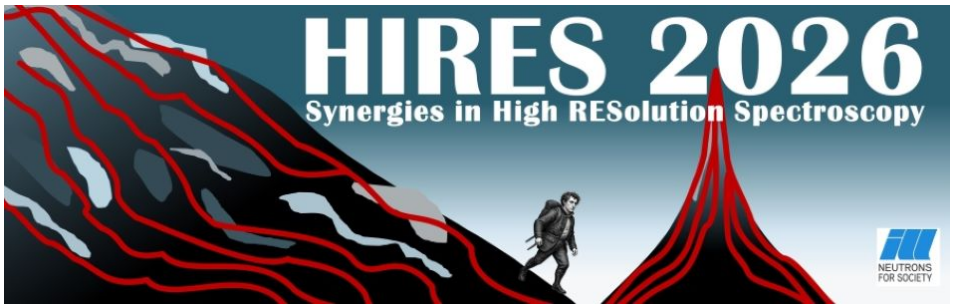
HIRES 2026



Report of Contributions

https://workshops.ill.fr/e/HIRES2026

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

Pressure dependent dynamical investigation of relaxations associated with hydrogen bonding in 1-propanol

Hydrogen bonds are ubiquitous in nature and play a central role in determining the microscopic dynamics of liquids. While water remains the most important hydrogen-bonded liquid, its peculiar behaviour and supercooling challenges motivate the study of simpler systems, such as mono-hydroxy alcohols,where hydrogen-bond dynamics are better separated from structural relaxation. Dielectric spectroscopy has shown that mono-hydroxy alcohols exhibit a dominant slow Debye relaxation, slower than the α-relaxation, and growing evidence suggests that poly-alcohols display a similar, though more merged, separation of processes. In this work, we investigate the relaxation dynamics of liquid 1-propanol and its 10% glycerol mixture above the glass transition using quasi-elastic neutron scattering (IN16B backscattering, wide-angle spin-echo, and IN5 time-of-flight) combined with dielectric spectroscopy. High-pressure measurements up to 6 kbar reveal that the slowest relaxation process shifts by orders of magnitude, whereas faster processes are largely unaffected, enabling their better separation. Selective deuteration demonstrates that this slow dynamic originates from intermolecular hydrogen bonds, while faster components are associated with methyl group motions and structural relaxation. Ongoing molecular dynamics simulations are used to calculate dynamic structure factors and support the interpretation of neutron and dielectric spectroscopy data, with the goal of disentangling the individual relaxation processes. Together, these experimental and computational efforts provide detailed insight into the pressure-,concentration-, and temperature-dependent hydrogen-bond dynamics of mono-hydroxy alcohols.

Session

Liquids

Primary author: Mr TIWARI, Anand Kumar (Institut Laue-Langevin)

Co-authors: Dr FARAGO, Bela (Institut Laue-Langevin); Dr JAKOBSEN, Bo (Roskilde University); Prof. NISS, Kristine (Roskilde University); Dr APPEL, Markus (Institut Laue-Langevin); Dr A. GONZALEZ, Miguel (Institut Laue-Langevin)

Presenter: Mr TIWARI, Anand Kumar (Institut Laue-Langevin)

Session Classification: Liquids

Contribution ID: **7** Type: **Poster**

Development of Spectroscopic Neutron Imaging towards Advanced Electrolyte Characterization

As developments in renewable energy continue, the advancement of energy storage devices is pressed towards further innovation to meet efforts towards net-zero emissions. With energy storage systems, Li-ion batteries (LIBs) are the most widespread in applications from consumer electronics to grid storage due to their high energy density and long lifetime. Electrolyte engineering (which involves a careful selection of solvents, salts, and additives) is one of the simplest modifications in LIB technology to make an immense impact on improving performance. In this work, we develop a technique in neutron imaging, specifically spectroscopic neutron imaging (SNI), that leverages energy transfer with the sample to achieve chemically sensitive contrast. We will showcase the development of SNI and its prospective applications to advanced electrolyte characterization.

Session

Instrumentation

Primary author: YOUNG, Robert (ISIS-STFC-UKRI)

Co-authors: Dr MORGANO, Manuel (ISIS-STFC-UKRI); Dr KOCKELMANN, Winfried (ISIS-STFC-UKRI)

Presenter: YOUNG, Robert (ISIS-STFC-UKRI)

Session Classification: Instrumentation

Contribution ID: **8** Type: **Oral**

Diffusion, search and attack motions of antibodies

A fundamental feature of the antibody structure is the flexible linker between the 3 fragments that allows great flexibility and simultaneous binding to epitopes of antigens and receptors. Combining dynamic light scattering, neutron spin-echo spectroscopy and PFG-NMR we determine characteristic internal fragment dynamics on top of translational and rotational diffusion under crowding conditions. Short-time and long-time translational diffusion show an effective hard sphere like behavior within a colloidal picture. Internal fragment motions are characterized as “attack” and “search” motions complemented by rotational fragment motions. We find that the “attack” motions exposing the binding domain are highly preserved from low to physiologically relevant concentrations and higher, while “search” motions and overall rotational diffusion are suppressed under crowding conditions. Hydrodynamic interactions change the friction between frag-ments determining relaxation times while interparticle interactions influence the strength of the entropic spring between fragments.
A direct comparison shows that the internal fragment motions have a significat contribution to QENS data on shorter scale.

Biehl, R., Kruteva, M., Czakkel, O. et al. Diffusion, search and attack motions of antibodies. Commun Biol 8, 1461 (2025). https://doi.org/10.1038/s42003-025-08995-9

Session

Biology/Health

Primary author: BIEHL, Ralf (Forschungszentrum Jülich)

Co-authors: KRUTEVA, Margarita (Forschungszentrum Jülich); CZAKKEL, Orsolya (Institut Laue Langevin); HOFFMANN, Ingo (ILL); RICHTER, Dieter (Forschungszentrum Jülich); STADLER, Andreas (Forschungszentrum Julich)

Presenter: BIEHL, Ralf (Forschungszentrum Jülich)

Session Classification: Biology/Health

Contribution ID: **9** Type: **Poster**

New developments and upgrade programm for the TOF spectrometer TOFTOF at the MLZ

Within this presentation we want to show new developments on sample environment dedicated for TOFTOF. Although we want to show and discuss our planed upgrade program for TOFTOF.

Session

Instrumentation

Primary author: WOLF, Marcell (TUM - MLZ)

Co-author: GARVEY, Chris (Technische Universität München)

Presenter: WOLF, Marcell (TUM - MLZ)

Session Classification: Instrumentation

Contribution ID: **10** Type: **Invited**

Dynamics and structure of proteins and lipids in context of diseases using neutron scattering and synchrotron radiation

A hallmark of amyloidosis such as Alzheimer's disease is the deposition of amyloid fibrils, which are self-assembled protein filaments with core regions rich in β-sheets, in various organs. Cytotoxicity underlying the pathogenesis of amyloidosis is partly caused by the disruption of cell membranes by binding of amyloid fibrils. Since amyloidogenic proteins form polymorphic fibrils with different levels of cytotoxicity, it is crucial to understand the structural and dynamical features of these fibrils and lipid membranes to gain insights into their physical properties leading to higher cytotoxicity. For this purpose, we have employed model systems of polymorphic amyloid fibrils of hen egg white lysozyme and membranes of DMPG and DMPC, and utilized elastic incoherent neutron scattering (EINS) and quasi-elastic neutron scattering (QENS) to characterize the molecular dynamics at the sub-nanosecond timescale while we have utilized vacuum ultraviolet circular dichroism (VUVCD) and small-angle X-ray scattering (SAXS) to characterize the structure of the fibrils and monomers.

In addition, we are now working on another protein, Notch2nl-B, which is involved in the expansion of the cerebral cortex and related to brain tumors. The modern-type (197I) is known to promote the brain tumor formation compared with the ancestral-type (197T), suggesting that possible changes in its structure and dynamics are associated with the pathogenesis of the brain tumor. We have employed VUVCD and SAXS to obtain structural information on this protein containing flexible regions, for which application of EINS/QENS is expected.

In this talk, we will present our recent findings on molecular dynamics and structure of the above systems relevant with the pathogenesis of the corresponding diseases.

Session

Biology/Health

Primary author: MATSUO, Tatsuhito (Hiroshima International University)

Presenter: MATSUO, Tatsuhito (Hiroshima International University)

Session Classification: Biology/Health

Contribution ID: **11** Type: **Poster**

Correlated Electron Dynamics and Magnetic Excitations in Topological and Intermetallic Quantum Materials

Understanding low-energy excitations and spin–charge correlations in quantum materials remains a key challenge in condensed matter physics. In this study, we investigate the magneto transport and structural properties of high-quality intermetallic single crystals (EuAuSb and DyMn6Sn6) alongside topological insulator thin films (Bi–Sb–Te–Se, BSTS) to explore the interplay between topology, magnetism, and electronic correlations. The intermetallic compounds exhibit complex magnetic ordering and anisotropic transport behavior arising from strong 4f–3d hybridization, while the BSTS thin films reveal weak antilocalization and linear magnetoresistance features associated with topologically protected surface states.

The combination of magneto transport data with high-resolution spectroscopic insights provides a comprehensive picture of charge carrier scattering and spin dynamics across these systems. We discuss the relevance of neutron-based techniques—such as spin-echo, backscattering, and TOF spectroscopy—for probing quasi elastic dynamics, magnetic fluctuations, and phonon–magnon interactions in such correlated systems. This approach emphasizes the powerful synergy between neutron spectroscopy and complementary transport and ARPES measurements in unraveling the microscopic origins of emergent quantum phenomena in intermetallic and topological materials.

Session

Hard Condensed Matter

Primary author: SHARMA, Vishnu (Indian institute of Technology (BHU) Varanasi)

Co-author: Prof. CHATTERJEE, Sandip (Indian institute of Technology (BHU) Varanasi)

Presenter: SHARMA, Vishnu (Indian institute of Technology (BHU) Varanasi)

Session Classification: Hard Condensed Matter

Contribution ID: **12** Type: **Oral**

A combined QENS and NMR study of the dynamics of the deep eutectic solvent ethaline

Over the past decade, Deep Eutectic Solvents (DESs) have garnered significant attention within the scientific community due to their remarkable functional properties. Yet their nanoscale organization remains challenging due to nanoscopic domains and dynamics heterogeneity.

We probed the molecular dynamics of the benchmark deep eutectic solvent ethaline, separating the motions of its two components choline chloride and ethylene glycol across a broad window of length and time scales (sub-nanometer to micrometers; picoseconds to milliseconds). Using pulsed-field-gradient NMR, time-of-flight QENS, and backscattering inelastic fixed-window scans (IFWS) on isotopically labeled samples, we obtained a species resolved view of the dynamics. At the micrometer scale, translational motion follows classical hydrodynamics: the two constituents exhibit distinct diffusion coefficients that reflect their different hydrodynamic sizes. This is no longer valid at the nanometer scale, where both components show similar short-range diffusivities, indicating strong supramolecular association. At sub-nanometer scales, we detect jump motions that precede Fickian diffusion and localized dynamics within transient molecular cages. The spatial amplitudes of these localized motions track each species molecular size and chemistry, while their correlation times differ from observations in other choline-based DESs (e.g., glyceline). Altogether, the results highlight how subtle differences in hydrogen-bonding propensity of the polyol donor control dynamics and why nanoscale behavior cannot be reliably inferred from macroscopic properties especially under varying environments such as confined media, interfaces, and porous catalysts.

Reference: M. N. Kamar et al. J. Chem. Phys. 163, 134506 (2025)

Session

Liquids

Primary author: Mr KAMAR, Mohammad Nadim (Institute of Physics of Rennes)

Co-authors: Dr MOZHDEHEI, Armin (Institute of Physics of Rennes); Dr DUPONT, Basma (Institute of Physics of Rennes); Dr LEFORT, Ronan (Institute of Physics of Rennes); Dr MORÉAC, Alain (Institute of Physics of Rennes); OLLIVIER, Jacques (Institut Laue-Langevin); APPEL, markus (ILL); MORINEAU, Denis (Institute of Physics of Rennes, CNRS-University of Rennes 1)

Presenter: Mr KAMAR, Mohammad Nadim (Institute of Physics of Rennes)

Session Classification: Liquids

Contribution ID: **13** Type: **Poster**

Promising features of praseodymium nanoferrites

Praseodymium-doped magnetite ($Pr_xFe_{3-x}O_4$, $x = 0.15$ and 0.45) was synthesized by co-precipitation from chloride precursors to investigate the influence of lanthanide substitution on structural and magnetic properties. Both compositions crystallize in a mixed spinel structure, space group Fd-3m (no. 227), and exhibit single-phase character, as confirmed by powder X-ray diffraction. Refined lattice parameters are 8.392(2) Å for $Pr_{0.15}Fe_{2.85}O_4$ and 8.388(2) Å for $Pr_{0.45}Fe_{2.55}O_4$, indicating slight lattice contraction with increasing Pr content. Average particle size ranges from 24 nm ($Pr_{0.15}Fe_{2.85}O_4$) to 17 nm ($Pr_{0.45}Fe_{2.55}O_4$). Mössbauer spectroscopy revealed modifications in the Fe^{2+}/Fe^{3+} ratio, suggesting partial occupation of tetrahedral and octahedral sites by Pr^{3+} ions and changes in the local electronic configuration. Magnetization measurements confirmed ferrimagnetic behavior with negligible coercivity and stable magnetic ordering up to room temperature. These results indicate Pr substitution alters the Fe^{2+}/Fe^{3+} balance, inducing deformation of oxygen polyhedra and increased magnetic anisotropy. The obtained Pr-doped Fe_3O_4 nanomaterials combine soft magnetic characteristics with strong potential for environmental remediation, enabling efficient adsorption of heavy metal ions and degradation of organic pollutants, while magnetic separability allows recovery and reuse. Thus, Pr-substituted magnetite is a promising class of eco-efficient nanomaterials for catalytic, magnetic, and wastewater treatment applications.

