
# 8th European Conference on Neutron Scattering

Hosted by the Heinz Maier-Leibnitz Zentrum (MLZ)
at Garching/ Germany
March 20th-23rd, 2023

## Book of Abstracts

We gratefully acknowledge our supporters - please don't forget to visit the EXPO in MW Yard 2!

# NEUTRONS FOR EUROPE

COME AND VISIT OUR COMMON STAND TO LEARN MORE ABOUT THE TWO FACILITIES*

The Institut Laue Langevin (ILL) - the European neutron source - is an international research centre at the leading edge of neutron science and technology. It is located in a setting of outstanding beauty in the cosmopolitan city of Grenoble in south-east France.

The Institute operates the most intense continuous neutron source in the world, supplying neutrons to a suite of high-performance instruments that are constantly being developed and upgraded. As a service institute, the ILL makes its facilities and expertise available to visiting scientists. Each year, over 1400 researchers from over 40 countries visit the ILL, performing more than 800 experiments and publishing about 600 scientific articles - 25% of which featured in high-impact journals, in 2022.

The European Spallation Source (ESS) is a multidisciplinary research facility based on one of the world's most powerful pulsed neutron sources. It's currently in the installation and commissioning phase. This is a pan-European project with Sweden and Denmark serving as host countries and will deliver transformative capabilities extending the technique to new domains of science. ESS will give scientists new possibilities in a broad range of research, from life science to engineering materials, from heritage conservation to energy and magnetism.

***On Monday, Tuesday and Wednesday between 13:30 and 14:00 there will be the opportunity to meet with Director General Helmut Schober, Science Director Giovanna Fragneto and Head of the Neutron Instrument Division Andrew Jackson, respectively.**

ill
NEUTRONS FOR SOCIETY

ess
EUROPEAN SPALLATION SOURCE

AS THE PRESENT AND FUTURE EUROPEAN NEUTRON SOURCES, THE ILL AND ESS WILL PLAY A KEY ROLE IN THE FUTURE DEVELOPMENT OF GLOBAL NEUTRON SOURCE SCIENCE


MODELLING - DETAILED-DESIGN - ANALYSIS - PROCUREMENT
MANUFACTURING - ASSEMBLY - INTEGRATION - TEST

Added Value Solutions (AVS) is an international company which aims at providing technology-based services to innovative and challenging projects. Founded in 2006, with Headquarters in the North of Spain, we are a global SME strongly focused on the development of outstanding devices, mechanisms, instruments and structures for research infrastructures worldwide.

**AVS's expertise covers design, manufacturing, assembly, tests and supply under ISO 9001 EN 9100, providing our customers all the way up from the conceptual design to the turnkey.**

AVS skills on engineering design, mechatronics and positioning in UHV, extreme magnetic fields / radiation / temperature, neutron instrumentation, opto-mechanics and detection make AVS the perfect partner for instrument construction at neutron sources. Our company is also very active in other fields like Fusion, Space, Particle Accelerators, Astrophysics and Lasers.

AVS develops neutron instrumentation for reactors and spallation sources worldwide, including ESS, ILL, ISIS, FRM II, HZB, LAHN, CHESS, ANSTO, NIST and more. Our portfolio includes all kind of turnkey instruments including TAS spectrometers, SANS instruments, TOF spectrometers and diffractometers.

AVS designs and develops all-size non-magnetic vacuum chambers, neutron guide selectors, sample positioning systems, guide fields and magnetic circuits, neutron collimation systems, double focusing monochromators and analysers, neutron detectors and complex shielding solutions.

www.neutronguide.com
www.boron10coating.com

S-DH

## Boron-10 Coatings for Detectors:

- Cascade
- Powtex
- Magic
- Dream

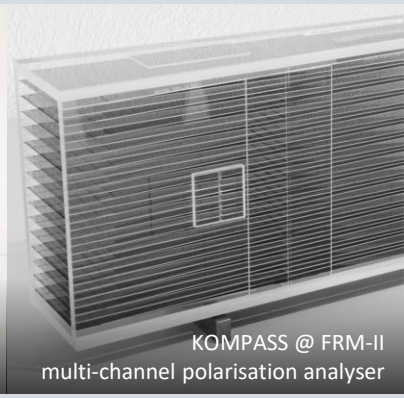
www.neutronguide.com

S-DH GmbH
Siemensstr. 34
69123 Heidelberg
Germany

SwissNeutronics

*Neutron optics from the finest art ...*

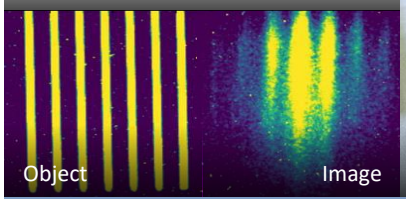
H14 @ ILL
neutron guide splitter

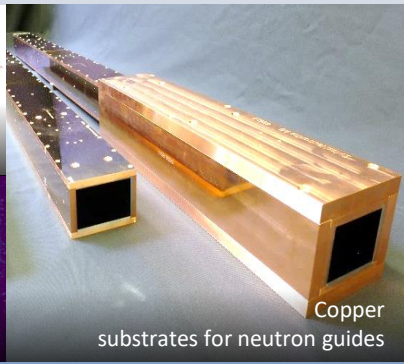


KOMPASS @ FRM-II
multi-channel polarisation analyser

*... to novel concepts*

Scheme of Nested Mirror Optic



Copper
substrates for neutron guides

*www.swissneutronics.ch*

# MON

| | | | | | |
|---|---|---|---|---|---|
| **09:00** | Welcome adresses | | | | |
| **09:45** | New structures and exotic properties of simple molecular systems under extreme conditions: using neutrons to explore planetary interiors (L. Bove) **MW 2001** | | | | |
| **10:30** | Coffee break MW Yards 1 & 3 | | | | |
| **11:00** | Neutron Methods **MW 0001** | Proteins & Peptides seen by Neutrons **MW 2001** | Engineering 1 **SCC 001** | Diffraction and beyond **SCC 002** | Frustrated Magnets 1 **SCC 3** |
| **12:30** | Lunch break (light lunch in MW Yards 1 & 3) | | | | |
| **14:00** | Magnetic Structures **MW 0001** | From Membranes to Kinetics and Dynamics **MW 2001** | Spectros-copy **SCC 001** | Magnetic Thin Films & Nano **SCC 002** | Glasses & Liquids **SCC 3** |
| **16:00** | Poster session (board numbers MO-XXX) **MW Yards 4 - 6** | | | | |

TUE

| | | | | | |
|---|---|---|---|---|---|
| **09:00** | Harnessing the power of neutron to quantify softness (A. Scotti) | | | | |
| **09:45** | Advances in Neutron Imaging (M. Strobl) **MW 2001** | | | | |
| **10:30** | Coffee break MW Yards 1 & 3 | | | | |
| **11:00** | Energy Materials **MW 0001** | Functional Materials 1 **MW 2001** | From Polymers to Thermo-dynamics **SCC 001** | Data Evaluation & Software 1 **SCC 002** | Frustrated Magnets 2 **SCC 3** |
| **12:30** | Lunch break (light lunch in MW Yards 1 & 3) | | | | |
| **14:00** | Neutron Sources: Developments and Foresight **MW 0001** | | European Neutron Sources: Status and Upgrades **MW 2001** | | |
| **16:00** | Poster session (board numbers TU-XXX) **MW Yards 4 - 6** | | | | |

| | |
|---|---|
| **19:00** | Public Lecture<br>R. Gebhard (Director of the Bavarian State Archaeological Collection) on neutrons and archeology<br>**MW 2001** |

# WED

| | | | | | |
|---|---|---|---|---|---|
| **09:00** | Vortices in unconventional superconductors (E. Blackburn) | | | | |
| **09:45** | Ultracold Neutrons as powerful probes in particle physics and cosmology (T. Jenke) **MW 2001** | | | | |
| **10:30** | Coffee break MW Yards 1 & 3 | | | | |
| **11:00** | Soft Matter Interfaces **MW 0001** | Super-conductors **MW 2001** | Engineering 2 **SCC 001** | Data Evaluation & Software 2 **SCC 002** | MS CANS 1 **SCC 3** |
| **12:30** | Lunch break (light lunch in MW Yards 1 & 3) | | | | |
| **14:00** | Polymers & Criticality **MW 0001** | Functional Materials 2 **MW 2001** | Neutron Optics (and Polarization) **SCC 001** | Fundamental Physics **SCC 002** | MS DEUNET 1 **SCC 3** |
| **15:30** | Coffee break MW Yards 1 & 3 | | | | |
| **16:00** | Bio-inspired Soft Matter Systems **MW 0001** | Bulk Magnetism 1 **MW 2001** | Imaging & Neutron Detection **SCC 001** | Source Materials **SCC 002** | MS DEUNET 2 **SCC 3** |

**19:00** Conference dinner
**Hofbräuhaus München, Platzl 9, 80331 München**

THU

| | | | | | |
|---|---|---|---|---|---|
| **09:00** | Spin-orbit excitons in transition metal oxides (C. Stock) | | | | |
| **09:45** | Disclosing the unknown deep inside biomembranes (V. Rondelli) **MW 2001** | | | | |
| **10:30** | Coffee break MW Yards 1 & 3 | | | | |
| **11:00** | Structure & Dynamics **MW 0001** | Bulk Magnetism 2 **MW 2001** | Cultural Heritage **SCC 001** | Sample Environment **SCC 002** | MS CANS 2 **SCC 3** |
| **12:30** | Lunch break (light lunch in MW Yards 1 & 3) | | | | |
| **14:00** | Award ceremonies and closing **MW 2001** | | | | |
| **16:00** | Guided tours of the FRM II **Meeting Point at Conference Office** | | | | |

# Monday, 20 March 2023

## Welcome adresses - MW 2 001 - Lecture hall (20 Mar 2023, 09:00 - 09:45)

**-Chairs: Martin Müller**

## Plenary - MW 2 001 - Lecture hall (20 Mar 2023, 09:45 - 10:30)

**-Chairs: Martin Müller; Werner Paulus**

### [531] New structures and exotic properties of simple molecular systems under extreme conditions: using neutrons to explore planetary interiors (09:45)

*Presenter: BOVE, Livia Eleonora*

Simple molecular systems, like water, methane, ammonia, hydrogen, and their mixtures are of para-mount importance for many fields, ranging from energy storage applications to condensed matter and planetary physics [1-2]. These systems are widespread on Earth, in various planetary bodies in the solar system and in newly detected water-rich exoplanets, and constitute an incredibly rich gas resource to be exploited. Due to their relatively simple stoichiometry and electronic structure they also repre-sent key systems for the understanding the physical-chemical behavior of more complex molecular systems. Under the extremely broad range of pressure and temperature conditions experienced in planetary interiors these simple molecular systems and their mixtures display a rich phase diagram, anomalous dynamical, thermal and transport properties, super-ionicity, plasticity and enhanced quan-tum effects [3-12]. In this talk I will review our recent experimental results on the structure and the dynamics of simple molecular systems under extreme conditions probed by neutron, x-ray and light scattering techniques, and will discuss their impact for planetary modelling and energy applications. [1] L. E. Bove et U. Ranieri, Phil. Trans. R. Soc. A 377: 0262 (2019). [2] W.L. Mao et al., Physics Today 60, 42 (2007). [3] S. Klotz, L. E. Bove et al. Nat. Mat. 8, 405 (2009). [4] L. E. Bove, R. Gaal, et al., PNAS 112, 8216 (2015). [5] S. Klotz, L.E. Bove, et al., Sci. Rep. 6, 32040 (2016). [6] U. L. Ranieri et al., Nature Com., 8, 1076 (2017). [7] S. Schaack et al., JPC C 122 11159 (2018). [8] U. L. Ranieri, et al. J. Phys. Chem. C, 123, 1888 (2019). [9] S. Schaack et al., PNAS, 10.1073/pnas.1904911116 (2019). [10] U. L. Ranieri, et al., Nature Com. 12: 195 (2021). [11] M. Rescigno et al., under submission (2023). [12] H. Zhang et al., J. Chem. Phys. Letters, in press (2023).

## Diffraction and beyond - SCC/0-002 - Taurus 1&2 (20 Mar 2023, 11:00 - 12:30)

**-Chairs: Johanna K. Jochum; Rasmus Toft-Petersen**

### [47] Construction of the DREAM Diffractometer at ESS (11:00)

*Presenter: FEYGENSON, Mikhail*

Neutron diffraction instrument DREAM is among the first instruments to be constructed at the European Spallation Source (ESS) in Lund, Sweden. The Diffraction Resolved by Energy and Angle Measurements (DREAM) instrument is being built as an in-kind contribution from the Jülich Centre of Neutron Science (Germany) and Laboratoire Leon Brillouin (France)1. The instrument views both cold and thermal neutron moderators. A solid Si bender will be reflecting the cold neutrons into the incident beam while transmitting the thermal neutrons. As a result, the neutron bandwidth will include both thermal and cold neutrons at their peak intensities, providing the Q-range of 0.01 – 25 Å–1 in a single frame, which is ideally suited for conventional powder diffraction, pair-distribution function and low-angle diffraction measurements. The long ESS pulse is shaped to the experimental needs by pulse-shaping choppers. The combination of pulse shaping and an unpreceded peak brightness of the ESS source provides a user with a particularly flexible choice between high resolution and high intensity. We note that the estimated highest resolution in the backscattering detector is Δd ~ 0.0003 Å, which will set a new world record in neutron diffraction. The highest-resolution diffraction will be available from the first days of ESS operation, using a dedicated detector. Another feature of the instrument is the neutron polarizer, which will enable half-polarization studies of magnetic nanoparticles at low scattering angles. The construction of the instrument at the ESS site has begun in December 2021. Two experimental caves, detector support frame, sample vessel, and control hutch have been completed. In this talk, I will remind the broad science case of DREAM, which still remains very relevant. The progress on manufacturing all instrument components will be discussed, including the most recent installation activities. We will outline our plans for the instrument commissioning with and without neutrons at the ESS site.

### [483] Recent upgrade at high resolution SANS diffractometer D16@ILL. (11:30)

*Presenter: CRISTIGLIO, Viviana*

D16 is one of ILL's 2-axis cold neutron diffractometer. In terms of Q-space and Q-resolution, D16 nicely fills the gap between the small angle instruments and classical diffractometers. Because of its special characteristics, D16 remains unequaled for the study of a wide range of systems in biology, physics, and material science. Its specifications have been optimized for the study of structures with relatively large periodicities of about 5 nm. These include large unit-cell lamellar organizations such as membranes or clays, two-dimensional membrane and surface lattice structures, colloidal and liquid structures, magnetic systems with large fluctuations giving rise to satellite reflections very close to Bragg peaks or small-angle scattering. The instrument geometry offers a variable vertical focusing which allows working in reflectivity or diffraction mode. The scattering geometry obtained with large, vertically oriented samples, profits the most from the large vertical cross-section of the beam at the sample position. A high-resolution SANS setup is used routinely in experiments requiring the 1% wavelength bandwidth and the high angular resolution of the instrument. In this presentation, the ENDURANCE II detector project will be presented as well as examples where a major gain would be provided by a large banana detector (protein arrangement at nm scale, nanoporous materials, semi-crystalline polymers, time-resolved and/or small sample experiments, as levitation, samples under mechanical stress). The new design, the major characteristics, performances and new directions of the instrument will be shown, as well as recent examples of research on D16.

### [393] Benchmarking the FLUKA predictions of the neutron flux delivered at the INES instrument and envisaged solution for reducing the background. (11:50)

*Presenter: QUINTIERI, Lina*

INES is a powder diffractometer operated at ISIS, in which thermal and epithermal neutrons are used to study elemental and isotopic composition of materials, with special application to cultural heritage studies. In this talk we present the comparison of the average neutron fluence rate measured at INES with the predictions based on the FLUKA_CERN simulations. The total integrated flux, the full energy spectrum and the spatial distribution of neutrons at the sample location have been calculated by coupling the FLUKA_CERN model of the ISIS Target Station 1 with the Mcstas instrument beam line one. Particularly interesting is the benchmarking of the predictions in the epithermal region of the neutron spectrum for its peculiar fundamental relevance for the INES beam line. A practical solution to reduce the background is also analysed and suggested as a valuable option of whom all the instruments fed by the water moderators in the ISIS-TS1 experimental hall could eventually benefit.

### [119] CERBERUS: The Multi-purpose Neutron Scattering Instrument at the First Target Station of the Spallation Neutron Source. (12:10)

*Presenter: FROST, Matthew*

The Neutron Scattering User Program at Oak Ridge National Laboratory in Oak Ridge, USA has long needed a single-crystal alignment station co-located with its Time-of-Flight Spectroscopy instrument suite. The First Target Station (FTS) at the Spallation Neutron Source (SNS) has an open beam port located at position 16a which looks at a poisoned-decoupled thermal-water moderator. The floor space in that area of the FTS instrument hall is limited and will only accommodate an instrument with a very compact design. We have identified an opportunity to utilize this flux and expand the experiment capability available at the SNS. The instrument will have two stations located at 20 meters and 31 meters. The availability of these two positions will provide opportunities to operate in three distinct modes: as an alignment station (SXA), a near-infrared Beryllium-filter spectrometer (BeFAST), and as a nuclear cross-section measurement station (XSM). We expect a new instrument of this type to complement existing capabilities at the SNS and HFIR and provide an opportunity to support new user communities and expand the scientific contributions of the SNS. Details of the expected instrument capability as well as a proposed layout and targeted user science cases will be presented. This research used resources at the High Flux Isotope Reactor and Spallation Neutron Source, a US Department of Energy, Office of Science User Facility operated by the Oak Ridge National Laboratory.

## Engineering 1 - SCC/0-001 - Lecture hall (20 Mar 2023, 11:00 - 12:30)

**-Chairs: Michael Hofmann; Sandra Cabeza Sanchez**

### [10] Monitoring the precipitation of the hardening phase in the new VDM® Alloy 780 by in-situ high-temperature small-angle neutron scattering, neutron diffraction and complementary microscopy techniques (11:00)

*Presenter: SOLIS, Cecilia*

The hardening phase precipitation process plays an important role in the development of new Ni-base superalloys. In the present work, we apply a powerful combination of advanced characterization techniques to characterize in-situ the $\gamma$' precipitation in the new VDM® Alloy 780. During the whole heat treatment process, in-situ time-of-flight (TOF) neutron diffraction (ND) unambiguously identified the $\gamma$' phase as well as its weight fraction and the misfit with the matrix while in-situ small-angle neutron scattering (SANS) provided precise precipitates' size analysis. Atom probe tomography (APT) and scanning electron microscope (SEM) provided detailed microstructural characterization and chemical composition of the phases necessary for a proper neutron scattering data evaluation. This contribution reveals more detailed information on the nucleation, growth, and Ostwald ripening processes starting from the early precipitation stage in bulk samples using the complementary microstructure investigation methods. The nucleation and growth kinetics of precipitates at 720 °C depend on heating rates and the size distribution obtained in the pre-heating history of the sample. A subsequent heat treatment step at 620 °C, typically used in Ni-base superalloys, does not lead to similar progressive precipitation or growth. The expected matrix-diffusion-controlled Ostwald ripening process of the $\gamma$' precipitates was in-situ monitored by SANS on full precipitation hardened sample at expected operating temperatures (750 °C) showing smaller coarsening kinetics than other reported Ni-based superalloys.

### [159] The effect of location in the build space on the mechanical properties in Ti-6Al-4V samples produced by EBM (11:30)

*Presenter: RAFAILOV, Gennady*

From all possible Additive Manufacture methods, the electron beam melting (EBM) of Ti-6Al-4V has the closest properties to the traditionally produced Ti-6Al-4V. Therefore, EBM Ti-6Al-4V can be used in many engineering parts, yet its material properties must be understood completely. In particular, the differences among properties of objects oriented vertically or horizontally with respect to the build direction were subject to large numbers of research work. In this work, we will compare and explain the difference in properties as a function of printing orientation in the entire range between vertical to horizontal orientations, by studying six Ti-6Al-4V rods at different angles with respect to the build direction. We will determine the variation in mechanical properties as a function of the building space. The mechanical response and deformation were analyzed by neutron scattering undertaken on the HIPPO diffractometer at Los Alamos National Laboratory. The texture was measured at different deformation levels i.e the texture variation for each rod was measured from as printed state to 10% strain, 14% strain, 17% strain, and failure. We will compare and explain the mechanical properties' relation to texture differences.

### [341] Advanced characterization of additive manufacturing samples through Bragg edge imaging (11:50)

*Presenter: MALAMUD, Florencia*

Additive manufacturing (AM) has gained significant importance in the past years and is regarded to have the potential to revolutionize the manufacturing processes of materials, enabling complex geometries that are not feasible to be built using conventional manufacturing processes. The increasing complexity of AM-built components demands advanced spatially-resolved characterization techniques to characterize the microstructure distribution with the corresponding three-dimensional spatial resolution. Bragg edge imaging (BEI) holds great potential in spatially resolved studies of engineering materials, and enables local crystallographic observations even in complex components. The technique is based on the wavelength-dependent effect of neutron diffraction at crystal lattice planes on the neutron transmission spectrum. The wavelengths of discontinuities (Bragg edges) in the neutron transmission spectrum, directly relate to respective lattice spacings, allowing crystalline phase identification and lattice strain analysis, while the overall wavelength-dependent transmission pattern provides information of other microstructural features as defects or texture variations. Here, different examples will be presented, related to the application of BEI for advanced microstructural characterization of additive manufacturing samples, layered specimens built by multimaterial laser powder bed fusion and complex metastable steel components built by LPBF with locally tuned microstructure.

### [56] Scaling and Fouling in Reverse Osmosis Wastewater Desalination – Operando Studies with Small-Angle Neutron Scattering (12:10)

*Presenter: SCHWAHN, Dietmar*

The treatment of water for potable use is one of the great challenges of our time. Reverse osmosis (RO) desalination is a widely used technology for the treatment of sea and wastewater. A main problem is scaling and fouling of the membrane surface, which prevents the optimal use of this technology [1]. Our goal is to investigate these phenomena at the microscopic level using operando SANS techniques under most realistic conditions in combination with H2O/D2O contrast variation. We will present

mineral scaling as well as silica and protein (BSA) fouling on the surface of polyamide membranes with the following results: (i) Aqueous silica dispersions form a crystalline cake layer of simple cubic order. The cake layer could be removed at larger crossflow. Only in one case did we observe irreversible cake layer formation, which has the characteristics of an unstable phase transition from otherwise first-order liquid-solid phase transitions [2]. (ii) Organic fouling of BSA dissolved in a model wastewater solution is determined by the immediate formation of stable organo-mineral colloids, i.e., composite particles of about micrometer size that increase only in number density. Their composition was about 50% protein and 50% minerals, mainly calcium phosphate and carbonate, as analyzed in previous in vitro SANS measurements [3]. [1] S.E. Bone et al, Joule 4 (2020) 1-23. [2] V. Pipich et al, Membranes (MDPI) 11 (2021) 413. [3] V. Pipich et al, Langmuir 29 (2013) 7607-7617.

## Frustrated Magnets 1 - SCC/3-Venus - Venus (20 Mar 2023, 11:00 - 12:30)

**-Chairs: Yixi Su; Ross Stewart**

### [184] Quantum spin liquid in the Ising triangular-lattice antiferromagnet NdTa7O19 (11:00)

*Presenter: PREGELJ, Matej*

Spin liquids–strongly correlated, yet disordered magnetic ground states–are extremely attractive from fundamental as well as application point of view [1,2]. While their realizations are scarce and not yet completely understood, they are praised as a platform for quantum computers. A classical spin liquid is predicted for the Ising antiferromagnetic triangular model, while additional non-commuting exchange terms should induce its quantum version. Here we present our discovery of quantum spin liquid in the triangular-lattice antiferromagnet NdTa$_7$O$_{19}$ [3]. Our refinement of magnetic susceptibility, magnetization, inelastic neutron scattering and electron paramagnetic resonance spectra reveals an Ising-type Kramers doublet ground state of Nd$^{3+}$ ions. The Curie-Weiss temperature imply exchange interaction of ~0.5 K, yet no magnetic reflections were found down to 40 mK. However, polarized neutron diffraction at 50 mK reveals diffuse magnetic scattering corroborating Ising correlations between the nearest neighbours. Finally, dynamical nature of the ground state down to 66 mK is confirmed by muons spin relaxation. Our study [3] shows the key role of strong spin-orbit coupling in stabilizing spin liquids resulting from magnetic anisotropy and highlights rare-earth (RE) heptatantalates RETa$_7$O$_{19}$ as a novel framework for realization of these states. [1] Y. Tokura *et al.* Nat. Phys. 13, 1056 (2017) [2] D. Basov *et al.* Nat. Mater. 16, 1077 (2017) [3] T. Arh *et al.* Nat. Mater. 21, 416 (2022)

### [145] Understanding synthesis-driven structure-property relationships in quantum materials (11:30)

*Presenter: GRAHAM, Jennifer*

Quantum materials are a broad class of systems that exhibit many unusual and exotic phenomena [1] in which the chemical and magnetic ground states can be deeply intertwined. For example, ZnV2O4 is an S = 1, cubic spinel which contains a geometrically frustrated pyrochlore sublattice. Previous studies have shown that the magnetic ground state for ZnV2O4 appears to be highly sample dependent, ranging from an antiferromagnet to an unconventional and highly frustrated spin glass [2-4]. We hypothesise that local deviations from the average chemical structure, which arise during the sample preparation, are at the heart of this problem. To explore this, we have prepared two powder samples of ZnV2O4 using different synthetic routes, a conventional solid-state route and a novel rapid microwave-assisted method [5]. In this talk we will explore how synthesis impacts the evolution of the chemical and magnetic ground states of ZnV2O4, using high-resolution powder neutron and X-ray diffraction and magnetometry to reveal the average structural and magnetic behaviour, and, X-ray pair distribution function analysis and diffuse neutron scattering data to understand the local structure. References 1. C. Broholm et al., Science 367 6475 (2020) 2. Y. Ueda et al., J. Phys. Soc. 66, 3 (1997) 3. S. Ebbinghaus et al. J. Alloys Compd., 370, 75 (2004) 4. A. J. Browne and J. P. Attfield, Phys. Rev. B, 101, 024112 (2020) 5. E. E Levin et al. Chem Mater. 31 18, 7151 – 7159 (2019).

