilllouin (LLB) has proposed to build a compact SANS instrument equipped with polarized neutrons on the new H15 cold guide, to complement the existing suite and mitigate the loss of the Orphée reactor in Saclay.
Following a relatively short design and procurement phase (2020-2023), the installation of SAM at the ILL began mid-2023 and was achieved by the end of February 2024. The instrument has detected its first neutrons on March 4th, 2024 and, following a 'hot commissioning' phase, has received its first users during the second ILL cycle with around 20 experiments performed.
We will discuss the main characteristics & performances of the instrument, which demonstrate its competitiveness with respect to world-leading SANS instruments already in operation. We will also show a selection of results obtained during the 'friendly user' program organized by the French Federation for Neutron Scattering (2FDN) and the ILL.

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Session Classification: Contributed talks

Contribution ID: **11** Type: **Oral**

L'étude de vieillisement des électrodes de batteries Li-ion par imagerie neutronique

Tuesday, 3 June 2025 13:45 (15 minutes)

L'imagerie neutronique, sensible aux noyaux atomiques plutôt qu'à la densité électronique, constitue un outil puissant pour l'étude des batteries Li-ion, permettant notamment d'observer des éléments peu détectables par les rayons X, comme l'hydrogène et le lithium-6. Dans cette étude, nous exploitons cette technique pour analyser la distribution locale du lithium et identifier les hétérogénéités de (dé)lithiation au cours du cyclage électrochimique, dans le but de mieux comprendre les mécanismes de vieillissement des électrodes de batterie.

Afin d'optimiser le contraste d'imagerie sans altérer les performances des batteries, nous explorons différentes modifications chimiques, notamment l'utilisation d'un électrolyte deutéré ou de lithium-6. L'imagerie *operando* est réalisée sur des cellules conçues pour cette technique permettant une observation simultanée de l'électrode positive, du séparateur et de l'électrode négative. L'évolution de la concentration en lithium dans les électrodes est systématiquement comparée entre des électrodes fraîches (non cyclées) et des électrodes vieillies sous divers régimes de cyclage, allant de lent (C/5 correspondant à une charge complète en 5 heures) à rapide (2C, une charge complète en 30 min). Ces travaux contribuent non seulement à une meilleure compréhension des mécanismes de dégradation des batteries Li-ion, mais aussi à l'amélioration des méthodologies d'imagerie et des conceptions expérimentales.

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Session Classification: Contributed talks

Contribution ID: **12** Type: **Poster**

Design of an Inelastic Neutron Spectrometer for the French ICONE project

Monday, 2 June 2025 18:15 (15 minutes)

ICONE (Innovative COmpact NEutrons facility) is a project of a French High-Intensity Compact Accelerator-driven Neutron Source (HiCANS) aimed at delivering an instrument suite for the French scientific community at the 2035 horizon. ICONE will produce neutrons by accelerating protons to an energy 25 MeV and impacting them on a Beryllium target. The resulting neutrons will then be moderated to a useful energy range of 2–100 meV, making them suitable for neutron scattering instruments.
One of the key challenges of HiCANS is the design and optimization of inelastic neutron scattering instruments. Indeed, the inherent need for beam filtering in direct and indirect geometries in order to analyze the energy transfer introduces a loss in neutron flux. To make full use of the produced neutrons on ICONE, a combination of simulation tools is employed to develop and optimize a virtual model of an inelastic instrument, which will then enable the calculation of instrument performance by the realization of virtual experiments using McStas, and the maximization of the signal/noise ratio using the OpenMC software packages.
The data generated will then be reduced using the SCIPP software package developed at ESS and analyzed, allowing direct comparison and benchmarking with previous experimental results obtained at LLB on the Orphée reactor. This conception will present the entire simulation chain and the first results obtained.

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Session Classification: Posters

Contribution ID: **13** Type: **Oral**

Effect of the magnetic metal site on the dipolar-octupolar pyrochlores Nd2Ru2O7 and Nd2Ir2O7

Tuesday, 3 June 2025 14:00 (15 minutes)

Pyrochlore oxides with the formula R2M2O7 (R representing a rare-earth element and M a metal ele-ment) consist of two interpenetrating pyrochlore lattices, and are a rich playground to stabilize unconven-tional magnetic frustrated phases [1]. In this family, Nd-based compounds exhibit intriguing physics due to the dipolar-octupolar nature of the Nd3+ ground state doublet [2]. In particular, at low temperature, they stabilize a peculiar dipolar-octupolar antiferromagnetic ground state which manifests as a so-called all in- all out state with a reduced ordered magnetic moment along the local ⟨111⟩ directions of the tetrahedra. When the M4+ metal ion carries a magnetic moment, its ordering can strongly impact the magnetic properties of the R3+ ion. For example, a fragmented state was discovered in Dy2Ir2O7 and Ho2Ir2O7 [3-4], stabilized by the molecular field induced by the antiferromagnetic ordering of the Ir4+ magnetic moments and the rare-earth. Recent studies suggest that ruthenate compounds may also stabilize fragmented states [5].
In this context, we are interested in the Nd2Ir2O7 and Nd2Ru2O7 compounds, which are expected to combine these physics. In both systems, the Nd3+ ion exhibits an all in - all out ordering with a reduced ordered moment [6-7], which reminds the dipolar-octupolar ordering of Nd2Zr2O7. However, our detailed study of the temperature dependence of the magnetic properties of both compounds using neutron diffraction (ILL D1B) and high resolution inelastic neutron scattering (ILL IN5), show that it is considerably affected by the presence of the metal ion.
While the metal ion orders into two different magnetic structures in both compounds (all in - all out in Nd2Ir2O7 [7] and easy-plane antiferromagnetic Γ5 in Nd2Ru2O7 [8]) and at two different temperature scales (150 K and 35 K respectively), our measurements combined with spin wave and mean field analysis show that the temperature dependence of the ordered moment and the spin excitations in both systems can only be understood by introducing in the Hamiltonian a coupling between the octupolar component of the Nd3+ ion and the metal. This term generates an octupolar moment and magnetic excitations at much larger temperature than in Nd2Zr2O7 and its existence provides an exciting new playground to study unconventional magnetic states with dipolar-octupolar rare-earth ions.

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Session Classification: Contributed talks

Contribution ID: **14** Type: **Oral**

Optical molecules in MFI-type zeolites: the unique assets of neutron scattering to complex systems

Tuesday, 3 June 2025 14:15 (15 minutes)

The modelling of adsorption or confinement of organic molecules in zeolite crystals is a long story, not only because of the infinite possibilities offered by the intrinseque properties of the guest molecules and of the framework topologies.
The simplest family of such inclusion compounds is probably the (dye@zeolite) one. A priori the properties arising from the inclusion of simple dyes, hyperpolarisable molecules or photochromes in the microporous channels mainly depends on the zeolite topology and not of charge compensating cations as for gas separation or catalysis process. However the structures generally inferred from ab initio calculations or/and powder XRD lack reliability.
I will present few examples showing assets of of neutron scattering for the comprehension of such systems.

