

Book of Abstracts

2nd to the 4th of July, 2025

Sola Strand Hotel Sola, Norway

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Neutron Scattering with Polarized Neutrons Combined with MD-Simulations: New Insights into Collective and Self Dynamics from Intermediate to Intermolecular Length Scales

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Neutron scattering is a unique technique to characterize structural and dynamic properties of matter. Particularly important is the potential, playing with isotopic labelling, of accessing different correlation functions (collective, self) or 'isolating' the signal of a given component or molecular group in a complex system. However, the coexistence of coherent and incoherent contributions to the scattered intensity is, in most of the situations, unavoidable. These contributions can only be separated by applying polarization analysis – which poses technical difficulties. The recent implementation of this capability in spectrometers, in particular in the case of PLET at ISIS with sub-meV resolution, opens the possibility of investigating problems / systems that could not be approached in a rigorous way until now. One of them is the question of the collective dynamics of liquids and glass-forming systems in the mesoscale or intermediate length scales region, i. e., at length scales larger than the intermolecular ones but not vet in the hydrodynamic regime. In this talk, new insights on the problem of how collective and self-dynamics evolve from intermediate to intermolecular length scales will be presented, considering systems with different intermolecular interactions. They have been provided by the application of spectroscopy with polarization analysis as well as using the NSE technique as an alternative and complementary way to address self- and collective dynamics. We will also show the great help of molecular dynamics simulations to interpret the experimental results.

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Nuclear quantum effects in liquid water explored using polarized QENS

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Although the influence of nuclear quantum effects (NQE) in the properties of liquid water is well-known, the magnitude of their effects depends strongly on the specific conditions and property considered. It has been suggested that this could be due to competing quantum effects, where proton delocalization in the direction of the H-bond would reinforce it, while delocalization in other directions would distort and therefore weaken the H-bonds [1]. While the effect of NQEs in the structure of liquid water remains controversial, both from the experimental and computational approaches, they are much stronger in the rotational and translational dynamics and the subject of intense theoretical and computational efforts [1,2]. We have used polarized QENS in LET to explore the extent of NQEs in light (H₂O) and heavy (D₂O) water at 278 K and compared the experimental spectra with classical simulations in order to separate the effect of NQEs from the classical isotopic mass effect. The self-dynamics of protons in H_2O and D_2O as obtained from the analysis of the incoherent dynamical cross section will be presented, together with an analysis of the possibilities and limitations of using this information to improve the classical potentials.

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[2] N. Stolte et al: "Nuclear Quantum Effects in Liquid Water Are Marginal for Its Average Structure but Significant for Dynamics", J. Phys. Chem. Lett. 2024, 15, 12144–12150.

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Polarized quasi-elastic neutron spectroscopy accessing molecular structural relaxations in water-ethanol mixtures with and without guest molecules

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Polarized neutron time-of-flight spectroscopy permits to access quasi-elastic scattering informing on picosecond time-scale diffusion. We have employed this method using LET at the ISIS Neutron and Muon Source to access the molecular structural dynamics in water-ethanol mixtures [1]. We also investigate the effect of a supramolecular gelator and of a paracetamol (PCM) drug added to these mixtures [2]. Our observations indicate an enhanced rigidity of the hydrogen bond network in the water-ethanol mixtures at the mesoscopic length scale compared to the molecular scale as the ethanol fraction increases, which is consistent with the hypothesis of small transient molecular clusters forming in the mixtures. When adding the supramolecular gelator, we find that, although this gelator significantly alters the macroscopic rheological behavior of the solvent at concentrations of 0.3 and 0.5 wt.%, it does not affect the hydrogen bond network at the microscopic level. In contrast, the addition of PCM at 5 wt.%, which does not change the macroscopic properties, modifies the structural dynamics of water-ethanol mixtures at length scales commensurate with and below the PCM-PCM correlation length in the mixture. This finding reveals the intricate interplay between solute, solvent, and gel interactions, demonstrating a lack of direct correlation between macroscopic rheological and microscopic diffusion properties in such complex systems. On the example of these hydrogen-bonded fluids, the results illustrate the benefit from unambiguously separating the self- and collective dynamics. The work with loaded drug molecules points towards a future interest in higher energy resolution at a similar range of momentum transfers.

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Probing polymer structure and dynamics through molecular

dynamics simulations and comparison with NSE and SANS spectra

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State-of-the-art experimental techniques such as small-angle neutron scattering (SANS) and neutron spin echo (NSE) spectroscopy provide valuable insights into the unique structural characteristics and segmental and diffusion dynamics of polymers in their molten state. However, there are often cases where analysing experimental findings with such methods is challenging. We mention for example the case of minor contamination of ring polymer melts by linear analogues which can significantly affect polymer relaxation but also the case of subtle structural differences along the polymer chain which can lead to different spectra.

Molecular dynamics (MD) simulations can effectively address these issues by allowing precise control over the sample's composition. Recent theoretical advancements and the availability of atomistic force fields enable the predictions of neutron scattering spectra from MD simulations with remarkable accuracy.

In this presentation, we will outline the theoretical framework for predicting SANS and NSE spectra based on the analysis of microsecond-long atomistic MD trajectories and we will illustrate the application of such a methodology with specific examples, including ring polyethylene oxide (PEO) melts [1], mixtures of PEO rings with linear counterparts [2,3], and polyethylene glycol/silica nanocomposites [4].