Session

Materials Science

Primary authors: Ms SZARKOWSKA, Kinga (University of Białystok); Dr KLEKOTKA, Urszula (University of Białystok); Dr OLSZEWSKI, Wojciech (University of Białystok); Ms BIERNACKA, Maria (University of Białystok); Prof. REĆKO, Katarzyna (University of Białystok)

Presenter: Ms SZARKOWSKA, Kinga (University of Białystok)

Session Classification: Materials Science

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

Effect Surface Chemistry on the Properties of Nanoconfined Water

In many natural and technological settings, water exists not as bulk liquid but as thin interfacial films or within nanopores, where its behavior is strongly influenced by surface chemistry. These constraints can significantly alter hydrogen-bonding compared to bulk water, raising the question of whether surface chemistry can be deliberately tuned to control interfacial water properties.
Our research tackles this challenge using periodic mesoporous materials (PMOs) whose pore walls are functionalized with organic bridges to create nanoscale patterns with adjustable repetition lengths, hydrophilicity, ionic surface charge and H-bonding capacity [1]. With pore diameters of ~4 nm, these systems provide precise models for studying how molecular-scale heterogeneity shapes the physics of surface water.
We will present results from recent work where the structure and dynamics of water confined in the nanopores or adsorbed on the inner surface of PMOs were investigated by the combination of various high resolution quasielastic neutron scattering experiments [2,3] with broadband dielectric spectroscopy [4] and Raman spectroscopy [5] covering thus extended temperature and time scales.

References

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2 A. Jani et al, J. Chem. Phys., 154, 094505 (2021)
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4 B. Malfait et al. J. Phys. Chem. C, 125, 16864 (2021)
5 B. Malfait et al. J. Phys. Chem. C, 126, 3520 (2022)

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Session

Liquids

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Presenter: MORINEAU, Denis (Institute of Physics of Rennes, CNRS-University of Rennes 1)

Session Classification: Liquids

Contribution ID: **15** Type: **Poster**

Characterization of the magnetic phase transitions in double perovskite Nd2NiMnO6

Through neutron powder diffraction, we confirm the double perovskite Nd_2NiMnO_6 adopts a monoclinic $P2_1/n$ structure with nearly complete B-site ordering of Ni^{2+} and Mn^{4+}. Below T_1 = 198 K, magnetic susceptibility and neutron data reveal the Ni^{2+} and Mn^{4+} sublattices undergo ferromagnetic ordering, driven by strong 3d-3d exchange interactions. Upon cooling through T_2 = 22 K, a secondary transition occurs, where we discover an additional noncollinear, symmetry-breaking order of Nd^{3+} moments. We propose this rare-earth canting stems from the competition between f-d and f-f Heisenberg exchanges, finely balanced in the perovskite framework. The ground state symmetry also implies significant Nd^{3+} easy-plane anisotropy and a decoupling of the antiferromagnetic spin canting from the transition metal lattice.
Between T_1 and T_2, anomalous frequency-dependent ac susceptibility appears, characteristic of reentrant spin-glass-like behavior, attributed to antisite disorder and competing interactions. Furthermore, analysis of isothermal magnetization reveals magnetic entropy changes, suggesting potential for magnetic refrigeration. A peak entropy change of 2.25 J $kg^{-1}K^{-1}$ at T_1 under a 7 T field was observed. The scaling of this entropy, alongside other critical exponents, confirms the ferromagnetic transition at T_1 is a mean-field second-order phase transition. Collectively, our results provide crucial details on Nd_2NiMnO_6's magnetism, reinforcing double perovskites as model systems for studying competing interactions, magnetocaloric effects, and reentrant spin-glass phenomena

Session

Magnetism

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Presenter: ATTAH-BAAH, John Matthias (Federal University of Sergipe, Federal University of Minas Gerais.)

Session Classification: Magnetism

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

ZETA+ : First successes

Neutron resonance spin echo (NRSE) was invented nearly thirty years ago and initially developed to study the lifetime of crystal lattice excitations. It was subsequently used to determine the distribution and mosaicism of a crystal. This technique also allows the measurement of small crystallographic distortions and micro-gaps (a few tenths of a μeV) between different excitations. These measurements can be performed on the crystallographic or magnetic responses of the crystal.

Recently, a third generation of NRSE (ZETA$^+$), was installed on IN22. Compared to the previous generation, it allows measurements down to zero Fourier time or Larmor phase, thus opening the way to exploring new domains for obtaining new information.

The first measurement performed with this new option was the determination of the relatively short lifetime of a phonon in $SrTiO_3$. The result obtained is a phono width of 337 μeV (τ = 3.9 ps) with an energy gap of 2.1 meV. This result could not be obtained with cold triple-axis or time-of-flight spectrometers because the excitation is located near the Γ-point, and therefore too close to different nuclear contributions, and the excitation width is to small. Furthermore, most of the NRSE signal exists only for short Fourier times, making any measurement impossible with previous NRSEs.

The second measurement consisted of determining the distortion of TbB_4 during its transition to its second magnetic phase below 24 K where the structure is expected to change from tetragonal to orthorhombic. Measuring the crystal distortion by Larmor diffraction at the nuclear Bragg peak Q = (400) reveals that the difference between $d_{(400)}$ and $d_{(040)}$ is $4.59(12)\times10^{-4}$.

These examples illustrate the capabilities of ZETA$^+$.

Session

Instrumentation

Primary authors: Dr BOURDAROT, Frederic (CEA-Grenoble); Dr BINISKOS, Nikolaos (CEA--Grenoble)

Presenter: Dr BOURDAROT, Frederic (CEA-Grenoble)

Session Classification: Instrumentation

Contribution ID: **17** Type: **Poster**

Origin of Proton Conduction in Hydrated Sulfonated Porous Aromatic Framework: Insights from IN5B and IN16B QENS measurements

Understanding water diffusion in subnanometer pores is essential for designing next-generation proton-conducting materials. Sulfonated porous aromatic frameworks (SPAFs) offer a unique platform for this by combining rigid, permanently microporous carbon scaffolds with adjustable -SO3H densities. Their high proton conductivities, often comparable to fluorinated polymers, indicate that hydration and nanoscale dynamics differ markedly from bulk water, yet the microscopic basis remains unclear.

We address this question using complementary QENS measurements on IN16B (backscattering, λ = 6.2 Å, ΔE ≈ 0.75 μeV) and IN5B (time-of-flight, λ = 4.9 Å, ΔE ≈ 80 μeV) at ILL to resolve water dynamics in two fully hydrated SPAFs (93% RH) with nominal degree of sulfonation (DoS) 50% and 80%. Across all temperatures, the QENS data are consistently described by two separable motions: fast, local reorientation (resolved on IN5B) and a slower, translational jump-diffusion (resolved on IN16B). Because of the higher resolution, IN16B used for extracting the narrow translational linewidth Γ1(Q,T) via IFWS (3 and 6 μeV), which is then fixed in IN5B fits to isolate the broader rotational linewidth Γ2 and the EISF.

DoS_80% shows systematically slower translational diffusion and longer residence times than DoS_50%, indicating stronger water-acid interactions and reduced translational connectivity at higher acid density. Localized reorientations remain in the ps range, but vary in amplitude with DoS. Together, the combined TOF+BS dataset provides a continuous ≈10 ps - 1 ns dynamical window that links pore-scale dynamics to macroscopic, humidity-dependent proton transport and demonstrates the power of complementary neutron spectrometers for resolving ion conduction mechanisms in porous conductors.

Session

Soft Condensed Matter

Primary author: Dr MOZHDEHEI, Armin (Institute of Physics of Rennes, CNRS-University of Rennes)

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Presenter: Dr MOZHDEHEI, Armin (Institute of Physics of Rennes, CNRS-University of Rennes)

Session Classification: Soft Condensed Matter

Contribution ID: **18** Type: **Poster**

Following the dark-recovery process of the pP-SB1-LOV protein with neutron backscattering spectroscopy.

Light is an important stimulus for many biological processes. While structural changes in photo-responsive proteins are studied using well-established techniques, the implications of dynamic transitions during the photo-switching process remain to be assessed. High-resolution neutron backscattering spectroscopy enables the study of protein dynamics on the pico- to nanosecond timescale.

In this contribution, the photocycle of the pP-SB1-LOV protein is investigated using neutron backscattering spectroscopy on two instruments: the IRIS time-of-flight inverted-geometry crystal analyser and the IN16B high-resolution backscattering spectrometer.

Experiments were conducted initially with ex-situ illumination, and later with in-situ illumination, to observe the dynamics of the stationary dark-adapted and illuminated states. Comparisons are drawn between the quasi-elastic neutron scattering (QENS) observables and QENS observables derived from molecular dynamics simulations using the MDANSE software package of these stationary states. Further, the dynamic transitions along the dark-recovery process were observed by fixed window scans as well as continuous QENS spectra.

Resolving the dynamics of photo-responsive proteins throughout their photocycle within the constraints of a neutron backscattering experiment demands careful consideration of experimental design and data analysis framework, which will be continued in a long-term proposal aiming to develop pump-probe experiments at IN16B.

Session

Biology/Health

Primary author: BOSSERHOFF, Theresa (JCNS-1 & ILL)

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Presenter: BOSSERHOFF, Theresa (JCNS-1 & ILL)

Session Classification: Biology/Health

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

MIRACLES, the new backscattering spectrometer at ESS

MIRACLES is the neutron time-of-flight backscattering spectrometer at the European Spallation Source (ESS), which will provide the highest energy resolution among the current instrument suite [**1**]. Key features of MIRACLES will be: a) high and tuneable energy resolution, allowing to disentangle complex dynamics in a single experiment; b) versatile sample environment, aimed to investigate kinetic processes and reproduce *in situ/in operando* conditions; c) future polarization analysis capabilities, whose importance is increasingly recognized e.g. in the liquid and soft matter community [**2**]. This contribution reports the design and development of MIRACLES key components during construction and approaching commissioning phase. Perspective on how such capabilities will open new scientific possibilities will be also presented, demonstrating how MIRACLES will be configured as a groundbreaking neutron scientific instrument.

[**1**] F. Villacorta *et al.*, *Rev. Sci. Instrum.* **96**, 045101 (2025). N. Tsapatsaris *et al.*, *Rev. Sci. Instrum.* **87**, 085118 (2016).
[**2**] B. Rosi *et al.*, *J. Chem. Phys.* **162**, 214902 (2025). J. Maiz *et al.*, *Macromolecules* **55**, 2320–2332 (2022). M. Golub *et al.*, *Crystals* **14** (8), 743 (2024).

Session

Instrumentation

Primary authors: ROSI, Benedetta Petra (ESS); PEREIRA, Jose (ESS Bilbao); CONDE ESTEBANEZ, Alexander (ESS Bilbao); BECK, Christian (ESS DMSC); MAZKIARAN, Idoia (ESS Bilbao); ARANDA, Ivan (ESS Bilbao); ZUGAZAGA, Aitor (ESS Bilbao); MARTÍNEZ, Roberto (ESS Bilbao); G. DEL MORAL, Octavio (ESS Bilbao); SIMELIO, Antoni (ESS Bilbao); BORDALLO, Heloisa (University of Copenhagen); VILLACORTA, Félix (ESS Bilbao)

Presenter: ROSI, Benedetta Petra (ESS)

Session Classification: Instrumentation

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

On the origin of the non-dispersive mode in glass-forming liquids: the case of squalane

In spite of its fundamental interest, the collective dynamics of molecular liquids and glass-forming systems at the mesoscale –and its relationship with self-dynamics– is still poorly understood [1,2]. Mesoscale means distances long enough compared to intermolecular dimensions but not yet in the hydrodynamic region. Neutron scattering experiments addressing the coherent dynamic structure factor S(Q,t) there are extremely challenging due to very weak intensities, strong incoherent contributions –even in deuterated samples— and multiple scattering [1,3]. As shown by us [1,3,4], it is possible to isolate S(Q,t) by NSE combining measurements on deuterated and protonated versions of the same molecule. This procedure has allowed us to proof the dominance at the mesoscale of a Q-independent process [3,5,6]. This process observed for S(Q,t) also appears in the self-motions at the mesoscale at shorter times than diffusion [3].
Experiments in [3,5,6] were restricted to high T in a narrow range where the non-dispersive mode can be described by a single exponential. To discern the origin of the non-dispersive process its complete characterization over a large T range is crucial, addressing questions as its connection with viscosity and/or diffusion, the impact of cooperativity on the T- dependence of the characteristic time and functional form, etc.
Here we present new NSE results on squalane, trying to contribute to answering these questions.
REFERENCES: [1] B. Farago et al, Phys. Rev. E 65, 051803 (2002); [2] Z. Shen et al, J. Chem. Phys. 159, 114501 (2023); [3] A. Arbe et al, Phys. Rev. Lett. 134, 098001 (2025); [4] Experimental Report 6-02-678; [5] A. Arbe et al, J. Chem. Phys. 158, 184502 (2023); [6] A. Arbe et al, Phys. Rev. Research 2, 022015 (2020)

Session

Liquids

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Presenter: ARBE, Arantxa (Centro de Fisica de Materiales (CSIC-UPV/EHU))

Session Classification: Liquids

Contribution ID: **21** Type: **Poster**

Spin Dynamics of $Ba_5Ru_3O_{12}$: An Inelastic Neutron Scattering and Machin Learned Force-Field Study

We have Performed an inelastic neutron scattering (INS) investigation on the trimer ruthenate $Ba_5Ru_3O_{12}$, that undergoes long-range antiferromagnetic ordering at T_N = 60 K. The INS spectra suggest two distinct spin-wave excitations one at 5.6 meV, which is less intence and a broader intense excitation around 10-15 meV. Notably, these magnetic excitations persist well above T_N, indicating short-range correlations in the trimer network. We have modelled this spectra using linear spin-wave theory (SpinW) in combination with machine-learning force-field (MLFF) calculations which suggest that $Ba_5Ru_3O_{12}$ hosts strong magnetic frustration arising from competing nearest and next-nearest-neighbor exchange interactions, exchange anisotropy, and strong spin–orbit coupling. These competing interactions stabilize a non-collinear magnetic structure which makes this compound different from all other compounds that belongs to the same ruthenate trimer family. Furthermore, our theoretical calculations of the isolated Ru_3O_{12} trimer ground state are consistent with the experimentally observed excitation energies, providing a unified understanding of the magnetic dynamics in $Ba_5Ru_3O_{12}$.