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Session Classification: Contributed talks

Contribution ID: **15** Type: **Invited Oral**

Surprises from polymer topology and hydrodynamics

Tuesday, 3 June 2025 08:45 (30 minutes)

Linear polymers in shear flow display a dominant mode of dynamics known as tumbling, around the vorticity axis, whereby the two ends exchange their places, accompanied by a temporary compression of the chain in the gradient direction. We will demonstrate that topological polymers respond to shear in dramatically different ways, emerging from a coupling between topology and hydrodynamics. In particular, we will discuss ring polymers as well as rings connected either chemically (bonded rings, BR) or mechanically (catenated rings, CR). Rings display vorticity swelling and an inflated phase that suppresses tumbling and Brownian motion. BRs tumble around an axis parallel to the gradient direction, whereas CRs show slip tumbling while maintaining their overall orientation and shape. These unusual phenomena all result from proper consideration of hydrodynamic interactions and they disappear if the latter are (artificially) switched off.

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Session Classification: Invited speakers

Contribution ID: **16** Type: **Oral**

One-dimensional hydride ion diffusion in the nitride-hydride catalyst Ca3CrN3H

Wednesday, 4 June 2025 11:00 (15 minutes)

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 substructure. Recently, the new nitride-hydride Ca_3CrN_3H was discovered and shown to be promising to be used as a catalyst for ammonia synthesis [1]. For the rational development of Ca_3CrN_3H, or related materials, towards such an application, a fundamental understanding of its hydride ion mobility is crucial, but such an understanding is at present lacking.

In this work, we investigate the nature of hydride ion mobility in Ca_3CrN_3H using quasielastic neutron scattering (QENS) and machine-learning molecular dynamics (MLMD). The combined analysis of QENS and MLMD data indicates vacancy-mediated hydride ion diffusion within the channel-like structure of Ca_3CrN_3H. This diffusion mechanism is characterized by correlated localized and long-range diffusion occurring on relatively fast timescales of approximately 10 picoseconds and 50 picoseconds, respectively, with a notably low activation energy of ~50 meV. Crucially, these findings suggest that the high catalytic performance of Ca_3CrN_3H for ammonia synthesis is partly due to the facile hydride ion transport from the bulk to the surface of the material, where the catalytic reaction takes place. Furthermore, the results highlight the potential for efficient hydride ion transport over macroscopic distances, positioning Ca_3CrN_3H as a promising fast ion conductor.

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Presenter: FINE, Lucas (ILL)

Session Classification: Contributed talks

Contribution ID: **17** Type: **Invited Oral**

The new D007 permanently-polarized diffuse scattering instrument at the ILL

Monday, 2 June 2025 14:15 (30 minutes)

The D7 neutron diffuse scattering instrument at the Institut Laue-Langevin [1] has been an important experimental tool in the study of disordered materials, making use of neutron polarization analysis to provide a clean and unambiguous separation of the magnetic, incoherent, and structural contributions to the scattering.
D7 has been disassembled, and the new D007 [2] started its commissioning in 2024. The upgrade promises an increase in flux by an order of magnitude with a comparable resolution.
Both diffraction and spectroscopic modes will be still available. In diffraction mode, the same momentum transfer range as D7 will be accessible (0.2 Å–1 ⊠ Q ⊠ 4.1 Å–1). The instrument may be converted into a polarized direct geometry time-of-flight spectrometer by adding a system of two choppers, and should offer a comparable energy resolution (0.1 meV ≤ ΔE ≤ 0.5 meV depending on the incident wavelength [3]).
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[2] G. J. Nilsen et al., Nuclear Instruments and Methods in Physics Research A 951, 162990 (2020).
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Presenter: MANGIN THRO, Lucile (ILL)

Session Classification: Invited speakers

Contribution ID: **18** Type: **Invited Oral**

Could fungi seeThe Last of Us? - Why and how we should study antifungal drugs using neutron reflection and lipidomics

Wednesday, 4 June 2025 10:00 (30 minutes)

Millions of people suffer life-threatening fungal infections, but there are no vaccines, and only a few antifungal agents, whose application is often restricted by toxicity, resistance and low bioavailability. Most antimycotic drugs target ergosterol residing in fungal membranes, but their precise mechanisms of action, toxicity and resistance development are still unclear. A fuller understanding of the function of the current drugs is critical for designing better, safer therapeutics in a world where climate change is a driving factor in the adaptation of pathogenic fungi to new geographical areas.

Candida glabrata is a non-pathogenic yeast in healthy humans, but the number of infections it causes has increased, making it urgent to understand its virulence and resistance. We have combined RNA interference to produce well-defined genetic modifications in C. glabrata strains (1) with lipidomic analysis to study the link between lipid composition and antifungal drug resistance.

Amphotericin (AmB) is a WHO essential medicine that has the broadest antifungal spectrum and has been used as the last line of defense against systemic fungal infections for more than 50 years, but its mechanism of action and resistance are still not well understood. We have used neutron reflection to elucidate the mechanism by which fungal cells become resistant to AmB in model fungal membranes (2,3) and membranes from C. glabrata strains with increased or decreased AmB resistance. Our integrative approach demonstrates how neutron techniques can provide insight into the molecular basis of antimicrobial activity and resistance with the long-term aim to improve therapies.

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(3) Delhom et al. Nanomaterials 2020 doi:10.3390/nano10122439

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Presenter: WACKLIN-KNECHT, Hanna (European Spallation Source ERIC)

Session Classification: Invited speakers

Contribution ID: **19** Type: **Poster**

Probing Hydrogen Diffusion in Coal for Geological Storage via Quasielastic Neutron Scattering

Monday, 2 June 2025 19:15 (15 minutes)

Underground hydrogen storage (UHS) in coal seams presents a compelling opportunity for scalable, low-carbon energy storage, yet the fundamental understanding of hydrogen transport in such complex porous media remains limited. In this study, we explore hydrogen diffusion in coal using quasielastic neutron scattering (QENS), a technique uniquely suited to capturing molecular-scale dynamics of hydrogen due to its large incoherent scattering cross-section. Our focus lies in characterizing how temperature, pressure, and coal heterogeneity affect hydrogen mobility and retention at the microscopic level. Through prior neutron spin echo (NSE) experiments on methane and macroscopic sorption studies in anthracite coal, we observed strong temperature dependence and time-dependent diffusivity indicative of heterogeneous transport pathways. Early-stage findings also suggest that hydrogen diffuses more rapidly than CH_4 and CO_2 due to its smaller size and weaker interaction with the coal matrix, a trend accompanied by slight coal matrix shrinkage upon hydrogen uptake. These preliminary insights highlight the need for multi-scale, high-resolution characterization of gas transport in coal. QENS offers the potential to resolve localized hopping and longer-range diffusion regimes, thereby advancing our understanding of hydrogen mobility in nanoporous carbonaceous systems and informing strategies for safe and efficient subsurface hydrogen storage.

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Presenter: HE, Xinxin (Pennsylvania State University)

Session Classification: Posters

Contribution ID: **20** Type: **Oral**

Accessing Diffusive Properties of Dilute Protein Solutions with Neutron Backscattering

Wednesday, 4 June 2025 11:15 (15 minutes)

Background:
Understanding the diffusive properties of colloidal suspensions is essential for exploring fundamental transport mechanisms, optimizing industrial formulations, developing advanced materials, and enhancing biomedical and pharmaceutical applications. Short-time diffusion is predominantly influenced by hydrodynamic interactions. Quasielastic neutron scattering (QENS) offers a non-invasive approach to studying these diffusive processes, free from the effects of multiple scattering or turbidity.

Methods:
Neutron Backscattering (NBS), due to its energy resolution and accessible q-range, enables the examination of short-time self-diffusion in colloidal suspensions. In particular, Fixed Window Scans (FWS) provide insight into the scattering function at specific energy transfers, achieving significantly higher count rates than full QENS spectra. This advantage allows for reduced acquisition times and facilitates the investigation of suspensions with weak scattering signals.