Direct comparison of the MD-extracted neutron scattering spectra against available experimental measurements conducted under identical conditions and system compositions will also be presented, revealing remarkable agreement between the two approaches.

References

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- [3] D.G. Tsalikis, and V.G. Mavrantzas, Macromolecules 53, 803-820, (2020).
- [4] E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, and V.G. Mavrantzas, Macromolecules 54, 4470-4487, (2021).

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Dynamics of Organic Ferroelectrics using Quasi-elastic Neutron Scattering Spectroscopy and Molecular Dynamics Simulations

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Organic ferroelectrics are important functional materials for their flexible structure, low cost and applications in quantum computing, energy storage materials, electronics and medical devices [1-2]. These materials are free from toxic elements and so sustainable alternatives to traditional ferroelectrics. Most of these organic ferroelectrics are either hydrogen bonded or halogen bonded, which play an important role in their ferroelectric properties [3-8]. Charge or proton transfer occur through chemically distinct donor-acceptor pairs connected through these bonds, which act as a bridge. In presence of an external field this transfer of protons changes the polarisation of these materials by changing geometry from centro-symmetric to non-centrosymmetric [2]. Microscopic understanding of the ferroelectricity, particularly dynamics of these hydrogen and halogen bonds are yet to be reported.

In this presentation we investigate some of these ferroelectrics, both hydrogen bonded and halogen bonded, such as croconic acid and 4,5- \neg -dichloro- \neg -2- \neg -methyl- \neg -imidazole (C4H4Cl2N2), respectively. The results of quasi-elastic and inelastic neutron scattering experiments will be compared with first-principles molecular dynamics and lattice dynamics simulations. It is found that strong anharmonicity present in both hydrogen and halogen bonds in these materials. Calculated Born effective charge tensor predicts that microscopic origin of ferro-electricity of this material is from H bonding of either O-H—H or N—H-N bonds forming bridges between molecular units.

We will present microscopic insight of the dynamics of this material using both INS and QENS spectroscopy complimented by first principles molecular simulations. The prospect of using machine learned potentials will be discussed.

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Dynamics of ionic liquids confined in porous glasses – A showcase for polarization analysis in QENS

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The structure and dynamics of the ionic liquid (IL) 1-ethyl-3-methylimidazolium acetate (EMIMAc) with small amounts of water in nanoporous glass are measured and compared to the bulk liquid. With X-ray diffraction the domain structure was determined, while neutron spin echo spectroscopy/neutron backscattering were employed to measure the dynamics. The experimental challenge is to separate coherent and incoherent contributions of elastic and inelastic scattering, resulting in a rather complex set of information from the different instruments. Differences in ordering in the bulk and in confinement could be observed, which also has an influence on the ionic mobility of the IL. Partial deuteration allowed to get insight into the mobility of the smaller molecule of the IL, and the influence of small amounts of water has been studied [1].

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Polarised neutrons for studying slow dynamics at European Spallation Source

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Polarised neutrons have long been used to study magnetic structures and dynamics in nanoto meso-scales [1]. In soft matter studies, polarisation analysis has recently been shown to be an important method to determine coherent and single-particle motions in QENS in the intermedia length scale where diffusion occurs [2,3]. Owing to the persistent push to advance the technology, polarised neutron has changed from a scarce resource that often requires an instrumentation expert to carry out measurements, to becoming a commonly available resource that can benefit a considerably wider research community. To date, 40% of instruments are providing polarised neutron capability.

To meet the coming user demand, eleven of the fifteen ESS instruments [4] under construction aim to offer polarised neutrons for user experiments, including three spectrometers CSPEC, MIRACLES, T-REX that are most suited to study diffusion and other slow dynamics. In conjunction with in-kind contributions and instrument grants, the ESS Polarisation Project will support nine of the eleven instruments to incorporate polarisation analysis capabilities [5]. Neutron spin filters based on polarised 3He technologies and polarising supermirror devices are selected according to the different neutronic requirements and constraints on each instrument. An update of the project will be presented with highlights on some of the instrumentation innovations and improvements.

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Development of Wide-angel polarized neutron capability at the China Spallation Neutron Source

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Polarized Neutron experiment capability have been established at the China Spallation Neutron Source (CSNS) over the past few years. Current commissioned neutron beamlines at the CSNS adopts in-situ 3He system as their analyzer, while only covering small angel and straight beam geometry. With the next phase beamline development planned and under development, wide-angle geometry polarization analysis becomes a necessity for future CSNS beamlines. Currently, the polarization group at the CSNS has developed a prototype wideangle insert for the planned diffractometer and spectrometer, as well as the core 3He glass cell. Multiple categories of science cases are surveyed to determined the future scope of the new beamlines and the corresponding polarized neutron insert parameter. In this talk, a brief introduction of the current CSNS wide-angle polarization analysis is introduced, along with the roadmap and future science cases discussions.

New instrumentation and polarization / 2

BL02 ToF Backscattering Spectrometer at J-PARC MLF -Polarization Neutron Experiment Prospects-

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The latest instrument specifications of the J-PARC MLF BL02 spectrometer are introduced, and the future of scientific research expected from the use of polarized neutrons will be summarized from the viewpoint of the instrument scientist in charge of the spectrometer.

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

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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. Based on this design, we explore transmission wide angle polarizer supermirror analyzer option through Monte-Carlo simulations [3]. At this conference, we will present our work towards performing polarization analysis with the high-resolution capabilities at the SPHERES instrument.