Session

Magnetism

Primary author: KUSHWAHA, Ekta (Rajiv Gandhi Institute of Petroleum Technology)

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Presenter: KUSHWAHA, Ekta (Rajiv Gandhi Institute of Petroleum Technology)

Session Classification: Magnetism

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

Structure and dynamics of oil/water interfaces in emulsions

Emulsions are an indispensable part of everyday life; they are used in a wide range of applications, including cosmetics, drug delivery, and food systems. Mixed interfaces in emulsions are common and are composed of proteins and low molecular weight emulsifiers like phospholipids.
The charge and nature of phospholipid head groups exert a significant influence on the interfacial structure and rheology of protein-stabilised emulsions, yet exert only a minor effect on their interfacial dynamics. A combination of lab based methods – such as drop tensiometry and interfacial rheology – and scattering methods – such as small angle neutron scattering (SANS) and neutron spin echo spectroscopy (NSE) – is employed in this presentation to facilitate the answering of research questions about structure and dynamics of complex interfacial systems containing proteins and two different phospholipids [1].
Phosphatidylcholine has been observed to be loosely bound to the interface in the presence of β-lactoglobulin molecules. In contrast, phosphatidylglycerol has been found to be partially bound to β-lactoglobulin molecules via hydrogen bonds or hydrophobic interactions.
The interfacial dynamics of the protein are inert for changes in interfacial structure, composition, and rheology, although structure and rheology have a strong influence on each other.

[1] T. Heiden-Hecht et al., Journal of Colloid and Interface Science 703 (2026) 139095

Session

Biology/Health

Primary authors: HOLDERER, Olaf (Forschungszentrum Jülich GmbH, JCNS at MLZ); HEIDEN-HECHT, Theresia; FRIELINGHAUS, Henrich; MÜLLER, Maren

Co-authors: CZAKKEL, Orsolya (Institut Laue Langevin); ZOLNIERCZUK, Piotr (Oak Ridge National Laboratory); FÖRSTER, Stephan (Forschungszentrum Jülich); PREVOST, Sylvain (Institut Laue-Langevin); SCHWÄRZE Kuno

Presenter: HOLDERER, Olaf (Forschungszentrum Jülich GmbH, JCNS at MLZ)

Session Classification: Biology/Health

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

Wide angle neutron polarization analysis time of flight spectroscopy at ISIS

In recent years, polarised neutron spectroscopy on multi-detector spectrometers has become possible with the advent of wide-angle neutron spin analysers, either using polarizing supermirror arrays (e.g. D007 (ILL), HYSPEC (SNS)) or 3He spin-filters (LET (ISIS), PASTIS (ILL)). Wide-angle neutron polarization analysis is particularly useful for studying materials with short-range or non-crystalline order. Most commonly, it has been employed to separate magnetic scattering in disordered magnetic materials from nuclear scattering using XYZ polarization analysis developed by Schärpf [1] in the mid-80s. At the same time, it was realised that polarized neutrons could also be employed in the study of soft-matter and biological materials due to their ability to distinguish single-particle dynamics (such as diffusion) from co-operative correlated motions via the separated coherent and incoherent neutron cross-sections in hydrogenous materials.

In this webinar I will introduce the technique of uniaxial polarization analysis and its application to high resolution spectroscopy (QENS) studies using LET at ISIS, and on the proposed SHERPA spectrometer. Since neutron polarization experiments always come with a major flux and counting-rate penalty, I'll discuss when (and when not) polarized neutrons are really necessary in QENS measurements, using examples from LET. Future prospects for high-resolution magnetic spectroscopy with polarization analysis will also be discussed.

[1] O Schärpf and H Capellmann (1993). The XYZ-Difference Method with Polarized Neutrons and the Separation of Coherent, Spin Incoherent, and Magnetic Scattering Cross Sections in a Multidetector. Physica Status Solidi (A), 135(2), 359–379. https://doi.org/10.1002/pssa.2211350204

Session

Primary author: STEWART, John ross

Presenter: STEWART, John ross

Session Classification: Instrumentation

Contribution ID: **24** Type: **Poster**

Describing NSE Data from Undulating Membranes: Recent Advances

The Zilman-Granek (ZG) stretched exponential [1] has been widely used to describe neutron spin echo (NSE) data from undulating membranes for more than 2 decades.
However, with the abilities of modern NSE spectrometers, it becomes necessary to go beyond the stretched exponential approximation.

Recently, we have published an expression for the dynamic structure factor of undulating vesicles, that explicitly takes into account their spherical geometry, their finite size and the effect of translational diffusion [2]. We compare these expressions to NSE data from simple vesicle membranes.

While the traditional stretched exponential yields drastically different values of the bending rigidity for vesicles made from the same type of lipids but extruded to different sizes, our new expression yields consistent results of the effective bending rigidity. However, at q<0.05 1/Å the observed bending rigidity decreases and it becomes apparent that additional effects need to be taken into account. While it is theoretically possible to disentangle these effects, it remains a challenge to do so with current experimental data.

Our expression allows for the consistent description of membrane undulations in terms of an effective bending rigidity wich is independent of the vesicle size. Measuring to sufficiently low q and sufficiently long fourier times, it becomes obvious, that the description in terms of a single bending rigidity is an oversimplification. However, the quantification of the influence of different effects remains difficult.

References

[1] A. G. Zilman, R. Granek, Phys. Rev. Lett. 77, 4788 (1996)
[2] R. Granek, I. Hoffmann, E. G. Kelley, M. Nagao, P. M. Vlahovska, A. Zilman, Euro. Phys. J. E, 47, 12 (2024)

Session

Soft Condensed Matter

Primary author: HOFFMANN, Ingo (ILL)

Co-authors: KELLEY, Elizabeth (National Institute of Standards and Technology); Prof. GRANEK, Rony (Ben-Gurion University of The Negev); NAGAO, Michihiro (NIST / University of Maryland)

Presenter: HOFFMANN, Ingo (ILL)

Session Classification: Soft Condensed Matter

Contribution ID: **25** Type: **Poster**

NSE as a Tool for Understanding the Dynamics of Self-Organizing Water–Monoalcohol Mixtures Toward Green Solvent Design

Surfactant-free microemulsions (SFME) are an emerging class of self-organized ternary liquids that develop mesoscale structure without conventional surfactants. Understanding their phase behavior and dynamics is crucial for applications in drug delivery, extraction, and chemical engineering.

In ternary mixtures, SFME formation arises from a delicate interplay of molecular architecture, hydrotropic interactions, and collective nanoscale dynamics. Here, we combine Neutron Spin Echo (NSE) spectroscopy with complementary PFG-NMR measurements to probe these dynamics across three representative systems: octanol–ethanol–water, 2-ethylhexanol–ethanol–water, and ethyl acetate–sodium salicylate–water. Together, these methods link structural organization with diffusive dynamics across multiple timescales. NSE resolves the q-dependent evolution of diffusion, enabling us to identify transient species and quantify characteristic aggregation lifetimes and correlation lengths. This integrated approach provides a direct comparison of how linear versus branched alcohols and non-ionic versus ionic hydrotropes modulate nanoscale dynamics.

In a SFME system, NSE measurements capture the shift in dynamics as the system transitions from pre-Ouzo aggregates (oil-in-water) to reverse aggregates (water-in-oil), providing insights into the motion of individual species across q-scales. The incoherent signal reflects NMR-like behavior, while the coherent signal highlights collective dynamics associated with aggregate formation.

Overall, NSE combined with complementary techniques reveals how molecular architecture and intermolecular forces control diffusion, aggregation lifetimes, and the emergence or suppression of structure in SFME systems.

Session

Soft Condensed Matter

Primary authors: Mr MALAYIL KALATHIL, Firoz (PostDoc Researcher); HOFFMANN, Ingo (ILL); PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique)

Co-authors: ALBA-SIMIONESCO, Christiane (LLB); PREVOST, Sylvain (Institut Laue-Langevin); ZEMB, Thomas (CEA/ICSM)

Presenter: Mr MALAYIL KALATHIL, Firoz (PostDoc Researcher)

Session Classification: Soft Condensed Matter

Contribution ID: **26** Type: **Poster**

FANTASTIC, an indirect geometry TOF spectrometer designed for the ICONE neutron source

The ICONE project of a French HiCANS is aimed at delivering an instrument suite for the French scientific community at the 2035 horizon. ICONE will produce moderated neutrons in the energy range of < 200 meV, making them suitable for use on neutron scattering instruments. A major challenge is the design and optimisation of instruments to make full use of the ToF flux. To address this, digital twins of the instruments are developed using advanced simulation tools to support performance prediction, optimisation, and virtual experiments.
FANTASTIC is an indirect geometry ToF spectrometer, meaning that the incident beam is polychromatic and the energy discrimination is made by a set of analysers placed after the sample. A total of 30 analyzers is foreseen with tunable take-off angle to select a range of final wavelengths. This allows to access a large (ħω, Q) space. A detailed digital twin of FANTASTIC has been implemented in McStas to evaluate and optimise instrument performance. The calculated energy resolution (FWHM) is in the range of 0.15meV(elastic) and 1 meV at ΔE=20 meV. The elastic Q-resolution lies between 1-4%.
Dedicated data-reduction workflows have been developed to treat the large volumes of ToF event data produced by such instruments. These routines, based on tools such as SCIPP, process NeXus data to compute (ħω,Q)and support both powder and single-crystal measurements with UB-matrix handling.
FANTASTIC is designed to tackle a wide range of scientific challenges, from frustrated magnetism to lattice dynamics. The instrument performance has been benchmarked against measurements from IN8@ILL and simulations of BIFROST@ESS. We will present the instrument design, digital-twin methodology, guide optimisation, resolution characterisation, and benchmarking results.

Session

Instrumentation

Primary author: KARYOS, Kyriakos (CEA/LLB)

Co-author: Mr FABREGES, Xavier (CEA/LLB)

Presenter: KARYOS, Kyriakos (CEA/LLB)

Session Classification: Instrumentation

Contribution ID: **27** Type: **Poster**

Using applied magnetic fields to induce unconventional magnetic order in the frustrated quantum magnet, clinoatacamite, Cu2Cl(OH)3

The natural mineral clinoatacamite, [Cu2Cl(OH)3], exhibits low-temperature, frustrated magnetic behaviour where competing interactions are responsible for novel magnetic properties. Attempts to establish the magnetic phases in this material have been undertaken and an unconventional applied field (H||b) phase diagram has been revealed [1]. Two critical transition temperatures at zero field have been identified with long range antiferromagnetic (AFM) order for T1 < 6K, and paramagnetic behaviour for T2 >18K. In-field magnetisation data collected between 6-18K reveal three distinct phases for H||b which are not completely understood. Until now, the phase diagram of clinoatacamite has not been probed for H||a*or H//c*. We will present neutron scattering measurements of single crystal clinoatacamite in applied fields up to 10T. With these measurements we have mapped out the phase diagram of the antiferromagnetic structure for H||a*.

I will be conducting TOF experiments in future to determine accurate exchange interactions in this frustrated materaial.

Session

Magnetism

Primary authors: ALLEN, Jackson (University of Wollongong); AVTAROVSKI, Juliana (University of Wollongong); RULE, Kirrily (ANSTO); TOBIN, Siobhan (ANSTO)

Presenter: AVTAROVSKI, Juliana (University of Wollongong)

Session Classification: Magnetism

Contribution ID: **28** Type: **Invited**

Universal behavior of mesoscopic dynamics in molecular liquids: spectroscopy with polarized neutrons and MD-simulations

In spite of its fundamental interest, the dynamics –collective and self—of molecular liquids and glass-forming systems at the mesoscale is still poorly understood. Quasielastic neutron scattering (QENS) is the ideal technique to carry on this kind investigations in a wide Q-range (Q: momentum transfer) due to the high energy resolution available. The problem is that the measured intensity always contains a combination of coherent and incoherent contributions, which can be very relevant at the mesoscale. The development of spectroscopy methods by using polarized neutrons –that allow separating both neutron components— has fueled a new revival of this topic of utmost importance in the general field of liquids. By means of the recently implemented neutron polarization analysis on a wide time-of-flight spectrometer (LET @ ISIS) and also by using the wide-angle neutron spin echo spectrometer WASP at the ILL, we have been able to separate coherent and incoherent neutron scattering in different liquids with different molecular interaction [A. Arbe et al., Phys. Rev. Research 2, 022015(R) (2020); A. Arbe et al., Phys. Rev. Lett.134, 098001 (2025)]. Our results show that, independently of the intermolecular interactions, all liquids follow some kind of universal behavior at the mesoscale: (i) density-density fluctuations decay –apart from hydrodynamic-like modes—through a non-diffusive exponential process; (ii) the fingerprint of the local molecular motions involved in this process can be observed in the short time regime of the incoherent intermediate scattering function. These results were interpreted with the help of massive MD-simulations carried on in different systems. In this talk I will give an overview of the current status of these investigations.

Session

Presenter: Prof. COLMENERO, Juan (Centro de Física de Materiales (CSIC-UPV/EHU))

Session Classification: Liquids

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

Dynamics of Polymer Rings in Ring-Linear Blends combining Rheology and Neutron Spin Echo Spectroscopy

We have investigated the dynamics of polyethylene-oxide (PEO) ring/linear blends of various molecular weight ratios. Both the blend viscosity as well as the microscopic dynamics were studied. The blend viscosity displays a maximum at intermediate ring volume fractions. For symmetric blends the relative viscosity maximum increases with the molecular weight of the polymers, while for asymmetric blends the viscosity maximum gets stronger, if the linear constituent becomes smaller than the ring. Applying neutron spin echo (NSE) spectroscopy on samples containing a fraction of labelled rings, we essentially observed the internal ring dynamics and its modifications as function of ring volume fraction ϕ_R. We observe an increased enslavement of the ring dynamics with higher host Mw. While this holds for all hosts above 10K, linear chains exhibiting only five entanglements are not able to impress its dynamics on the rings. In symmetric ring linear blends increasing ring enslavement well correlates with the increase of the viscosity enhancement observed. For asymmetric blends increasing host Mw in all cases leads to stronger enslavement. The observed increase of the viscosity found for shorter hosts does not find any parallel in the microscopic dynamics. Blends. At ϕ_R=0.5 the spectral shapes are still local reptation type, however, the decrease of constraints compared to the neat linear melts is more pronounced for the shorter host. The results qualitatively agree with available simulations validating them.