Results:
Using FWS, we analyzed dilution series of two model protein systems with concentrations reaching below 1 mg/ml. For highly concentrated protein solutions, our previously established analysis framework demonstrated quantitative agreement with center-of-mass diffusion obtained from full QENS spectra [1]. The reduced acquisition time also enables the study of kinetic processes [2]. For dilute suspensions, hierarchical diffusive processes contribute to the extracted $\gamma(q)$, necessitating a refined analytical approach. We present a method for disentangling these contributions and compare the results with collective long-time diffusion coefficients derived from dynamic light scattering.

Conclusion:
NBS-FWS provides access to short-time self-diffusive properties in dilute suspensions, which were previously inaccessible using classical NBS techniques. Advanced analytical methods enable the separation of distinct diffusion contributions, offering a more comprehensive understanding of colloidal dynamics.

References:
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[2] Under Review in Journal of Applied Crystallography

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Presenter: BECK, Christian

Session Classification: Contributed talks

Contribution ID: **21** Type: **Oral**

Microscopic view of hydrogen adsorption in size-variant nano-clay materials

Wednesday, 4 June 2025 11:30 (15 minutes)

Hydrogen is the carbon-free fuel par excellence because its combustion emits only water. Research has focused on H2 storage in lightweight materials for the needs of vehicles, excluding clays due to their weight. But large-scale terrestrial storage for industrial applications does not require the same specifications. In this context, clay minerals offer several interesting properties, such as large surface area, low cost, global abundance and environmental safety.

We investigate, at the microscopic level, H2 adsorption on synthetic 2:1 trioctahedral smectites of nanometric dimensions, specifically Laponite, and its precursor, pre-Laponite. Our aim is to understand the higher H2 sorption capacity of pre-Laponite, combining adsorption isotherm measurements, elastic and inelastic neutron scattering experiments and Grand Canonical Monte Carlo (GCMC) simulations.

The adsorption isotherms at 40 K, up to 1 bar, are fitted with a Langmuir contribution and a smoothest one. GCMC simulations show that the Langmuir model, accounting for the strongest binding sites, describes adsorption within the interlayer, as confirmed by small angle neutron scattering. Inelastic neutron scattering experiments were undertaken to probe the para-to-ortho rotational transition of H2, the energy of which is highly sensitive to its environment. At 40K, two adsorption sites are identified in the interlayer, with orientational potential wells of about 80K and 1300K, respectively. Based on wide angle neutron scattering analysis, the second site would be situated above the hexagonal cavity defined by Si tetrahedra. Quantum sieving effects were also evidenced comparing D2 and H2 adsorption. The highest adsorption in pre-Laponite compared to Laponite is attributed to the slightly more open interlayer space (sheet-to-sheet distance is 1 nm in pre-Laponite and 0.97 nm in Laponite).

The perspective of these results is the fine modulation of the interlayer space to optimize the storage of hydrogen in clays at low temperature and beyond, under pressure, at room temperature.

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Session Classification: Contributed talks

Contribution ID: **22** Type: **Oral**

Bowtie-Shaped Deformation Isotherm of Superhydrophobic Cylindrical Mesopores

Wednesday, 4 June 2025 11:45 (15 minutes)

Deformation of superhydrophobic cylindrical mesopores is studied during a cycle of forced water filling and spontaneous drying by in situ small-angle neutron scattering. A high-pressure setup is put forward to characterize the deformation of ordered mesoporous silanized silica up to 80 MPa. Strain isotherms of individual pores are deduced from the shift of the Bragg spectrum associated with the deformation of the hexagonal pore lattice. Due to their superhydrophobic nature, pore walls are not covered with a prewetting film. This peculiarity gives the ability to use a simple mechanical model to describe both filled and empty pore states without the pitfall of disjoining pressure effects. By fitting our experimental data with this model, we measure both the Young's modulus and the Poisson ratio of the nanometric silica wall. The measurement of this latter parameter constitutes a specificity offered by super-hydrophobic nanopores with respect to hydrophilic ones.

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Presenter: PICARD, Cyril (UGA)

Session Classification: Contributed talks

Contribution ID: **23** Type: **Invited Oral**

Altermagnetism and neutron scattering

Tuesday, 3 June 2025 09:15 (30 minutes)

Altermagnetism usually refers to the set of collinear compensated magnets at weak spin-orbit coupling whose crystal symmetries do not enforce spin degeneracy. In these systems, one expects an anisotropic pattern of spin splitting in momentum space in the electronic bands. In the magnon bands, one expects a similar pattern of chirality splitting. This talk will be dedicated to explaining how to characterize altermagnets using neutrons. It turns out that neutron scattering is an almost ideal tool for this purpose.

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Presenter: MCCLARTY, Paul (Laboratoire Léon Brillouin)

Session Classification: Invited speakers

Contribution ID: **24** Type: **Invited Oral**

Complex multi-q magnetic order and multiferroicity in spinel GeFe2O4

Wednesday, 4 June 2025 14:30 (30 minutes)

As they often stabilize with complex non-collinear magnetic structures, frustrated magnets are potential candidates for type-II multiferroism, where both magnetic and electric orders appear at the same temperature and are strongly coupled [1]. In these materials, the proper understanding of the coupling between spin and charge degrees of freedom is a key to identify the microscopic mechanism at the origin of the multiferroic properties [2]. Here we focus on the normal cubic spinel GeFe2O4, crystallizing in the Fd-3m space group. In this compound, the Fe magnetic ions form a pyrochlore sublattice, consisting of a network of corner-sharing tetrahedra prone to magnetic frustration [3]. In this talk I will present our recent study combining experiments (single-crystal neutron diffraction and inelastic neutron scattering) with meticulous modeling of the experimental data. I will show how this complementary approach has been successful to evidence, in this system, a non-coplanar spin texture described by a combination of 6 symmetry-equivalent propagation vectors [4]. We will also see how this complex multi-q magnetic order plays a crucial role in the emergence of ferroelectric properties recently observed at the magnetic transition temperature [5].

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Session Classification: Invited speakers

Contribution ID: **25** Type: **Invited Oral**

Nanometer-size superchaotrope ions or a new class of solubilizers

Tuesday, 3 June 2025 19:00 (30 minutes)

Superchaotropic nano-ions have recently captivated attention for their remarkable ability to adsorb onto hydrated neutral surfaces or bind strongly to some cavities of macrocyclic molecules.They indeed exhibit a range of fascinating behaviors:
1. Dramatically increasing the cloud point of non-ionic surfactant systems.
2. Triggering conformational changes in thermo-sensitive polymers in aqueous solutions.
3. Solubilizing weakly hydrophilic compounds in water.
4. Acting as molecular “glue” to link proteins.
5. Inducing phase transitions in lyotropic systems.
Nano-ions bridge the gap between surfactants, hydrotropes, and colloids, with their effects governed by charge density rather than specific chemical composition. Their chemistry, whether polyoxometalates or boron clusters, unlocks a spectrum of exciting possibilities for applications yet to be explored. These versatile compounds are poised to redefine boundaries in materials science, biochemistry, and beyond.