### [232] High-resolution spectrum of fractional excitations in Ce$_2$Sn$_2$O$_7$ (11:50)

*Presenter: SIBILLE, Romain*

A correlated liquid state was reported in the pyrochlore Ce$_2$Sn$_2$O$_7$. Its nature remained elusive, but with additional knowledge on the crystal-electric field scheme, the case of cerium pyrochlores was further investigated based on degrees of freedom having both magnetic dipole and magnetic octupole components. A number of recent studies all point towards a quantum spin ice (QSI) based on a manifold of ice-rule correlated octupoles to be stabilized in these materials. Theorists had conceptualized such an octupolar QSI, where quantum dynamics is endowed by couplings between other components of the ‘dipole-octupole’ pseudo-spins. This talk reviews findings reported so far on Ce$_2$Sn$_2$O$_7$, puts these in perspective with results on other cerium pyrochlores, and presents new experimental data that further hint at cerium pyrochlores being genuine representatives of QSI – the model 3D quantum spin liquid. In particular, we argue that excitations observed in Time-Of-Flight spectroscopy are associated with the fractional excitations of QSI. Using backscattering experiments performed on IN16B, we further confirm this conclusion. The improved energy resolution allows detailed comparisons with theories for spinon dynamics in QSI. It is predicted that the alternative vacuum of this condensed matter system is drastically different from that of our Universe, with phenomena arising from strong light-matter interactions. We observe a gapped spectrum with an edge structure corroborating the predictions for the effects of photons on the production of matter excitations.

### [171] Fractional Excitation-induced Phonon Renormalization in α-RuCl3 (12:10)

*Presenter: MERRITT, Adrian*

The quantum spin liquid (QSL) phase is of immense interest to condensed matter physicists, and have been studied for decades. With a Kitaev model that is exactly solvable and gives a QSL ground state, α-RuCl3 is a promising Kitaev QSL candidate. Above the critical magnetic field Bc~7T and below T~6K there is evidence for the fractional excitations in the QSL phase. Although previous inelastic neutron scattering measurements have focused on magnetic excitations, the phonon dispersions have not been well-studied. However, recent theoretical work has shown that the fractional excitations can induce phonon renormalization via the spin-lattice coupling, and would in particular affect the acoustic phonons. Our measurements have focused on the phonon dispersion in α-RuCl3 to observe this phonon renormalization effect. We have used high-quality in-house grown α-RuCl3 single

crystals for inelastic neutron and x-ray scattering measurements, combined with phonon dynamics calculations, to survey the acoustic phonons, in particular under magnetic fields. We will discuss our results with a focus on examining the low-energy acoustic phonon relevant to the phonon renormalization effect. Notably, our inelastic neutron scattering measurements under magnetic field will be compared with inelastic x-ray scattering measurements without a magnetic field and with DFT calculations of the phonon branches to clarify the behavior of these phonon branches in this phase of interest.

## Neutron Methods - MW 0 001 - Lecture hall (20 Mar 2023, 11:00 - 12:30)

**-Chairs: Christian Franz; Mogens Christensen**

### [7] Uniaxial Control of Quantum Matter (11:00)

*Presenter: SIMUTIS, Gediminas*

Quantum matter is characterised by competing and intertwined orders. Here I will present our recent advances in using uniaxial pressure as a clean “surgical” tool to tune quantum phases while simultaneously obtaining microscopic insights via scattering experiments. In particular, we address two directions - minimizing the background and enabling the tuning in-situ. First, we study spin order in cuprate superconductors characterized by small moments, which remains challenging for pressure studies. We overcome this challenge by designing a low-background uniaxial strain cell, optimizing the experiment based on neutron-tracing simulations and using aggressive focusing and energy analysis. We show that the spin order parameter in cuprates is uniaxial and coupled to the charge channel [1]. Second, to further improve the feasibility and speed of such experiments, we have designed a new in-situ uniaxial device for large-scale facility research based on an actuator-motor mechanism, efficient feedback loops and the sample-holder design enabling rapid exchange of the samples [2]. I will demonstrate the improved capabilities of this device reporting the control of charge order in cuprates and magnetic phases in skyrmion materials, respectively. [1] Simutis et al. in review and arXiv:2204.02304 (2022) [2] Simutis et al. in review and arXiv:2207.13194 (2022)

### [310] Recent advances in the development of holographic optical components for very cold and cold neutrons (11:30)

*Presenter: HADDEN, Elhoucine*

Milestone steps have been taken recently to meet the requirements of experimenters using cold (CN) and very cold (VCN) neutrons. In fact, despite the wide range of experiments that can benefit from the long wavelength neutrons, e.g. in the study of slow dynamics within large structures, or in the study of the neutron itself as a quantum object, their use remains limited compared to thermal neutrons. Aiming to make the realization of such experiments simpler and more accessible for a larger scientific community, we present our recent developments in the fabrication of thermally and mechanically stable optical components showing good diffraction efficiencies, and allowing for a good space management thanks to sufficiently large diffraction angles. We present the synthesis, recording process together with the light and neutron diffraction results of nanodiamond based nanoparticle-polymer composites holographic gratings [1, 2]. The diamond core has large coherent scattering and low incoherent scattering cross sections with low absorption, making it the best candidate for CN and VCN holographic optical elements. Furthermore, we highlight the impact of emerging phenomena i.e the grating decay along its thickness, the holographic scattering phenomenon and the influence of the wide VCN spectrum on the analysis of the neutron diffraction results. [1] Tomita et al. Physical Review Applied, 14:044056, 2020 [2] Hadden et al. Proc. SPIE, 12151:1215109-1-7, 2022

### [193] Recent Progress in the use of time-of-flight SESANS and other Larmor precession techniques on Larmor. (11:50)

*Presenter: DALGLIESH, Robert*

The neutron spin-echo system on the Larmor instrument at ISIS has now been operating for more than 5 years. The system was design by TU-Delft to be highly flexible for utilisation in a wide range of Larmor precession techniques including SESANS, SEMSANS, MIEZE-SANS, Larmor Diffraction and TOFLAR. The flexibility and complexity of the system has unfortunately led to some difficulties in routine operation that have taken time to resolve. It is now believed that the system can be operated in a reliable and reproducible manor and in recent cycles a significant number of SESANS experiments have been carried out with both expert and non-expert users. The wider collaborative effort between the groups at TU-Delft, ISIS, ORNL and Indiana University to develop simulations and standards for cross calibration of instruments has also made progress. Some recent results from Larmor and the development of standards will be discussed along with a brief review of some of the other projects that are ongoing on the beamline.

### [40] Fast neutron inelastic scattering technique for characterization of rare-earth elements in magnetic materials (12:10)

*Presenter: MELESHENKOVSKII, Iaroslav*

Recycling of rare-earth elements contained in magnetic materials is an important step towards sustainability of valuable resources. The challenges are many and such tasks require analytical techniques to characterize the composition of the waste flows. Characterization of the rare-earth elements in industrial scale is a new challenge to take up. The existing traditional methods used for determination of rare earth elements content are usually based on chemical analytical methods such as ICP-MS or –OES and non-destructive methods such as XRF and LIPS. However, the former require chemical dissolution of a part of a sample and the latter provide only a near surface information. Non-destructive methods based on PGNAA with cold or thermal neutrons reach their performance capabilities in such applications due to attenuation of the interrogation beam in bulk and dense waste flows. Fast neutron inelastic scattering prompt gamma activation (PGA-INS) technique has been proposed as a promising

technology to tackle the mentioned challenges. In this presentation, we discuss on the method physics, instruments and detection methodologies, present the preliminary experimental results acquired with the FaNGaS instrument installed the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching, as well as provide an outlook on the future research activities necessary for method application in industrial tasks.

## Proteins & Peptides seen by Neutrons - MW 2 001 - Lecture hall (20 Mar 2023, 11:00 - 12:30)

**-Chairs: Michaela Zamponi; Tommy Nylander**

### [89] Diffusive Dynamics of Bacterial Proteome as a Proxy of Cell Death (11:00)

*Presenter: PETERS, Judith*

Temperature variations have a big impact on the bacterial metabolism and death, yet an exhaustive molecular picture of these processes is still missing. For instance, whether the thermal death is determined by the deterioration of the whole or a specific part of the proteome is hotly debated. In our work, by monitoring the proteome dynamics of E. coli we show that only a minor fraction of the proteome unfolds at the cell death. First, we prove that the dynamical state of the E. coli proteome is an excellent proxy for the temperature dependent bacterial metabolism and death. The proteome diffusive dynamics peaks at about the bacterial optimal growth temperature, then a dramatic dynamical slowdown is observed which starts just below the cell's death temperature. Next, we show that this slowdown is caused by the unfolding of just a small fraction of proteins which establish an entangling inter-protein network—dominated by hydrophobic interactions— across the cytoplasm. Finally, we prove that the deduced progress of the proteome unfolding and its diffusive dynamics are both key to correctly reproduce the E. coli growth rate.

### [166] Hemoglobin diffusion and polymerization in HbFxHbS1-x compounds (11:30)

*Presenter: LONGEVILLE, Stéphane*

Sickle cell disease (SCD) is a genetic blood disorder, inducing severe anemia. It results from the polymerization of the oxygen-carrying protein hemoglobin found in red blood cells (RBC), which leads to a deformation of the cells to rigid, sickle-like shape under certain circumstances that will obstruct capillaries vessels, and will ultimately induce the disease of different organs. The hemoglobin (HbS), that is at the origin of this blood disorder, is a variant of normal human hemoglobin A0 (HbA0) whose sequence only differs by two amino acids over the 574 of the protein. Human that are homozygote of HbS gene (inherited from both parents) suffer from a severe anemia. SCD was the first identified molecular disease by Linus Pauling, in 1949 [1]. The pharmacological treatments for sickle cell disease include hydroxyurea, a molecule that promotes the synthesis of fetal hemoglobin (HbF) that leads to a hemoglobin mixture HbFxHbS(1-x) in blood with HbF partially or fully inhibiting HbS polymerization depending on its concentration. We have shown previously that diffusion inside the red blood cells is similar to that in solution at the same concentration [2]. From the concentration dependence of the diffusion coefficient and using a simple model developed for oxygen uptake in the lungs [3] we have stressed that not only the diffusion of hemoglobin is necessary to obtain the full oxygenation of the RBC during the limited time of transit in the capillary close to the alveolar sac [4] but the concentration of hemoglobin inside RBC corresponds to an optimum oxygen transport for an individual under physical activity. We investigated the structure and the dynamics of HbS and HbF mixtures to better understand 1- how HbF will inhibit HbS polymerization, under which concentration and partial oxygen pressure. The impact of oxygen partial pressure is fundamental, because in the body it differs from the alveoli (PO2=160 mm.Hg) down to the heart (PO2=10-20 mm.Hg). And 2- gain insight on the oxygen exchange process at the RBC level. We will present how the intermediate scattering function is strongly affected by the oxygen partial pressure and the fraction of HbF present in solution (x). Moreover, we will show how the free (non polymerized) Hb diffusion is affected by polymerization and discuss the physiological implications. [1] L. Pauling et al. Science 110, 543–548 (1949). [2] W. Doster and S. Longeville, Biophys. J. 93 (4) , 1360-1368 (2007) [3] A. Clark et al., Biophys. J., 47, 171 (1985). [4] S. Longeville et al., Scientific Report, 7, 10448 (2017)

### [130] Organisation of photosynthetic thylakoid membranes during simulated coral bleaching - a SANS study (11:50)

*Presenter: GARVEY, Christopher*

Small angle neutron scattering (SANS) is a non-ionizing and non-destructive statistical probe of structure. When applied to actively metabolizing cells it can provide a perspective on structural changes associated with cell physiology. Here we report on the application of SANS to understand environmentally induced physiological changes of corals. Corals bleach under a number of stresses, one of these being thermal stresses exemplified by the 2010, 2016 and 2017 bleaching events in Australia's Great Barrier Reef. The aim of this work is to utilize SANS to probe the arrangements of the intra-cellular membranes associated with photosynthetic apparatus of the symbiotic algae known as zooxanthellae or Symbiodinium living in hospice in coral cells. Here we report on the temperature induced rearrangements of photosynthetic membranes in Symbodium living within individual Aiptasia anemone specimens extracted from SANS data using a model of the structure. The SANS curve is a number of broad peaks superimposed on a Porod like decay. These shape, relative intensity and angular position of these features are analysed within a model of the organisation of membranes developed from electron microscopy. The results provide a simple perspective on the effects of temperature on the photosynthetic machinery of the symbiote.

### [78] Influence of polarisation analysis on buffer subraction (12:10)

*Presenter: SARTER, Mona*

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. The results and the implications for data treatment in the future will be discussed.

## From Membranes to Kinetics and Dynamics - MW 2 001 - Lecture hall (20 Mar 2023, 14:00 - 16:00)

**-Chairs: Christopher Garvey; Margarita Kruteva**

### [41] Planar lipid bilayers as model biological membranes for structural neutron studies (14:00)

*Presenter: FRAGNETO, Giovanna*

Cells, the basic units of living organisms, are well delineated and separated from the external environment by membranes. Capable of both enclosing the cellular constituents and allowing exchanges with the outside world, these membranes are only a few nanometers thick. To study the dynamics and function of these amazing objects, physicists first seek to understand their structure. This involves experiments on model systems, simpler and better controlled than real membranes, and can profit from a probe that is able to access different scales of size and time: thermal neutrons. Since the pioneering work in the seventies on cell membrane structure by neutron scattering, developments driven by constantly improving neutron instrumentation, coupled with development of measurement and analysis methods, have involved both the optimization of samples towards more biologically relevant model systems and include the use of more complex lipid mixtures up to natural extracts. A natural lipid deuteriation facility has been set-up at the ILL (http://www.ill.eu/L-Lab) and recent results on lipid production and characterisationn will be presented. Recent developments in the study of the structure of membranes will be presented including neutron and x-ray reflectometry study of the out-of-equilibrium fluctuations of phospholipid membranes induced by the active transmembrane protein bacteriorhodopsin (BR) [1] and the effect of phospholipase2 on lipid bilayers [Corucci et al., submitted]. Furthermore, the use of neutron scattering methods to study the interaction of the spike protein of SARS-CoV-2 virus will be presented [2], including results revealing the different roles of peptides present within the fusion domain and the role of intracellular calcium levels that could provide an indication to where and how the viral and host membranes fuse during SARS-CoV-2 infection [3]. *References* [1] Insertion and activation of functional Bacteriorhodopsin in a floating bilayer by T. Mukhina et al., JCIS (2021) [2] Lipid bilayer degradation induced by SARS-CoV-2 spike protein as revealed by neutron reflectometry, by A. Luchini et al. Scientific Reports (2021) [3] Strikingly Different Roles of SARS-CoV-2 Fusion Peptides Uncovered by Neutron Scattering", by A. Santamaria et al., J. Am. Chem. Soc. (2022).

### [484] Metabolically-incorporated deuterium in myelin from mice localized by neutron diffraction (14:30)

*Presenter: DEMÉ, Bruno*

Myelin is a natural and dynamic multilamellar membrane structure that continues to be of significant biological and neurological interest, especially with respect to its biosynthesis and assembly during its normal formation, maintenance, and pathological breakdown. To explore the usefulness of neutron diffraction in the structural analysis of myelin, we investigated the use of in vivo labeling by metabolically incorporating non-toxic levels of D2O via drinking water into a pregnant dam (D-dam) and her developing embryos. All of the mice were sacrificed when the pups (D-pups) were 55 days old. Myelinated sciatic nerves were dissected, fixed in glutaraldehyde and examined by neutron diffraction. Parallel samples that were unfixed (trigeminal nerves) were frozen for mass spectrometry (MS). The diffraction patterns of the nerves from deuterium-fed mice (D-mice) vs. the controls (H-mice) had major differences in the intensities of the Bragg peaks but no differences in myelin periodicity. Neutron scattering density profiles showed an appreciable increase in density at the center of the lipid-rich membrane bilayer. This increase was greater in D-pups than in D-dam, and its localization was consistent with deuteration of lipid hydrocarbon chains, which predominate over transmembrane proteins in myelin. MS analysis of the lipids isolated from the trigeminal nerves demonstrated that in the pups the percentage of lipids that had one or more deuterium atoms was uniformly high across lipid species (97.6% +/- 2.0%), whereas in the mother the lipids were substantially less deuterated (60.6% +/- 26.4%) with levels varying among lipid species and subspecies. The mass distribution pattern of deuterium-containing isotopologues indicated the fraction (in %) of each lipid (sub-)species having one or more deuteriums incorporated: in the D-pups, the pattern was always bell-shaped, and the average number of D atoms ranged from a low of ~4 in fatty acid to a high of ~9 in cerebroside. By contrast, in D-dam most lipids had more complex, overlapping distributions that were weighted toward a lower average number of deuteriums, which ranged from a low of ~3–4 in fatty acid and in one species of sulfatide to a high of 6–7 in cerebroside and sphingomyelin. The consistently high level of deuteration in D-pups can be attributed to their de novo lipogenesis during gestation and rapid, postnatal myelination. The widely varying levels of deuteration in D-dam, by contrast, likely depends on the relative metabolic stability of the particular lipid species during myelin maintenance. Our current findings demonstrate that stably-incorporated D label can be detected and localized using neutron diffraction in a complex tissue such as myelin; and moreover, that MS can be used to screen a broad range of deuterated lipid species to monitor differential rates of lipid turnover. In addition to helping to develop a comprehensive understanding of the de novo synthesis and turnover of specific lipids in normal and abnormal myelin, our results also suggest application to studies on myelin proteins (which constitute only 20–30% by dry mass of the myelin, vs. 70–80% for lipids), as well as more broadly to the molecular constituents of other biological tissues.

### [272] Timescale of SARS-Cov2 virions with human host cells (15:00)

*Presenter: JAKSCH, Sebastian*

The fusion of viral and host cell membranes is a pivotal step in the infection and life cycle of any virus. Despite the massive global research interest in SARS-CoV-2 many aspects of the fusion process are still only rudimentarily understood. Biological fusion

assays are widely applied to study different steps of viral-host membrane fusion, however, multidisciplinary approaches offer a broader range of parameters to study and the exact timescale of the fusion on a microscopical scale is still elusive. Here, we report the establishment of a new model system for viral fusion based on the neutron scattering behavior of tailored unilamellar lipid vesicles with specific membrane proteins, either SARS-Cov2 spike or ACE2 receptor proteins. Our target was to design individual vesicles from cellular material which only contain the membrane proteins included in the initial cellular plasma membrane and none of the organelle membranes within the cell. Thus, by protein expression on the cells, individual virion and target vesicles could be designed. The results of creating 100 nm unilamellar vesicles by extrusion were confirmed by several methods, among the dynamic light scattering as well as small-angle X-ray and neutron scattering. A contrast matched fusion experiment with SANS allowed us to determine the timescale of the fusion between SARS-Cov2 virions and human host cells.

### [421] Orange Carotenoid Protein: Effect of Internal Dynamics on Protein Functionality (15:20)

*Presenter: GOLUB, Maksym*

In cyanobacteria, photosynthesis is initiated by light absorption in protein complexes referred to as phycobilisomes (PBs). In excess light, photodamage to the photosynthetic apparatus is prevented by non-photochemical quenching (NPQ). This adaptive process responsible for high light tolerance is realized by the interplay between the light-harvesting PBs, a light-sensitive effector of NPQ called Orange Carotenoid Protein (OCP), and a regulatory Fluorescence Recovery Protein (FRP). The underlying structural processes are currently a field of intensive research[1-4]. It is well known that OCP exhibits a significant structural change upon photoactivation switching from the ground state (OCPO) to the active state (OCPR). However, the knowledge about the structural changes induced by light is insufficient to describe and understand OCP's functionality. A rarely considered aspect is the importance of internal protein dynamics. Using QENS, we probe the protein dynamics of the orange carotenoid protein in the observation time range from ~0.1 picoseconds to ~26 ps. Our measurements in the dark and under (in-situ-) blue light illumination directly reveal the dynamics in the ground and the active state of OCP, respectively. It is shown that the localized internal dynamics of amino acid residues are significantly enhanced upon photoactivation. This effect is attributed to the light-induced large-scale structural changes exposing larger areas of the protein surface to the solvent. A more open structure of OCPR also causes higher flexibility of structural elements like domain linkers and N-terminal extension. However, the latter enhancement of flexibility is significantly smaller than that observed before for the mutant OCPW288A [5]. That is an inspiring observation since the OCPW288A mutant mimics the overall structure of OCP in the active state, as shown by SANS [5]. Our observation from the QENS experiment suggests that the point mutation destabilizes a relatively rigid part of the protein structure rendering in-situ experiments indispensable to determine the proper active state dynamics. In the present study, we provide the first MD simulations that shed light on the observed difference in protein dynamic between OCP in the active state and its mutant OCPW288A. 1. Kirilovsky, D. and C.A. Kerfeld, Cyanobacterial photoprotection by the orange carotenoid protein. Nat. Plants, 2016. 2(12): p. 16180. 2. Gupta, S., et al., Local and Global Structural Drivers for the Photoactivation of the Orange Carotenoid Protein. Proc. Natl. Acad. Sci. U. S. A., 2015. 112(41): p. 5567-5574. 3. Moldenhauer, M., et al., Assembly of photoactive orange carotenoid protein from its domains unravels a carotenoid shuttle mechanism. Photosynth. Res., 2017: p. 1-15. 4. Golub, M., et al., Solution Structure and Conformational Flexibility in the Active State of the Orange Carotenoid Protein: Part I. Small-Angle Scattering. J. Phys. Chem. B, 2019. 123(45): p. 9525-9535. 5. Golub, M., et al., Solution structure and conformational flexibility in the active state of the Orange Carotenoid Protein. Part II: quasielastic neutron scattering. J. Phys. Chem. B, 2019. 123(45): p. 9536-9545.

### [27] Structural dynamics of substrate processing by the PAN-proteasome complex in solution: a time-resolved small angle neutron scattering study (15:40)

*Presenter: GABEL, Frank*

A multitude of structural biology techniques, including crystallography, NMR and cryo-EM, as well as single molecule experiments, have recently provided new and exciting mechanistic insight into protein substrate degradation by AAA+ ATPases and the proteasome. However, direct structural information on the conformational changes of the working complex and on the respective substrate state(s) and populations, during the active unfolding and degradation process in solution, remains scarce. We use time-resolved small angle neutron scattering (TR-SANS), in combination with selective macromolecular deuteration and solvent contrast variation, to obtain structural information on the respective components during the active degradation process in solution. By using the PAN-proteasome complex from the hyperthermophilic archaeon Methanocaldoccus jannaschii, it was possible to temperature-active and fine-tune the unfolding and hydrolysis process. Combined with online fluorescence, we were able to obtain separate structural information on the conformational state of PAN and on the GFPssrA substrate during the active reaction in solution. We find that PAN undergoes a reversible conformational contraction during the substrate unfolding process. GFP aggregates rapidly in the presence of PAN alone but is being hydrolyzed very efficiently once the proteasome is added to the reaction.

## Glasses & Liquids - SCC/3-Venus - Venus (20 Mar 2023, 14:00 - 16:00)

**-Chairs: Wiebke Lohstroh; Natalie Malikova**

### [30] Open problems in liquids dynamics: the role of neutron scattering (14:00)

*Presenter: GUARINI, Eleonora*

We review recent inelastic neutron scattering experiments aimed at the investigation of still open issues in the dynamics of liquids at the nanometer and picosecond scales. It is shown that the interpretation of experimental results is put on solid grounds by the application of modern methods of analysis and lineshape modeling which ensure the fulfillment of fundamental physical properties that the spectra must obey. This last condition, especially when studying weak signals in the dynamic structure factor, becomes crucial to avoid overinterpretations of the real information conveyed by scattering data. Moreover, we highlight the different roles that neutron data presently play in relation with molecular dynamics simulations, depending on the addressed physical problem and the nature of the sample, by including in the discussion the case of quantum liquids. In particular, we show how neutron measurements remain an indispensable benchmark in assessing the present capabilities of classical and quantum simulation methods. We also illustrate the potential of statistical methods, such as Bayesian inference, when applied to neutron data analysis and the opportunity they provide in establishing the spectral features without *ab initio* assumptions on the model lineshape, i.e., on the expected dynamical processes: an effective tool aimed at avoiding biases of confirmation which conventional and physically unconstrained analyses are sometimes exposed to.