Session

Soft Condensed Matter

Primary author: RICHTER, Dieter (Forschungszentrum Jülich)

Co-authors: Prof. VLASSOPOULOS, Dimitris (FORTH Heraklion); Dr HOFFMANN, Ingo (ILL Grenoble); Dr ALLGAIER, Jürgen (Forschungszentrum Jülich); PEPONAKI, Katerina (FORTH Heraklion); Dr KRUTEVA, Margarita (Forschungszentrum Jülich); Dr MONKENBUSCH, Michael (Forschungszentrum Jülich)

Presenter: RICHTER, Dieter (Forschungszentrum Jülich)

Session Classification: Soft Condensed Matter

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

Towards the development of polarization analysis with high energy resolution for SPHERES

Neutron polarization analysis provides profound additions of knowledge to the field of soft condensed matter research. The ability to separate the coherent and incoherent scattering contributions gives information on spatial correlations and collective motion, and information from single particles, respectively.
In this study, we focus on upgrading the SPHERES (SPectrometer for High Energy RESolution) backscattering instrument at JCNS [1,2] to meet the demands for high energy resolution and polarization analysis. Because of geometry constraints the polarization analyzer would need to be located between the sample and the Si111 analyzers. To meet this requirement, we investigate a transmission wide-angle supermirror polarization analyzer using Monte Carlo simulations [3]. We evaluate its performance in terms of transmission and polarization under realistic beam conditions and instrument geometry.
At this conference, we will present the resulting analyzer concept and discuss its implications for performing polarization analysis with the high-resolution capabilities of SPHERES.

[1] J.Wuttke, Rev. Sci. Instrum. 83, 075109 (2012)
[2] J.Wuttke, Rev. Sci. Instrum. 84, 115108 (2013)
[3] P. Böni, Nucl. Instrum. Methods Phys. Res. Sect. A 966, 163858 (2020)

Session

Instrumentation

Primary authors: BABCOCK, Earl (JCNS at the MLZ); ZAMPONI, Michaela (Forschungszentrum Juelich GmbH); HUANG, chuyi (Jülich Centre for Neutron Science)

Presenter: HUANG, chuyi (Jülich Centre for Neutron Science)

Session Classification: Instrumentation

Contribution ID: **33** Type: **Poster**

Non-Gaussian polymer dynamics on the scale of an entanglement strand

The research on Non-Gaussian (NG) dynamics in polymer melts has been largely focused on the decaging of polymer segments near the glass transition and was quantified in terms of the NG parameter. Recently, based on simulations, theoretical investigations led to quantitative determination of the NG parameter for the linear entangled polymers. We present a study on diffusion of short poly(ethylene oxide) (PEO) in a strongly entangled PEO melt1. Within the entanglement volume, the dynamics of the short PEO was found significantly Non-Gaussian. The COM MSD are sub-diffusive at short times until they have reached the size of the reptation tube d. Then, a crossover to Fickian diffusion takes place indicating cooperative chain motion within the entanglement volume d3. Thus, the host dynamics within the tube is not only cooperative but also significantly Non-Gaussian.

Quantitative comparison of the dynamic structure factors from unentangled and strongly entangled melts was performed for the poly(butylene oxide) (PBO)2. The spectra from entangled PBO can be very well described by the dynamic structure factor based on the concept of local reptation, including the Rouse dynamics within the tube and allowing for NG corrections. Comparing quantitatively the spectra from both polymers leads to the surprising result that their spectra differ only by the contribution of classical Rouse diffusion for the low molecular weight melt. The sub diffusive component is common for both the low and high molecular weight PBO melts, indicating that in both melts the same interchain potential is active, thereby supporting the validity of the Generalized Langevin Equation approach.

1. M. Kruteva et al. Macromolecules, 54(24), 11384 (2021)
2. M. Kruteva et al. ACS Macro Letters, 13(3), 335 (2024)

Session

Primary author: KRUTEVA, Margarita (Forschungszentrum Jülich)

Co-authors: RICHTER, Dieter (Forschungszentrum Jülich); HOFFMANN, Ingo (ILL Grenoble); ALLGAIER, Jürgen (JCNS); MONKENBUSCH, Michael (Forschungszentrum Jülich); ZAMPONI, Michaela (Forschungszentrum Juelich GmbH)

Presenter: KRUTEVA, Margarita (Forschungszentrum Jülich)

Session Classification: Soft Condensed Matter

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

The Role and Dynamics of Interstitial Water and Sodium in Hydrated Manganese Iron Prussian Blue Analogs: A Synergistic Study Combining NPD, QENS, and MLIP-MD

Manganese-iron Prussian blue analogs (MnFePBA) are promising cathode materials for sodium-ion batteries due to their high energy density, low cost, and facile synthesis. While most studies advocate dehydration to enhance cycling stability, recent findings suggest that hydration stabilizes a monoclinic phase with superior sodium diffusivity and greater capacity retention than the dehydrated rhombohedral phase.

However, the structure and reaction mechanisms of hydrated MnFePBA remain contested. Though the monoclinic unit cell is established, contradictions persist between computational predictions—placing interstitial water at body-center and sodium at face-center—and experimental observations from X-ray diffraction (XRD) and neutron powder diffraction (NPD). These discrepancies arise from the similar electron densities of oxygen and sodium in XRD analysis, while the inherent mobility of both species complicates site occupancy refinement even with NPD's superior scattering contrast.

We combine NPD, quasi-elastic neutron scattering (QENS), and machine learning interatomic potential molecular dynamics (MLIP-MD) to resolve these ambiguities. NPD on D_2O- and H_2O-hydrated samples confirms water at body-center sites and sodium at face-center sites. QENS experiments at IN16b and SHARPER (ILL) characterize sodium and water diffusion on nanosecond and picosecond timescales, respectively. Comparing dehydrated and hydrated samples, we extract sodium diffusivity and activation energy.

MLIP-MD simulations agree with experimental findings and reveal that the hydrated monoclinic structure enables significantly faster sodium diffusivity (10^{-12} m^2/s) than the dehydrated rhombohedral structure (10^{-18} m^2/s at 300 K), while elucidating distinct diffusion pathways for each species.

Session

Hard Condensed Matter

Primary author: YANG, YuanChi (CEA-Liten, CEA-Irig, UGA)

Co-authors: Ms PINEAU, Léna (CEA-Liten); Dr PERALTA, David (CEA-Liten); SUARD, Emmanuelle (Institut Laue Langevin); Dr MARKER, Katharina (CNRS SyMMES); Dr SIMONIN, Loïc (CEA-Liten); APPEL, markus (ILL); BERROD, Quentin (CNRS SyMMES); Dr LYONNARD, Sandrine (CNRS SyMMES); Dr VAN ROEKEGHEM, Ambroise (CEA-Liten); Dr JACQUET, Quentin (CNRS SyMMES)

Presenter: YANG, YuanChi (CEA-Liten, CEA-Irig, UGA)

Session Classification: Hard Condensed Matter

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

Atomic dynamics studied with INS, QENS and large-scale atomistic simulations

Neutron scattering is an ideal probe of the atomic structure and dynamics in solids, from fast ionic diffusion in solid-state electrolytes to lattice dynamics and thermal transport in thermoelectrics, or structural distortions in metal-halide perovskites. Many of these phenomena bridge the time-scales probed by quasielastic and inelastic neutron scattering (QENS/INS). This presentation will illustrate the complementarity of QENS -both coherent and incoherent- and INS, as well as opportunities to leverage machine learning and large-scale atomistic simulations. Examples will focus on fast ion diffusion in superionic conductors [1-5] and dynamic structural fluctuations in metal-halide perovskites [6-8]. We investigated a series of halide and sulfide fast Na+/Li+ ion conductors, using a combination of coherent/incoherent QENS, INS, ab-initio molecular dynamics (AIMD), and machine-learning molecular dynamics (MLMD). In several instances, we find that soft anharmonic phonon modes play an important role in facilitating ionic hops, reflecting the softness in the potential energy surface. Further, the different coherent/incoherent components of QENS, supplemented with large-scale MLMD simulations, provide detailed insights into the diffusion process.

[1] J. L. Niedziela, et al., Nature Physics 15, 73–78 (2019)
[2] M. K. Gupta, et al., Energy and Environmental Science 14, 6554-6563 (2021)
[3] M.K. Gupta et al., Advanced Energy Materials 12, 2200596 (2022)
[4] Q. Ren et al., Nature Materials 22, 999–1006 (2023)
[5] J. Ding et al., Nature Physics 21, 118–125 (2025).
[6] T. Lanigan-Atkins et al, Nature Materials 20, 977–983 (2021)
[7] X. He et al, PRX Energy 3, 013014 (2024).
[8] C. Mao et al. Physical Review Materials, 9, 065401 (2025).

Session

Hard Condensed Matter

Primary author: DELAIRE, Olivier (Duke University)

Presenter: DELAIRE, Olivier (Duke University)

Session Classification: Hard Condensed Matter

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

Self and collective dynamics in a highly crosslinked polybutadiene rubber

In recent years, a great effort has been put to investigate collective relaxations in liquids [1] and polymer systems [2] at mesoscopic scales. This has been experimentally achieved using neutron scattering methods, especially in combination with polarization analysis (PA) capabilities [3] allowing to disentangle incoherent and coherent contributions, or with computational methods [4]. Few neutron spectrometers currently allow PA, and the method has also limitations due to reduced neutron flux. Here we present the results of the investigation of a crosslinked rubber of deuterated 1,2-polybutadiene (d1,2-PB), where we use an alternative approach and combine different neutron spectrometers to separate self and collective dynamics [5]. In the neat polymer melt the collective segmental relaxation around the structure factor peak *S(Qmax)* shows de Gennes narrowing, with a collective relaxation time *τc(Q)* that increases without plateauing towards lower *Q*s. In the crosslinked d1,2-PB rubber, the peak at *S(Qmax)* is reduced and instead a strong low-*Q* peak emerges. Both the collective d1,2-PB relaxation rates around the former *S(Qmax)* and the relaxation around the new crosslink correlation peak are significantly slowed down compared to the melt. Finally, the cross-linking strands exhibit their own fast dynamics, which is well described by diffusion within a spherical Gaussian well.

Session

Soft Condensed Matter

Primary authors: ROSI, Benedetta (European Spallation Source); KRUTEVA, Margarita (Forschungszentrum Jülich); MONKENBUSCH, Michael (Forschungszentrum Jülich); ALLGAIER, Jürgen (Forschungszentrum Jülich); FALUS, Peter (ILL); OLLIVIER, Jacques (ILL); R. DE SOUSA, Nicolas (ANSTO); RICHTER, Dieter (Forschungszentrum Jülich)

Presenter: ROSI, Benedetta (European Spallation Source)

Session Classification: Soft Condensed Matter

Contribution ID: **39** Type: **Poster**

Using QENS to Probe the Dynamics of the Tau Protein under Liquid-Liquid Phase Separation

Tau is an intrinsically disordered protein (IDP) expressed in neurons. In contrary to well-folded proteins, IDPs lack a distinct stable 3D structure and sample a vast conformational space instead. Tau's biological function lays in its interaction with the microtubules. In patients with Alzheimer's disease, however, it is found to be part of protein filaments in the brain.
Solutions of tau can spontaneously demix into a dense phase (enriched in protein) and a light phase(depleted in protein) in a process called liquid-liquid phase separation (LLPS). In the presence of LLPS, tau has been found to aggregate more easily [1]. To understand diseases such as Alzheimer's disease on a molecular level, it might be important to shed light on the protein dynamics during LLPS and aggregation. Previously, we studied the dynamics of tau and its hydration water in monomers and fibers [2]. Here, we extend our efforts to elucidating tau dynamics under LLPS by quasi-elastic neutron scattering (QENS). The measured QENS signal represents the superimposed contributions of the protein center-of-mass translational diffusion, of the protein tumbling, of internal protein fluctuations on the level of the protein backbone and side chains, and of the solvent [3].
We will discuss results from a first experiment at the back-scattering spectrometer IN16B at the Institut Laue Langevin (ILL), in which we compared two tau solution (80 mg/mL), namely a homogeneous solution and a solution that underwent LLPS. Initial QENS data analysis indicates tau under LLPS is less mobile.

[1] Lin Y., et al., ACS Chem. Neurosci., 11, 615-627 (2020)
[2] Fichou Y., et al. Proc. Natl. Acad. Sci. U.S.A., 112, 6365-6370 (2015)
[3] Grimaldo M., et al. Quart. Rev. Biophys., 52, e7 (2019)

Session

Biology/Health

Primary author: SOMBRUTZKI, Finn (IBS and ILL Grenoble)

Co-authors: Dr SCHIRÒ, Giorgio (Insitut de Biologie Structurale); WEIK, Martin; SEYDEL, Tilo; Dr FICHOU, Yann (IECB / CBMN / Univ. Bordeaux)

Presenter: SOMBRUTZKI, Finn (IBS and ILL Grenoble)

Session Classification: Biology/Health

Contribution ID: **40** Type: **Poster**

Time-resolved QENS to investigate kinetically evolving samples

Neutron spectroscopy offers a unique access to diffusive properties of molecules on the nanosecond time scale. Next to structural properties, diffusive properties are also relevant for molecular interactions. In recent years, the interest in the investigation of kinetically evolving samples has been continuously increasing. While for other neutron scattering techniques, time-resolved measurements have been already well established in the past [1.], new technical and methodical developments permit now only recently to access kinetic measurements with a minute resolution in neutron spectroscopy [2.,3.].
Time-resolved quasi-elastic neutron spectroscopy (TR-QENS) can be used to investigate the diffusive properties during the kinetic transitions of the samples. In this contribution, we summarize our latest works to TR-QENS investigating samples during changes of control parameters such as temperature [4.] and time-dependencies after chemical changes in the samples including phase transitions from homogenous solutions towards protein crystals [5.,6.]. Next to the insights obtained for the individual samples investigated, the developed methods will provide new frameworks for future kinetic TR-QENS studies.