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Presenter: DIAT, Olivier (ICSM)

Session Classification: Invited speakers

Contribution ID: **26** Type: **Oral**

Fluids at an electrostatically active surface: Optimum in interfacial friction and hydroelectronic drag

Wednesday, 4 June 2025 17:00 (15 minutes)

Fluids at solid interfaces are central to key technologies in energy conversion, electrochemistry, and catalysis, yet their nanoscale dynamics remain only partially understood. On metallic surfaces, recent studies have revealed unconventional interfacial phenomena—including complex electrostatic screening, anomalous wetting behavior, and quantum friction—that call for new modeling tools bridging charge dynamics in the metal with molecular motion in the fluid. In this work, we introduce a molecular simulation framework based on Virtual Thomas-Fermi fluids, enabling a realistic, atomically-resolved treatment of interfacial transport that captures both charge relaxation in the metal and its coupling to the surrounding liquid. Applying this approach to water near metallic surfaces with tunable screening properties, we uncover a non-monotonic dependence of interfacial friction on metallicity, peaking when charge relaxation modes in the solid and fluid dynamically overlap. Furthermore, we report a direct observation of hydroelectronic drag, a momentum transfer mechanism rooted in dynamic electrostatic interactions at the interface. These results shed new light on interfacial transport under electrostatic coupling and open avenues for designing metal–fluid interfaces with tailored frictional properties. We further discuss how these predictions could be directly tested via inelastic neutron scattering experiments targeting interfacial charge–density correlations.

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Presenter: HERRERO GUILLEN, Cecilia (Institut Laue Langevin)

Session Classification: Contributed talks

Contribution ID: **27** Type: **Invited Oral**

Invisible nanodiscs and their formation process, by SANS

Tuesday, 3 June 2025 09:45 (30 minutes)

Membrane proteins are responsible of all the communication between living cells and their environment. Despite their basic and therapeutic interest, their are under-represented in our structural biology knowledge due to the intrisic difficulties presented by their production, purification and handling. Nanodiscs are a great tools to study them in their native lipidic environment, and to study the effect of the variation of this environment on their structure. In particular, BioSANS can make use of contrast variation in this aim. Here, as an example, we will present how the contrast variation can be used to study the nanodiscs formation process.Building on the pioneering work of Maric *et al.* our goal is to provide our users with adequat nanodiscs constituants, at required deuteration levels, to enable the SANS study of membrane protein conformation and the interplay with their surrounding lipidic environment.

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Presenter: MARTEL, Anne (ILL)

Session Classification: Invited speakers

Contribution ID: **28** Type: **Oral**

Near-Surface Concentration Profile of Sheared Semidilute Polymer Solutions

Wednesday, 4 June 2025 16:00 (15 minutes)

Controlling the structure of polymer solutions near a solid surface is crucial for many industrial processes as it significantly impacts solution flow and influences slip at the interface. To date, only a few techniques have been developed to experimentally investigate this type of interface at the nanometric scale of solid/liquid interactions. In this study, we probe the interface between a smooth sapphire surface and a semidilute polystyrene solution, using neutron reflectivity. A special setup for flow measurements under shear has been designed and optimized. Our results show that, at rest, polymer chains are globally depleted from the solid surface. Contrary to common assumptions, some polystyrene 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 is only vaguely confirmed in the literature.

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Presenter: LAFON, Suzanne (LIPHY, CNRS)

Session Classification: Contributed talks

Contribution ID: **29** Type: **Oral**

In Situ SAXS and SANS Monitoring of Both Nanofillers and Polymer Chain Microstructure under Uniaxial Stretching in a Nanocomposite with a Controlled Anisotropic Structure

Monday, 2 June 2025 16:15 (15 minutes)

We will show in this contribution how the combination of SANS and SAXS allows for a detailed monitoring of the respective evolutions of the structure of fillers by SAXS and conformation of polymeric chains by SANS under uniaxial stretching at various elongation ratios in a nanocomposite made of spherical magnetic nanoparticles of γFe2O3 dispersed in a matrix of polystyrene (PS) chains [1]. The chain conformation is directly obtained by SANS as we probed samples containing 25% PSH/75% PSD chains, taking benefit from the fact that the neutron scattering length density of PSD is similar to the one of γFe2O3 [2], while the structure of filler is directly probed by SAXS. We can make the structure of fillers in the nanocomposite before stretching very anisotropic thanks to the appliance of a magnetic field during the nanocomposite processing that induces the formation of nanoparticle chains aligned along the direction of the field, either parallel or perpendicular to the subsequent stretching. This gives rise to very anisotropic mechanical properties, and the structure of fillers evolves very differently [3].

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Presenter: Dr COUSIN, Fabrice (Laboratoire Léon Brillouin)

Session Classification: Contributed talks

Contribution ID: **30** Type: **Oral**

Fate of self-assembled lipid nanoparticles in a biomimetic medium

Wednesday, 4 June 2025 15:30 (15 minutes)

For two decades, pharmaceutical industries have developed a growing interest towards nanoparticles (NPs). The combination of pharmaceutical activity and nanoscale formulation offers many advantages such as better targeting and reduced toxicity of the drug, improvement of the pharmacokinetic to cite a few. However, the limited knowledge regarding some of their physicochemical characteristics following their administration in the body poses a barrier to their safe use. Despite the abundance of publications in the field over the past years, only a limited number of nanoparticles have received marketing authorization (1).

In this context, we propose to study a particular case of "soft" NPs formed by self-assembly in water of the squalene-Leucine-enkephalin (SQ-LENK) prodrugs. These amphiphilic nanomedicines are intended to alleviate pain in patients after intravenous administration without causing side effects (2). Indeed, these SQ-LENK NPs constitute a great alternative to other opioids like morphine since they displayed an important analgesic activity in vivo with a longer lasting effect. Moreover, it was observed that unlike morphine, they act on peripheral opioid receptors thus avoiding the central nervous system, commonly implicated in the occurrence of addiction phenomena (3).

Following previous studies on the influence of different linkers between squalene and enkephalin on the NP stability (4), this study aims to characterize the behavior of SQ-LENK NPs in a biomimetic environment. To replicate physiological conditions, the NPs were examined in various buffer solutions across a range of concentrations, resulting in different pH and ionic strength values. A combination of SAXS/WAXS and SANS techniques was then employed to investigate the evolution of the internal structure, size, shape and self-assembly state of SQ-LENK NPs in these buffered media.

The analysis finally revealed an equilibrium between SQ-LENK NPs, micelles and monomers (SQ-LENK bioconjugates composing the NP) depending on the buffer concentration. As a first result, the relative proportion of each compound in the suspension appears to be primarily governed by the pH. Variability in self-assembly can significantly impact the pharmacokinetics of these prodrugs, thereby influencing their therapeutic efficacy. Consequently, precise characterization of size distribution, morphology, and the nature of the self-assembled structures is essential for effectively controlling the activity of such NP formulations.

For now on, ongoing studies are focused on investigating the interactions between blood proteins and SQ-LENK NPs in buffered media in order to be one step closer to the biological media.

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Co-authors: Dr GOBEAUX, Frédéric (CEA); Dr LEPETRE-MOUELHI, Sinda (Institut Galien Paris-Saclay); Dr TESTARD, Fabienne (CEA)

Presenter: RONCIN, Hugo (CEA)

Session Classification: Contributed talks

Contribution ID: **31** Type: **Invited Oral**

Computational chemistry - scientific results and state-of the art software tools

Wednesday, 4 June 2025 09:30 (30 minutes)

The analysis of neutron data in the context of magnetic structure relies heavily on the fitting of the parameters of an effective Hamiltonian model. The complexity of the systems under study leads to the increase of the number of parameters of these models and a good starting guess for the fit becomes crucial. Ab initio calculations on these systems can provide quantitative estimate for the number of parameters to consider and for their values. In this talk I will show our recent developments in the context of the calculation of magnetic excitations from ab initio methods and put it in the more general framework of the role of simulations in the analysis of neutron data in the ILL and the development of an integrated data platform (C-Lab) for the neutron users.