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Poster session / 15

Additives in TiFe Metal-alloy Systems: Effect on Crystal Structure and Hydrogen Storage

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Hydrogen storage poses challenges in the hydrogen economy due to its low density. Titaniumiron (TiFe) alloys are promising for ambient-condition storage, reversibly absorbing hydrogen at room temperatures with volumetric capacities comparable to liquid H2 (~100 kgH2 m-3) [1]. However, low gravimetric capacity and oxide formation limit TiFe's standalone use. Elemental doping and mechanical processing have been proposed to address these issues. Theoretical studies suggest transition element dopants (e.g., Cr, V, Nb, Mn) enhance TiFe's hydrogen storage by altering lattice size and strain, facilitating H2 diffusion [2]. Limited research exists on TiFe doped with Ta, Nb [3,4] and correlations between crystallographic structure and storage properties remain unclear.

In this work, V- and Nb-doped TiFe alloys with varying stoichiometries were synthesized via vacuum arc melting (VAM). Structural characterization via PXRD and EXAFS revealed high agreement between refined crystallographic parameters. Pressure-composition-temperature (PCT) measurements demonstrated improved activation and kinetics with precise doping, linking dopant-induced lattice occupancy to hydrogen absorption. These findings advance mechanistic insights into transition-metal-doped TiFe for optimized storage.

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(4) Hydrogen storage properties of TiFe-based ternary mechanical alloys with cobalt and niobium. A thermochemical approach E.A. Berdonosova a, V.Yu. Zadorozhnyy b,c, M.Yu. Zadorozhnyy b, K.V. Geodakian a, M.V. Zheleznyi b, A.A. Tsarkov b, S.D. Kaloshkin b, S.N. Klyamkin a,.

Poster session / 3

Ion-transport in PFPE-based polymers - challenges in analysis

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We investigate battery relevant mechanically rigid M1I0 polymer and viscolelastic M1I3 polymer, with and without Li, to understand the interplay between dynamics/mechanics and

columbic efficiency in batteries. The polymer network consists of a PFPE backbone interconnected by urethane units containing H-bonds, with H atoms involved in N-H bond being responsible for polymer rigidity. When Li salt is added, Li cations bind to the oxygen atoms in the urethane units. In fact, FTIR revealed a lengthening of the C=O bond on addition of Li salt, which was attributed to weakening of H-bond, as Li cation formed Lewis acid complexation with the basic carbonyl oxygen site. This interaction is known also to increase barrier heights to rotation.

At the highest energy resolution QENS (at LET) revealed localized dynamics in all polymers. Amongst other fast motions, these could be a due to constrained motions of the hydrogenbonded units. While the extracted correlation times for M1I0, M1I3 and Li_M1I0 are similar, the correlation time for Li_M1I3 was twice as long. A similar trend is observed at the intermediate resolution. Interestingly, at the lower energy resolution which probes slightly faster dynamics, the pristine polymers still show localized motions, whereas polymers with Li salt show diffusive motions. At these temporal scales, H-bond breaking is possible which may result in decoupling of Li-ions, facilitating thereby Li-ion migration, also across the hydrogen-bond connected chains (intrachain migration).

The QENS signal unfortunately contains significant coherent contribution which limits the accessible Q-range for incoherent dynamics. At Q values below 1 Å-1, we account for the coherent contribution with a linear background. However, at higher Q values, we require characterizing the ratio of incoherent to coherent via polarisation methods. We plan polarized-QENS measurement in the future to widen the Q-range for our analysis and confirm our assumptions in the lower Q-range.

Poster session / 20

Polarization analysis on MIRACLES, the new backscattering instrument at ESS

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The new backscattering spectrometer MIRACLES at the European Spallation Source (ESS) will feature unprecedented performances combining high flux with tunable energy resolution, large accessible dynamical range, and the possibility to implement polarization analysis [1]. Here we report recent examples of how such polarization analysis could be particularly relevant to discriminate between self and collective dynamics in complex molecular systems [2,3]. In particular, we discuss recent results on polymer nanocomposites and we discuss how the capabilities of MIRACLES could open up new possibilities in this field.

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SUPER² - A Neutron Scattering and Atomistic Simulations for a SUPERior Understanding of SUPERionic Conduction

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Through recent years, the importance of functional energy materials has increased due to challenges originated by the climate change, which can be mitigated by transitioning from fossil-fuel to green technologies. Considering this, solid-state batteries have emerged as a promising candidates for technological application towards this energy revolution [1]. However, the ionic conductivity, which in batteries is related to the electric power and time of charge, still requires an improvement to reach real-life applications.

In this work we present the SUPER2 project, which aims to investigate the ionic diffusion mechanism of solid-state superionic conductors at the atomic-scale. Our goal is to create a robust but accessible methodology for data analysis and computational simulations, focusing our attention on the polarization analysis of neutron quasi-elastic coherent scattering. This methodology will be tested by studying the ionic diffusion mechanism of selected well-known ionic compounds, taking advantage of the improvements on experimental [2] and computational

techniques [3], to access longer time and spatial scales.

As a starting point to test our methodology, preliminary results obtained for the ionic conductor Li6.5La3Zr1.5Nb0.5O12 will be presented. Temperature dependent inelastic neutron scattering measurements found broad acoustic phonons even at T = 100 K. Geometry optimization calculations, using density functional theory, have been attempted, although the Li vacancies are unstable and difficult the convergence of the calculations.