### [448] New opportunities for liquid neutron spectroscopy at ISIS (14:30)

*Presenter: STEWART, Ross*

Quasi-elastic neutron spectroscopy of liquids is in common usage at the ISIS Neutron and Muon Source, UK, to examine incoherent (non-propagating) dynamical properties, such as diffusion constants and local internal molecular modes. However, it is much more difficult to measure coherent excitations in liquids with neutrons due to their kinematical constraints - namely the rather limited range of excitation energies at low momentum transfers, where the coherent liquid modes must be measured. As a result, coherent liquid spectroscopy is most commonly attempted using inelastic X-ray scattering. In principle, however, neutron spectroscopy should be able to provide much better data than IXS, since the energy resolution is generally much better, and the line-shape is a well-behaved Gaussian function rather than a Lorentzian. We will present recent data taken on the LET and MERLIN direct geometry neutron time-of-flight spectrometers on propagating excitation modes in liquids, including measurements under pressure. We will also present an instrument concept called BRILL, which is a recently-proposed direct geometry neutron time-of-flight spectrometer at ISIS, dedicated to the measurement of low-momentum transfer propagating excitations.

### [258] Unraveling the coherent dynamic structure factor of liquid water measured by neutron spectroscopy with polarization analysis: a molecular dynamics simulation study (15:00)

*Presenter: COLMENERO, Juan*

This work is focused on atomistic molecular dynamics (MD) simulations of water carried out at 300 K. The main goal was to better understand the experimental results of the coherent dynamic structure factor S(Q,$\nu$) of D$_2$O that were obtained by means of neutron scattering with polarization analysis and previously reported by us [1]. First, the simulations were directly validated by direct comparison of both imaginary part of the susceptibility χ''(Q,$\nu$) and S(Q) --calculated from the simulations-- with the corresponding experimental results. After that, we have considered the time domain S(Q,t) as well as its self- and distinct-contributions. We have also calculated S(Q,t) corresponding to a H$_2$O sample. The main results obtained are: (i) The Q-independent relaxation process identified in S(Q,$\nu$) in the mesoscopic range (Q$^0$-mode) is the responsible of the restructuring of the hydrogen bond (HB) network at times shorter than that corresponding to the molecular diffusion; (ii) the vibrational contribution identified at high frequency in S(Q,$\nu$) corresponds to a hydrodynamic-like mode propagating in a medium with fixed HB bonding pattern; (iii) in the crossover range from mesoscopic to intermolecular scales, diffusion also progressively contributes to the decay of density fluctuations; (iv) MD-simulations suggest that it would be basically impossible to measure S(Q,$\nu$) of H$_2$O in the mesoscopic range with the current neutron scattering capabilities. References [1] A. Arbe, G. Nilsen, J. R. Stewart, F. Alvarez, V. García-Sakai and J. Colmenero, Physical Review Research **2**, 022015 (2020).

### [497] Using neutrons for the study of amorphous materials: PDF analysis and titanium glasses (15:20)

*Presenter: GIRON LANGE, Esther*

The atomic-scale structure of liquids and glasses is crucial for understanding their material properties. However, amorphous materials lack of translational periodicity that leads to the Bragg peaks observed in the diffraction pattern for a crystal. Instead, the diffraction pattern is diffuse, and it is a challenge to solve the structure. The understanding of the neutron diffraction patterns measured for structurally disordered materials is achieved by means of Pair Distribution Function (PDF) analysis. This theory allows to obtain real-space structural information in the form of partial pair-distribution functions g(r) [1]. Due to the complexity of glassy and liquid systems, understanding their structures often requires of multiple techniques and PDF analysis on neutron diffraction experiments has efficiently been used in numerous systems [2][3]. One application where this technique is found useful is on the understanding of nucleation, crystal growth and the physical properties of glasses. This is of increasing interest among

industry due to the potential versatility of the material’s design. For this purpose, PDF analysis proves to be a powerful technique when combined with other techniques such as TEM, x-ray diffraction or NMR. Determining the structure of the systems, although still challenging, becomes possible. This information can lead to the design a priori of new families of glasses without the need of producing and testing many different materials. For example, in titanium glasses the presence of this metal has been observed to play a structural role on: (i) its optical properties (ii) inner crystal growth processes. These systems benefit from the negative neutron scattering length of titanium in contrast with its positive x-ray scattering length. Thus, a quantitative analysis of the short-range structure is possible when these two techniques are combined. [1] H. E. Fischer, A. C. Barnes, and P. S. Salmon. Neutron and x-ray diffraction studies of liquids and glasses. Rep. Prog. Phys., 69:233–299, 2006. [2] P. Salmon and A. Zeidler. Networks under pressure: the development of in situ high-pressure neutron diffraction for glassy and liquid materials. Journal of Physics: Condensed Matter, 27:133201, 2015. [3] U. Hoppe. Structure of titanophosphate glasses studied by x-ray and neutron diffraction. Journal of Non-Crystalline Solids, 353:1802–1807, 2007.

### [124] Experimental evidence for a dynamical crossover in liquid metals (15:40)

*Presenter: DEMMEL, Franz*

Cooling a liquid and avoiding crystallization the viscosity will increase dramatically and finally the viscous liquid will arrest into the glass state. This process is accompanied by a slowing down of the structural relaxation process. However, it is unclear whether there exists a particular, universal temperature range at which the slowing down sets in. We investigated the dynamics of liquid metals, ranging from rubidium over lead to aluminium, to scrutinize changes with temperature [1]. To this end we measured the temperature dependence of the collective particle dynamics at the structure factor maximum through inelastic neutron scattering. In addition, we investigated the intermediate scattering function, which becomes non-exponential towards the melting point. The Stokes-Einstein relation evidenced a change at the same temperature range where the collective dynamics showed a crossover [2]. Classical and ab initio simulations support these findings [2,3]. These results suggest a change in dynamics of the equilibrium liquid metal state well above the melting point and indicate a crossover from a fluid-like dynamics to a viscous liquid dynamics with decreasing temperature. The similarity of the changes in the studied monatomic metals is evidence for a universal character of this crossover. References: [1] F. Demmel et al, Phys Rev B 73 (2006) 104207 ; F. Demmel et al, J. Phys.: Condens. Matter 20 (2008) 205106; F. Demmel et al, J.Phys.: Condens. Matter 27 (2015) 455102; F. Demmel et al, Phys Rev E 73 (2006) 032202 ; F. Demmel et al, Phys Rev E (2012) 85 051204 [2] F. Demmel, A. Tani, Phys Rev E 97 (2018) 062124 [3] F. Demmel et al, Scientific Reports 11 (2021) 11815

## Magnetic Structures - MW 0 001 - Lecture hall (20 Mar 2023, 14:00 - 16:00)

**-Chairs: Martin Meven; Romain Sibille**

### [107] Controlling the magnetic structure in W-type Hexaferrites (14:00)

*Presenter: MØRCH, Mathias*

Hexaferrites are important metal oxides, widely used as both permanent magnets and microwave absorbers. Recently, hexaferrites have attracted great interest, because they show magnetoelectric effects at room temperature. [1,2] We have synthesized W-hexaferrites with varied Co/Zn ratio and investigated the magnetic order using neutron powder diffraction. In SrCo2Fe16O27 and SrCoZnFe16O27 a planar (Cm'cm') magnetic ordering was found, rather than the uniaxial (P63/mm'c') found in SrZn2Fe16O27, which is common in most W-type hexaferrites. Furthermore, in all three studied samples, non-collinear terms were present in the magnetic ordering, one of which is common to the planar ordering in SrCo2Fe16O27 and uniaxial ordering in SrZn2Fe16O27. These non-collinear terms could be a sign of an imminent transition in the magnetic structure, which is further supported by thermomagnetic measurements. The thermomagnetic measurements revealed magnetic transitions at 520 and 360 K for SrCo2Fe16O27 and SrCoZnFe16O27, and Curie temperatures of 780 and 680 K, respectively, while SrZn2Fe16O27 showed no transition, but a Curie temperature at 590 K. Conclusively the magnetic transition can be adjusted by fine-tuning the Co/Zn stoichiometry in the sample. We believe a stoichiometry near SrCo0.65Zn1.35Fe16O27 would have the magnetic transition at room temperature, possibly giving rise to room temperature magnetoelectric effects.[3] [1] Kitagawa, Yutaro, et al. "Low-field magnetoelectric effect at room temperature." Nature materials 9.10 (2010): 797-802. [2] Song, Y. Q., et al. "Spin reorientation transition and near room-temperature multiferroic properties in a W-type hexaferrite SrZn1. 15Co0. 85Fe16O27." Journal of Applied Physics 115.9 (2014): 093905. [3] Morch, M.I, Christensen M. "Controlling the Magnetic Structure in W-type Hexaferrites" Submitted

### [43] Revisiting the antiferromagnetic structure of $\rm Tb_{14}Ag_{51}$. The importance of distinguishing alternative symmetries for a multidimensional order parameter (14:30)

*Presenter: POMJAKUSHIN, Vladimir*

We revisit the antiferromagnetic structure of $\rm Tb_{14}Ag_{51}$ with the propagation vector [1/3,1/3,0] and parent space group P6/m using both magnetic symmetry and irreducible representation arguments. We have found a new magnetic structure under the hexagonal Shubnikov magnetic space group P-6′, which fits much better the experimental data. This new solution was obtained by constraining the spin arrangement to one of the three possible magnetic space groups of maximal symmetry that can be realised by a magnetic ordering transforming according to the 4-dimensional physically irreducible representation that is known to be relevant in this magnetic phase. The refined model, parameterised under P-6′, implicitly includes the presence of a third harmonic with the propagation vector at the gamma point [0, 0, 0], which has an important weight in the final result. The structure consists of 13 symmetry-independent Tb magnetic moments with the same size of 8.48(2)μB, propagating cycloidally in the ab-plane. The modulation has a substantial deviation from being purely sinusoidal due to the contribution of the mentioned third harmonic.

### [247] Nuclear Magnetic Ordering in Naphthalene (15:00)

*Presenter: STEINER, Jakob*

Analogous to electronic magnetism, a nuclear spin system can undergo a transition from a paramagnetic to a ferromagnetic or antiferromagnetic state subject to mutual dipole-dipole interactions. This exotic phenomenon, known as nuclear magnetic ordering (NMO), has only been observed in a few cases that form simple atomic single crystals. We recently developed a model to describe NMO in molecular crystals, which exhibit more ordering possibilities since each molecule contains more than a single spin. Our model predicts a ferromagnetic order in a naphthalene single crystal with thin disk-shaped domains perpendicular to the magnetic field with alternating polarization. The critical spin temperature to reach this order is below the uK range and is achieved by hyperpolarization of the naphthalene protons followed by an adiabatic demagnetization in the rotating frame (ADRF). The latter reduces the effective field on the spins to zero and transfers the high degree of Zeeman order into pure dipolar interaction. Using NMR studies, we were able to confirm the existence of NMO, but only neutron scattering could provide clear evidence of the nature of the order or the size and shape of the domains. To investigate these properties, we performed neutron reflectometry measurements. Due to the polarization dependent interaction cross-section of the neutrons and the polarized protons, we were able to observe Bragg reflexes on the domain boundaries and study the ordered state in detail.

### [316] Redetermination of the incommensurately modulated magnetic structure of CrAs (15:20)

*Presenter: FRIESE, Karen*

Chromium arsenide (CrAs) is considered a model system in which superconductivity and helimagnetism coexist. The superconductivity is induced by pressure and forms a dome-like phase region with a maximum TC of 2.2 K at about 1 GPa. The superconductivity occurs in the vicinity of an antiferromagnetical phase of CrAs which is incommensurate and described as a double helix in the literature. This model was first proposed on the basis of neutron powder diffraction data and assuming an analogous magnetic structure as the one observed for MnP [1]. Since the model was in reasonable agreement with the powder

diffraction data, it was henceforth considered to be correct for CrAs. We have investigated the magnetic structure of CrAs for the first time by means of neutron high-pressure single-crystal diffraction in clamp cells. The results clearly show that the established model of the magnetic structure of CrAs is not in accordance with the measured intensities and can be discarded. While our data do not allow an unambiguous identification of one singular model, we identify four candidate models based on a stringent use of group theoretical considerations and the subsequent refinement using magnetic superspace groups with the program Jana2006 [2]. Details of these models will be presented. Acknowledgments: This work was supported by the BMBF under project No.05K19PA2. [1] H. Watanabe et.al., J. Appl. Phys. 40,1128-1129 (1969). [2] V. Petricek et. al.,. Z. Kristallogr. 229, 345-352 (2014).

### [515] Magnetism and dynamics in multiferroic antiferromagnet Ba2CoGe2O7 (15:40)

*Presenter: DUTTA, Rajesh*

Multiferroic Ba$_2$CoGe$_2$O$_7$ is well known for having an unconventional metal-ligand *d-p* hybridization mechanism responsible for the magnetically induced ferroelectricity [1,2]. It exhibits many exotic quantum phenomena, and among them anisotropic spin excitations and self-tunable single ion anisotropy under external applied magnetic field have been observed recently, using inelastic neutron scattering (INS) technique [3]. A spin gap of about 0.1 meV has been observed under zero magnetic field and interpreted as an effect of spin-nematic interaction [4]. However, we have predicted such gap via linear spin wave theory by introducing the Dzyaloshinskii–Moriya interaction in the spin Hamiltonian. We have observed a spin gap of 0.105 meV in energy at 2 K under zero magnetic field and the gap energy decreases with increasing temperature. We enlighten the discussion on understanding the origin of the zero-field spin gap in details. References: [1] H. Murakawa, et al., “Comprehensive study of the ferroelectricity induced by the spindependent d-p hybridization mechanism in Ba$_2$XGe$_2$O$_7$ (X = Mn, Co, and Cu),” Phys. Rev. B 85, 174106, 2012. [2] H. Murakawa, et al., “Ferroelectricity induced by spin-dependent metal-ligand hybridization in Ba$_2$CoGe$_2$O$_7$,” Phys. Rev. Lett. 105, 137202, 2010. [3] R. Dutta, et al., “Spin dynamics study and experimental realization of tunable single-ion anisotropy in multiferroic Ba$_2$CoGe$_2$O$_7$ under external magnetic fields,” Phys. Rev. B, 104, L020403, 2021. [4] M. Soda, et al., “Spin-nematic interaction in the multiferroic compound Ba$_2$CoGe$_2$O$_7$,” Phys. Rev. Lett., 112, 127205, 2014.

## Magnetic Thin Films & Nano - SCC/0-002 - Taurus 1&2 (20 Mar 2023, 14:00 - 16:00)

**-Chairs: Stefan Mattauch; Andreas Michels**

### [170] Investigation of magnetic proximity effects in SU/FMI/SE heterostructures (14:00)

*Presenter: DALAL, Kamaldeep*

Topological states, potentially leading to the formation of Majorana fermions, have been predicted to emerge in heterostructures of an s-wave superconductor (SU) and a semiconductor (SE) with large spin orbit coupling and split band structure [1]. Incorporation of ferromagnetic materials, such as ferromagnetic insulators (FMI), into the het-erostructures constitutes a promising route for providing the Zeeman energy necessary for splitting the SE bands [2]. The initial step towards development of an intrinsically topological trilayer structure is to ensure the adequate strength of magnetic proximity effects at different combinations of FMI/SE and FMI/SU interfaces [3]. We use polarized neutron reflectometry to quantify the extent of the magnetic proximity at the FMI/SU and FMI/SE interfaces, which is crucial for entering the topological phase. We will pre-sent detailed depth resolved structural and magnetic profiles of different MBE grown heterostructures, e.g. InAs/EuS/InAs/Pb, InAs/Pb/EuS/Pb, and InAs/EuS/Pb. The data will be compared to structural and magnetic response information obtained from Scanning Tunneling Electron Microscopy (STEM) and SQUID VSM measurements. The understanding of these interfaces will help in the optimization of the final device structure. References: 1. Lutchyn, R. M., et. al., PRL, 7, 105 (2010) 2. Escribano, S. D., et. al., NPJ QM, 7, 81 (2022) 3. Liu, Yu, et. al., ACS N. Lett., 1, 20 (2019)

### [250] Proximity effect in DyCo thin films investiagted by Polarized Neutron Reflectometry (14:30)

*Presenter: LOTT, Dieter*

Amorphous Rare-Earth - 3d Transition Metal alloys (RE-3d TM) are fascinating magnetic materials due to the easy, straight-forward tunability of their magnetic properties, depending on temperature and the concentration ratio between the RE and 3d TM components. In this presentation, DyCox thin films sandwiched by two thin Ta layers are discussed that show various intriguing phenomena, e.g. a novel atomic exchange bias effect [1] or the appearance of compact skyrmions [2]. Previous XMCD measurements in transmission and TEY on the samples demonstrates that the bulk and the most upper surface moments of the DyCo films behaving differently in these samples. This results into a coupling between the both regimes. The detailed knowledge of the coupling behavior is crucial for the explanation of the observed phenomena, however, by the XMCD techniques only the upper surface (TEY) and the an average through the complete film (transmission) could be probed. Here, we will present comprehensive polarized neutron reflectivity studies carried out on MARIA of JCNS at the FRM-II (MLZ) that enabled us to probe the complete magnetic depth profile gaining a much better detailed view of the coupling behavior between surface/interface and the bulk parts. The study of the magnetic profile in dependence on temperature and magnetic field allowed us to gain important information about the magnetic states, particularly at the proximity to the Ta layers that are crucial for our understanding and may help us on the way to tailor the magnetic properties in this simple but magnetically very versatile system. [1] K. Chen, D. Lott, F. Radu, F. Choueikani, E. Otero, P. Ohresser, “Observation of an atomic exchange bias effect in DyCo4 film”, Scientific Reports 5, 18377 (2015) [2] K. Chen, D. Lott, A. Philippi-Kobs, M. Weigand, C. Luo and F. Radu, "Observation of compact ferromagnetic skyrmions in DyCo3 film", Nanoscale, (2020),12, 18137-18143,

### [187] Magnetism of pure and Fe-doped multiferroic CoCr2O4 thin films under strain (15:00)

*Presenter: SAERBECK, Thomas*

Mutliferroic materials are under investigation due to the prospect of controlling the magnetic state with electrical potentials or vice versa. We present an investigation of thin film multifferroic CoCr$_2$O$_4$ (CCO) in pure and Fe-doped form grown with different crystallographic orientation and strain on either MgAl$_2$O$_4$(001) (MAO) or Al$_2$O$_3$(0001) (ALO) substrates. Bulk CCO shows a ferrimagnetic transition temperature at about 95 K with 0.08 $\mu_\text{B}$/f.u. and a transition into a conical spin state with multiferroic character at 26 K [1]. The doping with Fe leads to different sublattice magnetizations, magnetic compensation and increased transition temperatures [2]. Both substrates accommodate epitaxial growth of CCO, while the lattice mismatch of about 3% leads to a compressive strain. CCO on MAO follows the orientation of the substrate with a (001) film normal. The oxygen sublattice match of the (0001) ALO plane leads to a (111) growth. Polarized neutron reflectometry, in combination with several complementary techniques, is used to investigate the chemical and magnetic morphology as a function of depth. The measurements reveal a homogeneous magnetization profile with a magnetization 0.18 $\mu_\text{B}$/f.u. at 2 K, which is higher than reported magnetizations in bulk. Despite the large strain, the substrate interfaces are sharp and structural and magnetic effects do not exceed 5 nm. We will compare these results to the magnetization behavior of thin film Fe-doped CCO. [1] Y. Yamasaki et al. PRL 96, 207204 (2006). [2] R. Padam et al. APL 102, 112412 (2013).

### [11] Magnetic order in skyrmion-hosting magnetic multilayers probed by small-angle neutron scattering and polarized neutron reflectometry (15:20)

*Presenter: UKLEEV, Victor*

Magnetic multilayers (MMLs) composed of alternating ferromagnetic / heavy-metal layers are one of the most technologically promising classes of skyrmion-hosting systems due to number of their advantages, such as skyrmion stability at room temperature

and their tunability via layer engineering [1]. Through the combination of broken inversion symmetry and spin-orbit-coupling at the asymmetric interfaces, Dzyaloshinskii-Moriya interaction (DMI) is induced that leads to stabilization of Néel-type skyrmions in finite magnetic fields [1]. In this study we utilized small-angle neutron scattering (SANS) and polarized neutron reflectometry (PNR) methods to probe the magnetic order in [Pt/CoFeB/Ru]$_N$ ($N$=10 and 40 repetitions) MMLs with bulk and layer-resolved sensitivities, respectively. Neutron scattering experiments with polarisation analysis are needed to clarify the relation between Néel (DMI-induced) and Bloch (dipolar-induced) domain walls, that seem to be inaccessible in relatively thick samples (hundreds of nm) by any other experimental technique [2]. Here, long-periodic magnetic stripe domains and orientationally disordered skyrmion phases were unambiguously observed by SANS and off-specular reflectivity. Furthermore, by using the parameters deduced from quantitative modelling of the PNR, we were be able to refine the Hamiltonian parameters used for micromagnetic models. [1] A. Fert, N. Reyren and V. Cros, Nat. Rev. Mater. 2, 17031 (2017) [2] W. Legrand, et al. Science Advances 4.7, eaat0415 (2018)

### [17] Resolving the complex spin structure in Fe-based soft magnetic nanocrystalline material by magnetic small-angle neutron scattering (15:40)

*Presenter: BERSWEILER, Mathias*

The present work focuses on the unique ability of magnetic small-angle neutron scattering (SANS) to quantitatively analyze the magnetic interactions, namely the exchange-stiffness constant and the strength and spatial structure of the magnetic anisotropy and magnetostatic fields in (Fe<sub>0.7</sub>Ni<sub>0.3</sub>)<sub>86</sub>B<sub>14</sub> alloy [1]. This particular compound is a promising HiB-NANOPERM-type soft magnetic nanocrystalline material, which exhibits an ultrafine-grained microstructure with an average particle size as small as 4 nm and an extremely small coercive field of ~ 4.9 µT. The neutron data analysis based on the micromagnetic SANS theory yields an exchange-stiffness constant of A<sub>ex</sub> = (10 ± 1) × 10<sup>-12</sup> J/m, a value that is 2-3 times larger than those reported previously for similar alloys [2]. The large value of A<sub>ex</sub> together with the small grain size and low anisotropy is believed to be responsible for the extreme magnetic softness of this alloy. Furthermore, the magnitude of the extracted anisotropy-field and longitudinal magnetization scattering functions allow us to conclude that the magnetization jumps at internal particle-matrix interfaces, and the ensuing dipolar stray fields, are the main source of the spin disorder in this material. This work was financially supported by the National Research Fund of Luxembourg (AFR grant No. 15639149 and CORE grant SANS4NCC). References: [1] M. Bersweiler *et al.*, IUCrJ **9**, 65–72 (2022). [2] D. Honecker *et al.*, Phys. Rev. B **88**, 094428 (2013).

## Spectroscopy - SCC/0-001 - Lecture hall (20 Mar 2023, 14:00 - 16:00)

**-Chairs: Robert Georgii; Robert Bewley**

### [82] First results on the Wide Angle Neutron Spin Echo (WASP) (14:00)

*Presenter: FALUS, Peter*

The first Neutron Spin Echo (NSE) instrument, IN11, was in user operation for 40 years. The newest spin echo instrument WASP took the relay and just had its first full year of user operation. I will use this occasion to review how the design of the wide angle NSE spectrometers has developed over the years. Apart from WASP, all non-resonant Neutron Spin Echo spectrometers use the basic IN11A design where the precession field is generated by long solenoids along the neutron beam. This construction limits the angular detector coverage and count rate of the instruments. Last century there have been two attempts to make a wide-angle coverage neutron spin echo in-strument. IN11C at ILL was equipped with a flattened solenoid downstream of the sample and it had a 30 degree-wide angular coverage The SPAN instrument[1] at HZB used a pair of coils in the anti-Helmholtz configuration creating an azimuthally symmetric magnetic field, which, in theory, could allow a nearly 360 degree detector coverage. WASP uses an improved SPAN construction, and it aims to have a 500 times higher detected intensity than IN11A while the resolution remains the same. The long construction has finished in 2018, and the instrument has seen 4 full cycles of user operation. The detailed characteristics of the instrument and the first scientific results[2-4] will be presented. References [1] C Pappas et al., Physica B: Condensed Matter, 283, 365-371 (2000). [2] P Luo et al. Nature Communications, 13, 2092 (2022) [3] H Frielinghaus et al., Frontiers in Physics, 10, 872616 (2022) [4] F Lundin et al.,J. Phys. Chem. C , 126, 16262−16271 (2022)

### [359] Crystof: A thermal spectrometer for HBS (14:30)

*Presenter: VOIGT, Jörg*

At JCNS we develop a technical design for a future high brilliance neutron source HBS. The very compact design of the neutron source allows to extract larger phase space volumes from the neutron moderators as compared to existing facilities, where the minimum distance between the moderator and extraction system and/or first choppers poses a significant constraint. In this presentation we discuss a concept for a compact hybrid chopper spectrometer, that images the neutron source via a large crystal monochromator onto the sample. The monochromator provides a narrow wavelength resolution also for short wavelength, which is difficult to realize at long pulse and continuous neutron sources. The secondary wavelength is resolved by a chopper close to the sample and the time-of-flight to the detector, leading to the name “Crystof” for this spectrometer. The instrument is optimized for neutron energy loss scattering in the energy range between 10 and 100 meV resulting in a compact secondary spectrometer that allows large solid angle coverage at acceptable cost for the detector system. We will compare the performance of such a concept to existing thermal time of flight spectrometers. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [117] BIFROST - An extreme environment cold neutron spectrometer at the European Spallation Source (15:00)

*Presenter: TOFT-PETERSEN, Rasmus*

Inelastic neutron scattering is instrumental in making key discoveries in a broad range of materials, such as superconductors, multiferroic materials and quantum magnets. However, the applicability of the technique is limited by inherently weak signals, leaving parametric studies as a function of sample environment parameters relatively inaccessible. BIFROST, currently under construction at the European Spallation Source (ESS), aims to drastically shift those limits of feasibility by combining a multiplexing crystal analyzer backend with an indirect geometry time-of-flight front end. Due to the peak brilliance and long pulse of the ESS source, the primary spectrometer enables an unprecedented polychromatic sample flux exceeding 10^10 n/s/cm2 at 5 MW accelerator power, with a primary spectrometer resolution ΔEi/Ei of 4 %, common in cold neutron spectroscopy. The multiplexing backend consists of 9 Q-channels with continuous angular sensitivity, each containing 5 fixed analyzers probing neutron energies below 5.0 meV. The analyser backend utilize position sensitive detectors to significantly improve energy resolution as compared to a normal triple-axis backend. By shaping the source pulse, an energy resolution well below 0.1 meV is obtainable even far from the elastic line while retaining a respectable flux on the sample. Instrument construction is making significant progress, with major components installed, and the instrument slated for completion by the end of 2023.