[1.] doi: 10.1016/bs.mie.2022.08.010
[2.] doi: 10.1016/j.nima.2011.11.090
[3.] doi: 10.1107/S1600576724003820
[4.] doi: 10.1021/acscentsci.2c01078
[5.] doi: 10.1107/S160057672500353X
[6.] doi: 10.1021/acs.cgd.9b00858

Session

Soft Condensed Matter

Primary authors: BECK, Christian (ESS DMSC); MOSCA, Ilaria (Institut Laue-Langevin); MATEO MIÑARRO, Laura; SEYDEL, Tilo; ROOSEN-RUNGE, Felix (Division of Physical Chemistry, Lund University); SCHREIBER, Frank (Universität Tübingen)

Presenter: BECK, Christian (ESS DMSC)

Session Classification: Soft Condensed Matter

Contribution ID: **41** Type: **Poster**

Integrated Computational Workflows for the MIRACLES Backscattering Spectrometer at ESS

Among the instrument suite which is currently constructed at the European Spallation Source (ESS), the time-of-flight backscattering spectrometer Miracles 1 will provide the highest energy resolution permitting diverse studies of molecular dynamics.
This poster contribution is focusing on the computational aspects of the spectrometer.
To support efficient and reproducible research, MIRACLES integrates a robust computational pipeline covering both the data reduction and scientific analysis.
Following data collection, mimicked by McStas simulations 2 of the instrument, Scipp 3 enables flexible, performant reduction of event-based neutron data, leveraging Python workflows tailored to MIRACLES' needs. The workflow further supports advanced analysis via the easy science software package 4.
By combining simulation, reduction, and analysis, the MIRACLES computational environment fosters rapid, transparent scientific insight and user engagement. We present an overview of these tools, illustrate typical workflows, and show how computational integration at ESS accelerates both instrument development and experimental science.

1 Félix J. Villacorta et al, Rev. Sci. Instrum. 96, 045101 (2025)

2 P. Willendrup, and K. Lefmann, Journal of Neutron Research, vol. 23, 2021

3 Simon Heybrock, et al, Scipp, doi.org/10.5281/zenodo.17513273

4 https://app.easyscience.software/

Session

Instrumentation

Primary authors: BECK, Christian (ESS DMSC); Mr JACOBSEN, Henrik (ESS DMSC); ROSI, Benedetta (European Spallation Source); VILLACORTA, Félix (ESS Bilbao); Dr ROD, Thomas

Presenter: BECK, Christian (ESS DMSC)

Session Classification: Instrumentation

Contribution ID: **42** Type: **Oral**

Atom-scale dynamics in germanium-based hybrid metal halide perovskites

Metal halide perovskites (MHPs) are currently receiving great attention because of their photophysical properties and concomitant promise for use in both solar cells and light emitting diodes, however, fundamental properties surrounding the atomic-scale dynamics remain unclear for these materials. In this contribution, we report on results from inelastic and quasielastic neutron scattering (INS and QENS) studies of the dynamics in the Ge-based hybrid MHPs MASn1-xGexI3, (x = 0, 0.25, 0.5, 0.75, 1; MA = methylammonium) and FAGeX3 (FA = formamidinium; X = I, Br). Of specific interest here, the Ge ions exhibit a polar off-centering distortion and it is of great interest to understand how this affects the materials' dynamical and photophysical properties.

For MASn1-xGexI3, the results show two modes of MA reorientations, with different geometry and time-scale, and that the pace of reorientations increases with increasing Sn concentration. The vibrational frequencies trend in the opposite direction and are related to the space group rather than directly to the Sn concentration, highlighting the importance of the structure. For FAGeX3, several vibrational modes related to the inorganic framework at 20 meV and below of FAGeI3 are blue-shifted compared to FAGeBr3, while several modes above the phonon gap at 65 meV and above are red-shifted, indicating that the type of halide ion influences the external (librational) and internal (vibrational) modes of the organic cation differently. Given the strong correlation between dynamics and electronic and optical properties of hybrid MHPs, such as charge carrier dynamics and photoluminescence etc., this new insight is important for the rational design of hybrid MHPs with specific functions.

Session

Materials Science

Primary authors: Prof. KARLSSON, Maths (Chalmers University of Technology); OJSTEDT, Oskar (Chalmers University of Technology); Dr LAVÉN, Rasmus (Chalmers University of Technology)

Presenter: OJSTEDT, Oskar (Chalmers University of Technology)

Session Classification: Materials Science

Contribution ID: **43** Type: **Oral**

Correlating QENS with Rheology in Polymer Nanocomposites

Polymer Nanocomposites (PNC) can enhance the mechanical properties over the host polymer. Greater understanding of their microstructure and dynamics is needed to effectively design PNC with improved characteristics. A model system of well-dispersed elongated silica nanoparticles in strongly adsorbed poly(ethylene oxide) is used to investigate the shape effects of nanoparticles with comparison to literature data for other silica particle systems. Quasi-elastic neutron scattering is used to obtain information about the polymer at the interface between the nanoparticles and bulk polymer. Interfacial polymer Rouse dynamics and the extent of the interface is obtained from two possible modifications of the Rouse model for the interface. The first of these suppresses longer range Rouse modes to account for additional topological constraint imposed by adsorption to the nanoparticle. The second of these modifications treats the interface as experiencing the same type of Rouse dynamics as the bulk, but on a longer timescale, indicated a higher relaxation time. These results are connected to rheology to explain the large effect of a small amount of nanoparticles commonly observed in PNC.

Session

Soft Condensed Matter

Primary authors: ROOKS, Jack (University of Delaware); Prof. FRATINI, Emiliano (University of Florence); Dr FERRARO, Giovanni (University of Florence); Dr OSTI, Naresh (Oak Ridge National Laboratory); Dr TAKAHITO, Osawa (Japan Atomic Energy Agency); FARAONE, Antonio (NIST Center for Neutron Research); Prof. WAGNER, Norman (University of Delaware)

Presenter: ROOKS, Jack (University of Delaware)

Session Classification: Soft Condensed Matter

Contribution ID: **44** Type: **Poster**

Neutron Scattering Opportunities in Hierarchical Graphene–Zeolite Hybrid Materials for Dye Adsorption

Hierarchical graphene–zeolite hybrid materials (MZN–GO and MGN) combine ~5 nm mesopores, sub-1.5 nm micropores, and heterogeneous carbon–zeolite interfaces containing –OH/–COOH groups, mixed sp^2/sp^3 domains, and defect-induced radical sites. These structural motifs strongly influence how confined water and organic dyes—here represented by Rhodamine 6G (R6G)—are adsorbed, organized, and transported within the pore network. Our preliminary BET, electron microscopy, and Raman/SERS studies reveal distinct confinement effects and interfacial interactions that cannot be captured by X-ray or optical probes alone.

Although neutron experiments have not yet been undertaken, this system offers compelling opportunities for QENS and contrast-matched SANS. Neutrons could directly resolve confined-water mobility, hydrogen-related dynamics, dye aggregation states, and pore-filling behavior—key parameters for understanding adsorption efficiency and guiding rational materials design.

We are actively seeking neutron-scattering collaborators interested in advancing the structure–dynamics relationships governing pollutant uptake in hybrid porous materials. Our team will provide well-defined materials and comprehensive physicochemical characterization. We welcome joint efforts to develop future neutron proposals that leverage the complementary sensitivities of QENS and SANS to advance materials science in confined environments.

Session

Materials Science

Primary authors: Ms KALYAN, Poonam (National Taiwan Normal University); LIU, Yi-Hsin (Natinal Taiwan Normal University); Prof. YEH, Yi-Chun (National Taiwan Normal University)

Presenters: Ms KALYAN, Poonam (National Taiwan Normal University); LIU, Yi-Hsin (Natinal Taiwan Normal University)

Session Classification: Materials Science

Contribution ID: **45** Type: **Poster**

Phonon–Lattice Coupling in Mn-Doped II–VI Nanostructures: A Neutron-Ready Platform

Mn-doped II–VI nanostructures provide a clean playground to study how lattice vibrations reshape electronic and spin states. In our recent work on 0D Mn-doped $(CdSe)_{13}$ clusters and 2D Mn-doped $CdSe(en)_{0.5}$ nanosheets, we observe giant magnetic moments and room-temperature giant Zeeman splitting, accompanied by strain-sensitive LO phonons and strong magneto-optical responses. Microstrain domains, ligand-induced distortions, and symmetry breaking in these crystals suggest that specific phonon modes modulate Mn^{2+} zero-field splitting and sp–d exchange, opening phonon-assisted spin-flip channels.

So far our picture comes from Raman, PL, EPR, and X-ray probes, which are effectively limited to $Q \approx 0$. The next step is to resolve how these strain-engineered phonons evolve across momentum and length scales using neutron spectroscopy (INS, NSE) and total scattering/PDF. We will outline our materials platform, key phonon signatures, and open questions on spin–phonon coupling, and we are actively seeking collaborators with neutron-scattering expertise to design and execute joint experiments on these nanostructures at large-scale facilities.

Session

Materials Science

Primary authors: Dr NARAYANAM, Nagaraju (Natinal Taiwan Normal University); LIU, Yi-Hsin (Natinal Taiwan Normal University)

Presenters: Dr NARAYANAM, Nagaraju (Natinal Taiwan Normal University); LIU, Yi-Hsin (Natinal Taiwan Normal University)

Session Classification: Materials Science

Contribution ID: **46** Type: **Oral**

Cooperative tracer chain dynamics in highly entangled polymer melts

The dynamics of short unentangled tracer chains in the melt of a highly entangled polymer matrix has been investigated using neutron spin echo spectroscopy [Zamponi et al., Phys. Rev. Lett. 126, 187801 (2021)]. Irrespective of the tracer chain length, the center of mass mean square displacement is subdiffusive at short times and crosses over to Fickian diffusion at longer times. The diffusion coefficients obtained on the molecular length scale are in very good agreement with results from macroscopic methods, but the dependence on the tracer chain length strongly deviates from the Rouse expectation. For all the different tracers, the cross-over to normal diffusion always occurs at the same mean square displacement, which corresponds to the tube diameter of the entangled host. This observation cannot be understood within the standard reptation model, where within the entanglement volume simple Rouse motion is assumed, but might be explained by cooperative chain motions, where the tracer chains move cooperatively with the host chains to an extent limited by the tube size.

Session

Soft Condensed Matter

Primary authors: ZAMPONI, Michaela (Forschungszentrum Jülich); KRUTEVA, Margarita (Forschungszentrum Jülich); MONKENBUSCH, Michael (Forschungszentrum Jülich); WILLNER, Lutz (Forschungszentrum Jülich); WISCHNEWSKI, Andreas (Forschungszentrum Jülich); HOFFMANN, Ingo (ILL); RICHTER, Dieter (Forschungszentrum Jülich)

Presenter: ZAMPONI, Michaela (Forschungszentrum Jülich)

Session Classification: Soft Condensed Matter

Contribution ID: **47** Type: **Oral**

Theory of Spin Seebeck effect and low-lying crystal field excitations in a Rare-Earth Iron Garnet

The spin Seebeck effect (SSE) is a phenomenon of thermoelectric generation that occurs within a device con- sisting of a bilayer of a metal and a ferromagnet. When Tb3Fe5O12(TbIG) is substituted for the ferromagnet, the effect was observed to go to zero at low temperatures, but increases to positive values with the application of a magnetic field. This is opposite to the expectation that the SSE should be suppressed by a magnetic field due to the increase in the magnon gap. We have provided a theory of this by calculating the low energy excitations, exploiting the parameters of Terbium Gallium Garnet Tb3Ga5O12(TGG) from the neutron-scattering studies and the close structural similarity between TGG and TIG. We show that when an external magnetic field is applied along the [111] direction of the crystal, the lowest Crystal Field level decreases with applied field and can carry a spin current. At low temperatures - defined by the energy of the CFE of a few mEV - this can result in an enhanced Spin Seebeck effect under applied magnetic field. While the experimental situation for low-lying magnetic excitations in TbIG is still not resolved, this makes a promising connection between the observation of low energy magnetic excitations and a low-temperature phenomenon of interest in spintronics.
This is theoretical work in collaboration with Bruno Tomasello (U. Catania) and Michiyasu Mori (JAEA, Tokai). It is closely related to more general studies with Stephan Gepraegs (Walter Meissner Institut, München), Danny Mannix (ESS, Lund) and Jack Thomas-Hunt (Aarhus)

Session

Hard Condensed Matter

Primary author: ZIMAN, Timothy (Institut Laue Langevin)

Presenter: ZIMAN, Timothy (Institut Laue Langevin)

Session Classification: Hard Condensed Matter

Contribution ID: **48** Type: **Poster**

Exploiting polarised neutron and ultrafast X-ray pump-probe synergies to reveal the spin and heat dynamics in spin caloritronics

Spin caloritronics are currently a science highight due to their potential exploitation in the next generation of spintronics applications. A prominent example are devices exploiting the spin Seebeck effect (SSE), where thermoelectric generation is achieved by a thermally induced spin-current, which is then converted into an electric charge current by the inverse spin Hall effect within the HM layer. At low temperatures the generation of a net spin current in the MI can be understood in terms of thermal excitation of chiral magnons 1. Therefore, the development of emerging technologies based on spin caloritronic physics, requires a high resolution microscopic understanding of their magnetic and heat dynamics. We present new insights into the dynamics of spin caloritronic materials, by exploiting the synergies of polarised neutron inelastic scattering at IN20 of the ILL and ultrafast X-ray pump-probe techniques using the LCLS XFEL. These studies were applied to prototype spin caloritronic materials, based on the rare-earth iron garnets of Tb3Fe5O12 and Gd3Fe5O12 (TbIG and GdIG). Polarised neutron inelastic scattering studies of single crystal TbIG can be correlated with the low energy chiral magnon modes responsible for the SSE in this material. In addition, our theoretical calculations highlight the Femtosecond X-ray pump-probe techniques were used to study the thermal 3 and magnetic dynamics induced in GdIG thin epitaxial films, using resonant X-ray magnetic scattering techniques. These results open new routes to investigate acoustic wave induced magnetic excitations with photon energy resolution beyond the current limits of RIXS.

Session

Magnetism

Primary author: MANNIX, Dan

Presenter: MANNIX, Dan

Session Classification: Magnetism

Contribution ID: **49** Type: **Poster**

Quasielastic neutron scattering study of clathrate hydrate formation from mixed gas fluxes (CH_4, H_2, C_2H_6) in nanoporous media.

Gas hydrates are crystalline solids formed by a three-dimensional network of cages formed by water molecules that are capable of trapping gas molecules inside. These compounds form when water and gases such as methane interact under low-temperature, high-pressure conditions. Current research increasingly focuses on synthesizing gas hydrates under milder conditions to develop them as gas storage systems, an approach particularly attractive for hydrogen. Promising strategies include forming hydrates inside nanoporous materials, where nanoconfinement effects can facilitate crystallization, or creating mixed methane/hydrogen hydrates, using methane as a seed to store hydrogen at pressures far lower than those required for pure hydrogen hydrates.