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Poster session / 11

Phonon Anharmonicity in Thermoelectric materials: Neutron Scattering and Ab-initio Insights

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Phonon properties are critical for optimizing thermoelectric (TE) materials. Conventional abinitio methods based on the harmonic approximation fail to capture temperature-dependent effects like lattice expansion and anharmonicity, causing prediction discrepancies for TE materials [1]. Anharmonic effects, reflected in phonon linewidth broadening and frequency renormalization, strongly influence thermal transport and TE performance.

This study combined experimental and computational techniques to investigate phonon properties in Mg Si [2]. A high-quality single crystal grown via the Bridgman method [3] was used for experiments on triple-axis spectrometers IN20 (ILL) and Eiger (PSI), covering temperatures from 300 K to 600 K [3]. High-purity powder samples were investigated by inelastic neutron scattering (INS) on MARI at ISIS. The stochastic temperature-dependent effective potential (sTDEP) method was used for ab-initio phonon calculations, incorporating higher-order force constants from density functional theory (DFT) with the SCAN meta-GGA functional [4,5]. This approach enabled predictions of phonon dispersion, linewidths, and temperature-dependent broadening.

Powder INS showed that the phonon density of states, closely matches the sTDEP predictions, demonstrating the model's accuracy in capturing lattice dynamics. Single-crystal INS revealed pronounced phonon linewidth broadening with increasing temperature, especially near the X-point, highlighting significant anharmonicity in Mg Si. Notably, the largest linewidth broadening with a FWHM of 0.39 meV at 600 K aligns with computational results.

This work provides a comprehensive understanding of phonon anharmonicity in Mg Si through INS experiments and advanced ab-initio calculations. Our findings underscore the importance of anharmonic effects in thermal transport and validate the sTDEP method for studying TE materials.

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Poster session / 29

Investigation of Li-ion self-diffusion in solid-state Li6.8La2.9Zr1.8Nb0.2O12 electrolyte material with polarized neutrons

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Solid-state batteries offer the promise of safer and higher energy density compared to contemporary Li-ion batteries, where the main hindrance to wide-scale commercial application is the lack of a suitable solid-state electrolyte material [1]. Li7La3Zr2O12 (LLZO) based materials show high promise as Li-ion conducting electrolytes for solid-state battery applications [2,3]. Despite the relatively high solid-state Li-ion conductivity, wide electrochemical stability window, and mechanical strength, the ionic conductivity of LLZO is still considerably lower than that of organic liquid-based electrolytes [3]. The partial substitution of Zr with Nb in LLZO has been shown to increase Li-ion conductivity through the formation of Li-vacancies and stabilization of the cubic phase [4,5]. To better understand the Nb-doping effect on the Li dynamics, a Nb-doped 7Li-isotope enriched LLZO, 7Li6.8La2.9Zr1.8Nb0.2O12 sample was investigated with polarized neutron scattering, performed on the LET spectrometer at ISIS, UK in the temperature range from 300 to 440 K. Neutron polarization analysis was used to separate the incoherent scattering dominantly caused by the dynamics of 7Li. The quasielastic incoherent scattering is fitted and analyzed to determine the presence of different 7Li-ion dynamics. The activation energy of the translational self-diffusion transport mode is determined and compared to other LLZO-based materials and with the values obtained by other methods. The mechanism for 7Li-ion jumps between the vacancies in the LLNZO crystal structure is analyzed and presented.

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Poster session / 10

Temperature-dependent neutron diffraction, magnetic, and ESR studies on MgFe2O4 nano-ferrite prepared via Sol-Gel auto-combustion using DL-alanine as a fuel

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The present work investigates the crystallographic and magnetic properties of post-annealed magnesium ferrite (MgFe2O4) powder using neutron diffraction within a comprehensive temperature range (10 - 300 K). The obtained crystallite and domain size variations show a robust correlation with the magnetic properties. Further, the magnetic behaviour was investigated using zero-field cooling (ZFC) and field-cooling (FC) magnetization. Further, temperature variation of magnetic domain size (Dm) and crystallite size are thoroughly examined. The observed reduction in domain size as the temperature decreases is attributed to the increase in the coercive field (HC). The magnetic moments for MgFe2O4 nano powder estimated through the Rietveld refinement of neutron diffraction patterns are consistent with the magnetic moment calculated from M(H) loops. Further, Electron Spin Resonance (ESR) technique is employed to investigate the magnetic behaviour of MgFe2O4 over a temperature range of 90 K to 300 K, focusing on dipolar and super-exchange interactions. The ESR spectra linewidth

 (ΔH_PP) of MgFe2O4 increases from 1225 Oe to 1870 Oe as the temperature decreases from 300 K to 90 K, indicating the enhancement of dipole magnetic interactions.

Poster session / 46

Polarized spectroscopy for dynamics at the JCNS

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The Juelich Center for Neutron Science along with the outstation in Garching at the Maier Leibnitz Zentrum (MLZ), supports many polarized spectroscopy instruments and developments from polarization analysis (PA) on wide angle time-of-flight to cold/thermal triple axis and Neutron Spin Echo (NSE) and work towards PA for high resolution backscattering. Existing polarized spectroscopy instruments suitable for slow dynamics study include the Diffuse Neutron Scattering (DNS) spectrometer, and Juelich NSE "Phoenix." The JCNS has constructed the SNS-NSE at Oak Ridge and has also collaborated with HZB to implement wide-angle polarization analysis at the NEAT instrument in Berlin. The presently commissioned ToF spectrometer TOPAS will provide PA for higher energies and short time scales. The bispectral instrument TREX in Lund (ESS) will have adaptable energy resolution for a larger dynamic range. The DNS WAPA project will improve the resolution to allow routine inelastic experiments with cold neutrons. Finally PA on SPHERES will allow high resolution QENS to probe ns dynamics.