Primary author: REBOLINI, Elisa

Presenter: REBOLINI, Elisa

Session Classification: Invited speakers

Contribution ID: **32** Type: **Poster**

Dynamics of the critical phonon modes in quantum paraelectric SrTiO3

Monday, 2 June 2025 18:30 (15 minutes)

The proximity of $SrTiO_3$ to a ferroelectric quantum critical point (FE QCP) has become a promising new branch of the study of quantum critical phenomena. New forms of quantum order have been reported in $SrTiO_3$, different from the quantum paraelectric state via dielectric measurements. The critical point here is associated with a soft optical phonon mode responsible for the ferroelectric instability.
We report our recently performed triple-axis inelastic neutron scattering experiments on single-crystal $SrTiO_3$ at the temperature and pressure region of interest. These were the first direct measurements deep into the enigmatic "quantum polar-acoustic state" in the vicinity of the FE QCP. Measurements are taken at and around $q = 0$ in multiple directions in reciprocal space to explore the transverse acoustic and soft optical phonon modes and their hybridization. In addition, we explore how pressure affects the underlying phonon modes in $SrTiO_3$. We also present first-principles calculations in the low-temperature tetragonal phase, in comparison with the experimental observations. Our explorations directly address the coupling of the soft optical mode with the acoustic phonons, and its response to external pressure. We believe this could help us understand the importance of anharmonic lattice dynamics and quantum fluctuations in $SrTiO_3$.

Acknowledgement The experiments were carried out with the support of the Institut Laue-Langevin, Grenoble, France through the approval of beamtime for proposals 7-02-212, 7-02-213, 7-02-219 and 7-02-223 on IN8 and the support of Paul Scherrer Institute for proposal 20230501 on EIGER. The calculations were performed with the support of IDRIS high-performance computer centre for the calculation time under the GENCI project n_A0150801842. The authors would like to thank G. G. Guzmán-Verri, P. B. Littlewood, E. Artacho, J. Lashley, M.B. Lepetit, and T. Weber for their generous help and discussions.

Primary author: DENG, Shiyu (Institut Laue-Langevin)

Co-authors: IVANOV, Alexandre (ILL); WILDES, Andrew (Institut Laue Langevin); Dr HAINES, Charles R.S. (School of Physics, University of East Anglia,); COAK, Matthew (University of Birmingham); Dr SAXENA, Siddharth S. (University of Cambridge); Dr NIKITIN, Stanislav (Paul Scherrer Institute); FENNELL, Tom (Paul Scherrer Institut); PIOVANO, andrea (ILL)

Presenter: DENG, Shiyu (Institut Laue-Langevin)

Session Classification: Posters

Contribution ID: **33** Type: **Oral**

Emergent Polar Metal Phase in a Van der Waals Mott Magnet

Wednesday, 4 June 2025 16:15 (15 minutes)

We report the emergence of a polar metal phase in layered van der Waals compound $FePSe_3$. This Mott insulator with antiferromagnetic order offers a unique opportunity to fully tune an insulator into a polar metal state with pressure, without doping-induced disorder or impurities. Our synchrotron and neutron diffraction data unambiguously show a structural transition and loss of the inversion symmetry. We also observed the suppression of magnetic ordering and an insulator-to-metal transition correspondent with this structural transformation. The loss of the inversion symmetry combined with the pressure-induced metallicity in $FePSe_3$ offers a new platform to investigate polar metallicity at accessible pressures. Moreover, the high-pressure metallic phase shows unconventional resistivity deviating from the Fermi-liquid description, close to the magnetic critical transition pressure at sufficiently low temperatures, which strongly suggests underlying quantum criticality. Our work not only explores the comprehensive temperature-pressure phase diagram of $FePSe_3$ but also provides insights for further investigation of van der Waals strongly correlated magnetic compounds.

The paper is available open-access: arXiv: 2501.13635v1

Primary author: DENG, Shiyu (Institut Laue-Langevin)

Co-authors: WILDES, Andrew (Institut Laue Langevin); Dr WANG, Bosen (Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences); Dr KIM, Chaebin (Department of Physics and Astronomy, Seoul National University); HAINES, Charles R.S. (School of Physics, University of East Anglia,); Dr LIU, Cheng (Cavendish Laboratory, University of Cambridge); Dr JARVIS, David M. (Institut Laue-Langevin); Dr DAISENBERGER, Dominik (Diamond Light Source); Dr LAMPRONTI, Giulio I. (Department of Earth Sciences, University of Cambridge); Dr HAMIDOV, Hayrullo (Navoi State University of Mining and Technologies); Prof. PARK, Je-Geun (9Department of Physics and Astronomy, Seoul National University); Dr CHENG, Jinguang (Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences); Dr WARREN, Mark R. (Diamond Light Source); COAK, Matthew (University of Birmingham); Dr YANG, Pengtao (Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences); SAXENA, Siddharth S. (University of Cambridge); KLOTZ, Stefan; HANSEN, Thomas (DIFF); Mr ZHANG, Xiaotian (Cavendish Laboratory, University of Cambridge)

Presenter: DENG, Shiyu (Institut Laue-Langevin)

Session Classification: Contributed talks

Contribution ID: **34** Type: **Oral**

Ninety years of ripening in small angle scattering instrumentation and exploitation methodogy

Wednesday, 4 June 2025 17:30 (15 minutes)

SAXS emerged in India in the group of Raman, then in the fifties of Kratky centered on the study of the empty cell by André Guinier in France and a dialogue of Kratky and Porod with Svedberg about proteins in solution. In the seventies and eighties absolute scaling at low-q and asymptotic laws at high-q started to be measured and were concomitant to the birth of science at nano-scale. Thermodynamics came in when the osmotic compressibility could be measured as well as simulated by Hayer when SAXS and SANS could be done on the same sample. We will give a brief history of the field, the case of off-equilibrium lipid nanopartiscles important for vaccines and gene therapy for which small angle scattering in small volume and broad q-range is crucial for progress.

Primary author: ZEMB, Thomas (CEA/ICSM)

Presenter: ZEMB, Thomas (CEA/ICSM)

Session Classification: Contributed talks

Contribution ID: **35** Type: **Oral**

Coupling Centrifugation with Neutron Scattering for In Situ Structural Control

We present a novel in situ sample environment for neutron scattering, inspired by soft matter techniques but to our knowledge never before implemented at large-scale facilities. Based on controlled centrifugation, this setup enables the application of accelerations from 1000 to 5000 g, generating stable density gradients that induce phase transformations and nanophase separation directly within the beamline. These structural changes can be monitored in real time, with the system returning to its initial state once rotation ceases — opening new pathways to study irreversible, gravity-driven phenomena. The prototype consists of a vertical centrifuge holding eight Hellma cells in a rotating disk. Validated on the D22 SANS instrument at ILL, the setup has demonstrated its potential for the purification and densification of dilute colloidal dispersions of ludox type. This new tool paves the way for advanced investigations of soft matter systems and colloidal interactions and may serve as a versatile platform for the analysis of multi-populations samples, fluid extraction and selective separation under controlled acceleration.