### [315] Marmot : Multiplexed Analyzer system with continuous energy analysis (15:20)

*Presenter: STEFFENS, Paul*

The Marmot project is a new type of multiplexed secondary spectrometer for cold triple axis instruments. It is based on a novel concept of energy analysis, using a large array of bent silicon blades and a position sensitive detector. By its particular geometry, it allows for continuous analysis of the neutron energy in a wide energy range (about 3.5 to 7 meV) and with a large divergence. Tests on a prototype prove that the design works very efficiently, while keeping the background low, and with an energy resolution equal or better than conventional focusing analysers. It will be installed at the cold TAS Thales at the ILL and may be of interest also for other applications in neutron spectroscopy. We will disuss the design and its particularities with respect to other concepts of multiplexed spectrometers.

### [202] SHERPA: a backscattering instrument with polarisation analysis (15:40)

*Presenter: SILVERWOOD, Ian*

Polarisation analysis (PA) has been growing in popularity to separate the coherent and incoherent scattering contributions in complex systems. For quasielastic spectroscopy, PA has been used with neutron spin-echo, triple axis, and direct geometry time of flight spectrometers. However, crystal analyser backscattering instruments are the workhorses of quasielastic neutron scattering (QENS), due to high signal, high resolution and low cost. PA has not been implemented on backscattering instruments to date. SHERPA (Spectrometer for High Energy Resolution Polarisation Analysis) is proposed as a near-backscattering instrument with single axis polarisation analysis for the ISIS neutron source. It will be well-suited to study diffusion and molecular dynamics in aqueous systems, proteins, polymers, MOFs, proton conductors and adsorbed phases, amongst others. Initial simulations suggest that SHERPA would out-perform LET at the equivalent resolution by a factor of 130 in detected intensity. The design uses pyrolytic graphite crystal analysers exploiting the prismatic effect (FARO design$^{1}$). Polarisation and analysis are proposed with supermirror cavities. The factors influencing these decisions will be presented with McStas simulations of the preliminary instrument. 1:Rev. Sci. Instrum. 90, 075106 (2019); https://doi.org/10.1063/1.5089642

## Poster Session MONDAY: Posters, beer and pretzels - Yards 4 - 6 (20 Mar 2023, 16:00 - 18:00)

### [39] The Electron Microscopy Facility at the MLZ (board MO-001)

*Presenter: APPAVOU, Marie-Sousai*

In order to provide our users the possibility to complete their neutron scattering data with real space images we will present the Electron Microscopy possibilities at MLZ consisting of a Cryogenic transmission electron microscope Cryo-TEM (JCNS) and an Environmental Scanning Electron Microscope ESEM (JCNS & Hereon). TEM yield real space images of soft matter systems, particularly in cryogenic environment, in terms of size measurements and distribution of particles, shape, self-assembly systems and aggregates; virtually it may complete and enhance any SANS, reflectometry and macromolecular crystallography on soft matter investigation. Moreover, the MLZ is, since recently, also equipped with a Thermo Fischer Quattro S Environmental Scanning Electron Microscope (ESEM) operated in conjunction/cooperation by JCNS and Hereon. Beyond conventional SEM imaging on Material Science samples, the ESEM offers the possibility to work under relatively high pressure and in the presence of humidity and this, without having to subject the sample to any preliminary coating. This will allow investigations of soft matter system with water content. Additionally the ESEM is eqipped with an EDX detector for elemental analysis. The instruments as well as the extended suite of preparation equipment will be described.

### [340] A compact high-temperature furnace for SANS magnets (board MO-003)

*Presenter: AL-FALOU, Abdel*

Many modern high performance alloys feature ferromagnetic elements like Co or Ni. With SANS being a principal technique to investigate the nanostructure of these compounds in in-situ conditions, the ever present magnetic scattering can be of similar magnitude as the nuclear signal. Magnetic fields combined with high temperatures can hence be a key ingredient for studies of Co or Ni based superalloys or Steel samples. We present a prototypical furnace that has been designed to fit the small-scale dimensions (80mm bore) of the available 2.5T magnet at SANS-1, MLZ. The innovations lie in a light-weight and compact design, with watercooling utilizing a 3-D printed Copper structure that is press-fitted to the aluminum dewar. The heating mechanism is based upon often-applied Joule heating of Nb-foils, although the implemented elements differ considerably in size from existing ones. The internal scaffold is exclusively made of ceramics, which display ideal thermal stability, electric and magnetic irresponsiveness. Samples with sizes of 10mm are anticipated. Preliminary testing has confirmed the benchmarks set by previous ovens in the regime of 1000°. Simulations predict a possible temperature of more than 1700°. A run with maximum power however is still a work in progress due to safety measures. The oven, by its small size and application to metallurgic samples, also makes excellent use of the *SANS-1MAX* upgrade program that is planned for the upcoming years.

### [430] Aqueous solutions of heterocyclic amines: structure and thermodynamics (board MO-005)

*Presenter: ALMÁSY, László*

Heterocyclic amines, such as piperidine and N-methylpiperidine aggregate in aqueous solutions due to hydrogen bonds between hydration water molecules. No such aggregation occurs in the mixtures of these amines with other hydrogen-bonded solvents, such as methanol or ethanol. This difference highlights the active role of water solvent in promoting the self-aggregation. However, the role of various contributions in thermodynamic functions due to specific interactions, van der Waals forces, and the effect of the size and shape of the molecules remains open. In the present communication we explore and discuss the family of solutions of pyrrolidine, piperidine, and their methylated counterparts in water and in methanol, as revealed by thermodynamic measurements as well as by direct visualization of the mesoscopic stucture employing small-angle neutron scattering. While the limiting partial molar enthalpies of solutions of pyrrolidine, N-methylpyrrolidine, piperidine, and N-methylpiperidine in methanol follow closely the trend assessed from theoretically calculated molecular interaction energies, their behavior is markedly different in water solutions, and can be described by taking into account an empirical hydrophobic hydration term. Small angle neutron scattering evidenced that the aqueous amine solutions are microheterogeneous on the nanometer-order length scale. Various models are considered to describe the structural arrangement of the hydrated amine molecules. The tendency of approaching phase separation increases in the order: N-methylpiperidine < N-methylpyrrolidine < piperidine < pyrrolidine.

### [79] Effect of pressure on the micellar structure of PMMA-b-PNIPAM in aqueous solution (board MO-007)

*Presenter: ALVAREZ HERRERA, Pablo*

Amphiphilic diblock copolymers feature self-assembly behavior in aqueous solution. In particular, poly(methyl methacrylate)-b-poly(N-isopropylacrylamide) (PMMA-b-PNIPAM) forms core-shell micelles upon heating above the cloud point of PNIPAM (Tcp) [1]. Previously, it was found that pressure strongly affects the dehydration extent of PNIPAM homopolymers in aqueous solution [2]. Here, we present the effect of pressure on the micellar structure of PMMA-b-PNIPAM in aqueous solution by small-angle neutron scattering (SANS). In temperature-resolved experiments, we find that the micellar shell strongly dehydrates above Tcp at atmospheric pressure. In contrast, at 75 MPa, it remains hydrated, and the micelles form highly correlated aggregates. We also characterized the micellar structure in a pressure-resolved experiment at 31.8 °C. We find that, after crossing the co-existence line, the micellar shell appreciably shrinks, despite it remains partially hydrated. Thus, pressure is a tool to modify the micellar structure and the aggregation behavior of the micelles. [1] C.H. Ko, C.M. Papadakis et al., Macromolecules. 2021, 54, 384. [2] B.-J. Niebuur, C. M. Papadakis et al., ACS Macro Lett. 2017, 6, 1180.

### [87] Development of a “Newton shutter” prototype for use in Neutron Scattering (board MO-009)

*Presenter: ARNOLD, Tom*

The scientific case of the FREIA instrument at ESS is partly based on the measurement of reflectivity with very fast time-resolution. The novel elliptical guide design delivers up to 3 collimated beams onto the sample position and thereby enables the possibility of quickly changing the incidence angle without moving the sample. However, it remains technically challenging to achieve sequential selection between beams at a speed that will allow the full potential of the instrument to be achieved. The ZOOM instrument at ISIS is intended to measure scattering from very large-scale structures, something that will only be possible by using focusing optics: a system of CRLs coupled with a fast aperture. This aperture has strikingly similar requirements to the FREIA shutters since it will need to be able to close to create a small aperture as the neutron pulse reaches the focal wavelength of the lenses. Here we present the design and testing of a prototype shutter system that is capable of opening and closing in between or during beam pulses. The shutters are able to select which pulses to accept in any arbitrary pattern and open or close within a few milliseconds. By incorporating a slit into the shutter, it is also able to generate a change in aperture size mid-pulse. Testing has been performed on the ZOOM beamline demonstrating that the performance meets the requirements of both instruments. To illustrate the potential application of these shutters on the FREIA instrument we also report on recent experiments examining the digestion of triolein films. While this complex process can be followed using existing reflectometers, the Q-range available at the required time resolution severely limits our ability to interpret the development of the digestion process.

### [61] Polarized 3He for science with neutrons at the JCNS in Garching (board MO-011)

*Presenter: BABCOCK, Earl*

The 3He group has developed in-situ polarizers for many JCNS instruments including MARIA, TOPAS, KWS1, POLI, and KWS2 and will provide another two polarizers for the ESS for DREAM and TREX. We develop all 3He cells and magnetic systems in house, as well as the laser sources for the FRM2-based devices. We have also work towards wide angle analysis with C-shaped analyzer cell. The status and concepts of the various installations will be discussed.

### [281] Magnetization process in large grain ferromagnets studied by polarized neutron imaging (board MO-013)

*Presenter: BACKS, Alex*

Polarized neutron imaging (PNI) uses Larmor spin precession to spatially resolve bulk magnetic properties [1]. In recent years, it has been advanced with applications like visualizing magnetic domains [2] or vector-fields [3]. Grain oriented silicon steels, which are used as magnetic core material, have grains and magnetic domains in the mm to cm range and a preferential magnetization axis. Here, we present PNI measurements of the the magnetization process in a thin sheet in applied fields up to 4.5mT. In the remanent state, part of the sample shows stripe magnetic domains, which are aligned with the rolling direction and appear to be uniform through the thickness of the sample. A different part is highly disordered, but reorganized into similar stripe domains above 3.0mT. In addition, the crystal grain structure plays a visible role. The experiment required perpendicular magnetic fields for retaining the polarization and achieving the sample magnetization, However, since field variations outside the sample affect the neutron spin, we have used finite element and ray tracing simulations in the experimental planning and data analysis, to account for additional spin rotations. Our results provide a direct observation of the magnetic domains during magnetization, and highlight the capability of PNI to investigate macroscopic inhomogeneities of magnetic materials. [1]: M Strobl et al., Journal of Phys. D: Applied Physics 52 (2019) [2]: K. Hiroi et al., Physica B: Condensed Matter 551 (2018) [3]: A. Hilger et al., Nature Communications, 9.1 (2018)

### [225] Take it up a notch - Sample Environment at SINQ (board MO-015)

*Presenter: BARTKOWIAK, Marek*

Following the successful guide upgrade at SINQ [1], PSI continues to improve the instrumentation to take advantage of the performance gain. The resulting boost in signal to noise enables faster data aquisition and allows more demanding experiments. This could be experiments allowing for smaller samples sizes, at extreme conditions, with increased complexity or combinations of all three. The increasing complexity of the scientific questions can often only be addressed by tuning multiple control parameters or combining results from complementary measurement techniques. For example, the measurements of low-energy magnetic excitations are often performed under a combination of extreme conditions, such as high magnetic field, ultralow temperatures and high pressures. The sample environment group at SINQ has expanded their activities to be able to meet this demand. I will provide an overview of the ongoing sample environment projects and newly available equipment including a cryomagnet for multi-parameter studies. Further more, I will discuss the opportunities and challenges. [1] T. Geue, F. Juranyi, C. Niedermayer, J. Kohlbrecher, J. Stahn, U. Gasser, M. Yamada, C. Klauser, M.Kenzelmann, C. Rüegg & U.Filges (2021) SINQ—Performance of the New Neutron Delivery System, Neutron News, 32:2, 37-43, DOI: 10.1080/10448632.2021.1916267

### [254] Dynamic cluster formation, viscosity and diffusion in monoclonal antibody solutions (board MO-017)

*Presenter: BECK, Christian*

Antibodies play a crucial role in the immune response of mammals. Monoclonal antibodies (mAbs) are particularly relevant for therapeutics due to their high specificity and versatility. The pharmaceutical challenge is to formulate highly concentrated mAb solutions to achieve a significant therapeutic effect, while keeping their viscosity below the subcutaneous injectability limit [1], thus rendering their administration to patients less difficult and painful. Since the understanding of macroscopic viscosity requires an in-depth knowledge on protein diffusion and dynamic cluster formation [2,3], we study the self-diffusion of five mAbs (produced and characterized at Lonza AG) in aqueous solution as a function of antibody type, concentration and temperature, by quasielastic neutron scattering (QENS). QENS allows to determine the hydrodynamic mAb cluster size [4] and to probe the internal mAb dynamics. A subset of mAbs was studied using small angle neutron scattering (SANS) to understand the nature of mAb-mAb interactions. Complementary information is provided by MD simulations and rheology measurements. As a reference, we use polyclonal antibodies from bovine serum [5]. [1] C. Berteau, et al., Med. Dev. (Auckland, NZ), vol. 8, p. 473, 2015 [2] S. von Bülow, et al., PNAS (USA) 116, 984 (2019). [3] M. Heinen, et al., Soft Matter 8, 1404 (2012). [4] M. Grimaldo, et al., Quart. Rev. Biophys. 2019, 52, e7 (2019). [5] M. Grimaldo, et al., J. Phys. Chem. B 118, 7203 (2014).

### [331] Analysis Frameworks for Quasi-Elastic Neutron Scattering with Discrete Energy Transfers (board MO-019)

*Presenter: BECK, Christian*

Quasi-elastic neutron scattering (QENS) allows to probe with a high energy resolution the total scattering function as a function of energy and momentum transfer $\hbar\omega$ and $q$, respectively. Classical QENS spectra are often captured with quasi-continuous energy transfers with acquisition times of several hours. Since the spectrometers are constantly upgraded, new measurement techniques are available. The possibility to move the monochromator in a neutron backscattering spectrometer with a constant velocity allows to probe the scattering function at a specified energy transfer. In principle, such measurements were possible also previously by changing the monochromator temperature, which however requires more time. These fixed window scans (FWS) result in high quality data with acquisition times of only a fraction of the one necessary for full QENS spectra. However, since only discrete energy transfers are available, the established approach, based on analyzing the energy dependence for each momentum transfer $q$ individually, does fail. Here, we present new analysis frameworks for the FWS overcoming the mentioned limitations by combining different energy transfers. By including data from the new installed diffraction data, we have developed an approach determining the volume fraction of the solutes based on the data collected. The combination of this knowledge with established analysis frameworks allows to automatize the analysis frameworks and reduce the input parameters nedeed.

### [263] BEER@ESS: Versatile instrument for engineering studies (board MO-021)

*Presenter: BERAN, Premysl*

The time-of-flight engineering diffractometer BEER [1], which is under construction at the European Spallation Source (ESS), will offer new opportunities for investigations of engineering materials and components using a multi-scale approach and under near-processing conditions. BEER combines the high brilliance of the ESS source with large instrument flexibility. The diffractometer includes a novel beam-shaping technique, the so-called modulation technique [2]. By a time-encoded extraction of several short pulses from the long ESS pulse, a substantial intensity gain of up to an order of magnitude compared to a pulse shaping method (one pulse extraction) for high-crystal-symmetry materials can be achieved without compromising the resolution. More complex crystal symmetries or multi-phase materials can be investigated by the standard pulse shaping method. The variable chopper set-ups and advanced extracting techniques [3] offer broad intensity/resolution ranges that can be adjusted for the experiment's needs. The combination of diffraction, small angle scattering, and even imaging techniques in quasi-simultaneous measurement opens a multi-scale investigation approach without the necessity to change the instrument. [1] K.H. Andersen, et al., Nuclear Instruments and Methods in Physics Research Section A. 957 (2020) 163402. [2] M. Rouijaa, et al., Nuclear Instruments and Methods in Physics Research, Section A. 889 (2018) 7-15 [3] J. Saroun, et al., J. Phys.: Conf. Ser. 746 (2016) 012011

### [334] The backscatter detector system of PERC (board MO-023)

*Presenter: BERNERT, Karina*

The instrument PERC is currently under construction at the FRM II. It aims to measure the beta spectrum of neutron decay more precisely than its predecessors PERKEO II and PERKEO III, enabling the determination of several correlation coefficients in neutron beta decay with an improved precision by one order of magnitude. Of particular interest is the so-called beta asymmetry parameter A which describes the anisotropic emission of electrons in the decay of polarized neutrons. PERC aims to measure A with an unprecedented precision of $\Delta A = 4 \times 10^{-5}$ making it possible to determine the CKM matrix element $V_{ud}$ most precisely and test the unitarity of the CKM matrix. PERC will observe neutron decay in an 8 m long neutron guide and a high magnetic field will guide the charged decay products to the main detector, positioned downstream of the experiment. In order to achieve the targeted precision, it is important to identify backscattering events, in which the electron only deposits a part of its

energy in the detector, as this would otherwise alter the measured spectrum. The magnetic field guides backscattered electrons downstream, where a detector system will identify the backscattering events by the coincidence time. The backscatter detectors will consist of two scintillation detectors and SiPM arrays on the backside for readout. Due to the high background in the area of the backscatter detector system, spatial resolution is necessary to avoid random coincidences. Using the Monte Carlo simulation tool Geant4 I compare different possible setups in their energy and spatial resolution to identify the optimal design. I present the results of these simulations and the status of the development of the detectors.

### [223] How Polymorphism and Ligand Binding modulate G-quadruplex Fast Dynamics (board MO-025)

*Presenter: BERTINI, Luca*

G-quadruplexes (G4s) formed by the human telomeric sequence AG3(TTAG3)3 (Tel22) play a key role in cancer and ageing. G4 structures are known to display a variety of topologies, which are determined by several factors, resulting in structural polymorphism. Neutron Scattering techniques are a valuable tool to investigate how G4 structural polymorphism and ligand binding affect their sub-nanosecond dynamics. Within this context, we combined FTIR spectroscopy to monitor the Tel22 conformation and EINS to assess the corresponding dynamical properties. K+ and Na+ stabilized G4s were found to be in the parallel and mixed parallel-antiparallel topologies, respectively, with the latter resulting to be dynamically more stable. This result is compatible with the presence of ordered hydration-water structures in the antiparallel conformation. Complexation with the model ligand BRACO19 (BR19) resulted in an overall increase of Tel22 mobility. Such a dynamical enhancement, which is uncorrelated to the G4 topology, can be ascribed to a preferential binding of water molecules to Tel22 rather than to BR19.

### [18] Amphiphilic surfactants as model additives for engine friction reduction (board MO-027)

*Presenter: BOGGIO-ROBUTTI, Beatrice A. M.*

The annual global cost of friction and wear is estimated to be €2.5 trillion and represents a significant energy loss. Organic friction modifiers (OFMs) are amphiphilic surfactants utilised to minimise engine losses with the aim of enhancing vehicle fuel economy. Conventionally, OFMs are thought to adsorb at metallic surfaces forming compact monolayer surface films. These reduce friction by creating planes of low shear resistance between contacting metallic surfaces. It is challenging to reproduce the conditions found within a combustion engine and probe the interfacial structure of adsorbed OFMs in-situ. Therefore, much research so far has been conducted under static or mild conditions. In this work, the self-assembly and interfacial behaviour of Ethomeen 18/12 (E1812) has been investigated through use of conventional techniques, neutron scattering, and an in-house, custom tribometer rig. This allows for in-situ neutron and X-ray scattering under sheared lubrication conditions. Doping with water and small biofuel-related polar molecules has shown a strong effect on both micellisation patterns and friction-reducing performance. E1812 has been shown to adsorb at the iron oxide/dodecane-*d26* interface, forming layers of different thickness and degree of solvation depending on concentration and doping regimes. The behaviour of these solutions was also observed under shear, to follow the changes in lubricant film structure directly.

### [487] Interface engineering of 11B4C-containing Ni/Ti multilayer optics (board MO-031)

*Presenter: BROEKHUIJSEN, Sjoerd*

Ni/Ti is the material system of choice for non-polarizing reflective multilayer neutron optics such as monochromators, wave guides, and focusing devices. The reflected intensity as well as neutron energy range from state-of-the-art multilayers are hampered by an interface width limiting the optical contrast. Our previous work has shown that incorporation of low-neutron-absorbing 11B4C gives significant improvement in reflectivity, as a result of reduced interfaces widths, although at the expense of a lower optical contrast between the layers. In this work we have designed multilayers to maximize the optical contrast between individual layers and minimize the interface width by incorporating 11B4C at different positions in the multilayer stack. By co-depositing 11B4C in the Ni layer only, an excellent optical contrast is achieved while inhibiting the formation of crystallites in the Ni layer as well as intermetallics between both layers. Another design involves the addition of ultra-thin 2 Å 11B4C layers between the Ni and Ti layers, reducing the interface width by inhibiting the formation of intermetallics at interfaces. Since the reflectivity performance depends exponentially on the ratio of interface width to multilayer period depth-dependent designs are needed. We demonstrate how a depth-graded supermirror requires a compound design where thicker layers are grown with pure Ni/Ti and thinner layers incorporate 11B4C.

### [508] High-brilliance and high-flux neutron cold source based on elongated rectangular moderators. (board MO-033)

*Presenter: IOFFE, Alexander*

It is known [1] that optimized low-dimensional liquid para-H2 moderators can deliver 2-3 times higher cold neutron brightness compared to volumetric para-H2 moderators. We present a new analytic approach to calculate the brightness of liquid para-H2 moderators. It is shown that the brightness gain is the near-the-surface effect, so that narrow cold moderators shaped as elongated rectangular parallelepiped provide a substantially higher cold neutron brightness compared to the para-H2 moderator optimized for ESS [1]. The obtained results are in excellent agreement with MCNP calculations. As the brightness gain of such narrow moderators is associated with a decrease in neutron beam intensity, the moderators' assembly with the well-developed

total surface will provide wide intense neutron beams while maintaining the high brightness of the narrow moderator. This can achieved by the suggested staircase moderator geometry. Inhomogeneous thermal neutron flux distribution around the reactor core or the target of a spallation source sets a limit to potential brightness gains. This can be partly overcome by the stacked staircase moderator geometry that allows for the brightness gain up to 2.5-3.5 relative to the single flat moderators of the same width. [1] K. Batkov et al., Nuclear Instr. Meth. A 729 (2013) 500.

### [32] The role of neutron diffraction in understanding magnetization tuning of MnCO3 by Amino Acids incorporation (board MO-035)

*Presenter: CASPI, Elad Nisan*

Incorporation of organic molecules into the lattice of inorganic crystalline hosts is a common phenomenon in biomineralization and is shown to alter various properties of the crystalline host. Recently, we manipulated magnetism in MnCO$_3$ by admitting a specific single amino acid into its lattice matrix. Bulk measurements showed a clear negative (positive) correlation between amount of incorporated acid and Néel temperature (low temperature magnetic susceptibility under high magnetic field). Preliminary neutron diffraction results supported these findings and added to them clear observation of significant reduction in ordered magnetic moment values as well as splitting of oxygen atomic positions as the amount of incorporated amino acid is increased. Advanced, high resolution neutron diffraction data further suggest stress anisotropy caused by the amino acid as it is incorporated into the lattice, manifested by a high stress component along the hexagonal unique axis. These findings support the weakening of the super-exchange interactions in MnCO3 by multiple mechanisms, e.g. lattice distortion, lattice stress, and anisotropic bond-length expansion. It may be that this is the first time that the magnetic properties of a host crystal are tuned via the incorporation of amino acids, and neutron diffraction is a key method to explain the fundamental process of it.