Poster session / 45

Polarized neutron scattering capabilities on the cold triple axis spectrometer Sika in ANSTO

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Manipulating and filtering the neutron spin on neutron scattering instruments allows to extract unique insights on the properties of materials. Triple-axis spectrometers have proven to be one of the most flexible neutron scattering instruments to accommodate such experimental conditions. We will present the cold triple axis spectrometer Sika [1,2] and its capalibities for polarized neutron scattering experiment at the Australian Nuclear Science and Technology Organization (ANSTO). The National Synchrotron Radiation Research Center (NSRRC) in Taiwan has been responsible for operating this instrument, as per the agreement established between NSRRC and ANSTO. We will share the latest technical development and scientific achievements with polarized neutrons on Sika, such as identifying spin incoherent contribution to quasi-elastic neutron scattering (QENS) [3], identiying a weak ferromagnetic component of magengtic materials [4], determining the chirality of helimagnet, and so on.

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Hard condensed matter / 27

Ionic diffusion in superionic compounds studied with coherent and incoherent QENS and large-scale atomistic simulations

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Neutron scattering is an ideal probe of the atomic structure and dynamics in solids, from fast ionic diffusion in solid electrolytes to lattice dynamics in thermoelectrics or ferroelectrics. These dynamics 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].

The design of new solid-state electrolytes (SSEs) for future solid-state batteries hinges on identifying key diffusion mechanisms that can improve material performance. While static structural descriptors have been correlated with fast diffusion, the host framework flexibility and vibrations and their complex dynamic coupling with mobile ions remain insufficiently understood. Phonons describe the atomic dynamics in crystalline materials, a convenient basis to encode possible minimum energy pathways for ion migration, and provide insights into correlated ion jumps. 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 intricate details of the diffusion process. These results offer detailed microscopic insights into the dynamic mechanisms of fast ion diffusion in solid-state electrolytes.

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Hard condensed matter / 21

Accurate Estimation of Self- and Collective-Motion from Molecular Dynamics Simulation

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The self-diffusion coefficient for an ionic conductor is routinely estimated from molecular dynamics simulations by "fitting a straight line" to observe the mean-squared displacements (MSDs). Typically, this fitting is performed without considering fundamental concepts of displacements, such as their heteroscedasticity and correlation, leading to a sub-optimal estimation method. Meanwhile, the collective-diffusion coefficient is rarely determined from simulation, with a preference for assuming that the ionic motion is completely uncorrelated. However, this is not necessarily the case for many classes of materials.

I will present a Bayesian scheme for estimating the self-diffusion coefficient from a single simulation trajectory with high statistical efficiency and accurately estimating the uncertainty in the predicted value [1]. I will then discuss how this approach may be used to find the collective-diffusion coefficient. Throughout this seminar, I will introduce kinisi, a software package developed to improve the analysis of molecular dynamics simulation [2], and highlight the relevance of this work to inform the analysis of polarised QENS measurements.

You may enjoy this seminar if you are interested in diffusion, applied mathematics, molecular dynamics simulations, or open-source software.

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Hard condensed matter / 5

Phonon dynamics of CsAg5Te3-based thermoelectric materials by combining first-principles and neutron scattering

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Low lattice thermal conductivity is critical to thermoelectric materials and thermal barrier coatings. Combining first-principles calculations and neutron scattering experiments using CSNS@MPI as well as J-PARC@AMATERAS, we study the phonon dynamics properties of the recently synthesized low thermal conductivity material CsAg5Te3 [1]. Our results demonstrate that the liquid-like heat transfer could indeed exist in a well-ordered crystal. The low lattice thermal conductivity is mainly originated from its weak chemical bonding and strong phonon anharmonicity. Particle-like phonons and heat-carrying wave-like phonons contribute differently at different temperatures and the coupling between them leads to the nearly temperature independent behavior of lattice thermal conductivity [2]. In addition, we also study

the lattice structure, chemical bonding, harmonic as well as anharmonic phonon dynamics, and lattice thermal conductivity of the tetragonal -CsCu5Se3 by using first-principles calculations. The weak temperature dependence of the lattice thermal conductivity is carefully explained [3].

Keywords Phonon dynamics, Dynamic structure factor, First-principles, Inelastic neutron scattering, Boltzmann transport

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Hard condensed matter / 23

Potential of neutron spectroscopies in studies of complex hydrides for hydrogen storage applications

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Complex hydrides, such as Mg(BH4)2, have been studied for solid-state hydrogen storage application due to the high content of hydrogen per mass and volume in these compounds. Additionally, chemically bounded hydrogen and lower operational pressures offer significant safety advantages over the traditional storage methods in pressurized or cryogenic tanks. However, hydrogen release and re-absorption in the complex hydrides remains a problem as it still requires elevated operational temperatures (100 - 400 °C) impractically high rehydrogenation pressures, sluggish kinetics of hydrogen sorption reactions as well as complex reaction pathways.