Primary authors: ALBA-SIMIONESCO, Christiane (LLB); PREVOST, Sylvain (ILL)

Co-authors: LEGENDRE, Frédéric (LLB); LAVIE, pascal (LLB); TESSIER, Olivier (LLB); HOFFMANN, ingo; PLAZANET, Marie (Liphy); MALAYIL, Firoz (ILL); ZEMB, Thomas (ICSM)

Presenter: ALBA-SIMIONESCO, Christiane (LLB)

Session Classification: Contributed talks

Contribution ID: **36** Type: **Invited Oral**

BIFROST: an indirect geometry spectrometer at ESS

Wednesday, 4 June 2025 09:00 (30 minutes)

The first neutrons from the European Spallation Source are expected to arrive on November 9, 2025.BIFROST will be the first operating spectrometer at ESS. BIFROST is an indirect geometry instrument. It will explore quantum materials, for example, to understand the role of magnetism in superconductors, as well as to measure phonon and magnon spectra in functional materials. The instrument will be ready for startup at ESS (delivered to ESS in september 2025). In 2026, there will be an initial commissioning period with test measurements, followed by a second period for the first scientific measurement. I will review the key features of BIFROST and discuss the expected first science.

Primary author: Dr BOURGES, Philippe (LLB CEA Saclay)

Presenter: Dr BOURGES, Philippe (LLB CEA Saclay)

Session Classification: Invited speakers

Contribution ID: **37** Type: **Invited Oral**

HP-QENS reveals how plastic water is

Monday, 2 June 2025 13:45 (30 minutes)

1 IMPMC, CNRS-UMR 7590, Université P&M Curie, 75252 Paris, France
2 Physics Department, Università di Roma La Sapienza, piazzale Aldo Moro 5, 00196, Roma, Italy
3 LQM, Physics Department, Ecole Politecnique Federale Lausanne, Lausanne, Swiss.

Over the past decade, computer simulations [1–3] have predicted the existence of a novel and intriguing phase of water, termed "Plastic water." This phase was expected to emerge along the melting line between liquid water and ice VII, as well as in water mixtures under extreme pressure–temperature (p–T) conditions [4]. In this phase, water molecules remain organized in a regular crystalline lattice while retaining the freedom to reorient, resulting in a hybrid state between that of a solid and a liquid. While plasticity is commonly observed in crystals of globular molecules like methane—where rotational motion persists within the crystal at high temperatures prior to melting—its occurrence in water ice is highly unusual.

Beyond plastic ice, theoretical studies predict several exotic high-pressure phases of water with similar (bcc-type) streuctures but profoundly different proton dynamics: quantum tunneling in the symmetric phase, molecular reorientation in plastic ice, long-range proton diffusion in the superionic phase, among them. High-pressure quasielastic neutron scattering (HP-QENS) offers a uniquely sensitive probe of these dynamic processes, enabling direct observation and experimental confirmation of these elusive phases.

Our recent HP-QENS experiments under high pressure have unveiled varying degrees of plasticity in high-pressure ice phases [5], water–ammonia ice mixtures [6], salty ices [7], methane and hydrogen-filled ices [8,9], and confined amorphous ice [10]. In this talk, I will discuss how plastic water arises in diverse environments and under varying p–T conditions, how plasticity is linked to the "glassy" behavior of water, and the implications of the existence of plastic ices for the geodynamics of icy moons.

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Primary author: BOVE, Livia

Presenter: BOVE, Livia

Session Classification: Invited speakers

Contribution ID: **38** Type: **Invited Oral**

1D nanoporous membrane boosts the ionic conductivity of electrolytes

Monday, 2 June 2025 14:45 (30 minutes)

Solid-state batteries have attracted significant interest as promising candidates for high energy density and safe battery technology. However, they commonly experience low ionic conductivity at ambient temperature, which limits their power density. This study addresses this issue by developing a porous separator with one-dimensional (1D) nanometric channels that confine non-flammable ionic liquid-based electrolytes (ILLi). We achieve 1D macroscopic ionic transport by confining the electrolytes within Vertically Aligned Carbon NanoTubes (VA-CNT) composite membranes. Employing quasi-elastic neutron scattering techniques, we conduct a multiscale analysis of the diffusive motion of both bulk and confined electrolytes. By extracting diffusion coefficients spanning from the molecular to macroscopic scale, we gain insights into the transport properties of IL-Li. Our results show that nanometric confinement allows to lower the operational temperature of these electrolytes by up to 20 K compared to the non-confined electrolytes. At ambient temperature, we show a tenfold increase in conductivity under 1D CNT confinement. Molecular Dynamics simulations shed light on the underlying physics, showing a unique intermolecular organization of the IL-Li under confinement. Specifically, the molecules form a core–shell structure, resulting in the creation of quasi-1D transport channels. This study presents promising avenues for exploring the use of 1D materials in energy storage applications.

Primary author: BERROD, Quentin (CNRS SyMMES)

Co-authors: Dr PINCHART, Camille (LLB); ZANOTTI, Jean-Marc (Laboratoire Léon Brillouin (CEA-CNRS) / CRG SHARP); Dr MODESTO, Nino (SyMMES); Dr RAMOS, Raphael (CEA Liten)

Presenter: BERROD, Quentin (CNRS SyMMES)

Session Classification: Invited speakers

Contribution ID: **39** Type: **not specified**

PhD award

Tuesday, 3 June 2025 19:30 (30 minutes)

Session Classification: Invited speakers

Contribution ID: **42** Type: **not specified**

SAMBA: The first Small-Angle Neutron Scattering Instrument for the ICONE Compact Source

Wednesday, 4 June 2025 14:00 (30 minutes)

1 Université Paris Saclay, Laboratoire Léon Brillouin, UMR 12 CNRS-CEA, CEA-Saclay,91191, Gif-sur-Yvette, France

The ICONE project aims to develop a compact neutron source (HiCANS – High Current Accelerator-driven Neutron Source) to serve the needs of the French scientific community. Within this framework, the SAMBA instrument (Small Angle Measurements for Broad Applications) is being designed to provide versatile and efficient small-angle neutron scattering (SANS) capabilities, tailored to the characteristics of compact sources, including moderate flux and wide wavelength bandwidths.
SAMBA is optimized to maximize measurement efficiency across a broad range of scattering vectors (Q), using a modular collimation system. Monte Carlo simulations (McStas) have been employed to optimize the instrument geometry and predict its performance in terms of flux, resolution, and accessible Q-range.This presentation will outline the current design specifications and performance estimates for SAMBA. Beyond presenting the instrument, this session is intended as an opportunity to engage with the scientific community: feedback and discussions are highly encouraged to refine SAMBA's capabilities and better align the final design with the diverse needs of future users across soft matter, disordered materials, and nanostructured systems research.