To advance these technologies, it is essential to understand how gas hydrates form and how guest molecules behave inside their cavities. Quasielastic neutron scattering is well suited for this, as can probe molecular motions on the picosecond to nanosecond scale. This makes it possible to follow the evolution of gas molecules from the initial mobile stages of nucleation to the regime where they become localized and behave as free rotors at low temperatures.
In this work, gas hydrate formation was monitored inside a high surface area activated carbon using pure methane and two gas mixtures: methane–hydrogen (80%/20%) at 50 bar, and methane–hydrogen–ethane (5 bar of ethane plus 50 bar of the previous mixture). The aim was to study the dynamics of methane and ethane during hydrate formation and to assess whether hydrogen can be incorporated into methane or methane–ethane hydrates. The entire process was followed using quasielastic neutron scattering on the IN5 spectrometer at the Institut Laue-Langevin.

Session

Materials Science

Primary authors: Dr CZAKKEL, Orsolya (Institute Laue Langevin); Mr RAMÍREZ CEREZO, Víctor (Institute Laue Langevin/ University of Alicante)

Presenter: Mr RAMÍREZ CEREZO, Víctor (Institute Laue Langevin/ University of Alicante)

Contribution ID: **50** Type: **Oral**

Magnetic studies in a rare earth Kitaev candidate

We use IN5 and WASP to characterize the magnetic ground state of single crystal SmI_3, a 2D honeycomb magnet proposed as a possible f-electron Kitaev system. The ground state is established as a ferromagnetic correlated quantum spin liquid, however, both of these experiments identify low energy scattering at positions away from the zone center. Our work demonstrates the applicability of combining techniques from these complimentary instruments as a crucial step in measuring the spin liquid continuum scattering in a low-moment system.

Session

Magnetism

Primary authors: TAM, David (Institut Laue-Langevin); FJELLVAG, Oystein (institute for Energy Technology)

Presenter: TAM, David (Institut Laue-Langevin)

Session Classification: Magnetism

Contribution ID: **51** Type: **Oral**

Spinon continuum of a triangular lattice ising candidate

Rare-earth trihalides are attracting attention in the field of quantum matter for their potential to exhibit exotic ground states arising from interactions among magnetic moments, including competing interactions or geometrical frustration. While the late rare-earth halides adopt a honeycomb structure, the early rare-earth trihalides adopt a 3D UCl3-type structure, with ABAB stacked triangular lattices and a short cation distance along the [001] direction. We have investigated a cerium trihalide that behaves as a 1D Ising magnet with antiferromagnetic interactions along the chains. Neutron spectroscopy is a crucial tool for investigating magnetic excitations, and we investigate the spinon continuum of the 1D magnet.

Session

Magnetism

Primary author: FJELLVAG, Oystein (institute for Energy Technology)

Co-author: TAM, David (Institut Laue-Langevin)

Presenter: FJELLVAG, Oystein (institute for Energy Technology)

Session Classification: Magnetism

Contribution ID: **52** Type: **Invited**

Enhanced dynamics in disordered non-Kramers spin ice Ho2(Ti1−x-Hfx)2O7

The Ho2Ti2O7 compound is a frustrated magnet that does not stabilize an ordered ground state down to the lowest reachable temperature, but instead, enters a correlated but disordered phase called spin ice below about 2K. The excitations out of the spin ice state, described as emergent magnetic monopoles, exhibit extremely slow dynamics at low temperature.
In spin ices such as Ho2Ti2O7, where the magnetic element is a non-Kramers ion (integer J), the crystal electric field (CEF) ground state is a non-protected doublet. It has been proposed that in that case, quantum fluctuations induced by non-magnetic disorder can push the system toward a Quantum Spin Liquid phase (QSL). This phase is characterized, inter alia, by much faster dynamics.
To investigate this potential new QSL phase we have introduced non-magnetic disorder in Ho2Ti2O7, through a controlled substitution of Ti4+ ions by Hf4+ ions, with substitution rates from 0 to 40%.
X-ray and neutron diffraction measurements confirm that the crystal structure and the spin ice correlations are preserved up to at least 30% of substitution but a broadening of the crystal electric field levels is observed in inelastic neutron scattering measurements, as expected in the presence of local disorder.
To probe the dynamics, we have performed AC susceptibility and neutron spin echo (NSE) experiments down to 50 mK, which allows us to explore more than ten decades of time. These measurements reveal that the dynamics in the substituted compounds is accelerated by several orders of magnitude in the spin ice regime and up to 30 K, where quantum tunneling effects are relevant. This strongly suggests that disorder enables quantum fluctuations in the system and opens the way to the stabilization of a QSL phase at lower temperature.

Session

Hard Condensed Matter

Primary authors: LHOTEL, Elsa (Institut Néel CNRS); BUJAULT, Nathan (Institut Neel, CNRS & Univ. Grenoble Alpes)

Co-authors: SIBILLE, Romain (Paul Scherrer Institut); Dr PORÉE, Victor (SOLEIL)

Presenter: LHOTEL, Elsa (Institut Néel CNRS)

Session Classification: Hard Condensed Matter

Contribution ID: **53** Type: **Poster**

GERSEMI – Gaining Enhanced Resolution with Spin Echo for Multiscale Investigations. A high resolution Neutron Spin Echo instrument for the ESS

Neutron spin echo (NSE) spectroscopy is an essential quasi-elastic neutron scattering (QENS) method to probe dynamics in condensed matter. It gains access to a region of time and length scales which is complementary to other QENS techniques and high-resolution methods (e.g. PFG-NMR, photon correlation spectroscopy), and allows to cover unique science cases in various fields, including protein domain motions and biomembrane fluctuations, polymer chain dynamics, magnetic relaxations, and many more.

Here we present the conceptual design of GERSEMI, a high-resolution NSE spectrometer for the European Spallation Source (ESS). The instrument design suitably exploits the long and strong pulse of ESS and feature unique characteristics including: strong flux at long wavelengths, allowing to reach high resolution even on weakly-scattering samples; flexibility induced by the time-of-flight structure, including the possibility to access a wide Q-range with tunable resolution dQ/Q; broad and intense band of simultaneously available wavelengths, boosting capabilities which are currently prevented or limited on other NSE instruments (e.g. kinetic measurements, surface and interface dynamics, and more).

Along with the conceptual idea, we will present diversified scientific cases from a wide community, which will demonstrate the strong benefit from the realization of GERSEMI at ESS.

Session

Instrumentation

Primary authors: NOFERINI, Daria (ESS); ROOSEN-RUNGE, Felix (Division of Physical Chemistry, Lund University); HOFFMANN, Ingo (ILL); BERTELSEN, Mads (ESS); ROSI, Benedetta (European Spallation Source)

Presenter: NOFERINI, Daria (ESS)

Session Classification: Instrumentation

Contribution ID: **54** Type: **Oral**

High-pressure QENS: identifying plastic phases in planetary ices

Simple molecular systems such as hydrogen, water, ammonia, and methane are the main constituents of the Ice and Gas Giants (Uranus and Neptune), many icy moons, and numerous Neptune-like exoplanets. Space missions have also revealed dissolved salts (e.g., NaCl, KCl) in several icy-moon plumes. Although chemically simple, these systems display rich and sometimes unexpected physical behavior under extreme conditions. Water is especially intriguing due to its anomalous properties, largely driven by its ability to form strong directional hydrogen bonds. In liquid water these bonds form and break on picosecond timescales, coupling translational, rotational, and vibrational motions. Understanding its fast dynamics is key to describing intermolecular interactions. Changing H-bond strength — by adding ammonia, salts, or other bonding species — significantly modifies water's behavior. High pressure compresses molecular environments, accessing regions of the interaction potentials otherwise unreachable, while high temperature alters H-bond lifetimes and can induce exotic diffusive regimes. In this talk, I show how high-pressure quasi-elastic neutron scattering (HP-QENS) is a unique tool to directly observe the plastic phases of planetary-relevant ices. These mesophases retain crystalline order while allowing rapid molecular rotation. I will summarize results for Ice VII 1, ammonia hydrates at different compositions (AMM 2, AHH 3), and LiCl hydrates 4.

1 Rescigno et al., Nature (2025), DOI:10.1038/s41586-025-08750-4

2 Zhang et al., JPC Lett. (2023), DOI:10.1021/acs.jpclett.3c00092

3 Ninet et al., ILL (2023), https://doi.ill.fr/10.5291/ILL-DATA.7-02-215

4 Nicholls et al., ILL (2025), https://doi.ill.fr/10.5291/ILL-DATA.7-04-202

Session

Hard Condensed Matter

Primary author: RESCIGNO, Maria

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Presenter: RESCIGNO, Maria

Session Classification: Hard Condensed Matter

Contribution ID: **55** Type: **Poster**

Bayesian Inference for Neutron Spin Echo Measurement

Neutron spin echo (NSE) spectroscopy offers detailed access to microscopic dynamics but is limited by low flux, long acquisition times, and substantial noise. We introduce a Bayesian inference framework based on Gaussian Process Regression (GPR) that reconstructs high-quality spin-echo signals from sparse, noisy, and irregularly sampled measurements by leveraging correlations in reciprocal space. Tests on synthetic data and experimental dendrimer NSE results demonstrate that GPR effectively suppresses noise, fills in missing intensities, and improves overall accuracy, enabling shorter acquisitions and supporting high-throughput or real-time experiments. The approach generalizes to other scattering techniques with low signal-to-noise ratios, expanding the capabilities of neutron spectroscopy more broadly.

Session

Instrumentation

Primary author: TUNG, Chi-Huan (Oak Ridge National Laboratory)

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Presenter: TUNG, Chi-Huan (Oak Ridge National Laboratory)

Session Classification: Instrumentation

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

KVASIR: A backscattering neutron spectrometer for hard condensed matter at ESS

We present the instrument concept for KVASIR, a backscattering indirect time-of-flight neutron spectrometer for the European Spallation Source (ESS). KVASIR will probe low lying excitations in single crystals of hard condensed matter. The instrument follows the FARO/SHERPA concept, using mosaic prismatic PG analyzer crystals. KVASIR is simultaneously optimized for high resolution of energy- and momentum transfer, δE = 4 μeV and $\delta\mathbf{q}$ = 0.03 \AA^{-1} (FWHM), respectively. Detailed ray tracing simulations, considering the true geometry and aberrations of the analyser configuration, achieve δE = 5.7 μeV and $\delta\mathbf{q}$ = 0.03 \AA^{-1}. The proposed concept has room for both polarisation analysis and extreme sample environments. With this instrument, we can enable inelastic neutron scattering studies of single crystal hard condensed matter, with a particular focus on quantum properties, at yet unseen spatial and dynamic precision under extreme conditions.

Session

Instrumentation

Primary authors: DAVIDSEN, Amalie (Nanoscience Center, Niels Bohr Institute, University of Copenhagen, Denmark); KRIGHAAR, Kristine (Niels Bohr Institute); PETIT, Sylvain (LLB CEA-CNRS-Université Paris-Saclay); DEEN, Pascale (European Spallation Source); LEFMANN, Kim (University of Copenhagen)

Presenter: DAVIDSEN, Amalie (Nanoscience Center, Niels Bohr Institute, University of Copenhagen, Denmark)

Session Classification: Instrumentation

Contribution ID: **57** Type: **Invited**

From Molecular Mobility to Macroscopic Recyclability – A Multiscale Study on Vitrimers

Vitrimers are redefining the boundaries between thermosets and thermoplastics by combining permanent network integrity with true recyclability enabled by dynamic covalent chemistry. Yet, the key question remains: how does molecular mobility at the smallest length and time scales translate into macroscopic reprocessability? In this work, we unravel this connection through a multiscale dynamics driven investigation of a fully bio based vitrimer composed of glycerol triglycidyl ether and a vanillin derived imine hardener operating via catalyst free imine metathesis.

Molecular dynamics spanning from localized vibrational motions to cooperative segmental relaxations are captured by a powerful combination of broadband dielectric spectroscopy, mechanical spectroscopy, and neutron scattering. Dielectric relaxation fingerprints are directly correlated with viscoelastic response and neutron derived vibrational and quasielastic dynamics, allowing us to trace how microscopic mobility governs network rearrangements under thermal and mechanical activation. Special emphasis is placed on the low frequency vibrational density of states and the Boson peak as ultra sensitive probes of local elasticity and network integrity during recycling.

By correlating molecular scale mobility with macroscopic thermomechanical performance before and after reprocessing, this study provides direct experimental evidence for the preservation of dynamic and mechanical functionality upon vitrimer recycling. The results establish a fundamental structure dynamics property relationship for vitrimers and highlight the decisive role of molecular mobility in enabling sustainable, recyclable thermosetting polymers for high performance applications.

Session

Primary authors: SZYMONIAK, Paulina (Bundesanstalt für Materialforschung und –prüfung (BAM)); KRUTEVA, Margarita (Forschungszentrum Jülich); ZORN, Reiner; SCHOENHALS, Andreas

Presenter: SZYMONIAK, Paulina (Bundesanstalt für Materialforschung und –prüfung (BAM))

Session Classification: Soft Condensed Matter

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

Status Update about T-REX: The Bispectral Chopper Spectrometer at ESS

T-REX is a bispectral direct geometry spectrometer currently under construction at the ESS. T-REX looks at both the thermal and cold moderators at ESS, enabling users to study excitations with incident neutron energies ranging from 2 to 160 meV. A key feature of T-REX is its advanced XYZ polarisation analysis capability, which greatly enhances the scope of possible experiments on a direct geometry spectrometer.

This talk will present the scientific capabilities of T-REX and benchmark its performance against existing direct geometry spectrometers in Europe. In addition, a status update on the instrument's construction will be given, highlighting technical progress and key milestones achieved.