Due to the high neutron scattering cross-section of H, neutron spectroscopy is a distinguishable tool in the investigation of complex hydrides for hydrogen storage applications. It can offer unique insights into hydrogen absorption and desorption mechanisms, revealing fundamental interactions and transformations within these materials. This talk will introduce the use of neutron spectroscopies and their combination with vibrational spectroscopies, such as Raman scattering, to explore the structural and dynamic properties of hydrides in characterization of their structure and hydrogen dynamics highlighting recent progress in the field.

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Mechanisms of proton and hydride-ion diffusion in materials for energy applications investigated using quasielastic neutron scattering

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Hydrogen diffusion plays a key role in many materials of high interest for science and society; examples are proton conducting materials for utilization in environment friendly and efficient hydrogen fuel cells, and materials that can store hydrogen or facility important, industrial catalytic processes. However, fundamental questions surrounding the mechanism of hydrogen diffusion and its correlation with the materials' functional properties, such as proton conductivity and/or catalytic performance, remain to be elucidated for most of these materials. In this contribution, I will report on our recent studies of the mechanistic detail of hydrogen diffusion in two different classes of energy relevant materials, using quasielastic neutron scattering (QENS) together with computer simulations. The first example concerns a study of the brownmillerite type proton conducting oxide Ba2In2O5(H2O), which shows potential for being used as an electrolytic membrane in intermediate-temperature solid oxide fuel cells, whereas the second example concerns a study of the nitride-hydride Ca3CrN3H, which shows promise as a catalyst for ammonia synthesis. The combined analyses of experimental and theoretical data allow us to determine the mechanism of hydrogen diffusivity – stretching from protonic to hydridic species – in both classes of materials, and develop design criteria for new, potentially better performing materials for specific applications.

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Diffusion in Nb-Doped LLZO and Bismuth Vanadium Oxide Using ML-Driven Simulations

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Liquids, soft matter, and biophysics / 25

Influence from polarised QENS for proteins in solution – Ideas for data treatment for normal and polarised QENS

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Protein dynamics play a vital role in biology. Quasi elastic neutron scattering is an ideal method to access these dynamics. Normally data analysis is performed based on the assumption that the scattering spectrum is incoherent. In order to be observe the full range of protein dynamics it is necessary to perform the experiments in solution. This solution is usually a fully deuterated buffer, while the protein remains protonated. It is generally assumed that while the buffer leads to a coherent contribution, this can be taken into account during data analysis by subtracting the buffer contribution from the sample spectrum. Up until recently there was no way to experimentally verify this assumption. Polarised QENS experiments on LET allow for the coherent and incoherent contributions to be separated. By comparing the results from the polarised QENS experiment and the standard analysis method from unpolarised QENS it was possible to experimentally check this assumption. This has shown that the pure incoherent spectrum obtained from polarisation analysis does not match the results for normal QENS.

I will present ideas on how to treat normal QENS data to take the coherent contribution into account during data analysis. Both approaches that are currently available and ideas for how simulations could help with this in the future.

Liquids, soft matter, and biophysics / 13

Lipid acyl tail dynamics measured using conventional and polarized quasielastic neutron scattering

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Lipid molecules are basic building blocks for biological membranes, which are highly dynamic and provide a platform for various biological functions. From a materials point of view, these membranes are a visco-elastic entity. Viscosity of membranes regulates the transport of lipids and proteins in the membrane which determine the time necessary to maintain the functions. Chemically distinct lipid molecules are known to form membranes with different compositions depending on the secretory pathway. For example, more unsaturated lipids prepare membranes in early secretory pathways where the membrane viscosity is relatively lower, while more sterols and saturated lipid molecules are known for membranes in a late secretory pathway where the membrane viscosity is higher. Although biology uses different lipid compositions to maintain membrane viscosity, the molecular mechanisms of regulating the membrane viscosity are not well understood. In a previous neutron spin echo result, the slow component of the lipid acyl tail correlation relates to the transport of the lipid molecules and relates to the molecular origin of the membrane viscosity. Here, we employ quasielastic neutron scattering to measure lipid acyl tail correlation dynamics for saturated lipid membranes by utilizing isotope substitution and polarization analysis to separate coherent and incoherent components at the lipid acyl tail correlation peak. The results show that the timescale of the relaxations for self-motion of hydrogen is slightly faster than the collective dynamics in 10 ps and longer time scales. We will provide the analysis results together with some neutron spin echo data.

New instrumentation and polarization / 47

TREX: a polarized bi-spectral spectrometer at ESS

Author: Mo Aouane

T-REX is a bi-spectral direct geometry neutron chopper spectrometer, currently being constructed at the ESS. The instrument is a collaboration between Forschungszentrum Jülich and Consiglio Nazionale delle Ricerche (CNR). It is a very versatile instrument and will mainly focus on probing single crystals in the scientific areas of low dimensional, topological and frustrated materials, quantum magnets, high temperature superconductors, multifunctional oxides, and many more.

The instrument will measure a wide dynamic range with good wave-vector resolution over the energy transfer range from 20 µeV to 140 meV. Measurements will use non-polarized and polarized neutrons, for both cold and thermal neutrons. Thermal neutron polarization is achieved with the SEOP setup. Neutron spin analysis in XYZ is performed with the magic PASTIS setup.