Primary author: CHENNEVIERE, Alexis (Laboratoire Léon Brillouin, CEA Saclay)

Presenter: CHENNEVIERE, Alexis (Laboratoire Léon Brillouin, CEA Saclay)

Session Classification: Invited speakers

Contribution ID: **43** Type: **not specified**

News from LLB

Thursday, 5 June 2025 09:00 (10 minutes)

Primary author: DESMEDT, Arnaud

Presenter: DESMEDT, Arnaud

Session Classification: Research Infrastructures

Contribution ID: **44** Type: **not specified**

News from ESS

Thursday, 5 June 2025 08:30 (10 minutes)

Primary author: FRAGNETO, Giovanna (European Spallation Source ERIC)

Presenter: FRAGNETO, Giovanna (European Spallation Source ERIC)

Session Classification: Research Infrastructures

Contribution ID: **45** Type: **not specified**

News from ILL

Thursday, 5 June 2025 08:40 (10 minutes)

Primary author: JESTIN, Jacques (ILL)

Presenter: JESTIN, Jacques (ILL)

Session Classification: Research Infrastructures

Contribution ID: **46** Type: **not specified**

News from 2FDN

Thursday, 5 June 2025 08:50 (10 minutes)

Primary author: PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique)

Presenter: PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique)

Session Classification: Research Infrastructures

Contribution ID: **47** Type: **not specified**

EMBL

Thursday, 5 June 2025 11:00 (10 minutes)

Primary author: DJINOVIC CARUGO, Kristina (EMBL)

Presenter: DJINOVIC CARUGO, Kristina (EMBL)

Session Classification: Research Infrastructures

Contribution ID: **48** Type: **not specified**

Batteries hub

Thursday, 5 June 2025 11:10 (10 minutes)

Primary author: LYONNARD, Sandrine (CNRS SyMMES)

Presenter: LYONNARD, Sandrine (CNRS SyMMES)

Session Classification: Research Infrastructures

Contribution ID: **49** Type: **not specified**

FAIR data

Thursday, 5 June 2025 11:20 (10 minutes)

Primary author: PERRIN, Jean-Francois

Presenter: PERRIN, Jean-Francois

Session Classification: Research Infrastructures

Contribution ID: **50** Type: **not specified**

Machine learning in materials science, institutional intiatives, and example of applications

Thursday, 5 June 2025 11:30 (10 minutes)

Primary author: JAKSE, Noel (SIMAP Grenoble-INP-UGA)

Presenter: JAKSE, Noel (SIMAP Grenoble-INP-UGA)

Session Classification: Research Infrastructures

Contribution ID: **51** Type: **not specified**

ESRF

Thursday, 5 June 2025 10:00 (10 minutes)

Primary author: DAILLANT, Jean (ESRF)

Presenter: DAILLANT, Jean (ESRF)

Session Classification: Research Infrastructures

Contribution ID: **52** Type: **not specified**

PSI

Thursday, 5 June 2025 09:30 (10 minutes)

Primary author: KENZELMANN, Michel (Paul Scherrer Institut)

Presenter: KENZELMANN, Michel (Paul Scherrer Institut)

Session Classification: Research Infrastructures

Contribution ID: **53** Type: **not specified**

EMFL

Thursday, 5 June 2025 09:50 (10 minutes)

Primary author: SIMON, charles (LNCMI CNRS)

Presenter: SIMON, charles (LNCMI CNRS)

Session Classification: Research Infrastructures

Contribution ID: **54** Type: **not specified**

CERN

Thursday, 5 June 2025 09:40 (10 minutes)

Primary author: FREEMAN, Sean (CERN)

Presenter: FREEMAN, Sean (CERN)

Session Classification: Research Infrastructures

Contribution ID: **55** Type: **not specified**

Neutron detectors

Wednesday, 4 June 2025 17:15 (15 minutes)

Primary author: GUERARD, Bruno (ILL)

Presenter: GUERARD, Bruno (ILL)

Session Classification: Contributed talks

Contribution ID: **56** Type: **Oral**

ICONE: instrument suite status

Wednesday, 4 June 2025 16:30 (15 minutes)

Since the shutdown of the Orphée reactor, France is missing a national neutron facility to support its scientific community. Neutron sources worldwide are progressively transitioning from traditional reactor-based sources (such as ILL, Orphée, and FRM II) to pulsed sources (ESS, SNS, J-PARC). In parallel, the development of High Current Accelerator-driven Neutron Sources (HiCANS) offers a cost-effective route for building high-performance pulsed neutron sources on a smaller scale.

In this context, CEA and CNRS are working on the ICONE project, which aims to establish a French HiCANS facility designed to serve the national scientific community, prepare for optimal use of the ESS and train the younger generation. The project is in the "Avant Projet Détaillé" phase, during which the complete design of the facility is being developed.

A key aspect of this effort is the development of an instrument suite in collaboration with the community. This is done by collecting needs, collaborating on specific aspects through the API-CONE call for proposals held in 2024 and the input of the Scientific Council. The planned suite consists of 10-12 instruments, installed on two targets optimized for flux (SANS, reflectometry, ...) or resolution (diffraction, inelastic neutron scattering, ...).

This presentation will provide an overview of the ICONE project and discuss the details of the instrument suite, with a focus on the specificities and opportunities arising from the pulsed nature of the source.

Primary author: FABREGES, Xavier (Laboratoire Léon Brillouin, CEA/CNRS Saclay, France)

Presenter: FABREGES, Xavier (Laboratoire Léon Brillouin, CEA/CNRS Saclay, France)

Session Classification: Contributed talks

Contribution ID: **57** Type: **Oral**

Grazing Incidence Small Angle Neutron Scattering (GISANS) applied on soft matter systems

Wednesday, 4 June 2025 13:30 (30 minutes)

Institut Max von Laue- Paul Langevin (ILL), 71 Avenue des Martyrs, 38042 Grenoble, France (vagias@ill.fr)

The concept of softness is encountered in different materials of the everyday life, although its precise quantification is still far to be achieved. In thin films of soft matter, quite often compounds that are energetically incompatible have to be mixed. The softness of the emerging thin films stems from the interactions of the underlying compounds. Such interactions play a key role in the mixing of the underlying building blocks and the microstructure. The microstructure of the soft matter thin films in turns determines the macroscopic properties of the material, such as stiffness, viscosity or apparent yield stress. Controlling these properties is fundamental for application in the pharmaceutical field, in health-care products, soft robotics and actuators as well as in the stabilization of emulsions. Grazing Incidence small-angle neutron scattering is a valuable fundamental method to probe soft materials at interfaces. The large scattering volume being probed by the shallow incident angles, the isotope sensitivity of neutrons as probes and large penetration power of neutrons renders GISANS ideal to access buried nanostructured on films of soft matter. In this talk, I will show examples of the use of GISANS to investigate different cases from soft matter systems at interfaces, including ordered micellar assemblies of pluronic surfactants, orientation of lamellae in multiblock copolymer films, alignment of phospholipid membranes, inorganic colloids at air-liquid interfaces, as well as stimuli-responsive polymer brushes under extreme hydrostatic pressure.

Presenter: VAGIAS, Apostolos (D22 co-responsible)

Session Classification: Invited speakers

Contribution ID: **58** Type: **Poster**

Thermal conductivity in terbium-based compound : KTb3F10

Wednesday, 4 June 2025 15:45 (15 minutes)

KTb3F10 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 (C4n 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 W/m/K which is expected in amorphous materials such as glass. More interestingly, the thermal conductivity curve at low temperatures is not proportional to T3 as expected for a system where only phonons conduct heat but instead comprises a local extremum. 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 KTb3F10 and emphasize the microscopic signature of such coupling.