### [486] Implications of Surfactant Hydrophobic Chain Architecture on the Surfactant-Skin Lipid Model Interaction: a Neutron Diffraction Study (board MO-037)

*Presenter: CHEN, Yao*

Although surfactants have been widely used in skin care and other related applications, our knowledge about how surfactants interact with stratum corneum (SC) lipids remains limited. Our group has systematically studied how surfactants interact with a lipid SC model by neutron diffraction and molecular dynamics (MD) simulations, focusing on examining the impact of surfactant molecular architecture and surfactant types. The surfactant-SC mixed membrane was constructed by an equimolar mixture of ceramide/cholesterol/fatty acids and surfactant at 1% molar ratio of total lipids. The arrangements of water and surfactant molecules in the membrane were obtained through neutron scattering length density (NSLD) profiles via contrast variation method, mean-while, MD simulation clearly demonstrated the mechanism of hydration change in the surfactant-model SC mixed membrane. Surfactants significantly enhanced the membrane hydration and reduced the amount of phase-separated crystalline cholesterol, showing a strong dependence on surfactant chain length, branching, and double bond. The result clearly demonstrates how surfactant architecture affects its interaction with the SC membrane, providing useful guidance for either choosing an existing surfactant or designing a new one for surfactant-based transdermal application. We have recently extended this system by studying the configuration of zwitterionic, cationic and non-ionic surfactants in model SC membranes by neutron diffraction. The hydration and molecular arrangement change significantly with the type of surfactant.

### [489] Conformal deposition of BxC thin films for solid-state neutron detectors (board MO-039)

*Presenter: CHOOLAKKAL, Arun Haridas*

10B-based solid-state neutron detectors are a viable replacement to 3He detectors. Neutron irradiation of 10B produce charged detectable ions of 4He and 7Li. The detector efficiency using a planar thin film neutron converter configuration is limited by self-absorption of the conversion products in the layer. A 3D configuration, which allows for the conversion products to exit the converter, offers possibility for a higher detection efficiency. The fundamental challenge with a 3D architecture is to deposit conformal films of converter material on high aspect ratio pixelated sensor-chips. In addition, a low temperature process is required since the detector requires ohmic contacts which needs to be coated before converter layer deposition. We report conformal CVD of BxC thin films on sensor-chip substrates with 10:1 aspect-ratio morphologies, using triethylboron (TEB, B(C2H5)3) as single source CVD precursor at 450° C deposition temperature. Step coverage (SC) calculated from cross-sectional scanning electron microscopy measurements shows that films were conformal with a SC of 1. Quantitative analysis using time-of-flight ERDA reveals that the as-deposited films are B rich carbide material with 82.5 at.% B, 15.6 at.% C and < 2 at.% impurities. Promising neutron detection test results of structured diodes will be presented. By utilizing 10B enriched TEB, this result will open the way for efficient solid state n-detectors incorporating 3D-structured 10B4C converter material.

### [118] Experimental Setup for Neutron Pulse Measurement at Early-stage ESS Test Beamline (board MO-041)

*Presenter: CHULAPAKORN, Thawatchart*

A dedicated test beamline (TBL) is being built to provision the commissioning of the ESS spallation source. The functionality of the beamline employs “camera obscura” principle, which allows to observe both thermal and cold neutrons emitted from different parts

of the so-called *butterfly moderator*. The layout of TBL simply consists of a tapered collimator and a changeable pinhole with diameters of 1-10 mm. During the early stage of commissioning, the proton energy will be 570 MeV, corresponding to 100 kW and expectedly generate thermal-cold flux of 10<sup>5</sup> n/cm<sup>2</sup>/s on the TBL instrument. Besides the spatial neutron emission, this contribution will detail how the neutron pulse shapes will be measured, e.g. by Bragg diffraction from a monochromator crystal, Bragg dip transmission or the *pinhole time-of-flight method*.

### [278] On the use of perfect Si crystals in the development of innovative neutron optics (board MO-043)

*Presenter: COURTOIS, Pierre*

We present recent developments in the field of innovative neutron optics using perfect Silicon single crystals. A multiplexed array prototype analyzer has been constructed for the cold neutron triple axis spectrometer ThALES. The prototype consists in an array of 17 Si stacks of 2 mm of thickness. Each stack is composed of 2 plastically bent Si(111) blades with a bending radius of 2 m. The prototype was tested on the instrument showing the high performance of this device and the continuous energy analysis with good resolution that can be achieved. The technique of plastic deformation at high temperature was also used to produce high quality Si mosaic crystals with a mosaic distribution close to 0.2°. Such crystals exhibit excellent neutron properties and would represent an alternative to replace Ge mosaic crystal monochromators. Finally, we have developed appropriate techniques to prepare Silicon 3He neutron spin filter cells entirely built from perfect Si crystals. Experimental relaxation times T1 were found to be close to expected values. We aim to build large banana Si 3He NSF cells to be installed in the PASTIS3 device for wide angle XYZ polarization analysis.

### [266] A novel uniaxial pressure cell for neutron scattering studies of quantum magnetism. (board MO-045)

*Presenter: DEEN, Pascale*

The study of condensed matter is often achieved by perturbing the system thus creating a resultant change in material properties that provides an insight into the atomic scale interactions. One such perturbation is pressure. Pressure offers a convenient way to perturb quantum spin liquids and tune quantum phase transitions by altering the atomic positions and thereby the dipolar interactions and ionic orbital overlap. Varying the balance between the magnetic interactions, exchange and dipolar interaction including anisotropic crystal field effects, can lead to the creation of novel states of matter. Pressure can be applied in an isotropic manner, hydrostatically, or via tension or compression, known as uniaxial pressure. While hydrostatic pressure tunes all bond lengths symmetrically, uniaxial pressure allows an assymetric distortion of the crystal lattice. The application of uniaxial pressure for neutron scattering studies of quantum systems is particularly difficult since the neutron scattering signals are often weak and broad in S(Q,**ω**). We have developed a novel uniaxial pressure cell for the study of quantum magnets by neutron scattering. The cell is particularly suitable for inelastic neutron scattering and polarisation analysis of magnetically diffuse signals. The details of the pressure cell will be outlined with examples from recent experiments on the archetypal frustrated compound, Ho2Ti2O7 (HTO), in which we were able to modify the magnetic interaction parameters enabling an optimisation of the dipolar spin model to HTO.

### [322] HYMN – A novel unified toolbox for in-situ magnetic hyperthermia experiments using neutron scattering (board MO-047)

*Presenter: DEMBSKI-VILLALTA, Michal*

One of the most promising use cases of magnetic hyperthermia, is the use of magnetic nanoparticles (MNPs) for cancer therapy. In this treatment, MNPs are immersed into tumours and by heating with external magnetic fields, typically 100-900 kHz, destroy cancer cells. Since it is a clinical application the optimization of field parameters and in turn, the heating power, is crucial to maintain both safety and high efficiency. Safety dictates an upper limit of applied magnetic field exists. Hence, for successful application, the heating power needs to be improved by the optimization of MNPs structure. What is more, recent studies have shown a huge increase in magnetic heating by the excitation of transversal spin modes in MNPs, in low GHz range. An ideal tool for the characterization of such MNPs is small angle neutron scattering (SANS), with the extended functionality provided by the MIEZE technique. The aim of our ERUM-Pro HYMN project is to develop a novel, unified experimental and computational toolbox for in-situ magnetic hyperthermia experiments under clinical conditions, utilising the SANS and MIEZE-SANS technique, combined with nanomagnetic simulations. This will be achieved by the development of two custom-made setups for operation in the 100-450 kHz (up to 30 mT) as well as 0.5-4 GHz (up to 2 mT) range. We present first SANS results, where we used in-situ RF heating at 450 kHz to examine the dynamic structure formation of magnetite nanocubes with 12, 34 and 53 nm size.

### [172] miniADAM: the extension of the SuperADAM reflectometer family. (board MO-049)

*Presenter: DEVISHVILI, Anton*

The superADAM reflectometer at the ILL has been recently upgraded with a low takeoff angle extension. The new extension represent a stand alone simplified two axis diffractometer operating at 3.2Å. It is designed with speed in mind and provides faster measurement at higher Q-vectors which would not normally be accessible at a longer wavelength. The basic overview of the instruments infrastructure will be presented together with some preliminary results.

### [103] Innovative neutron guide replacement at the Institut Laue Langevin: The H24 (thermal) and H15 & H16 (cold) neutron guides. (board MO-051)

*Presenter: DEWHURST, Charles*

High-performance instrumentation projects rely on high-performance neutron guide infrastructure. During the extended reactor outage (2021 – 2023) we have replaced the H1-H2 beam-tube, in-pile optics and three new guides with innovative geometries to provide intense neutron beams to new or upgraded instrumentation. The upgraded IN5 (2019) time-of-flight spectrometer and its new elliptically focussing H16 cold-neutron guide demonstrates the best-use of phase-space and boasts huge gains in intensity, in particular at shorter wavelengths, while focussing onto much smaller samples. The new H24 thermal-guide uses a rather elegant concept of a common-curved-trumpet exploiting two radii of curvature to naturally diverge and expand the guide to be split into two distinct branches with four dedicate end-of-guide positions for instrumentation. The new H15 cold- guide has a rather complex opposing-curved expanding section, referred to as ‘the trumpet’ serving two important purposes: The first is to spatially expand the neutron guide allowing the guide to be split into multiple individual guide branches and dedicated end-of-guide beam positions. The second is that the opposing curve leaves a ‘fingerprint’ correlation between the divergence profile and spatial position at the end of the trumpet. Importantly, this allows guide branches to be more widely separated in angle therefore allowing space for substantially more instrumentation down-stream.

### [355] Effects of NSAIDs on the Dynamics and Phase Behavior of DODAB Bilayers (board MO-053)

*Presenter: DUBEY, Purushottam*

Dioctadecyldimethylammonium bromide (DODAB) show rich phase behaviour at different temperature and concentration [1]. We have studied the effects of Non-steroidal inflammatory drugs (NSAIDs), aspirin (Asp) and indomethacin (Indo), on the phase behaviour and the dynamics of DODAB lipid bilayer using quasielastic neutron scattering techniques (QENS). Elastic window scan showed that Asp and Indo shift coagel to fluid phase transition at lower temperatures, compared to pure DODAB. While cooling, Asp and Indo suppress the intermediate gel phase, found in pure DODAB. QENS data analysis showed that only internal motion exists in the coagel phase whereas in the fluid phase DODAB involves both lateral and internal motions. In the coagel phase, although the rotational diffusion coefficient of DODAB is almost twice with both NSAIDs, the dynamically active hydrogen fraction in DODAB becomes twice for Asp but remains the same for Indo. In the fluid phase, lateral motion decreases in the presence of Indo, whereas, Asp does not affect lateral diffusion. DODAB's internal diffusion remains unchanged in presence of Indo, whereas, Asp enhances the internal diffusion of DODAB. This study reveals that NSAIDs, Asp and Indo affect DODAB lipid bilayer phase and dynamics uniquely. [1] F.-G. Wu, N.-N.Wang, Z.-W Yu. Langmuir, 25, 13394−13401 (2009). [2] P. S. Dubey, H. Srinivasan, V. K. Sharma, S. Mitra, V. Garcia Sakai and R. Mukhopadhyay, Scientific Reports, 8, 1862 (2018).

### [122] Library of models for fitting Quasi Elastic Neutron Scattering data (board MO-055)

*Presenter: DURNIAK, Celine*

We report on a library of models for Quasi Elastic Neutron Scattering (QENS) data. This development, initiated by SINE2020 Workpackage 10 on Data Treatment, was to develop an exhaustive library of dynamical models in order to increase interoperability and modularity for rapid prototyping. Different building blocks are provided to users and can be combined, convoluted and plugged into different frameworks, such as Mantid Workbench [1], for visualizing and fitting. A similar approach was used for Small Angle Scattering with SasView, SasModels and its marketplace [2]. The library has been developed under an open-source license. The models are written in Python for easy integration in workflows. In order to help users, a few examples of data analysis using different standard fitting engines are provided as Jupyter notebooks [3]. Tools are also provided to help those interested in adding models or sharing examples of data treatment to the project. [1] O. Arnold, et al., Nuclear Instruments and Methods in Physics Research A 764, 156 (2014) [2] www.sasview.org and marketplace.sasview.org/ [3] jupyter.org/

### [423] In-situ investigation of the rolling texture influence in the AZ31 magnesium alloy with a strain diffractometer (board MO-057)

*Presenter: FARKAS, Gergely*

The influence of the basal texture of the hot-rolled sheet of the AZ31 magnesium alloy on the activity of individual deformation mechanisms and its implication on the mechanical response of the material was studied using a combination of advanced in-situ experimental techniques. Neutron diffraction coupled with acoustic emission (AE) was employed to monitor the twinning activity and the evolution of its dynamics from nucleation toward twin growth. The in-situ neutron diffraction experiments were performed by using the biaxial diffractometer TKSN-400 installed in the HK-9 horizontal neutron channel of the LVR-15 research reactor employing the axial geometry. The lattice strain evolution analysis confirmed the microplastic behavior of the sample compressed in the sheet normal direction suggested by the AE response. The in-situ EBSD experiments provided direct observation of the deformed microstructure, presenting an important confirmation of the hypothesis drawn from the indirect neutron diffraction and AE measurements.

### [198] Effect of microstructure on mechanical properties and residual stresses in interpenetrating aluminum-alumina composites fabricated by squeeze casting (board MO-059)

*Presenter: FIORI, Fabrizio*

Aluminum-alumina composites with interpenetrating network structure are interesting structural materials due to their high resistance to elevated temperature and frictional wear, good heat conductivity, enhanced mechanical strength and fracture toughness. In this paper aluminum-alumina bulk composites and FGMs are manufactured by pressure infiltration of porous alumina preforms with molten aluminum alloy (EN AC-44200). The influence of the interpenetrating microstructure on the macroscopic bending strength, fracture toughness, hardness and heat conduction is examined. Special focus is on processing-induced thermal residual stresses in aluminum-alumina composites due to their potentially detrimental effects on material performance in structural elements under in-service conditions. The residual stresses are measured experimentally in the ceramic phase by neutron diffraction and simulated numerically using a micro-CT based Finite Element model, which takes into account the actual interpenetrating microstructure of the composite. The model predictions for two different volume fractions of alumina agree fairly well with the neutron diffraction measurements. [1] J.Maj, M.Basista, W.Węglewski, K.Bochenek, A.Strojny-Nędza, K.Naplocha, T.Panzner, M.Tatarková, F.Fiori, Mat. Sci. Engng. A 715 (2018) 154–162

### [127] The upgarded cold neutron diffraction instrument DMC (board MO-061)

*Presenter: FJELLVAG, Oystein*

The cold neutron diffractometer DMC at SINQ, Paul Scherrer Institute, Switzerland, has recently undergone a major upgrade, and I will present the highlights. The cold neutron guide is upgraded, and DMC is now equipped with a large 2D neutron detector. Special features are high detection efficiency, large solid angle coverage and two-dimensional readout. For powder diffraction experiments we observe an order of magnitude higher count rate, still maintaining the low background of the old DMC instrument, expanding the experimental possibilities which were not feasible at SINQ so far. The 2D detector also opens for single crystal diffraction experiments and especially efficient mapping of large areas of reciprocal space and diffuse scattering. Features of the DMCpy software used for date treatment will also be presented.

### [503] Intermediate Magnetic Phase of Charge-Stripe Ordered La2NiO4.11 and the probable trigger for static magnetic ordering. (board MO-063)

*Presenter: FREEMAN, Paul*

In La-based cuprates the low superconducting transition temperature is accompanied with having only a partial gaping of the magnetic excitation spectrum [1]. This allows the magnetic excitations of La-based cuprates to be studied to lower energies than in other cuprate materials [1], and are often compared to those of charge-stripe ordered La$_{2-x}$Sr$_{x}$NiO$_{4+\delta}$ [2,3]. Inelastic neutron studies of La-based cuprates have observed two striking observations at base temperature, a low energy kink in the magnetic excitation spectrum [4], and an offset between the centring of low energy magnetic excitations and the magnetic Bragg peaks[5]. A combined neutron scattering and μSR study of charge-stripe ordered La$_{2}$NiO$_{4.11}$, shows similar effects as in La-based cuprates[4,5]. In La$_{2}$NiO$_{4.11}$ there is an offset between the wave vectors of the magnetic Bragg reflections and the low energy magnetic excitations in the ordered phase. Whilst the temperature evolution identifies an intermediate magnetic phase, and determines the probable trigger for static magnetic order in charge-stripe ordered La$_{2-x}$Sr$_{x}$NiO$_{4+\delta}$ . [1] M. Kofu, et. al., Phys. Rev. Lett. 102, 047001 (2009). [2] J, M. Tranquada et. al. Nature 375, 561 (1995). [3] H. Yoshizawa et. al., Phys. Rev. B 61, R854 (2000). [4] Zhijun Xu, et. al, Phys. Rev. Lett. 113, 177002 (2014). [5] H. Jacobsen, et. al., Phys. Rev. Lett. 120, 037003 (2018).

### [460] Recent developments of pyrolytic graphite monochromators (board MO-065)

*Presenter: FREUND, Andreas*

The application of HOPG (highly oriented pyrolytic graphite) as an efficient monochromator and filter material for neutron instrumentation has been discovered more than 50 years ago. Despite the fact that HOPG has been in use for such a long time, there is still room for improvements regarding its implementation in neutron beam optics. The features of a novel concept called POSI (pyrolytic-graphite-on-silicon) based on careful x-ray characterization of the HOPG crystals and proven technology show that the efficiency of HOPG monochromators can be increased while decreasing complexity and cost. Moreover, by combining HOPG and bent perfect silicon crystals the functionality of monochromator and analyzer systems is expanded from separate single devices to dual systems or bichromators augmenting the potential of experimental applications. The presentation will include a review of the state of the art, recent results obtained with mechanical tests, x-ray and neutron diffractometry of POSI systems and an outlook on future perspectives. Andreas K. Freund*(1), Dawn Krencisz (2), Mike Crosby (2), Changyong Chen (2), Brian Kozak (2), Pavol Mikula (3) and Gergely Farkas (3) (1) Consultant, 40 Rue Auguste Poirson, 33000 Bordeaux, France (2) Momentive Technologies, 22557 Lunn Rd, Strongsville, Ohio, OH 44179, USA (3) Nuclear Physics Institute, ASCR, 250 68 Řež, Czech Republic *Corresponding author, kafreund8@gmail.com

### [457] Scattered Neutron Imaging as a Technique to Compliment Traditional Radiography and Total-scattering Methods. (board MO-067)

*Presenter: FROST, Matthew*

The use of neutron scattering techniques to understand characteristics of materials at the nanoscale has matured to a point where the subtlest of reciprocal space features can be quantified. In contrast, radiographic imaging using thermal and cold neutrons is entering adolescence, garnering substantial interest by science communities external to traditional scattering disciplines and receiving large initial investments by neutron facilities new and old, large and small. Given this substantial investment in instrumentation technology dedicated to radiography as well as its uniqueness in beam configuration, an opportunity has arisen to develop Scattered Neutron Imaging (SNI) as a complimentary technique that can operate in a nominally parasitic mode at most neutron radiography instruments. Preliminary concepts have been simulated and a few have been tested that provide insight into the capability and performance of this only recently tenable technique. Results of those simulations and tests will be presented, as well as potential future implementations of the technique for instruments at North American neutron facilities. This research used resources at the High Flux Isotope Reactor and Spallation Neutron Source, a US Department of Energy, Office of Science User Facility operated by the Oak Ridge National Laboratory.

### [280] Magnetic phase transitions in frustrated epsilon-Fe$_2$O$_3$ polymorph (board MO-069)

*Presenter: GARCIA-MUÑOZ, Jose Luis*

The epsilon phase of Fe$_2$O$_3$ (ε-Fe$_2$O$_3$) presents captivating properties and it is receiving extraordinary attention due to its great application potentials. It stands out for its huge coercive field (up to 2 T at room temperature), millimeter-wave ferromagnetic resonance, remarkable non-linear magneto-optical effect, magneto-electric coupling [1], and room temperature ferroelectricity [2]. It has been much less studied than other iron (III) oxides because its formation requires special conditions [1]. ε-Fe$_2$O$_3$ presents a complex noncentrosymmetric structure (Pna2$_1$) with three distinct octahedral and one tetrahedral environments for Fe sites. We present a neutron-based investigation on the rich magnetic phase diagram and properties of geometrically frustrated ε-Fe$_2$O$_3$ nanoparticles. The nature of the incommensurate magnetic order, attributed by some authors to a spiral ground state [5], was investigated in zero and applied magnetic fields, and reinterpreted in the light of the models confronted to neutron data [6]. The study illustrates the interplay between the huge magnetic anisotropy, frustration and the stabilization of the super-hard ferrimagnetic phase in the 150-500 K interval. [1] M. Gich et al., Nanotech. 17, 687 (2006). [2] M. Gich et al., Adv. Mater. 26 (2014) 4645. [3] J. A. Sans et al. Nature Comms (2018), 9, 4554. [4] J.L. García-Muñoz et al., Chem. Mater. 29, 9705 (2017) [5] Yu. V. Knyazev et al. Phys. Rev.B 101, 094408 (2020). [6] A. Romaguera et al., submitted

### [494] Disposition of small molecules in stacked bilayers of stratum corneum lipids by neutron diffraction and selective deuteration (board MO-071)

*Presenter: GARVEY, Christopher*

The stratum corneum (SC) is a thin layer of anucleated cells in a lipid matrix and forms the outermost layer of skin, often depicted with a brick-and-mortar structure.[1] Understanding the molecular basis of the barrier properties of skin has important implications for diseased states such as atopic dermatitis and for topical application of therapeutics. The self-assembly of the intercellular lipid matrix forms an important aspect of the barrier properties of the SC, and it is mainly composed of ceramides, cholesterol and free fatty acids. Together, these lipids form two lamellar structures with periodicities (d) of 6 nm (short periodicity phase - SPP) and 13 nm (long periodicity phase - LPP).[2] The ceramides dictate the formation of these lamellar phases and in particular the ceramide EOS is important due to its exceptionally long structure, having an unsaturated fatty acid esterified to an ω-hydroxy fatty acyl chain. Our lipid matrix model, consisting of a 1:1:1 molar ratio of cholesterol, free fatty acids and ceramides, has a ceramide mixture of ceramide NS and ceramide EOS. In this study we have used neutron diffraction (D16 – ILL), over range of scattering vectors which span classical diffraction measurements to the range usually associated with small angle scattering to probe the localization of a small molecule, salicylic acid, within oriented lipid stacks. We used contrast variation of sorbed water to solve the phasing problem of unit cell reconstruction and provide a reconstruction of the scattering length density (SLD) profile of the lamellar/1D unit cell. By modulation of the SLD contribution of the salicylic acid to the overall profile by deuteration we are able to provide an insight of the localization of salicylic acid within the profile. References [1] P.M. Elias, Epidermal Lipids, Barrier Function, and Desquamation, Journal of Investigative Dermatology 80, (1983) S44-S49. [2] J. A. Bouwstra, G. S. Gooris, J. A. van der Spek and W. Bras, J. Invest. Dermatol., 1991, 97, 1005-1012.

### [132] Role of methyl substitutions in maintaining the fluid phase of a phospholipid (board MO-073)

*Presenter: GARVEY, Christopher*

The fluid lamellar phase of lipid bilayers is associated with the normal function of the plasma membrane. The extension of the range of the fluid phase can support an increase of the operational range of environmental conditions for the normal physiological functioning of the membrane. A range of enzymes may be utilized to provide to the lipid bilayer with a means of adapting to changes in environmental conditions. Methyl substitution is particularly common in Archaea and may have useful biotechnological

applications.[1, 2] The effect of such substitutions and their localization have been explored with molecular dynamics simulations.[3] In this study we examine and compare the changes in dynamics and structure with humidity and temperature of stacked bilayers of 1,2-diphytanoyl-sn-glycero-3-phosphocholine (diphytanoyl-PC), a lipid containing 4 methyl substitutions on a C16 carbon chain, and 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) for experimental comparison with simulations. We have utilized the cold triple-axis spectrometer MIRA (Heinz Maier-Leibnitz FRM II, Garching, Germany) as a two-circle neutron diffractometer with low background to study the packing of lipid molecules into bilayer stacks as a function of humidity. The backscattering spectrometer EMU (ANSTO, Lucas Heights, Australia) provides information about the short range motions of lipid chains that occur within the short time scales of < 1ns. DPPC exhibits clear gel-to-fluid transition while diphytanoyl-PC exhibits dynamics consistent with a fluid phase over a wide range of temperatures. [1] A. Gulik, V. Luzzati, M. De Rosa, A. Gambacorta, J. Mol. Biol., 182 131 (1985). [2] A. Gambacorta, A. Gliozzi, M. De Rosa, World J. Microbiol. Biotechnol. 11, 115 (1995). [3] D. Poger, B. Caron, A.E. Mark, J. Phys. Chem. B 118, 13838 (2014).