The chopper system enables poly-chromatic illumination of the sample and variable acquisition time frames by means of a specially developed FAN chopper that suppresses selectively the unwanted subpulses. The secondary spectrometer features a vacuum path of 3m from sample to detector, which will cover a dynamic range that extends from 0.05 Å-1 < Q < 10 Å-1, thus exploring a wide range of the reciprocal space. The novel Multi-Grid detector system is covered in a separate abstract. We will give an overview over the current built status of the instrument, timeline to completion and features offered to the user community.

New instrumentation and polarization / 39

SHERPA: a spectrometer for high-resolution polarization analysis

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SHERPA is a proposed near-backscattering instrument that will replace the IRIS spectrometer on the first target station at ISIS. By exploiting the prismatic effect of the PG(002)crystals in the secondary spectrometer, it promises huge gains in count-rate versus current ISIS instruments. This will facilitate routine polarization analysis on both small samples and weakly scattering materials. It is expected that SHERPA will revolutionize the study of a broad range of systems, from biomolecules to catalysts to energy materials.

New instrumentation and polarization / 19

MDANSE: Molecular Dynamics Analysis for Neutron Scattering Experiments – Recent Developments

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MDANSE (Molecular Dynamics Analysis of Neutron Scattering Experiments) [1,2,3] is an open-source software project developed to allow users to generate simulated neutron scattering observables from MD trajectories relevant to inelastic and quasi-elastic neutron scattering experiments. The MDANSE project began in 2015, supported by the SINE2020 program, and was initially developed by software engineers and researchers at the ILL. Over the last few years, new versions of MDANSE have been released, such as the alpha and beta releases of v2.0, the first versions to use Python3. We are now aiming for the first stable release of v2.0 in mid-2025. The significant changes in the new version include a brand-new graphical user interface, improved plotting options, new analysis calculations, and support for more MD trajectory formats. Additionally, to improve the overall user experience, a more intuitive user interface, updated online documentation, and tutorials [3,6] are being developed. Our presentation will include a history of the MDANSE program, an overview of current developments, our online documentation and tutorials, a roadmap of planned features, a live demonstration of MDANSE, and a Q&A session.

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New instrumentation and polarization / 38

Polarization analysis aspects of Neutron Spin Echo Spectroscopy

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In neutron polarization analysis studies changes of neutron beam polarization are observed, which are exclusively due to the interaction of the neutron spin with a sample studied. The interactions can be of two types: with nuclear spins and with magnetic fields inside the sample i.e. primarily between the nuclei. In NSE spectroscopy the behavior of the neutron beam polarization along neutron paths outside the sample is analyzed using special magnetic field configurations. In addition, the NSE configuration can also be specially adapted to the neutron spin changes inside the sample, in order to maintain its capability to analyze neutron energy changes in the scattering event on the sample. These configurations are different for samples of different magnetic behaviors such as paramagnetic, ferromagnetic, antiferromagnetic etc. In nonmagnetic samples, i.e. without strong internal magnetic fields between the nuclei, the standard NSE configuration operates unperturbed and also provides full polarization analyzed neutron scattering information at the same time as probing the quasielastic behavior. Actually, the polarization analysis information is always present in the standard raw data collection files at ILL, and even old data that have not been evaluated for polarization analysis can also be revisited and reevaluated for extracting the polarization information too, which was eventually not a point of interest at the time the data were taken. This revisiting feature could be of interest, for example in some polymer samples. The full, combined polarization and NSE quasielastic analysis method has been recently utilized for the study of intermediate length range correlations in water and heavy water over distances corresponding to 2-5 times the average intermolecular spacing.

Hard condensed matter / 41

Recent developments in resonant spin echo techniques for quasi-elastic neutron scattering

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We present recent developments in resonant spin echo techniques, focusing on Neutron Resonance Spin Echo (NRSE) and Modulation of Intensity with Zero Effort (MIEZE). These techniques have emerged as powerful tools for quasielastic neutron scattering, offering unique advantages over traditional methods such as backscattering and conventional Neutron Spin Echo (NSE). We will provide a comprehensive overview of the differences between these techniques, highlighting their strengths and limitations.

The presentation will showcase examples of the application of MIEZE to quasielastic and inelastic scattering, demonstrating its capabilities in probing dynamic processes in various systems. We will also discuss the differences between MIEZE and NRSE/NSE, particularly in terms of incoherent background and sample environment.

Furthermore, we propose the combination of MIEZE with polarization analysis to enhance the technique's sensitivity and selectivity. Additionally, we will discuss the concept of wideangle MIEZE, which promises to expand the technique's scope and applicability.

This presentation aims to stimulate discussion and explore the potential of resonant spin echo techniques in advancing our understanding of complex systems and phenomena. By highlighting the latest developments and proposed innovations, we hope to inspire new research directions and collaborations in the field of quasielastic neutron scattering.

Hard condensed matter / 12

Interfacial and bulk molecular and magnetic diffusive modes in iron oxide nanoparticles

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A QENS study on IN16B (ILL) together with elastic and inelastic fixed-window-scans up to 380 K on humid citrate-coated iron oxide nanoparticles with a diameter of 6 nm show the presence of two diffusive species in the interface region. A comparison between hydrogenated and deuterated samples collected on EMU (ANSTO) allows for an assignment to ligand- and water dynamics. In a global fit approach, we find the citrate molecules to rotate with an activation energy of Ea = 240 meV and a prefactor of 0 = 0.21 ps, while surface water diffuses translationally with an activation energy of Ea = 190 meV and a prefactor of 0 = 0.12 ps, significantly slower than bulk water.