Session

Instrumentation

Primary author: AOUANE, Mohamed

Co-authors: Prof. ORECCHINI, Andrea (Physics and Geology Department - University of Perugia); Dr FRANZ, Christian (Forschungszentrum Jülich); VOIGT, Joerg (Forschungszentrum Jülich GmbH)

Presenter: AOUANE, Mohamed

Session Classification: Instrumentation

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

Combining Inelastic Neutron Scattering with Nuclear Magnetic Resonance Spectroscopy for Molecular Hydrogen Endofullerenes

Endofullerenes consist of supramolecular complexes in which fullerene cages, consisting only of carbon atoms, completely confining single atoms or molecules, or in rare cases, multiple atoms or molecules. Endofullerenes are practical realisations of the classic "particle in a box" problem of quantum mechanics, in which confinement leads to energy quantization. We have studied the quantised translational-rotational dynamics of the confined H_2 molecules in the endofullerenes $H_2@C_{70}$ and $2(H_2)@C_{70}$. The allowed dynamical states of the endohedral hydrogens are heavily restricted due to the Pauli Principle. The effect of this is the existence of spin isomers and a metastable rotational state of H_2 at cryogenic temperatures. The translational and rotational excitations of these systems have been measured using IN5 and IN1-Lagrange spectrometers at the ILL-Grenoble.

In the INS spectrum we are able to directly observe transitions between corresponding translational and rotational states.

This measurement allows us to observe interactions between the protons which would be invisible to conventional solution state NMR. The complementary of the NMR experiments means we can deduce information about the positioning and orientation of the confined molecules within the fullerene cage. The combination of INS and NMR measurements allows the study of molecular confinement, spanning both the quantum and classical regimes.

Session

Hard Condensed Matter

Primary author: MCNULTY, Geoffrey (ILL)

Co-authors: BACANU, George R.; Dr VYAS, Vijyesh K. (University of Southampton); Mr HOLLAND, Simon D. (University of Southampton); OLLIVIER, Jacques (Institut Laue-Langevin); Dr WHITBY, Richard J. (University of Southampton); ROLS, Stephane; Dr LEVITT, Malcolm H. (University of Southampton)

Presenter: MCNULTY, Geoffrey (ILL)

Session Classification: Hard Condensed Matter

Contribution ID: **60** Type: **Oral**

Rheo-NSE: Probing dynamics of entangled polymer blends under shear.

Polymeric fluids are one of the most fascinating areas in soft matter physics. Entangled polymer systems exhibit complex, non-Newtonian viscoelastic behaviour arising from topological constraints that restrict chain motion. These entanglements result in characteristic plateau moduli and long relaxation times. To directly access molecular relaxation under shear, we used an updated cone–plate shear cell compatible with in-situ Rheology–Neutron Spin Echo (Rheo-NSE) and Rheology–Small Angle Neutron Scattering (Rheo-SANS). The cell features a non-magnetic design, an improved motor enabling precise speed control, and a dedicated filling protocol for highly viscous samples. In addition, enhanced sealing for operation at high shear rates.

A key challenge in Rheo-NSE is Doppler-induced phase shift arising from velocity gradients that project onto the scattering vector ($\vec{Q}$), causing beam depolarization and restricting the accessible Fourier time. To address Doppler shift, we performed extensive simulations to optimize instrument settings and quantify operational limits in accessible Fourier times, shear rates, and Weissenberg numbers. Using these simulations to take into account Doppler scattering on a pixel-by-pixel basis will significantly increased the effective measurable dynamic range or the available intensity depending the experiment's requirements. We optimized the experimental parameters by analysing static NSE data of the entangled polybutadiene (PBD) melt.

This integrated approach establishes Rheo-NSE as a quantitative probe for polymer dynamics, providing molecular insight into non-linear visco-elasticity in polymer blends, melts, and wormlike micelles, critical for understanding fundamental polymer physics, polymer processing, and material design.

Session

Soft Condensed Matter

Primary author: TEJASVI, Aastha (Department of Physics and Astronomy, Uppsala University)

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Presenter: TEJASVI, Aastha (Department of Physics and Astronomy, Uppsala University)

Session Classification: Soft Condensed Matter

Contribution ID: **61** Type: **Oral**

Extending MIEZE spectroscopy towards thermal wavelengths

Recent advances in neutron instrumentation have been motivated by a need for highest energy resolution over a wide range of momentum transfers to investigate new and exotic ground states without long-range order or well defined excitations, such as for example quantum spin liquids. One line of development has been towards multi-analyzer spectrometers, such as the CAMEA spectrometer, which has recently gone into user operation at the Paul Scherrer Institute.

Here, we are suggesting an extension of the MIEZE technique towards shorter wavelengths, that will increase the accessible energy and momentum transfers at the spectrometer RESEDA, towards 20.5meV and 3Å−1 respectively.

Session

Instrumentation

Primary authors: JOCHUM, Johanna (TUM-FRM2); KELLER, Thomas (Max Planck Institute for Solid State Research); FRANZ, Christian (Forschungszentrum Jülich); Prof. PFLEIDERER, Christian (TUM-FRM2)

Presenter: JOCHUM, Johanna (TUM-FRM2)

Session Classification: Instrumentation

Contribution ID: **62** Type: **Oral**

Update on VESPA, the vibrational neutron spectrometer at the ESS

We present an update on the design of VESPA, the neutron vibrational spectrometer of the European Spallation Source (ESS). VESPA is a broad-band indirect-geometry spectrometer designed to measure molecular vibrations and address a wide range of research areas highly relevant to society and industry, such as renewable energies or catalysis. The large neutron flux of the ESS will enable VESPA to routinely perform in-situ experiments and measure novel materials that are only available in limited quantities.

VESPA will give access in a single ESS pulse to an extended energy transfer range, 0–1000 meV. It will provide a large neutron flux in the low energy region, < 85 meV, and in the so-called "fingerprint region" of the spectra, 60–220 meV. This is achieved by the combination of a direct view of the ESS thermal moderator, partial view of the cold moderator, and the presence of a supermirror guide with elliptic profile and with high m-values, m = 3–5. Three high-speed double disc choppers in optically blind configuration will allow to divide the long ESS pulse into three subframes and to flexibly control the primary spectrometer energy resolution contribution from 0.5% to 2.5% of the incident energy, thus allowing to trade neutron flux for resolution depending on the scientific requirements.

The secondary spectrometer of VESPA is constituted of 16 spectroscopy modules and 4 diffraction banks in backscattering and equatorial positions. Each spectroscopy module is constituted of a focusing analyzer made of highly oriented pyrolytic graphite crystals, a cryo-cooled beryllium filter, and an array of high-pressure 3He position sensitive detectors. The design of the spectroscopy module has recently been updated to further increase the solid angle coverage up to 7.0 sr.

Session

Instrumentation

Primary author: PERRICHON, Adrien (ESS)

Co-authors: JOHANSSON, Alexander (ESS); POPLAND, Helen (ESS); WHITELEGG, Liam (ESS); DI FRESCO, Lorenzo (CNR); HARTL, Monika (ESS); SENESI, Roberto (CNR); CAMILLERI LLEDÓ, Rosa (ESS)

Presenter: PERRICHON, Adrien (ESS)

Session Classification: Instrumentation

Contribution ID: **63** Type: **Poster**

Bending and thickness fluctuations of phospholipid membranes: joint SAXS/SAXS/NSE analysis with stochastic models

Scattering studies are among the few methods that can be used to analyze the structure and dynamics of phospholipid membranes at nanometer scales. However, the available structural information is indirect, as it consists of correlation functions: space-correlation functions for elastic scattering (e.g. SAXS or SANS), and space-time correlation functions for inelastic scattering (e.g. NSE). An essential and challenging aspect of any scattering study is therefore the development of models to convert scattering data into structural and dynamical insight. Here we report on a family of time-dependent stochastic models that can be used for the structural and dynamical analysis of bending and thickness fluctuations in phospholipid membranes, possibly with included proteins. The methods are illustrated with the joint SAXS/SANS/NSE analysis of unilamellar vesicles prepared from phospholipids extracted from porcine brain tissues 1, as well as on red blood cell membranes containing band3 proteins 2.

1 C.J. Gommes, P. Dubey, A. Stadler, B. Wu, O. Czakkel, L. Porcar, S. Jaksch, H. Frielinghaus, O. Holderer, Gaussian model of fluctuating membrane and its scattering properties, Phys. Rev. E 110 (2024) 034608;

2 C.J. Gommes, O. Matsarskaia, J. Pusterla, I. Graf von Westarp, B. Wu, O. Czakkel, A.M. Stadler, Model for small-angle scattering analysis of membranes with protein-like inclusions, J. Appl. Crystallogr. 58 (2025) 1571-1581.

Session

Biology/Health

Primary authors: STADLER, Andreas (Forschungszentrum Julich); Dr WU, Baohu (Forschungszentrum Jülich); GOMMES, Cedric; FRIELINGHAUS, Henrich; GRAF VON WESTARP, Igor; Dr PUSTERLA, Julio; HOLDERER, Olaf (Forschungszentrum Jülich GmbH, JCNS at MLZ); MATSARSKAIA, Olga; CZAKKEL, Orsolya (Institut Laue Langevin); Dr DUBEY, Purushottam Shashikumar (Forschungszentrum Jülich); Dr JAKSCH, Sebastian (ESS); PORCAR, lionel (LSS)

Presenter: STADLER, Andreas (Forschungszentrum Julich)

Session Classification: Biology/Health

Contribution ID: **64** Type: **Oral**

The influence of dipolar interactions on the critical dynamics in nickel

The study of critical phenomena has always been deeply connected with magnetism in solid state materials. Nickel, one of the three archetypical room temperature ferromagnets, is understood to be an itinerant system with a high degree of localization regarding its magnetically active electron states. We report a high-resolution neutron spectroscopy investigation of nickel (Ni) near its Curie temperature T_{C}, extending measurements to unprecedentedly small wavevectors $q_{\mathrm{min}} = 6.6{\cdot}10^{-3}$ $unicode0x212B^{-1}$ and achieving an energy resolution of $\Delta E = 4.9\,\mu\mathrm{eV}$. This was achievable using the RESEDA spectrometer in MIEZE mode, a variant of the neutron resonant spin-echo technique.

Our analysis of the spin-wave dispersion reveals that the dipolar wavevector $q_{\mathrm{D}} = 6.4 \cdot 10^{-3}$ $unicode0x212B^{-1}$ is approximately half of the previously reported value, but strictly non-zero to rationalize the observed excitations. The spin wave stiffness $D(T)$ is in good agreement with literature, but most importantly, we uncover evidence that the linewidth of the spin waves follows the dynamical scaling characteristic of a dipolar ferromagnet rather than an isotropic one. In contrast, the linewidth of the fluctuations above T_{C} exhibit scaling consistent with the Resibois–Piette function and renormalization-group predictions, despite the itinerant ferromagnetic nature of Ni. This observation suggests a pronounced localization of the $3d$-electrons responsible for magnetic scattering.

Session

Magnetism

Primary author: BEDDRICH, Lukas (Jülich Centre for Neutron Science at MLZ)

Co-authors: JOCHUM, Johanna (TUM-FRM2); Dr SÄUBERT, Steffen (Research Neutron Source Heinz Maier-Leibnitz (FRM II), Technical University of Munich); FRANZ, Christian (Forschungszentrum Jülich); BÖNI, Peter (Technical University Munich)

Presenter: BEDDRICH, Lukas (Jülich Centre for Neutron Science at MLZ)

Session Classification: Magnetism

Contribution ID: **65** Type: **Poster**

Real-Time Magnetic Dynamics in a Frustrated Quantum Magnet Polymorph

Motivated by the growing effort to identify entangled quantum states in real materials, we investigate magnetic correlations across unprecedented energy and time scales in two archetypal frustrated spin-1/2 systems: a triangular-lattice antiferromagnet driven by geometric frustration, and a cubic-lattice antiferromagnet where frustration arises from quenched disorder. Both phases are realized in polymorphs of $Ba_3CoNb_2O_9$. Remarkably, we observe spin-liquid-like behavior in both cases, clearly distinct from classical long-range magnetic order or frozen spin-glass\ice states. These results provide the first direct time-domain evidence to address key open questions in quantum many-body physics (QMP), such as the reliability of long-time numerical predictions and the emergence of disorder-induced spin-liquid phases.

This poster highlights state-of-the-art approaches for probing real-time magnetic dynamics, combining complementary experimental methods with overlapping timescales: conventional Neutron Diffraction/Spectroscopy, Wide Angle Neutron Spin Echo, and Muon Spin Rotation. Our study provide new insights to QMP and point towards promising methodological development opportunities for the broader measurement-science community.

Session

Magnetism

Primary author: XU, Fanjun (HZB)

Presenter: XU, Fanjun (HZB)

Session Classification: Magnetism

Contribution ID: **66** Type: **Invited**

Structural relaxation and nano-domain dynamics in highly concentrated electrolytes for zinc anode batteries

Due to their intrinsic non-flammable nature, aqueous batteries are regarded as desirable alternatives to lithium-ion batteries which use non-aqueous electrolytes. Metallic zinc has long been regarded as an ideal anode material for aqueous batteries systems. Highly Concentrated Zinc Electrolytes (HCZEs) are a new type of Water in BiSalt Electrolytes (WIBSE) which might enable practical zinc anode batteries, improving their cycle life and energy density.1 HCZEs contain both a zinc salt and Li(TFSI) at very high concentrations, where TFSI is bis(trifluoromethanesulfonyl)imide. Ultimately, the effectiveness of HCZEs is believed to be due to i) the reduction of zinc hydroxide formation by depletion of water in the zinc ion solvation shell, through the segregation of water molecules in the solvation shell of the lithium ions, as well as ii) to the suppression of water activity.2 Using neutron scattering methods, we investigated the molecular structure and relaxation dynamics in HCZEs. The relation between these results and the macroscopic transport properties, viscosity and conductivity, will be discussed.3

1 F. Wang, *et al.*, Nature Materials, **17**, 543 (2018).
2 F. Wang, *et al.*, Adv Energy Mater, **11**, 2102016 (2021).
3 A. Faraone, *et al.*, J. Phys. Chem C, **128**, 12121 (2024).

Session

Liquids

Primary authors: FARAONE, Antonio (NIST Center for Neutron Research); Dr DURA, Joseph A. (NIST Center for Neutron Research); FALUS, Peter (ILL); GARCIA SAKAI, Victoria (ISIS Pulsed Neutron and Muon Source); Dr HEADEN, Thomas F. (ISIS Pulsed Neutron and Muon Source); SEEL, Andrew G. (ISIS Pulsed Neutron and Muon Source); Dr TAKEUCHI, Saya (Materials Science and Engineering, A. James Clark School of Engineering, University of Maryland); Prof. WANG, Fei (Department of Materials Science, Fudan University)

Presenter: FARAONE, Antonio (NIST Center for Neutron Research)

Session Classification: Liquids

Contribution ID: **67** Type: **Poster**

Nested mirror optics for neutron resonant spin-echo instrument RESEDA

RESEDA is a neutron resonance spin-echo (NRSE) spectrometer at FRM II that provides a flexible range of possible energy and momentum transfers by offering two modes of operation: the NRSE option, which has the advantage of providing larger spin-echo times and the possibility to measure at large scattering angles, and the MIEZE option, which is robust against depolarizing conditions at the sample position. The recent upgrades at RESEDA focused on improving the energy resolution of the MIEZE option and on adapting the instrument for the use of thermal neutrons. The potential result of these upgrades is access to MIEZE at large momentum transfers, allowing investigation of a new range of phenomena such as frustrated magnetism.