### [49] Dynamic spin-state order in perovskite-like LaCoO$_3$ (board MO-075)

*Presenter: GAZIZULINA, Alsu*

LaCoO$_3$ exhibits two crossovers at T$_{SS} \approx$ 100 K and T$_{MI} \approx$ 500 K observed in various physical properties such as thermal expansion and electric susceptibility. These crossovers are typically associated with the temperature dependent population of excited spin states of the Co$^{3+}$ ion, which evolves upon heating from the low-spin (LS), S = 0, to high-spin (HS), S = 2, configuration. Since the CoO$_6$ octahedra expands around the larger HS sites, a static LS-HS order was proposed by Goodenough in the 1960's [1] but was never confirmed experimentally. More recent models suggest that spin states form a 3D checkerboard-type short range order near the room temperature, which is formed due to different sizes of these spin states [2-4]. A corresponding dynamic distortion of the crystal lattice mimics closely the Co-O breathing mode. Using inelastic neutron scattering to study the lattice dynamics of LaCoO$_3$ over a wide temperature range, 5 K ≤ T ≤ 700 K, we find strong phonon renormalization of low- as well as high-energy phonon modes with periodicities corresponding to the proposed superlattice. [1] P. M. Raccah and J. B. Goodenough, Physical Review 155, 932 (1967). [2] J. Kuneš and V. Křápek, Physical Review Letters 106, 256401 (2011). [3] V. Křápek et al., Physical Review B 86, 195104 (2012). [4] J. Kuneš et al., Physical Review B 89, 115134 (2014).

### [252] Non-reciprocal magnons in non-centrosymmetric MnSi (board MO-077)

*Presenter: GEORGII, Robert*

Spin waves in chiral magnetic materials are strongly influenced by the Dzyaloshinskii-Moriya interaction, resulting in intriguing phenomena like nonreciprocal magnon propagation and magnetochiral dichroism. We studied the nonreciprocal magnon spectrum of the archetypical chiral magnet MnSi and its evolution as a function of magnetic field in all magnetic phases. Using inelastic neutron scattering, the magnon energies and their spectral weights are determined quantitatively after deconvolution with the instrumental resolution [1,2]. [1] T. Weber, J. Waizner, G. S. Tucker, R. Georgii, M. Kugler, A. Bauer, C. Pfleiderer, M. Garst, and P. Böni, Phys. Rev. B 97, 224403 (2018). [2] T. Weber, J. Waizner, G. S. Tucker, L. Beddrich, M. Skoulatos, R. Georgii, A. Bauer, C. Pfleiderer, M. Garst, and P. Böni, AIP Advances 8, 101328 (2018).

### [230] Metal as insulation winding high-temperature superconducting split pair coil to improve the protection against quenches (board MO-079)

*Presenter: GHANATHE, Madhu*

High-temperature superconducting split pair magnet for neutron scattering environment with the metal-as-insulation (MI) winding technique enables mechanical strength with quench risk reduction. Quench protection is crucial for superconducting magnet system's reliable and safe operation. High-temperature superconductors enable a rapid rise to the maximum magnetic field, compressed dimensions, and are cooled by dry cryostat. However, the risk of quenching, the sudden drop in the magnetic field or thermal runaway is still a unsolved problem. A new demonstrator of metal-insulated HTS cable is used to study the quenching mechanism for quench protection. This process maps out into three phases, Simulations, constructing a demonstrator, and analyzing; we addressed the first phase with research and development planning using the finite element method COMSOL to simulate the upcoming HTS with metal insulated technology. For quench protection of high-temperature superconducting (HTS) magnets, we have chosen the metal-as-insulation (MI) winding technique by co-winding the bare HTS tape with a metal ribbon which has high electric resistivity and mechanical strength.

### [73] Neutron coating development applied to non-depolarizing CuTi supermirror (board MO-081)

*Presenter: GOMEZ GUZMAN, Jose Manuel*

In the last two years the neutron optics group of FRM II has successfully sputtered non-depolarizing m=2 Cu/Ti supermirrors, which have been prepared with a standard DC magnetron sputtering facility. Control on the roughness grow and interdiffusion allowed us to get a very good maximum angle of total reflection (ca. 0.21°/λ) and polarized neutron reflectivity above 90%, as measured at the instrument GINA, located at BNC in Budapest. No difference between R+ and R- components was found within the statistical error bars. By using R+ and R- we were able to calculate the Spin Asymmetry (SA) of the sample defined as SA =

(R+ - R-)/(R+ + R-). The magnetic behavior of the Cu/Ti coating was checked by means of SQUID measurements at the WMI in Garching to be slightly ferromagnetic with magnetic moment of 10-3 Bohr-magneton/atom. For comparison, Ni/Ti and Ni(Mo)/Ti supermirrors were also measured, finding magnetizations of 0.55 Bohr-magneton/atom for Ni and 0.11 Bohr-magneton/atom for Ni(Mo), in agreement with data found in the literature. By knowing the structure of the sample, the simulation programs GenX and SimulReflec were used to distribute the magnetization measured by SQUID along the whole supermirror structure in order to check which would be the theoretical SA delivered by such a model, and whether this could be compatible to the one measured experimentally. The result of such simulations denotes, besides some discrepancies, the compatibility of the theoretical model with the experimental SA result. Moreover, GenX and SimulReflec were also used to calculate the theoretical Spin Flip Reflectivity (i.e. depolarization) that this magnetization would deliver, finding a maximum value of a few times 10-6.

### [300] Investigations on the kinetics of the Liquid-Liquid Phase Separation of the Myelin Basic Protein (board MO-083)

*Presenter: GRAF VON WESTARP, Igor*

Liquid-liquid phase separation (LLPS) of intrinsically disordered proteins has attracted a wide attention in the biological and biophysical community, and it is considered as a ‘hot’ topic. We investigated the kinetics of the LLPS of the myelin basic protein (MBP) over several orders of magnitude in time. MBP is essential for the integrity of myelin sheaths ensuring flawless neuronal signal propagation. MBP is intrinsically disordered and under appropriate solvent conditions, it is able to perform a so-called Liquid-Liquid Phase separation (LLPS). Dense liquid-like MBP phases being in contact with biomimetic membranes have been observed by neutron reflectometry. Hence, it is assumed that LLPS is necessary for physiological function of MBP. Despite intensive research, the nucleation and droplet growth of intrinsically disordered proteins such as MBP during the LLPS are not yet understood. Hence, we want to provide important information about LLPS kinetics. In our experiments, crowding by polyethylene glycol (PEG) induces the LLPS of MBP. TR-SAS allowed us to follow the evolution of nucleating droplets from ~ 0.1 sec to 3 min, while the long-time behaviour of µm-sized droplets was monitored by DLS giving indications for Ostwald ripening as Rh ~ t^1/3.

### [286] Unravel the structuring of meat analogues by neutron scattering (board MO-085)

*Presenter: GUAN, Tong*

The current unsustainable meat consumption makes a growing number of meat consumers turn to plant-based meat alternatives (PBMAs). To facilitate the transition towards a plant-based diet with its health and environmental benefits, the demand for an accurate reproduction of meat-like structure, texture and mouthfeel in PBMAs is pressing. High Moisture Extrusion Cooking (HMEC) is one of the methods to produce PBMAs. During HMEC, mixtures of plant proteins, dietary fiber and fat undergo heat- and flow-induced denaturation and subsequent plastification and texturization. The key to reproduce meat-like structures are the plastification and texturization which take place in a cooling die attached to the end of extruder. However, the “black-box” characteristics of the extrusion process make the understanding this process difficult. Small Angle Neutron Scattering (SANS) is a promising tool to unravel the mechanism of PBMA structurization. Here, we show the results of SANS measurements on different PBMA recipes, applying contrast variation to elucidate the role of the different components in the texturization of PBMAs. We also provide insight of in-situ SANS with a customized neutron-transparent cooling die. Crucially, this setup will help shed light on the plastification and texturization mechanism throughout the entire cooling process of extrusion. We expect to obtain a detailed insight into the structuring and thereby to pave the way towards a more sustainable nutrition.

### [371] ESS/ISIS Support Laboratories – how we best support the neutron scattering users through collaboration (board MO-087)

*Presenter: HARTL, Monika*

ESS/ISIS Support Laboratories – how we best support the neutron scattering users through collaboration K. Michel, M. Sharp, H. Schneider, M. Hartl G. Stenning, S. Langham, S. Youngs, M. Jura Facility Staff involved in supporting neutron scattering users in laboratories during their beamtime need possibilities for scientific and technical exchange, as well as personnel development opportunities and informal discussions. This is already quite common among the sample environment groups (ISSE) and deuteration labs (DEUNET) supporting the neutron scattering community. A strong collaboration between the Support Labs Groups at the ESS and ISIS grew from an in-kind project, and has now evolved to an exchange on relevant topics such as lab operations and development projects, safety incidents, trends in lab usage/scientific area, lab tours. Given the success of this collaborative relationship between the two facilities, both partners are keen to extend this exchange to similar groups at other facilities, and as such a workshop is planned for spring 2023 at ISIS. The workshop will be open for all other interested parties at facilities to participate in the exchange and discussion. Within this poster we will show an overview over the ISIS and ESS support user laboratories and touch on areas where collaboration is extremely useful. Among the many benefits, the sharing of expertise and new development as well as a better understanding of the users needs and how it changes are key. Another important aspect is the clarification of what support labs will do for the users, so users will know before beamtime what they can expect.

### [160] Monte-Carlo simulations of the new radiation shielding at the thermal beamport SR8 @ FRM II with SERPENT 2 (board MO-089)

*Presenter: HAUF, Christoph*

The thermal beamport SR8 at the research neutron source Heinz Maier-Leibnitz in Garching will be optimized to allow the simultaneous operation of three independent monochromatic powder diffractometers. SPODI will continue to be one of the world-leading high-resolution powder diffractometers. FIREPOD will be a dedicated high throughput instrument, well suited for a broad range of fast parametric studies. ERWIN will be a highly versatile multi purpose diffractometer for both powder as well as single crystals. Due to the unique characteristics of each instrument, the optimized beamport SR8 will be able to cater for a wide range of experimental demands and will substantially increase available beam time for neutron powder diffraction. To exploit the full capabilities of each instrument a complete rebuilt of the primary neutron optics at the beamport SR8 is necessary. This requires an entirely new radiation shielding around the neutron guides and monochromators. In this contribution, the results from detailed Monte-Carlo simulations to optimize the biological SR8-shielding are presented. Employing the SERPENT2 code, the full radiation transport of neutrons, as well as gamma radiation through the different shielding materials is simulated. While taking boundary conditions such as available space, floor load and costs into consideration, the underlying detailed CAD-based model is iteratively optimized to achieve a total dose rate lower than the desired limit of 3µSv/h outside the shielding.

### [188] The small-angle scattering instrument SANS-1 at MLZ (board MO-091)

*Presenters: HEINEMANN, Andre, MÜHLBAUER, Sebastian*

We present the developments and improvements of the SANS-1 instrument, a joint TUM and Hereon project [1] since the first user experiments in 2012. The classical pinhole SANS-1 features now two velocity selectors and an ultra-fast TISANE chopper, efficiently allowing to tune flux, resolution, duty cycle and frame overlap, including time resolved measurements with repetition rates up to 10 kHz. The signal to noise ratio has been significantly improved by upgrading the collimation line with new compound apertures. A second key feature is the large accessible Q-range facilitated by the sideways movement of the primary 1m$^2$ detector. Particular attention is hence paid to effects like tube shadowing and anisotropic solid angle corrections that arise due to large scattering angles on an array of single $^3$He tubes, where a standard solid angle correction is no longer valid. SANS-1 also features now a sample stage equipped with a heavy-duty 1-ton goniometer, allowing hosting a wide range of different sample environment like a set of sample changers, magnets, ovens, a bespoke dilatometer for in-situ rapid quenching/heating and stress analysis [2] and a dedicated HF-coil system for nanomagnetic hyperthermia [3]. We present a wide range of adapted sample environments, like a high T furnace that works as an insert for the 2.5T magnet, a future high field magnet and a pressure cell for GISANS. We also present the upgrade plans for a second detector array and a changed guide concept for a massive Q-range extension. [1] S. Mühlbauer et al., NIMA 832, 297-305, (2016) [2] TA Instruments, DIL805A/D/T Quenching dilatometer [3] NB Nanoscale, D5 HF-Generator for Magnetic Hyperthermie

### [23] Where does an enzyme reside in a sponge? (board MO-093)

*Presenter: HOLDERER, Olaf*

The substrates of enzymes are often insoluble in water. Protein molecules, however, are usually hydrophilic. Nature overcomes this problem by compartmentalization of the cytoplasm and by generating huge interfaces between polar and apolar regions inside the different relevant organelles. For biotechnological applications an approach mimicking this compartment formation has already been successfully employed . This is the use of microemulsions being thermodynamically stable mixtures of water and oil forming nanoscale compartments stabilized by surfactants and sometimes co-surfactants. Enzymes within a microemulsion can on the one hand be affected in their structure and function by the complex environment of the microemulsion and on the other hand, with their presence, alter the phase structure of the microemulsion and the properties of the amphiphilic interface. We were curious how a combination of laboratory and scattering techniques makes it possible to shed light on this complex situation. We discuss the cases of two enzymes inside bicontinuous microemusions as examples: the lipase from *Candida antarctica B* (CalB) and the diisopropyl fluorophosphatase (DFPase) from the squid *Loligo vulgaris*. The time-averaged structure was determined from SANS measurements and on the nanosecond time scales the fluctuations of the amphiphilic film were probed with NSE. The results show, that adsorption/desorption mechanisms of CalB at the surfactant monolayer lead to a stiffening of the interface while in the case of DFPase the interface remains unaffected. The approach we suggest makes it possible to comprehensively investigate the biotechnological usability of enzymes in microemulsions.

### [456] The Materials and Physics Support group at ESS (board MO-095)

*Presenter: HOLMES, Alexander*

In 2027, ESS will welcome its first users. To be able to support their experiments, the Materials and Physics Support group has already started to procure and integrate an ambitious list of sample environment systems (SES), from the simplest wet cryostat to the most advanced magnet. In our scope, SES for low and high temperatures, magnetic and electrical fields, high-pressure and thermo-mechanical processing are included as well as the corresponding labs and workshops. In addition, we will offer scientific support in the corresponding domains of expertise and offline (out of the beam) measurements.

### [99] LoKI & FREIA: The UK in-kind contribution to the first 15 instruments at ESS (board MO-097)

*Presenter: HOUSTON, Judith*

The UK in-kind contribution to the first 15 instruments at ESS includes small-angle neutron scattering and reflectometry instruments. As one of two SANS beamlines under construction, LoKI has been designed specifically with the needs of the soft matter, materials, and bio-science communities in mind. For example, its high flux and wide simultaneous Q-range will make it ideal for performing spatially-resolved and time-resolved studies. This will be one of the first instruments to be operational at ESS and we will present the current status with the installation which has been making significant progress on site over the last year. FREIA is a reflectometer with horizontal sample for liquid interfaces and specialising in soft-matter and time-resolved measurements. The novel design uses an elliptical guide to deliver a wide divergence beam onto a fixed sample position. From this beam up to three different collimated beams can be extracted meaning that the incident angle can be quickly changed without moving the sample. This instrument will be one of the latter instruments at ESS, but already most major components have been ordered and some early installations have taken place.

### [307] Li/Ni disorder of electrochemically cycled NCA-type battery cathodes (board MO-099)

*Presenter: HÖLDERLE, Tobias*

The replacement of combustion engines with battery-powered electric drivetrains is one of many essential steps to reduce greenhouse gas emissions on the way to a green future, leading to an increasing demand on Li-ion batteries with higher capacities and energy\power densities. Thus, different kinds of mixed lithium transition metal oxide cathode materials have been developed, like high nickel content Li$_{x}$Ni$_{0.8}$Co$_{0.15}$Al$_{0.05}$O$_{2}$ (NCA), with high power\energy densities at lower costs and increased safety due to minimized amounts of costly and reactive Co[1]. However, Ni-containing LIBs show poor thermal stability, capacity\ power fading and an efficiency loss due to the blocking of the 2D diffusion pathways of Li-ions caused by mixed occupations of Li/Ni (cation mixing) in the cathode, actively discussed in literature[2]. Facing cation mixing ex situ neutron powder diffraction at the high-resolution powder diffractometer SPODI (FRM II) was applied on extracted NCA materials harvested from a series of 18650-type cells charged to different states. The collected structural data was modeled using full-profile Rietveld refinement and obtained results were discussed dependent on its electrochemical behavior. A decreasing character of Li concentration upon cell charging along with charge-independent transition metal occupations revealed the absence of cation mixing in the NCA cathode during the discharge from 4.2 to 2.5V in full cell configuration against graphite negative electrode. [1] A. Purwanto, C.S. Yudha, U. Ubaidillah, H. Widiyandari, T. Ogi and H. Haerudin, Materials Research Express, 2018 [2] O. Dolotko, A. Senyshyn, M.J. Mühlbauer, K. Nikolowski and H. Ehrenberg, Journal of Power Sources, 2014

### [414] Proton Dynamics in Potassium Dihydrogen Phosphate (KDP) at Pressures up to 2.5 GPa by Inelastic Neutron Scattering (board MO-101)

*Presenter: IVANOV, Alexandre*

In the crystal structure of KDP (KH2PO4) the phosphate tetrahedra are linked together by a net of O-H-O hydrogen bonds. At ambient pressure and temperature protons are disordered in a two-minimum potential along the bonds. At a temperature of 123 K a ferroelectric phase transition takes place related to the locking of protons in one of these two energy minima. We used inelastic neutron scattering to follow pressure and temperature variation of bond-stretching and bond-bending vibrations of hydrogen. A compact high-pressure cell of a generic “piston-cylinder” type has been designed in order to make use of a special scattering geometry of the neutron spectrometer IN1-Lagrange at ILL with large solid angle open for scattered neutrons. The most informative energy range for hydrogen bond vibrations stays above the vibration range of the cell materials what makes the consequences of trade-off on sample volume and attainable pressure experimentally less penalising. The proton vibration spectra in KDP up to quasi-hydrostatic pressures of 25 kbar and temperatures around the phase transition have been recorded and analysed.

### [277] SKADI: Small-Angle Neutron Scattering at ESS (board MO-103)

*Presenter: JAKSCH, Sebastian*

SKADI [1] is a small-angle neutron scattering instrument being constructed at the European Spallation Source (ESS). This TOF instrument with 20 m collimation and 20 m sample detector distance will cover 3 orders of magnitude in Q-space simulateneously (10$^{-3}$ to 1 Å$^{-1}$), offer polarised scattering, as well as a versatile sample area of 3$\times$3 m $^2$. With a flux of approximately 8$\times 10^8$ n s$^{-1}$ cm$^{-2}$, due to a very efficient reflector-type neutron extraction, experiments with high flux requirements will be feasible, but also high resolution experiments with a more confined collimation. Thanks to a new scintillation-type detector [2], a semi-transparent beamstop allows measurements of very low Q-values. The large sample area, accessible from the top and by a side door, allows for very flexible, custom built sample environments for complex experimental setups, especially suited to in-situ experiments. [1] JAKSCH, Sebastian, et al. Technical Specification of the Small-Angle Neutron Scattering Instrument SKADI at the European Spallation Source. Applied Sciences, 2021, 11, 8, p. 3620. [2] JAKSCH, Sebastian, et al. Recent developments SoNDe high-flux detector project. NOP 2017 proceedings. 2018. S. 011019.

### [221] MIEZE spectroscopy at shorter wavelengths (board MO-105)

*Presenter: JOCHUM, Johanna K.*

We present a MIEZE (Modulation of intensity with zero effort) set-up for high-resolution neutron spectroscopy at momentum transfers up to 3□$^{-1}$, energy transfers up to ~20meV and an energy resolution in the µeV-range using both thermal and cold neutrons. One prominent advantage of MIEZE compared to classical neutron spin-echo is the possibility to investigate spin-depolarizing samples or samples in strong magnetic fields without loss of signal amplitude and intensity. This allows for the study of spin fluctuations in ferromagnets, and facilitates the study of samples with strong spin-incoherent scattering. The use of thermal neutrons increases the range of validity of the spin-echo approximation towards shorter spin-echo times. In turn, the thermal MIEZE option for greater ranges (TIGER) closes the gap between classical neutron spin-echo spectroscopy and conventional high-resolution neutron spectroscopy techniques such as triple-axis, time-of-flight, and back-scattering. To illustrate the feasibility of TIGER we present the details of an implementation at the beamline RESEDA at FRM II by means of an additional velocity selector, polarizer and analyzer.

### [287] Establishment of the SEC-SANS option at KWS-2 in MLZ (board MO-107)

*Presenter: KANG, Jia-Jhen*

The small-angle neutron scattering (SANS) diffractometer KWS-2 at the neutron source Heinz Maier-Leibnitz (MLZ, Garching, Germany) is operated by the Jülich center of neutron science (JCNS), with applications focusing on soft matter, colloidal particles, micelles, nanocomposites, and polymer gels. In recent years, we are working on the establishment of a new sample environment – the in-situ size exclusion chromatography (SEC) directly followed by SANS measurements, the SEC-SANS setup. The motivation is the growing demand from users interested in bio-molecular systems where the single-particle structure is the investigation target. However, many of such systems are prone to form aggregates, which then coexist with the interested single ones. Thus, an in-situ separation is necessary shortly before SANS data collection, for the sake of obtaining the scattering of individual particles. While the powerful technique of combining in-situ chromatography with small-angle scattering has been widely applied with X-ray sources, the SEC-SANS option has the advantage of the opportunity for contrast matching so that observation on specific domains is possible. At KWS-2, the SEC-SANS setup is equipped with two pumps that allow simultaneous elute and rinse of two columns, in an attempt to increase beamtime efficiency. After elution, the biomolecules are directed to a specially designed flow cell for SANS measurement. A UV-vis spectrometer is installed right before the cell, serving to indicate the arrival of the targeted biomolecules at the neutron beam, and the exposure is triggered.

### [351] NIST/IBBR Biomolecular Labeling Laboratory (BL2) (board MO-109)

*Presenter: KELMAN, Zvi*

One of the major obstacles in acquiring data and developing new techniques for macromolecular studies, is the production of high purity, well behaved, samples. The primary mission of the Biomolecular Labeling Laboratory (BL2) is to provide users the environment, equipment, and expertise necessary to produce stable isotope labeled biomolecular samples to be used for structural and biophysical studies such as small angle neutron scattering (SANS), nuclear magnetic resonance (NMR) and mass spectrometry. The BL2 capabilities and the mechanism to access the facility will be presented.

### [461] Extensive small angle neutron scattering (SANS) studies of Mucin polyelectrolyte solutions (board MO-111)

*Presenters: RAMYA, Koduvayur A., J. GARVEY, Christopher*

Mucins and mucin-like molecules[1] are an important group of biomacromolecules characterized by a charged and highly glycosylated linked peptide backbone. The fundamental structural unit is a bottle-brush-like morphology organized into higher level aggregates or networks forming a gel which is resistant to flow. The electrostatic interactions between polymer chains are of interest to understand the transport properties of these gels since gel forming attractive interactions are opposed by the electrostatic chain repulsion. In this study we have examined dilute solutions of the particles formed by pig gastric mucin (PGM) in increasing ionic strength by small angle neutron scattering (SANS) over an extended range of scattering vectors to encompass the hierarchical nature of the PGM particles. Ultra small angle neutron scattering measurements made on the Bonse-Hart type diffractometer KOOKABURRA[2] (ANSTO, Lucas Heights, Australia) are sensitive to the radius of gyration of the particles and the electrostatic interactions between particles. Conventional pin-hole SANS measurements were made on the two SANS instruments BILBY[3] and QUOKKA[4] (also ANSTO). These measurements were sensitive to the electrostatically mediated intra-particle mucin chain correlations and thus the degree of compaction within the particle. The dependence of the scattered intensity over the extended range of scattering vectors in this study reveals the interrelationships between chain and particle electrostatic interactions. References: 1. Pinzón Martín, S. et al. Front Chem 7, 710 (2019). 2. Rehm, C. et al. J Appl Crystallogr 51, 1 (2018). 3. Sokolova, A. et al. J Appl Crystallogr 52, 1 (2019). 4. Wood, K. et al. J Appl Crystallogr 51, 294 (2018).

### [509] A new method to find optimal neutron moderator size based on instruments' parameters (board MO-113)

*Presenter: KONIK, Peter*

Last decade saw an introduction of low-dimensional neutron moderators, made up of almost pure para-hydrogen. Thanks to the large difference between scattering cross-sections for thermal and cold neutrons, such moderators shaped as tubes or disks can provide a significant brilliance gain over traditional voluminous cold sources. Studies at ESS [1] showed potential gains of 2-3 times in useful neutron flux when reducing the moderator height from 12 to 3 cm. Gain factors are especially prominent for the high-resolution instruments exploiting well-collimated beams. Unfortunately, such small moderators in many cases cannot fully illuminate the guide entrance, which in turn leads to non-uniform divergence beam profile at the sample position. Larger neutron moderators with lower brilliance are thus preferrable for some neutron instruments. We present a general framework that allows to estimate the required moderator size basing on such instrument parameters as sample size, angular resolution and collimation distance. Phase space considerations are the basis of this method, while extensive Monte-Carlo simulations have been used to further prove it. This framework is especially useful for newly built neutron sources, or ones where the cold neutron source upgrade is happening. It can also be used in reverse, allowing to find optimal instrument parameters for a given moderator size, providing full sample illumination and maximal sample flux with minimal background. [1] Andersen K. H. et al. J. Appl. Cryst. 51 (2018) 264.