Further, various magnetic QENS signals are identified when considering the entire Q-range from Q=0.2 Å-1 up to Q=1.7 Å-1. Based on structure factor evaluations, dynamic features, and the temperature behavior, we identify to our knowledge for the first time in QENS data uniquely superparamagnetic relaxation in the low Q-regime for Q< 0.3 Å-1, a weak signal with spin glass behavior for 0.6 < Q < 1.0 Å-1 originating from the magnetic shell near the surface of the nanoparticles, and a magnon excitation with an energy of 22 µeV at 150 K in the range of the magnetic Bragg peak 1.2 < Q < 1.4 Å-1.

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QENS Study of the Interface Dynamics of Wet IONP

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Iron oxide nanoparticles (IONPs) are extensively used in many different fields ranging from heterogeneous catalysis to biochemistry. Optimizing their performance especially under humid conditions where water interactions significantly influence the functional behavior depends on an understanding of the atomic-scale dynamics of surface-bound species. The interface dynamics can be probed by QENS in the form of energy-resolved spectra (ERS) and fixed window scans (FWS). Adequate data treatment is essential for elucidating these processes, particularly when dynamics from different molecules coexist.

We have synthesized citrate-capped IONPs and equilibrated them at relative humidities (RH) ranging from 8% to 98%. The water surface coverage varies from monolayer to multilayer. ERS and FWS of these samples were measured on IN16B in the temperature range of 2–380 K. A global fitting procedure with shared parameters between the ERS and FWS fits was

used to analyze ligand and water dynamics, [1] as well as magnetic relaxations in 8% RH IONPs. [2] Extending this approach to the 85% RH sample, analysis of FWS also reveals distinct dynamical regimes in temperature space. While below 150 K there are signs of a weak magnetic process, water and ligand dynamics become observable above 200 K, evolving into a rapid decrease in elastic intensity. We interpret this feature as a pre-melting phase transition in hydration water. Before the phase transition, the dominant process can be described by Fick's law with a diffusion coefficient at 245 K of $1.57 \times 10^{-12} m^2 s^{-1}$. This is much slower than would be expected from any residual supercooled water on the surface.

Our analysis demonstrates that the interfacial dynamics of citrate-capped IONPs can be probed under application-relevant, wet conditions by QENS.

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Accelerating barocalorics research through polarised QENS

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Heating and cooling currently accounts for 50% of global final energy consumption and is responsible for more than 40% of energy related CO₂ emissions. As the planet warms, the demand for cooling increases, and without new environmentally friendly cooling devices, we risk runaway global warming. The most promising solid state replacement technology is based on barocalorics, where pressure drives an adiabatic temperature change at phase transitions with a large change in entropy.

Over the last 10 years, a huge range of barocalorics have been identified, but to engineer optimised materials for applications it is vital to understand what generates the large entropy changes. In addition to using diffraction to explore the configurational entropy, QENS and INS provide essential information about the dynamics, where vibrational entropy can sometimes be the dominant contribution.

We have used QENS and INS to explore ammonium sulfate and adamantane under hydrostatic pressure, but these used different samples since INS measurements require them to be perdeuterated. In the future we look forward to using polarised LET to enable us to extract the QENS and phonon scattering separately from the same sample measurement, even in samples where deuteration would be prohibitive. Since the lowest energy dynamics contribute most significantly to the calculated entropy, being able to cleanly separate the QENS and phonon signals will significantly impact the interpretation.

We had hoped to present our first pLET data, but unfortunately our experiments had to be cancelled due to instrument problems. Nevertheless, we are very excited to learn more about polarsiation analysed QENS, the instrumentation, the modelling and the data analysis, and are looking forward to discussions at the meeting.

Interplay of Cooperativity and Lattice Dynamics in Spin Crossover Compounds

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Cooperativity plays a crucial role in shaping the spin crossover (SCO) transition behavior, influencing its abruptness, hysteresis, and thermal response—features that are critical for applications such as solid-state barocaloric cooling. Previous studies have demonstrated a strong link between intermolecular interactions (e.g., hydrogen bonding, – stacking) and cooperativity. However, the connection between lattice dynamics and cooperative behavior remains largely unexplored.

In this work, we investigate the structural and dynamic origins of cooperativity in the SCO complex Fe(PM-BiA) (NCS) (PM = N-2'-pyridylmethylene, BiA = 4-aminobiphenyl), which exists in two polymorphs: an orthorhombic phase (Pccn) showing an abrupt spin transition (high cooperativity) around 177 K, and a monoclinic phase (P2 /c) exhibiting a gradual transition (low cooperativity) near 208 K.

To gain insight into the role of lattice dynamics, we employ a combination of inelastic neutron scattering, nuclear inelastic scattering, and quasi-elastic neutron scattering to probe complete lattice vibrations, Fe-specific phonon density of states, and local dynamic motions across a wide energy scale. Notably, we identify a Fe–N stretching phonon mode that couples strongly with the degree of cooperativity, suggesting a direct link between specific vibrational dynamics and the sharpness of the transition. By correlating these findings with spin-state changes, we quantify the electronic, vibrational, and configurational entropy contributions and their relationship to cooperativity. Our results offer new insight into how lattice dynamics mediate cooperativity in SCO transitions and provide a foundation for designing advanced caloric materials.