As one of the next steps in the instrument's development, it was proposed to install nested mirror optics (NMOs) at the instrument to allow neutron beam focusing at several places such as radio-frequency (RF) flippers or the sample position 1. Focusing at the RF flippers will allow the use of smaller AC field coils while increasing neutron beam size, thus improving RF flippers performance and increasing total neutron flux. Focusing the beam at the sample position would allow efficient experiments with samples with small cross sections, such as those used in high-pressure measurements or single crystals that are difficult to grow. For the MIEZE mode, this also helps to suppress phase aberrations, allowing measurements at large scattering angles.

In this contribution, we present the plans for NMO integration into RESEDA with the preliminary simulation results.

1 C. Herb et al., Nuclear Inst. and Methods in Physics Research, A 1040, 167154 (2022)

Session

Instrumentation

Primary authors: METTUS, Denis (TUM-FRM2); Mr SCHÖNLEITER, Florian (TUM); JOCHUM, Johanna (TUM-FRM2); KREUZER, Lucas (TUM-FRM2); PFLEIDERER, Christian (TUM-FRM2)

Presenter: METTUS, Denis (TUM-FRM2)

Session Classification: Instrumentation

Contribution ID: **68** Type: **Oral**

From Atomic Motion to Catalytic Function: Unraveling Hydrogen Dynamics in MoS_2 through High Resolution Neutron Techniques

Hydrogen gas is a key energy carrier for a decarbonized energy system, especially when generated by water electrolysis. Molybdenum disulfide (MoS_2) offers a cost-effective alternative to platinum catalysts for the hydrogen evolution reaction (HER) 1, though its performance remains limited by slow hydrogen dynamics and incomplete understanding of adsorption and reactivity mechanisms. This study employs quasi-elastic (QENS), neutron spin-echo (NSE) and inelastic neutron scattering (INS) with XPS, XRD and EDX to elucidate how chemical doping and electrochemical activation control atomic-scale hydrogen motion in MoS_2 nanopowders and affect catalytic behavior [2,3]. Classical and ab initio molecular dynamics simulations support interpretation of these results 4.

For pristine MoS_2, QENS and NSE reveal distinct hydrogen and water mobilities operating on different time scales. INS identifies vibrational modes of water and S-H bonds, whose intensities rise after electrolysis, indicating enhanced surface hydrogenation and hydroxylation. Nitrogen doping greatly accelerates hydrogen diffusion, consistent with defect-induced, highly mobile adsorption environments. Complementary XPS, XRD and EDX confirm structural and electronic modifications underpinning the enhanced dynamics. Continuing work on Co-doped MoS_2 aims to further tune hydrogen transport pathways through compositional design.

1 Cao et al., ACS Nano 15, 11014–11039 (2021)
2 Yang et al., J. Phys. Chem. C 17, 10917–10925 (2019)
3 Verma et al., Mater. Today: Proc. 102, 241–246 (2024)
4 Abidi et al., J. Phys. Chem. C 125, 17058–17067 (2021)

Session

Materials Science

Primary author: GERAKIANAKI, Aliki (Institute Laue Langevin)

Co-authors: TRAEGER, Franziska; FOUQUET, Peter (ILL); PIOVANO, andrea (ILL)

Presenter: GERAKIANAKI, Aliki (Institute Laue Langevin)

Session Classification: Materials Science

Contribution ID: **69** Type: **Poster**

CSPEC: the Cold Chopper Spectrometer of the European Spallation Source

The initial suite of instruments at the European Spallation Source (ESS), currently under construction in Lund, will include five spectrometers, among them CSPEC, a cold chopper spectrometer. CSPEC is delivered as a French-German in-kind contribution, led by the Laboratoire Léon Brillouin, Saclay, France, and the Technische Universität München, Germany.

CSPEC will be the first cold chopper spectrometer to operate on a long-pulsed spallation source, offering significant advantages in signal-to-noise ratio and enabling innovative measurement schemes. The instrument will utilise cold neutrons in the 2–20 Å wavelength range, with a tunable energy resolution of ΔE/E = 5–1%. CSPEC's science case is broad, serving diverse research communities including magnetism, soft matter, energy materials, and life sciences.

The instrument is specifically designed to address time-dependent processes under realistic experimental conditions (for example, electrolytes subjected to an external electric field). Taking advantage of the high flux delivered by the ESS, together with the novel opportunities offered by repetition-rate multiplication (RRM), CSPEC will be able to follow kinetic processes with time resolution of minutes for transient phenomena, or of ms for stroboscopic time-resolved measurements. It will also enable the study of materials whose synthesis yields samples too small for current capabilities. In this contribution, I will outline the instrument layout and expected performance, and provide the latest updates from the construction site.

Session

Instrumentation

Primary author: NOFERINI, Daria

Co-authors: MOREIRA, Fernando Yamil (ESS); DA SILVA, Jackson; OLSSON, Mats (ESS); LONGEVILLE, Stéphane; LOHSTROH, Wibeke; DEEN, pascale (European Spallation Source)

Presenter: NOFERINI, Daria

Session Classification: Instrumentation

Contribution ID: **70** Type: **Poster**

Upgrade of the Neutron Spin Echo Spectrometer at NIST Center for Neutron Research

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) has been operating a neutron spin echo spectrometer since the later ‘90s. Recently, through a collaboration among the University of Delaware, the University of Maryland and the NCNR with a strong support from the Jülich Center for Neutron Science, the instrument was significantly upgraded using funding from the Midscale Research Instrumentation-1 program of the National Science Foundation (NSF Proposal 1935956). This project supported the installation of a new neutron velocity selector, a new single V cavity polarizer, the replacement of the old precession coils with super conducting precession coils of optimized shape, Pythagoras coils, and a new detector. The upgrade aims for a 2.5x increase of the magnetic field integral, which translates in a dynamic range extension to Fourier times up to 250 ns for routine operations and the possibility to reach 700 ns in particular cases. Data acquisition rates are expected to increase by a factor 5 for a given dynamic range. All new components were delivered and installed, and cold commissioning has been performed. When the NCNR reactor resumes operation (anticipated spring 2026), the instrument hot commissioning will commence.

Session

Instrumentation

Primary authors: Dr NAGAO, Michihiro (NIST / University of Maryland); FARAONE, Antonio (NIST Center for Neutron Research); Dr MALISZEWSKYJ, Nicholas (National Institute of Standards and Technology); Mr BROCKER, Christophy (National Institute of Standards and Technology); MONKENBUSCH, Michael (Forschungszentrum Jülich); KOZIELEWSKI, Tadeusz (Forschungszentrum Jülich GmbH); HOLDERER, Olaf (Forschungszentrum Jülich GmbH, JCNS at MLZ); Dr NEUMANN, Dan (National Institute of Standards and Technology); WAGNER, Norman (University of Delaware)

Presenter: Dr NAGAO, Michihiro (NIST / University of Maryland)

Session Classification: Instrumentation

Contribution ID: **71** Type: **Oral**

Lifetimes of spin excitations with three-axis spin-echo

Special care is needed for spin echo spectroscopy of spin excitations. Even in the case of antiferromagnets (AF), which do not depolarize the neutron beam, the scattering on spin excitations induces neutron spin flips that affect the spin echo signal. We review three cases from TRISP at the FRM II. The first case is a straightforward example of magnons in the uniaxial AF MnF2, where by proper choice of the scattering plane the well known exponential decay of the spin echo polarization vs. tau is observed. The second example involves critical scattering in the classical AF Rb2MnF4, where the interference of different spin flip channels leads to a complicated oscillations of P(tau), such that the simple exponential analysis fails. The third example, critical fluctuations in close to quantum criticality in CeCu5.8Au0.2 is more challenging. In this case, in addition to the neutron spin flips from the critical scattering, a strong incoherent background originating from the Cu moments obscures the signal further. There is no analytical expression for P(tau) for the latter two cases. However, incorporating a ray-tracing model of the spectrometer and the sample into the fit makes the analysis straightforward and transparent.

Session

Magnetism

Primary author: KELLER, Thomas (Max Planck Institute for Solid State Research)

Co-author: Prof. KEIMER, Bernhard (MPI for Solid State Research)

Presenter: KELLER, Thomas (Max Planck Institute for Solid State Research)

Session Classification: Magnetism

Contribution ID: **72** Type: **Poster**

Portable devices for adding Spatial-Intensity-Modulation-mode capabilities to polarized neutron beams at FRM-II

The Modulated IntEnsity with Zero Effort (MIEZE) resonant spin-echo technique, implemented at the RESEDA instrument at the FRM II, allows measurements of depolarizing samples with high energy resolution and has its optimum resolution at small scattering angles, i.e. SANS geometries. With the recent adaptations towards thermal neutrons, and possibility to move the detector to large scattering angles, a large range of momentum transfers becomes accessible at RESEDA, greatly increasing the flexibility of the instrument. This, however, requires addressing the Larmor phase aberrations originating from the finite sample size, the effect of which becomes prominent outside of the SANS regime. By incorporating Magnetic Wollaston prisms (MWPs), a device which can produce controlled spatial modulations of intensity, it is possible to compensate Larmor phase aberrations, thereby extending the MIEZE resolution to any desired scattering angle. The spatial intensity modulation mode (SIM-mode) device incorporates MWPs with a radio-frequency (RF) spin flipper in a single modular unit, providing great flexibility of achievable modulations. Such SIM-mode devices could be then used at different instruments at FRM II, for example improving resolution of polarized SANS or diffraction instruments, or enabling the study of intra-particle mode-entangled neutron beams which has potential use in probing many-body quantum entanglement in materials 2. In this contribution, we provide an update on the construction progress of SIM-mode devices intended for use at FRM II, describe the details of their operation, and discuss the various possibilities they offer.

1 Fankang Li, J. Appl. Cryst. 55, 90-97 (2022).

2 J. Leiner et. al., Phys. Rev. Appl. 22, L031005 (2024).

Session

Instrumentation

Primary author: LITTLEHALES, Matthew (TUM)

Co-authors: METTUS, Denis (MLZ); Dr LEINER, Jonathan (ORNL); JOCHUM, Johanna (MLZ); Prof. PFLEIDERER, Christian (TUM-FRM2)

Presenter: LITTLEHALES, Matthew (TUM)

Session Classification: Instrumentation

Contribution ID: **73** Type: **Poster**

Neutron Scattering Characterisation of Gel Systems for Cleaning Delicate Artwork

Gels with tailored confining and release properties of solvents are essential tools for cleaning sensitive precious artefacts. Understanding thoroughly the transport phenomena at the molecular level in these systems is crucial for improving formulations, not only for cultural heritage conservation but also for applications such as drug delivery. To this end, we used QENS to probe the polymer-network dynamics and the transport of confined water in hydroxyethylmethacrylate (HEMA) hydrogels. Our investigation focused on the effects of crosslinking (chemical vs physical) and water content. The results show a distribution of relaxation processes in the polymer network, mainly linked to the side-chains. Water dynamics occur as a hydrogen-bond governed process with a jump-diffusion mechanism, and the interaction with the polymer matrix significantly slows the dynamics compared with bulk water and other confined systems. Such a strong interaction results as well in a fraction of water that appears as immobile at the investigated timescale. Higher hydration levels are associated with an increased mobility of both the water and polymer network. At equal water content, physical gels show slower relaxation and a smaller explored space than chemical gels, for the pHEMA network. Water mobility is strongly reduced in chemical gels at low hydration, while at high hydration the mobilities converge, albeit with shorter residence times in chemical gels. More recently, we have extended our investigations to castor-oil organogels, using SANS and QENS. These systems are suistainable and specifically designed for tackle the challenge of cleaning water sensitive artifacts in modern and contemporary art.

Session

Soft Condensed Matter

Primary authors: FARAONE, Antonio (NIST Center for Neutron Research); NOFERINI, Daria; CHELAZZI, David (University of Florence); FRATINI, Emiliano (University of Florence); POGGI, Giovanna (University of Florence); BAGLIONI, Piero (University of Florence)

Presenter: NOFERINI, Daria

Session Classification: Soft Condensed Matter

Contribution ID: **75** Type: **Poster**

Polarization and Analysis for High Energy Resolution On SPHERES: technical aspects

We have been working to develop the instrumentation concept for PA HEROS. The application of PA to high resolution neutron backscattering requires many considerations for the instrumental realization. We have been studying these aspects from incident beam polarization to polarization transport in the primary and secondary spectrometer and PST chopper to novel implementation of a wide angle polarization analyzer (WAPA). The practical aspects of polarized 3He type WAPA vs. super mirror (SM) transmission WAPA and rigorous simulation of performance have been performed, We have commissioned the construction of an SM tWAPA prototype to test the implementation of several innovations of the proposed tWAPA solution. Of particular note are a modular geometry matched to the SPHERES secondary spectrometer and detector geometry, and a novel radial magnetic cavity concept for the SM tWAPA to both provide high >300G saturation field for the SMs over a large vertical angle/height (ca. 30°/40 cm) and full horizontal scattering angle (140°) of SPHERES and also serve as the polarized neutron guide field in the secondary spectrometer. A section of this new SM magnetic system has also been produced for testing. This poster will provide an overview of the technical considerations and study as well as the status of prototyping and testing.

Session

Instrumentation

Primary author: BABCOCK, Earl (JCNS at the MLZ)

Co-authors: Dr SOLTNER, Helmut (ITE FZ-Juelich); VOIGT, Joerg (Forschungszentrum Jülich GmbH); ZAMPONI, Michaela (Forschungszentrum Juelich GmbH); HUANG, chuyi (Jülich Centre for Neutron Science)

Presenter: BABCOCK, Earl (JCNS at the MLZ)

Session Classification: Instrumentation