## [391] MARIA – The high-intensity polarized neutron reflectometer of JCNS (board MO-115)

*Presenter: KOUTSIOUMPAS, Alexandros*

The high-intensity reflectometer MARIA of JCNS is installed in the neutron guide hall of the FRM-II reactor, and is using a velocity selector (4.5Å<λ<40Å) with a resolution of 10%. By using Fermi-Chopper the wavelength resolution can be increased to 1% or 3%. The beam is polarized by a double-reflecting super mirror (4.5Å<λ<12Å) and in the vertical direction the elliptically focusing neutron guide increases the flux at the sample position reducing the required sample size or measuring time. A flexible Hexapod, as sample table, can be equipped with an electromagnet (up to 1.1T) or a cryomagnet (up to 5T), low temperature sample environment, a UHV-chamber ($10^{−10}$ mbar range) for the measurement of Oxide MBE samples, and various soft matter solid/liquid interface cells connected to a “sample robot” for automatic solvent contrast exchange and remote controlled heating/cooling. Together with the 400x400 mm² position sensitive detector and a time-stable ³He polarization spin filter based on SEOP technique, the instrument is well suited for investigating specular reflectivity (up to 7-8 orders of magnitude), off-specular scattering from structures down to the monolayer regime. The GISANS option can be used to investigate lateral correlations in the nm range. Due to the large detector even grazing incidence diffraction measurements are possible. Furthermore the high intensity allows for kinetic measurements down to a few seconds over a dynamic range of 3-4 orders.

## [25] Monoclinic symmetry of the hcp phase of Cobalt (board MO-117)

*Presenter: KOZŁOWSKI, Paweł*

The hexagonal close packed phase of cobalt (hcp-Co) is associated with numerous stacking faults while the face centered cubic phase of cobalt (fcc-Co) has considerably less stacking faults, as shown e.g. in [1]. Two domains of hcp-Co stacked one above the other with a stacking fault in between are usually delimited by a small interface region of a few fcc-Co layers as shown e.g. in [2,3]. The crystal structures of hcp-Co and fcc-Co should be considered together because the crystallites of these two phases are often clustered together in the same grains of cobalt. The gradual ferromagnetic spin reorientation in hcp-Co between 230 $^\circ$C and 330 $^\circ$C reported in [3] suggests that this phase could not have a hexagonal symmetry. This hypothesis is verified positively by synchrotron radiation and neutron powder diffraction [4]. The crystal structure of the hcp phase of cobalt is described by the monoclinic symmetry with the magnetic space group C2'/m'. In this monoclinic crystal structure the former hexagonal [001] axis is no longer perpendicular to the hexagonal layers. The monoclinic structure is an approximate description of the multitude of stacking faulted hcp-Co domains coexisting with fcc-Co domains. [1] O. S. Edwards and H. Lipson, Proc. R. Soc. Lond. Ser. A-Math. Phys. Sci. 180, 268 (1942). [2] O. Blaschko, G. Krexner, J. Pleschiutschnig, G. Ernst, C. Hitzenberger, H. P. Karnthaler, and A. Korner, Phys. Rev. Lett. 60, 2800 (1988). [3] E. Bertaut, A. Delapalme, and R. Pauthenet, Solid State Commun. 1, 81 (1963). [4] P. Kozlowski, P. Fabrykiewicz, I. Sosnowska, F. Fauth, A. Senyshyn, E. Suard, D. Oleszak and R. Przenioslo - in preperation.

## [80] Correlation of structure and dynamics in Cu-Ti melts (board MO-119)

*Presenter: KREUZER, Lucas*

Binary Cu-Ti alloys feature a large, undercooled liquid region and a high glass-forming ability (GFA). Thus, they provide the rare possibility to obtain two component bulk metallic glasses (BMGs), which is mainly addressed to special properties of the Cu-Ti system i.e., in the melt, it features a positive excess volume, whereas it still has a negative enthalpy of mixing. Although, the scientific interest in Cu-Ti-based BMGs increased, the relevant atomic mechanisms responsible for such good GFA are still to be explored. In our study, we discuss the temperature-dependent dynamical and structural properties of Cu-Ti melts, within a compositional range of 24 to 69 at% Ti. Electrostatic levitation is used to process the Cu-Ti samples without any container, which enables to obtain data about viscosity, density, and atomic structure with high accuracy. We found a non-monotonous trend of the viscosity, with the highest values at intermediate Ti contents. The measurement of the (weighed) self-diffusion coefficient of the pure Cu and Ti melts and of the Cu7Ti24 alloy confirms the viscosity results. Notably, this dynamical trend is not reflected by the macroscopic packing fraction, meaning a high viscosity does not necessarily correlate with a dense packing. In contrast, on the

atomic scale, diffraction measurements with x-rays and neutrons reveal a denser, local packing and a pronounced chemical short-range order, which is based on attractive interactions between Cu and Ti. These short-range interactions can explain the high viscosity, while the macroscopic packing fraction is rather governed by long-range interactions.

### [29] Detailed study of the neutron scattering from highly oriented pyrolytic graphite (board MO-121)

*Presenter: KRIGHAAR, Kristine*

Pyrolytic graphite (PG) has a high Bragg reflectivity for neutrons and is therefore much used for monochromators and analyzers in all types of backscattering and triple-axis spectrometers (TAS). PG can also be the source of background signals since it has low velocity phonon branches. If interpreted as Bragg scattering, these phonon branches will appear as broad spurious background signals. This has led to some backscattering instruments installing cooling to obtain better signal background ratio, but the need for cooling for TAS is disputed. We here present an investigation of the total scattering features of PG at different temperatures. We used a diffractometer to obtain a 2D scattering map of a PG analyzer crystal. Intensities span 5 orders of magnitude and consist of Bragg diffraction, powder rings, phonon scattering and surprisingly also a signal that appears as specular reflectivity at high q. We present a model of all features in the data using McStas UNION, and a new general Born-von Karman phonon description for McStas, we can effectively map scattering features in instruments as a function of both temperature and nominal analyzer energy. Our results show that while backscattering instruments do need cooling, TAS do not, due to a different orientation of the phonon scattering cloud. We argue that our McStas model will be useful to investigate scattering geometries of a wide range of instruments and determine possibilities of spurious signals and phonon contamination.

### [445] Spin Reorientation and Rare-earth ordering in Rare-earth Orthoferrites and Orthochromites (board MO-123)

*Presenter: MALIK, Vivek*

Temperature-induced spin reorientation in orthoferrites (RFeO$_3$) and orthochromites (RCrO$_3$) has recently attracted a lot of attention because of its various potential applications. Spin reorientation in these oxides can be utilized to design functional devices like magnetic switches, magnetic read/write heads, etc. This work presents the results of spin reorientation and rare-earth ordering in rare-earth orthoferrites and orthochromites. The magnetic structure of different orthoferrrites and orthochromites has been analyzed using neutron diffraction measurements. Role of Fe(Cr)-Fe(Cr), R-Fe(Cr), and R-R exchange interactions is identified to understand the complex magnetic structures.

### [377] Hydrogen storage chemistry: the path of phase transformation in 6Mg(NH2)2:9LiH:12LiBD4 during hydrogen-emission reaction (board MO-125)

*Presenter: KUZNETSOVA, Anastasiia*

Hydrogen storage technologies in low weight hydrides promise an aid with the global aim of CO2-emissions reduction. High mass energy densities are needed e.g. for heavy-load long distance mobility like trains, trucks, and airplanes. One of the potential reaction based systems is Mg(NH2)2+LiH with a reversible hydrogen capacity of 5.6 wt.% below 200oC. The kinetics of hydrogen desorption/reabsorption is one of the cornerstones of hydrogen storage materials characteristics. The formation of an intermediate phase with LiBH4 improves it. It is speculated that subsequent melting of e.g. α-phase Li4(BH4)(NH2)3 or β-phase Li4(BH4)2(NH2)2 improves the hydrogen diffusion. The mixtures described in literature are denoted 6:9:x, 6Mg(NH2)2:9LiH:xLiBD4, where x grows from 0.5 to 12. It has been shown that the increase of x leads to faster reaction kinetics at the cost of loss of mass hydrogen capacity (for 6:9:12 down to 2.3 wt.%). Neutron diffraction measurements at the diffractometer HRPT at PSI were conducted on the ball milled mixture 6Mg(NH2)2:9LiH:12LiBD4. Measurements were performed at several temperatures (RT, 50, 80, 90oC) in a vanadium container and during heating up to 180oC in a steel container while pumping out the released hydrogen. The phase composition was determined in the as-prepared state and in-situ during heating up to the melting transition. The disappearance of precursors and appearance of new ones was registered after cooling back down to the room temperature.

### [86] MDMC: a new program to refine force field parameters against experimental data (board MO-127)

*Presenter: LANG, Franz*

We present a newly developed program that combines molecular dynamics (MD) simulations with an optimisation protocol. e.g. using Monte Carlo (MC) methods, in order to determine the force field parameters values that lead to the best agreement with experimental data. The program is currently focussed on classical MD simulations and quasi-elastic neutron scattering (QENS) data, such as dynamic structure factor measurements. However, the program is designed to be extensible to other simulation engines and measurable data types.

### [155] Silicon detector for neutron beta decay measurements with PERC (board MO-129)

*Presenter: LEBERT, Manuel*

The PERC facility is currently under construction at the FRM II in Garching, Germany. It will serve as an intense and clean source of electrons and protons from neutron beta decay for precision studies. It aims to improve the measurements of the properties of weak interaction by one order of magnitude and to search for new physics via new effective couplings. PERC's central component is a 12 m long superconducting magnet system that has been delivered. It hosts an 8 m long decay region in a uniform field. An additional high-field region selects the phase space of electrons and protons, which can reach the downstream detector to minimize systematic uncertainties. The downstream detector and the two upstream backscattering detectors will initially be scintillation detectors with (silicon) photomultiplier readout. In a later upgrade, the downstream detector will be replaced by a pixelated silicon detector. We present the current design status of this silicon detector prototype.

### [133] European Spallation Source Polarisation Development (board MO-131)

*Presenter: LEE, Wai Tung Hal*

Polarised neutrons will be a capability offered to users in many ESS instruments. Of the currently approved 15 instruments [1], 12 aim to have the capability [2]. They include 1 imaging instrument, 2 SANS instruments, 2 reflectometers, 3 diffractometers, and 4 spectrometers. In conjunction with in-kind contributions and external grants, the ESS Polarisation Project will support 10 instruments. Polarised 3He based neutron spin filter will provide shared-use polarisers and analysers. Both Metastable Optical Pumping and Spin-Exchange Optical Pumping methods will be used, the latter will focus on in-situ polarisation applications. Depending on the benefits and the feasibility, selected instruments will use polarising-supermirror based polariser or analyser. Due to the generally wide-bandwidth nature of time-of-flight instruments at the ESS, adiabatic fast passage spin flipper, a.k.a. gradient field radio-frequency spin-flipper will be the primary method of choice. We will adopt innovative designs where applicable for the equipment. Even at an early stage of ESS operation, the neutron flux will be on par with some of the polarised neutron instruments at major facilities. The polarisation developmental effort is underway in parallel to instrument construction, with the aim of delivering polarised neutrons for first-science experiments as instruments are entering operation. Our first 3He polariser is currently under construction, that will provide shared use as lab-based polariser and analyser on SKADI and LoKI instruments. We will report our latest development in this presentation. [1] K. Andersen *et. al.*, Nucl. Instrum. Methods Phys. Rev. A 957,164302 (2020). [2] W.T. Lee *et. al.*, Report on ESS Polarisation Workshop, ESS-3549713 (2020).

### [72] Topochemical polymerization under high pressure: threshold distance and selectivity (board MO-133)

*Presenter: LI, Kuo*

Unsaturated molecular crystal can polymerize into extended carbon structure like diamond nanothread and graphene nanoribbon under external pressure, which is called pressure-induced polymerization (PIP). PIP has an obvious topochemical feature, with the structure of the polymeric product similar with the reactant. By analyzing the crystal structures of many reactants, we conclude that alkynes have a threshold distance of ~3.0 A before the PIP. For acetylene, the distance include an intrinsic threshold of 2.3 A and thermal displacement of ~0.8 A. The threshold distance also depends on the reaction path. To realize a perfect topochemical PIP, an ordered doping of "inert" atom and a suitable intermolecular stacking with strong intermolecular interaction are necessary.

### [245] CSPEC : Development of the cold chopper spectrometer of the ESS. (board MO-135)

*Presenter: LOHSTROH, Wiebke*

The European Spallation Source (ESS), expected to be the world’s most powerful neutron source, is currently under construction in Lund. Among the endorsed instruments foreseen for day one instrumentation at ESS, is the cold time-of-flight spectrometer CSPEC [1]. CSPEC is a joint proposal from the Technische Universität München (TUM), Germany, and the Laboratoire Léon Brillouin (LLB), Saclay, France. Experiments in an electric field, or laser excited light harvesting proteins, are still in an exploration stage, mainly due to the lack of flux at the instruments available today. CSPEC will benefit from the high brilliance of the ESS spallation in addition to the cumulative flux provided by repetition rate multiplication (RRM) that results in large flux gains making it possible to probe time-dependent phenomena with millisecond to second time resolution. The unique pulse structure of the ESS with its long pulse duration (2.86 ms) and a repetition rate of 14 Hz requires new concepts for the instrumentation to make optimum use of the available source time frame. With an instrument length of ~160 m, moderator to sample, a wavelength range of $\Delta \leq 1.7$ Å can be probed within each ESS time period via RRM. The energy resolution can be tuned in the range of $\Delta E/E = 6$ - 1%, and CSPEC will use cold neutrons in the range 2 - 20 Å. The guide is optimised to enhance signal to noise and will be able to focus on samples ranging from several mm^2 to several cm^2 in area. The large detector area, with a radius of 3.5 m, -30 o < 2θ< 140° and 3.5 m in height. In addition the sample chamber will, via the use of a gate valve, enable experiments under real and transient conditions. CSPEC is in the manufacturing phase and we will present the current design layout, expected performance and progress towards final construction. [1] P.P. Deen *et al.*, *CSPEC: The cold chopper spectrometer of the ESS, a detailed overview prior to commissioning*, Review of Scientific Instruments 92, 105104 (2021).

### [513] Structure and Dynamics of Huntingtin. A Segmental Labelling Approach (board MO-137)

*Presenter: LUND, Xamuel Loft*

Huntington’s Disease (HD) is a genetically inheritable neurodegenerative disorder caused by a mutation in the gene encoding the protein Huntingtin (Htt). The mutation causes an increase in CAG trinucleotides in the first exon, which increases the number of

glutamines in the poly-glutamine (Poly-Q) tract of the intrinsically disordered N-terminal region of the protein. HD symptoms only manifest in individuals with a poly-Q tract of more than 35 consecutive glutamines. The length of the Poly-Q tract beyond the threshold is correlated with the age of onset and the severity of the pathology. The exon-1 of Htt is a low complexity region that contains the N-terminal 17 residues, the poly-Q tract and a proline rich region. My project aims at elucidating the structural differences between non-pathogenic and pathogenic Htt exon-1 constructs using Small-Angle Neutron Scattering (SANS) measurements in amino-acid specific deuterated samples. Profiting of the distinct scattering properties of deuterium and hydrogen, we aim at extracting valuable structural information of the Poly-Q region. Constructs with specific deuteration patterns (Gln/Pro) are produced using the Cell-Free protein expression system. Cell-Free expression is used to control the animo acid composition and avoid secondary effects of the expression such as scrambling, in order to avoid isotopologues of partly deuterated protein samples. SANS data, collected at the D22 Beamline at ILL, and Small-Angle X-ray Scattering (SAXS) data measured at Soleil and ESRF Synchrotrons are combined with atomistic models to derive unique structural information of different Htt constructs. Synergistic analyses of the data are performed using the ensemble optimization method (EOM). Currently, eleven SANS samples have been measured for pathogenic (HttQ36) and non-pathogenic (HttQ16) constructs of the protein and ensemble analyses are in progress.

### [265] Inelastic magnetic scattering and hydrogen dynamics in H3O-Jarosite (board MO-139)

*Presenter: MACHUCA-BEIER, Lukas*

The mineral jarosite KFe3(OH)6(SO4)2 is a frustrated antiferromagnet. It exhibits long range magnetic order (LRO), when cooled below TN = 60 K, due to DM interaction. The mineral is a classic example of a 2D geometric frustration Kagome lattice. It has earlier been discovered that a substitution of H3O or D3O for K on the A-site prevents LRO. Instead, a spin glass transition sets in at Tg = 14 K. In contrast, substitution with NH4 (or ND4) only suppresses TN slightly. The objective is to understand the mechanics behind this selective suppression of LRO, which is yet to be understood. It has been hypothesized that H-disorder and/or H-dynamics could play a role in this effect. Moreover, Fe vacancies may lift the geometrical frustration locally. Thus, we performed inelastic neutron scattering experiments on powders of D3O-, H3O-, and ND4-jarosite to investigate the magnetic dynamics and hydrogen dynamics to understand the lack of LRO in H3O/D3O jarosite. The samples were characterized by 2H MAS to assess sample purity especially defect concentration and substitution on the A site. By comparing data from susceptibility, MAS-NMR and inelastic neutron scattering we aim to unveil the mechanics behind the glass transitions in H3O/D3O jarosite.

### [69] Quasielastic Neutron Scattering Study in Poly(tetrahydrofuran-co-epychlorohydrin) Based All-Polymer Nanocomposites (board MO-141)

*Presenter: MAIZ, Jon*

Single-Chain NanoParticles (SCNPs) are nano-objects obtained by intra-molecular cross-linking of individual macromolecular chains (‘precursors’). Due to their ultra-small size, softness and internal compartmentalization, they are good candidates for nanotechnology, e.g., for SCNPs was to form part of all-polymer nanocomposites (NC), i. e., mixtures where such nanoparticles are dispersed in a (linear) polymeric matrix. We study by quasielastic neutron scattering (QENS) a mixture consisting of 75 wt% poly(tetrahydrofuran-co-epychlorohydrin) (P(THF-co-ECH)) linear precursor chains and 25 wt% of P(THF-co-ECH) based SCNPs. Two samples are investigated, where one of the components is protonated (h) and the other one deuterated (d). Thus, with our QENS experiments we can discern how the dynamics of both components are mutually affected. In order to cover a wide dynamic range, we have combined a backscattering spectrometer (IN16B) and a time-of-flight (IN5) instrument. The Q-range accessed (approx. $0.2 \leq Q \leq 2$ Å-1) corresponds to relatively local length scales of observation. We observe the development of dynamic heterogeneity in the intermediate scattering function of the NC components, which grows with increasing time. Local motions in the precursor matrix of the NC are accelerated with respect to the reference bulk behavior, while the displacements of SCNPs’ hydrogens display enhanced deviations from Gaussian and exponential behavior compared with the pure melt of SCNPs.

### [75] Tuning hydrogel properties: counterion specific effects and addition of nanoplatelets (board MO-143)

*Presenter: MALIKOVA, Natalie*

Hydrogels are at the forefront of scientific attention especially in the biological and biomedical fields providing the basis for stimuli-responsive artificial tissues etc. We study physically crosslinked hydrogels based on ionenes, positively charged polymer chains, for which strong counterion-specific effects have been observed previously [1]. The nature of the ionene counterion modifies significantly the rheological properties of the hydrogels. Small angle scattering data (SAXS, SANS) reveal different mesh sizes for the cross-linking polymer networks and help to rationalized the observed elastic moduli and their concentration dependence [2]. Further, introduction of charged clay nanoplatelets into the hydrogel is possible [3]. Nanoplatelets organise in a regular face-to-face stacking manner, with a large repeat distance, following rather closely the hydrogel mesh-size (20-30nm). The degree of nanoplatelet ordering in the hydrogel is very sensitive to the negative charge location on the clay platelet (different for each clay type). Increased nanoplatelet ordering leads to an improvement of the elastic properties of the hydrogel, especially for concentrations close to the cgc. On the contrary, the presence of dense clay aggregates (tactoids), destroys the hydrogel network. [1] N. Malikova, A.-L. Rollet, et al, PCCP 17, 5650-5658 (2015). [2] C. Hotton, N. Malikova et al, submitted. [3] C. Hotton, N. Malikova et al, JICS 604, 358-367 (2021).

### [412] Development of a large-area curved Trench-MWPC 3He detector for D16 neutron diffractometer at ILL (board MO-145)

*Presenter: MARCHAL, Julien*

The D16 instrument is a versatile cold-neutron diffractometer operating at the ILL. It benefited from a number of upgrades over the years, such as the installation of a large-area 3He Multi-Wires Proportional Chamber (MWPC) in 2014. This detector provides a resolution of 1 x 1 mm2 over an area of 32 x 32 cm2. After 8 years of operation, the detector is now being replaced by a new curved detector covering a wider active area while still maintaining a high spatial resolution. Its 86° angular coverage will make it possible to perform time-resolved experiments with a large q-range. This new detector is based on the Trench-MWPC detector technology developed at the ILL. In the Trench-MWPC design, cathode electrodes consist in curved aluminium blades with teeth machined along one side of the blade. These blades are stacked on top of each other to form trenches inside which anode wires are stretched. In the D16 Trench-MWPC, 6 modules are mounted side by side in an 3He-filled curved vessel. Each module consists of 192 cathode blades spaced with a pitch of 2 mm and 192 anode wires with a pitch of 1.5 mm. The radius of curvature of the cathode blades is 1150 mm providing a parallax-free resolution of 0.075° horizontally along the 86° angular coverage of the 38 cm high detector. The various fabrication and mechanical inspection steps of the D16 Trench-MWPC detector modules and pressure vessel are presented as well as experimental results obtained during the characterisation with neutrons.

### [33] Magnetic excitations in the zigzag-chain compound KCu$_4$P$_3$O$_{12}$ (board MO-147)

*Presenter: MATSUO, Masashi*

We report on the results of inelastic neutron scattering (INS) of KCu$_4$P$_3$O$_{12}$. Cu$^{2+}$ ions carry $S = 1/2$ spins. Four types of nearest-neighbor exchange interactions form the eight-spin zigzag-chain ($J_1 - J_2 - J_3 - J_4 - J_3 - J_2 - J_1$ chain). We evaluated the exchange interactions as $J_1 = -8.5$ meV (antiferromagnetic), $J_2 = -2.7$ meV, $J_3 = -3.9$ meV, and $J_4 = 6.2$ meV (ferromagnetic) from magnetic susceptibility and magnetization curves at several temperatures using a data-driven technique based on machine learning proposed by Tamura and Hukushima. In the eight-spin zigzag-chain with the values of the exchange interactions, the ground state (GS) is the spin-singlet state. The first-triplet, second-triplet, third-quintet, and fourth-triplet excited states (1ES, 2ES, 3ES, and 4ES, respectively) are located at 2.9, 4.2, 6.7, and 8.5 meV, respectively. We performed INS experiments on KCu$_4$P$_3$O$_{12}$ powder using the HRC spectrometer at J-PARC (Proposal ID 2020B0026). We used incident neutrons with the energy 15.3 and 25.4 meV. Excitations at 5.5 K are most apparent at around $\omega =3$ meV and $Q = 0.7$ □$^{-1}$. The 3 meV excitation exists in a wide $Q$ range, indicating cluster excitation, and corresponds to the excitation from GS to 1ES (2.9 meV). Excitations are seen up to about 6 meV, indicating the existence of the excitation from GS to 2ES (4.2 meV). We can see weak excitations around 9 meV, corresponding to the excitation from GS to 4ES (8.5 meV). Probably, we also observed the excitation from 1ES to 3ES (3.8 meV) at high-temperature data. As a result, the calculated energies of 1ES, 2ES, 3ES, and 4ES from GS are consistent with the experimental results. We will discuss the $Q$ dependence of the INS intensity.

### [186] Port-GISANS: A portable GISANS booster for revealing the structure of complex soft matter interfaces and biomembranes. (board MO-149)

*Presenter: MEHLER, Filip*

Grazing incidence small angle neutron scattering (GISANS) has the potential to reveal highly relevant scientific questions in many areas of science. Examples include biomembranes, responsiveness of lipid membranes to external stimuli in situ such as exposure to light for photolipids and hydration, in-plane structure of DNA composites and micellar nanoreactors. These experiments are often limited by the neutron flux and/or signal to noise ratio. This may be overcome with dedicated GISANS instrumentation but currently experimental capabilities are limited. To overcome this, we are developing Port-GISANS, which will be a module to enable high quality GISANS experiments on existing and future small-angle neutron scattering (SANS) instruments. Port-GISANS will enable high quality surface scattering experiments with neutrons and allow high quality GISANS measurements at ESS from day one. The idea of the concept is to focus the incident neutron beam along the surface normal of the sample. Focusing the beam onto the sample will considerably increase the incident flux (at least by a factor of 10). Focusing compromises on divergence, resulting in a limited depth resolution. For many systems, e.g. thin films and single interfaces this is acceptable, as all in-plane scattering originates from the layer of interest. In this presentation we will present the conceptual and technical design of the Port-GISANS adapter and benchmark ray tracing simulations to show its potential and performance.