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[2] Stephen L. Chamberlain and L. R. Corruccini, Phys Rev B 71, 024434 (2005)
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Primary author: DEMORTIER, OLIVIER (Laboratoire Léon Brillouin, CEA Saclay)

Co-authors: IVANOV, Alexandre (ILL); FAUQUÉ, Benoît (Collège de France); ROESSLI, Bertrand (Paul Scherrer Institut); RESSOUCHE, Eric (Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38042 Grenoble, France); DAMAY, Francoise (LLB); LE BERRE, Françoise (Institut des Molécules et Matériaux du Mans); Dr BOURDAROT, Frederic (CEA-Grenoble); LHOSTE, Jérôme (Institut des Molécules et Matériaux du Mans); SIBILLE, Romain (Paul Scherrer Institut); PETIT, Sylvain (LLB CEA-CNRS-Université Paris-Saclay); FENNELL, Tom (Paul Scherrer Institut); COLIN, claire (Institut Néel, CNRS & Université Grenoble Alpes)

Presenters: IVANOV, Alexandre (ILL); FAUQUÉ, Benoît (Collège de France); ROESSLI, Bertrand (Paul Scherrer Institut); RESSOUCHE, Eric (Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38042 Grenoble, France); DAMAY, Francoise (LLB); LE BERRE, Françoise (Institut des Molécules et Matériaux du Mans); Dr BOURDAROT, Frederic (CEA-Grenoble); LHOSTE, Jérôme (Institut des Molécules et Matériaux du Mans); DEMORTIER, OLIVIER (Laboratoire Léon Brillouin, CEA Saclay); SIBILLE, Romain (Paul Scherrer Institut); PETIT, Sylvain (LLB CEA-CNRS-Université Paris-Saclay); FENNELL, Tom (Paul Scherrer Institut); COLIN, claire (Institut Néel, CNRS & Université Grenoble Alpes)

Session Classification: Contributed talks

Contribution ID: **59** Type: **Oral**

Structure and dynamics in Surfactant-free microemulsions

Firoz Malayil Kalathil, Marie Plazanet, Ingo Hoffmann, Sylvain Prévost, Thomas Zemb & Christiane Alba-Simionesco.

Ternary mixtures of oil, water and an hydrotrope can lead to complex and usable organization in terms of reactivity or solubility. This is the case of aqueous solutions of ethanol and oil, typically found in all kind of liquors, cosmetics or solvents for liquid-liquid extraction.
The archetypical case of this family is the ternary mixture of water, ethanol and octanol. A rapid dilution of the monoalcohols binary mixture with water takes the system into the biphasic region, where a metastable emulsion of oil droplets forms, known as the « Ouzo » effect. Before reaching this phase, a thermodynamically stable region was also identified close to the critical point and described as pre-Ouzo region 1.
Our work aims at providing a quantitative description of the whole phase diagram of this system from a microscopic point of view. For this purpose, we mainly combined X-ray small angle scattering, quasi-elastic neutron scattering and PFG-NMR. Our investigations enabled us to characterize the organization and the diffusion of each molecular species in the various regions. The main structural parameters describing the different phases could be identified and related with the regimes observed in self and collective diffusion.
The fine tuning of such phases was eventually addressed in exploring temperature effects or subtle chemical substitution on the monoalcohol.

Fig. 1 : phase diagramm (wt.%) of the ternary mixture octanol/ethanol/water. The binary region is colored in grey ; the Widom line starts from the critical point (red dot) and corsses the monophasic region toward the ethanol-water binary line ; the Lifshitz line delimitates the onset of structural organisation ; the minimum hydrotrope concentration (MHC) indicates the minimum quantity of ethanol required to form a monophasic solution as soon as octanol is added to water ; the dynamics was investigated along the blue dotted line.

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[3] F. Malayil Kalathil, PhD thesis, 2025.

Primary author: PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique)

Presenter: PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique)

Contribution ID: **60** Type: **not specified**

Inclusion au travail : briser les tabous des handicaps (in)visibles.

Bénédicte Henry Canudas & Ketty Beauvois (CEA Grenoble), Catherine Chazette (ILL)

L'inclusion au travail : un droit, une nécessité
Cette intervention débutera par un cadrage clair : définition de l'inclusion professionnelle et rappel des obligations légales. Car inclure, c'est permettre à chacun de s'épanouir au sein de son environnement de travail, sans se heurter à des barrières invisibles ou à des biais systémiques.

Le défi des handicaps invisibles : 80 % des handicaps en France
Soit dix millions de personnes concernées par des troubles non visibles (maladies chroniques invalidantes, troubles sensoriels, psychiques, cognitifs, musculo-squelettiques…) qui impactent leur quotidien professionnel. Loin d'être un sujet marginal, il s'agit d'un enjeu sociétal qui exige une vraie révolution des mentalités.

Témoignages croisés pour changer de regard
• Le vécu raconté en poésie d'une personne concernée (douleur et adaptation créative).
• Le récit audio d'un collaborateur ayant accompagné un collègue avec une maladie invalidante.

Passer à l'action
Nous conclurons par des solutions concrètes :
• Aménagements de poste
• Bonnes pratiques pour le maintien dans l'emploi
• Moyens pour créer des environnements réellement inclusifs.

Un plaidoyer pour transformer les défis en opportunités collectives.

Presenter: BEAUVOIS, Ketty (CEA Grenoble)

Session Classification: Inclusion

Contribution ID: **61** Type: **Poster**

The ICONE project: towards a new neutron source in France for materials science and industry

Monday, 2 June 2025 19:30 (15 minutes)

HiCANS, High Current Accelerator-based Neutron Sources, is a concept proposed several years ago which aims at revisiting how neutron sources suitable for neutron scattering could be built 1. The concept of HiCANS relies on technical progress in accelerator technology, neutron moderator design and neutron instrumentation developments to be able to propose a source using a low energy accelerator, in the tens of MeV of energy, while still being able to provide competitive neutron instrumentation. There are currently in Europe three main projects of HiCANS proposals, HBS in Germany, ARGITU in Spain and ICONE in France.
In 2024, the CEA and the CNRS have been mandated to write a Technical Design Report for a HiCANS source, namely ICONE, following a first Avant-Projet Sommaire published in 2023 [2].
We will present the different key aspects of HiCANS sources: accelerator, target-moderator assembly and neutron instrumentation. We will focus on the current status of the foreseen instruments on the ICONE project. Detailed Monte-Carlo simulations have been performed to be able to project as precisely as possible what performances can be expected on different instruments.
The long-term goal is to eventually build a user facility, ICONE, which would offer a suite of 10 neutron scattering instruments to the French community. We aim at achieving performances comparable to the instruments which were operated around the ORPHÉE reactor.

1 LENS Report Low Energy Accelerator-driven Neutron Sources (Nov. 2020) [https://www.lens-initiative.org/wp-content/uploads/2021/02/LENS-Report-on-Low-Energy-Accelerator-driven-Neutron-Sources.pdf]
[2] ICONE, Une Nouvelle Source de Diffusion Neutronique Française. Avant-Projet Sommaire (2023) [https://2fdn.cnrs.fr/wp-content/uploads/2023/09/ICONE-digital.pdf]

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Presenter: OTT, Frederic (IRAMIS / Laboratoire Léon Brillouin CEA-CNRS)

Session Classification: Posters

Contribution ID: **62** Type: **not specified**

Neutron detectors

The XtremeD, D16, and D20 instruments have recently been equipped with large-area, curved, position-sensitive 33He neutron detectors based on the Trench-MWPC (Multi-Wire Proportional Chamber) technique, initially introduced at the ILL in 2017. These detectors offer a unique combination of wide angular coverage, high spatial resolution, and excellent counting rate capabilities. Their development, along with selected characterization results, will be presented. The specific features of the Trench-MWPC design provide several advantages over conventional MWPCs, which will be described and discussed.

Presenter: GUERARD, Bruno (ILL)

Session Classification: Contributed talks