### [387] Area detector prototype for the hot single crystal diffractometer HEiDi (board MO-151)

*Presenter: MEVEN, Martin*

The HEiDi single crystal diffractometer at the hot source of the MLZ's FRM II offers high thermal and hot flow, high resolution and a large Q range. These properties make it an excellent tool to obtain detailed structural information for a wide range of current scientific topics. Within the framework of two recent projects funded by the BMBF, great efforts have been made to expand the capabilities of the instrument. These include optimized neutron optics for short wavelengths (e.g. λ = 0.87 Å) to maximize the flux

and signal-to-noise ratio for studies on small samples << 1 mm³. as well as diamond anvil and clamp cells for high-pressure experiments up to the GPa range and down to low temperatures [e.g. A. Grzechnik et al. J. Appl. Cryst. 53(1), 1-6 (2020)]. In addition, a position-sensitive 2D detector (PSD) is under development in cooperation with the JCNS of the FZJ. The PSD prototype is based on 6Li glass for neutron-photon conversion and fifteen position sensitive multi-anode photomultiplier tubes (MaPT) with a sensitive area of 48 x 48 mm³ and 16 x 16 pixel each. The design offers high sensitivity at short wavelengths (~70% at 0.9 Å) and a sensitive area of 23° x 13° (width x height). This ensures the detection of weak signals and (e.g. incommensurate or magnetic) superstructure reflections as well as a faster and more efficient sample characterization and data collection. Further details of the PSD concept as well as other planned extensions will be presented in the conference contribution.

### [42] Signature of defect-induced symmetry breaking in magnetic neutron scattering (board MO-153)

*Presenter: MICHELS, Andreas*

The antisymmetric Dzyaloshinskii-Moriya interaction (DMI) plays a decisive role for the stabilization and control of chirality of skyrmion textures in various magnetic systems exhibiting a noncentrosymmetric crystal structure. A less studied aspect of the DMI is that this interaction is believed to be operative in the vicinity of lattice imperfections in crystalline magnetic materials, due to the local structural inversion symmetry breaking. If this scenario leads to an effect of sizable magnitude, it implies that the DMI introduces chirality into a very large class of magnetic materials$-$defect-rich systems such as polycrystalline magnets. Here, we show experimentally that the microstructural-defect-induced DMI gives rise to a polarization-dependent asymmetric term in the small-angle neutron scattering (SANS) cross section of polycrystalline ferromagnets. The results are supported by analytical and numerical predictions using the continuum theory of micromagnetics. This effect, conjectured already by Arrott in 1963, is demonstrated for nanocrystalline terbium and holmium (with a large grain-boundary density), and for mechanically-deformed microcrystalline cobalt (with a large dislocation density). Analysis of the scattering asymmetry allows one to determine the defect-induced DMI constant, $D = 0.45 \pm 0.07 \, \mathrm{mJ}/\mathrm{m}^2$ for Tb at $100 \, \mathrm{K}$. Our study proves the generic relevance of the DMI for the magnetic microstructure of defect-rich ferromagnets.

### [95] Localization of Dye Molecules in Surfactant Assemblies via SANS Contrast Variation (board MO-155)

*Presenter: MUELLER, Wenke*

The heteroaggregation between azo dyes and surfactants is an interesting phenomenon. The responsivity of the dye spectrum to changes in their chemical environment is often used to monitor alterations in a solution state by means of UV/vis-spectroscopy. However, little attention was paid to the morphology of dye/surfactant assemblies. Small-angle neutron scattering (SANS) with contrast variation permits the elucidation of assembly-morphology and the unambiguous localization of dye-molecules within surfactant micelles. We studied the interaction between the commercial, anionic azo dye Blue and the cationic surfactant DTAB in an alkaline buffer. Solutions of Blue and DTAB phase-separate above a Blue:DTAB ratio of 1:2.5. Below this ratio, stable solutions form with the absorption spectrum of Blue depending on the concentration of DTAB. To better understand underlying mechanisms, the morphology of assemblies in the 1-phase region was studied with SANS. Moving from the precipitation threshold to the surfactant-rich side leads to a shrinking of assembly size and a reduction in its anisometry. SANS contrast variation was applied by matching DTAB to the solvent and revealing the scattering signal arising from Blue only. For all sample compositions, we unambiguously located Blue on a surface-layer of the dye-surfactant micelle. This work demonstrates the feasibility of SANS contrast variation for dye/surfactant-systems and relates findings to UV/vis spectroscopic investigations.

### [175] Development of a unique testing machine for in-situ neutron measurements at elevated temperatures and mechanical loading (board MO-157)

*Presenter: MUTSCHKE, Alexander*

To investigate superalloys under application conditions, which are often a combination of very high tensile loads, and temperatures in oxidizing environments, a new testing machine has been developed for use at several neutron instruments at the FRM II. The testing machine is designed to investigate the material behavior up to 100 kN. Different specimen grips were developed to perform tensile, compression, and fatigue tests to investigate the important material properties of newly developed alloys. The testing machine can be used for ex-situ experiments in the lab but is easily transferrable to different neutron instruments like STRESS-SPEC, SPODI, or SANS-1 at the MLZ. In-situ neutron diffraction experiments under tensile loading at different temperatures have already been performed at STRESS-SPEC and have demonstrated the functionality of this new, highly versatile sample environment.

### [347] Propagation-based phase contrast neutron imaging in McStas (board MO-159)

*Presenter: NAVER, Estrid*

Propagation-based phase contrast imaging is an established method in X-ray imaging. Recent results show that this approach with a Paganin type filter [1],[2] increases neutron image contrast significantly. We demonstrate that we can use this to distinguish materials with low neutron absorption. The neutron experiments were performed at BOA (SINQ@PSI [3]) using the neutron microscope [4]. These data were used to benchmark an implementation of wave propagation in McStas [5]. As proof-of-concept we applied the method to a sample of micrometre thin Al and Zr alternating layers, each of low neutron absorption. We showed

that the individual layers can be distinguished using propagation-based phase contrast, despite the divergent and polychromatic beam. In order to accurately simulate the formation of the phase contrast via sample interaction and wave propagation, a wave description of the neutron was implemented in McStas. This enabled us to simulate the phase difference of the wave gained when passing through the sample and the wave propagation between sample and detector and to replicate the experimental data. [1] D. M. Paganin et al., arXiv, 1909.11186 (2019) [2] M. Østergaard et al., arXiv, 2210.01403 (2022) [3] M. Morgano et al., Nucl Instrum Methods Phys Res A 754, 46-56 (2014) [4] P. Trtik et al., Physics Procedia 69, 169-176 (2015) [5] P. K. Willendrup, and K. Lefmann, J Neutron Res 22, 1-16 (2020)

### [458] Quantitative analysis of magnetic domain sizes in electrical steel (board MO-161)

*Presenter: NEUWIRTH, Tobias*

Electrical steel sheets comprising the magnetic core of electrical machines suffer from energy losses during reversal of magnetization depending on the mobility of the magnetic domains, which is influenced by the treatment of the electrical steel sheet during. Residual stress induced during the manufacturing process (e.g. by blanking the sheets) causes a degradation of domain mobility due to the magneto-elastic effect. Conversely, deliberately induced residual stress may be used to guide the magnetic field. However, there is a shortage of spatially resolved techniques able to probe the magnetic domain constellation in bulk samples of technically relevant dimensions. Neutron grating interferometry (nGI) gathers, among other things, information about ultra-small-angle-neutron scattering caused by a sample. Based on the high penetration of neutrons in electric steels and their high sensitivity to magnetic fields, nGI is the technique of choice for analysing the local effect of induced stress on the magnetic domains in a material. By varying the probed length scale and scattering direction, the correlation function of the considered sample as well as its anisotropy can be recovered and quantitative information about the domain size and shape can be extracted. We will show how residual stress affects magnetic domains when applying an external magnetic field and discuss theoretical models applicable to describe the system.

### [279] CAMEA — A multiplexing analyzer for neutron spectroscopy (board MO-163)

*Presenter: NIEDERMAYER, Christof*

CAMEA (Continuous Angle Multiple Energy Analysis) is a novel crystal analyzer concept optimized for neutron detection efficiency in the horizontal scattering plane [1]. The design comprises consecutive, upward scattering analyzer arcs set to analyze different neutron energies and an array of position sensitive detectors. CAMEA enables rapid mapping of excitations and is in particular compatible with the geometrical restrictions imposed by extreme sample environments. A focusing arrangement of the analyzer crystals together with distance collimation facilitate prismatic analysis of the scattered neutrons [2] and result in a quasi-continuous energy coverage with improved energy resolution. As part of the upgrade program of the Swiss Spallation Neutron Source SINQ, an elliptical neutron guide and a large double focusing monochromatic was installed resulting in a fivefold increase of the neutron flux at the sample position. We will present the spectrometer design, engineering solutions for the analyzer detector system and first data taken during the initial operation phase of the instrument. The results demonstrate the large performance gain for overview studies of low-energy dynamics. [1] F. Groitl et al., Review of Scientific Instruments 87, 035109 (2016). [2] J. O. Birk et al., Review of Scientific Instruments 85, 113908 (2014).

### [177] Design study of a 1-m$^{2}$ Position Sensitive Neutron Detector (PSND) (board MO-165)

*Presenter: NOWAK, Gregor*

Modern neutron Multi-Wire-Proportional-Chambers (MWPC) operating with $^{10}$B$_{4}$C films as solid-state-converter can surpass the performance of ones based on $^{3}$He in terms of position resolution and count rate capability at similar detection efficiency [1,2]. The use of large area coated converters on thin foils forces to develop a mechanical concept to avoid deformations of the neutron sensitive surface due to their own weight and due to acting electrostatic resulting from HV in operation. This concept must allow a parallel stacking of the converter elements in mm distance in order to accumulate conversion efficiency as needed for perpendicular neutron incidence geometry. HZG has introduced [1] and investigated as a contribution to the ESS the idea of stabilizing the converter elements by gas pressure gradient between both sides of the converter to counteract the forces resulting from operation. This concept is applied to the design study of a 1-m$^{2}$ PSND with a position resolution of 2 mm. The MWPC consists of up to 24 $^{10}$B$_{4}$C coated 0.3 mm thick Aluminum parallel stacked converters with a detection depth < 12 mm each. The deposition method of $^{10}$B$_{4}$C coatings with thicknesses up to 10 µm on pretreated Al substrates was elaborated [2, 3]. The delay-line read-out of the detector coupes for up to 170 kcps per detector plane. [1] European Patent: EP 17184906.0 (filed at 04.08.2017) [2] European Patent Application 2 997 174 (14.07.2014) [3] G. Nowak, et al. J. Appl. Phys. 117, 034901 (2015)

### [469] Residual stresses in AISI 316 L stainless steel manufactured via powder bed fusion (board MO-167)

*Presenter: NÉMETH, Gergely*

Powder Bed Fusion, especially Selective Laser Melting (SLM), has gained high acclaim among material engineers in the recent years since it brings a new possibility of production of engineering components with complex shapes. Additionally, by further rotary swaging, the mechanical properties of the components can be enhanced alongside the reduction of some characteristic defects of

the SLM process. On the other hand, the anisotropy, brought by the SLM itself, present in the workpieces (WPs) and the further mechanical treatments can give rise to complex residual stress (RS) distribution within the WPs. In this study, the RS distribution in AISI 316 L stainless steel samples, prepared by SLM method with different laser cladding orientations and levels of rotary swaging, were examined by neutron diffraction multi-linear scanning technique. According to results, only SLM manufactured WPs exhibit in general a centrosymmetric distribution of RS with tensile character at the periphery and compression character in the center of samples, in every measured direction. However, the detailed differences of RS between samples can be most probably attributed to the different build directions of the WPs. The additional cold rotary swaging process then destroys the symmetric distribution of RS in directions perpendicular to the processing route, while the symmetry is kept, and the RS gradient is increased in the parallel direction.

### [64] NMX Macromolecular Diffractometer at the European Spallation Source (board MO-169)

*Presenter: OKSANEN, Esko*

The NMX Macromolecular Diffractometer is optimised for small samples and large unit cells dedicated to the structure determination of biological macromolecules by crystallography. Neutron macromolecular crystallography is mainly driven by its ability to locate hydrogen atoms in biological macromolecules. NMX is a macromolecular diffractometer that uses the time-of-flight (TOF) quasi-Laue technique. The typical wavelength band is 1.8-3.55 Å, but wavelengths up to 10 Å are available. The collimation system tailors the beam size and divergence to the needs of the experiment. The sample is mounted on a six-axis robotic arm that allows the orientation to be optimised. The detectors are also mounted on robotic arms, which allows their positions to be optimised for the experiment. This allows data collection from crystals with unit cells up to 300 Å or more. The detector technology is based on gas-electron multipliers (GEMs) with Gd as a neutron converter. This combines large detector area with high spatial resolution and time-of-flight capability.

### [482] d 5 -off-centering induced ferroelectric and magnetoelectric correlations in trirutile-Fe 2 TeO 6 (board MO-171)

*Presenter: PAL, PIKESH*

We present the rare existence of d5 off-centering induced weak ferroelectric polarization and demonstrate its correlation with observed magnetoelectric (ME) properties in the G type (TN~210 K) antiferromagnet Fe2TeO6 compound.

### [45] Thermal Neutron Three Axes Spectrometer PUMA: Recent Instrumentation Development (board MO-173)

*Presenter: PARK, Jitae*

PUMA is the thermal neutron three-axes spectrometer (TAS) at MLZ. Owing to the dynamical double-focusing technique and compact neutron optics with wide beam divergence, PUMA is mainly characterized as one of the highest neutron flux TAS. In addition, PUMA is equipped with the early generation multi-analyzer and -detector setup, which is suitable for a type of time-dependent kinetic measurements, known as a stroboscopy. Along with the He-3 polarizer after the monochromator and deflector before the analyzer on the top of the multiplexing setup, one can perform a novel type polarized neutron scattering experiment by measuring spin-flip and non-spin-flip channels at a time. Since 2021, PUMA is co-operated by the Institute of Quantum Materials and Technologies of the Karlsruhe Institute of Technology (IQMT, KIT) and the Technical University of Munich (TUM) within the framework of a collaboration contract. As the first joint instrumentation project, we recently started developing a nested mirror optics (NMO) focusing technique on PUMA to further enhance the signal-to-noise ratio in measurements with a smaller sample size (less than 5 x 5 mm). This new optics will also help us to reduce background signals from a massive sample environment such as a magnet or high-pressure cell.

### [44] Dynamics of Furanosides: Inelastic Neutron Scattering and Raman Study of Methyl-β-D-Ribofuranoside (board MO-175)

*Presenter: PASCARIU, Matei*

The biological functionality and structure of DNA and RNA,[1] as well as the activity of various nucleoside-processing enzymes,[2] are all deeply linked to the properties of the underlying five-membered ring sugars, particularly furanosides. The study of five-membered rings is more challenging because of the strain of the ring in all conformations which leads to a small energy difference between twisted and envelope forms, ultimately giving rise to pseudo-rotation.[3] This is opposed to a six-membered ring, in which there is enough freedom to adopt a strain free chair conformation with bond lengths, bond angles, and dihedral angles kept at minimum energy. While much effort has been put into the conformational study of five-membered rings,[4,5] the dynamics of such sugars, including ring-puckering, intermolecular hydrogen bonding, hydroxyl group dynamics, rotations of methyl groups and other effects, are still unclear and need further research. To this aim, in the current work, inelastic neutron scattering on TOSCA[6,7] and Raman spectroscopy are employed to learn more about the dynamics and various interactions in methyl-β-D-ribofuranoside. The empirical data will be compared to simulated spectra using Density Functional Theory in order to provide a better understanding of this biomolecular building block. [1] A. G. Evdokimov et al., *J. Phys. Chem. A*, 1999, **103**, 744; [2] V. E. Marquez, Jr. et al., *Nucleosides, Nucleotides, Nucleic Acids*, 2001, **20**, 451; [3] J. Laane, *Vibrational Spectra

and Structure*, ed. J. R. During, Marcel Dekker, Inc., New York 1972, 26-50; [4] J. B. Houseknecht et al., *J. Phys. Chem. A*, 2003, **107**, 5763; [5] Z. Dzakula et al., *J. Am. Chem. Soc.*, 1996, **118**, 12796; [6] R. S. Pinna et al., *Nuclear Inst. And Methods in Physics Research, A*, 2018, **896**, 68; [7] S. Rudić et al., *Molecular Physics*, 2012, **110**, 1609.

### [2] Surface distortion of Fe dot-decorated TiO2 nanotubular templates using ToF-GISAS (board MO-177)

*Presenter: PAUL, Dr. Neelima*

Physical properties of nanoclusters, nanostructures and self-assembled nanodots, which in turn are concomitantly dependent upon the morphological properties, can be modulated for functional purposes. Here, in this article, magnetic nanodots of Fe on semiconductor TiO2 nanotubes (TNTs) are investigated with time-of-flight grazing incidence small-angle neutron scattering (TOF-GISANS) as a function of wavelength, chosen from a set of three TNT templates with different correlation lengths. The results are found to corroborate with the localized scanning electron microscopy (SEM) images. As we probe the inside and the near-surface region of the Fe-dotted TNTs with respect to their homogeneity, surface distortion, and long-range order using TOF-GISANS, gradual aberrations at the top of the near-surface region are identified. Magnetization measurements as a function of temperature and field do not show a typical ferromagnetic behavior but rather a supermagnetic one that is expected from a non-homogeneous distribution of Fe–dots in the intertubular crevasses.

### [203] Structural features of a new oxygen deficient perovskite oxygen ion conductor explored by neutron scattering (board MO-179)

*Presenter: PAULUS, Werner*

Oxygen ion conductors are materials of major interest for a series of application in the area of solid state ionics. In particular, oxides with brownmillerite type structure (A2BB'O5) have attracted much attention, showing oxygen ion mobility down to ambient temperature. Brownmillerite type frameworks containing B-cations with saturated or empty electron shells (d0 or d10 configurations) present a special case, as they impose a fixed oxygen stoichiometry, making them good candidates to study oxygen diffusion mechanisms on a microscopic level. In this context, we have synthesized a new phase (Sr2ScGaO5), having pure oxygen ion conductivity. Depending on the synthesis route, it adopts two polymorphs: the orthorhombic brownmillerite, consisting of alternating octahedral and tetrahedral layers, or an oxygen deficient cubic perovskite structure. Once synthesized, both phases are surprisingly kinetically stable, rendering them as a model system to study oxygen diffusion mechanisms. We report here on a multi-technical approach to characterize structural changes as a function of temperature. High-resolution structure analysis has been performed using X-rays (synchrotron and laboratory) and neutron diffraction methods, combined with neutron PDF analysis for local environment. To better understand the oxygen mobility mechanisms, these studies were complemented by Raman and impedance spectroscopy. Corallini S. et al, J. Phys. Chem. C 2015, 119, 11447-58. Ceretti M. et al, Crystals 2016, 6 (11), 146. Corallini S. et al. Inorg. Chem. 2017, 56, 2977-84. Ceretti M. et al., Inorg. Chem. 2020, 59, 13, 9434-42

### [302] Progress of MIRACLES experimental activities, the backscattering spectrometer at ESS (board MO-181)

*Presenter: PEREIRA, Jose*

MIRACLES is the neutron backscattering spectrometer of the European Spallation Source [1]. The instrument will display a flexible tuning of the energy resolution, that allows exploration of a broad range of timescales, from the nanosecond to the picosecond, along with an unprecedented wide dynamic range and a versatile selection of energies for quasielastic and inelastic scattering experiments in the cold neutron range. Our focus now is to describe how the scientific and technical requirements of the instrument are taking shape, with substantial progress in the development of design concepts for the neutron scattering components and experimental areas. Here, progress in the MIRACLES detector and data acquisition system, and evaluation of potential improvements in the analyzer system, that includes prototyping and testing measurements in the spectrometer IN16B at ILL, will be outlined. Furthermore, a description of the layout and ergonomics of the sample preparation areas will be detailed. These efforts will help to give final shape to the scattering system and the experimental station of the MIRACLES spectrometer. [1] K. H. Andersen, et al., "The instrument suite of the European Spallation Source", Nucl. Instrum. & Meth. A 957, 163402 (2020).

### [35] Proton dynamics in proton-conducting brownmillerite-based barium indate oxides (board MO-183)

*Presenter: PERRICHON, Adrien*

Proton-conducting oxides are an important class of materials for next-generation, intermediate-temperature solid-state electrolytes in e.g., proton conducting fuel cells. While most development efforts have been directed toward materials exhibiting the cubic perovskite structure, in recent years several promising alternative structures have emerged. One of these is the pseudo-cubic structure obtained upon hydration of brownmillerite-type barium indate phases. Unlike in cubic perovskites, pseudo-cubic barium indate phases exhibit several proton sites with distinct local environments. In this context, we report on a comprehensive study of the proton local environments and dynamics in the model system BaInO$_3$H, using inelastic and quasielastic neutron scattering techniques and ab initio molecular dynamics simulations. We show that, while the signature of up to four proton sites can be detected in the vibrational spectra, the diffusive proton dynamics can be described through the two main proton sites: the H(1) "perovskite-like" proton site and the H(2) proton site characteristic of the pseudo-cubic structure. We show that preferential motions, already observed at room-temperature, are hydroxyl reorientations for H(1) and proton transfers for H(2). We also show

that the activation of the more energetic counterpart motions of H(1) and H(2) is necessary to observe interexchange between sites and long-range diffusion in the nanosecond timescale.

### [325] Electric field-induced assembly of magnetic nanoparticles in ferrofluids (board MO-185)

*Presenter: PETRENKO, Viktor*

Stimuli responsive materials, which can self-assemble depending on the environment, are of great interest. In this context nanoparticles offer unique opportunities as they can be custom designed and it is very important to understand the assembly mechanisms to control the resulting structures, which is crucial for the synthesis of materials with controllable properties. It is well known, that properties of ferrofluids can be controlled by external magnetic field. However, inhomogeneous distribution of magnetic particles in non-polar ferrofluids was observed recently under external electric fields and formation of large aggregates was concluded in such systems. And it was also concluded, that electric fields, similar to magnetic fields, could be a driven force to induce the assembly of magnetic nanoparticles (MNPs) in bulk and at the interface. Thus, it was shown by SANS that aggregation process depends on the electric field strength. Impact of temperature on such aggregation was also concluded according to SANS experiments. Maximum changes in the magnetic structures of the particles under application of both magnetic and electric fields were observed by SANSPOL. Assembling of MNPs from non-polar ferrofluid on a planar surface and further evolution of the interface structure under electric field application were studied by NR. The reason of the observed effects is related to the polarization of the particles in the electric field and their interaction as dipoles.

### [305] Neutron Depth Profiling Measurements to Study Lithiation Mechanism of LiAl Electrodes (board MO-187)

*Presenter: PHAM, Thien An*

Metal alloys, such as LiAl, are gaining more interest as anode materials for lithium ion batteries because they exhibit a high theoretical capacity while being inexpensive. Aluminium has an almost three times higher specific capacity with 993 mAh/g in relation to the commonly used graphite anode. [1] During Lithiation, aluminium begins to form a solid solution with lithium, the so called alpha-LiAl phase. Once the solubility limit is reached upon lithiation, the alpha-LiAl undergoes a phase transition to the beta-LiAl phase. [2] Al electrodes were electrochemically lithiated to different state of charges in coin cells with Li metal as counter electrode. X-ray diffraction measurements were conducted on the disassembled anodes with the goal to understand the lithiation mechanism and to determine the fractions of alpha- and beta-LiAl phases. The Rietveld refinements yield that the samples charged to SoC25 show a higher amount of alpha-LiAl. Simultaneously, the amount of beta-LiAl in the samples increases with higher SoC as expected. Additional neutron depth profile measurements were performed in NPI CAS Rez at the CANAM infrastructure to determine the Li distribution throughout the lithiated samples. First results have confirmed that the lithiation of the aluminium starts at the surface where a higher Li concentration was identified. The higher charged sample also shows a stronger lithiation in the bulk of the Al anode. This shows that the whole anode is lithiated with a concentration gradient from surface to bulk material. In the lower charged sample, no Li was detected near the backside of the anode, indicating that pristine aluminium is there still present. Additional operando diffraction measurements are planned to further investigate the early stages of the lithiation and the nucleation of the beta-LiAl. This work was performed as collaboration between TUM (Heinz Maier-Leibnitz Zentrum, FRM II) and RWTH Aachen (ISEA) in the frame of the BMBF project ExcellBattMat cluster. Literature [1] Wang, H., et al. (2020). Journal of Materials Chemistry A 8(48): 25649-25662. [2] Liu, D. X. and A. C. Co (2016). J Am Chem Soc 138(1): 231-238.

### [385] Slowing down 14 MeV fusion neutrons (board MO-189)

*Presenter: PIETROPAOLO, Antonino*

The monochromatic neutron filed generated by $^{3}$H($^{2}$H,n)$^{4}$He reactions is typically used in fusion-related experiments. mainly devoted to material damaging, plasma diagnostics development and cross sections measruements. As a matter of fact, the monochromatic 14 MeV neutrons can be slowed down to obtain thermalised neutrons with the typical spectrum of a spallation neutron source, i.e. a maxwellian peak and an epithermal tail extending up to the maximum energy available. Although the golden standard for the production of intense neutron beams for scattering applications is fission and spallation, nevertheless exploiting the monochromaticity of the source may be an added value. Indeed, obtaining moderated neutron beams at a 14 MeV accelerator-driven neutron source with intensities such that a few neutron techniques might be made available, may represent a unique possibility to perform in the same site fusion-related investigations on materials applying dedicated neutron scattering techniques on material that, upoin 14 MeV neutron irradiation likely are heavily activated, making the transportation to other neutron site not feasibile over long periods. In this contribution, the strategy to obtain a moderated neutron field from 14 MeV source neutorns is discussed, showing both experimental measurements and Monte Carlo simulations. Some prediction on moderator brightness are provided for a 250 kW accelerator-driven 14 MeV fusion neutron source, currently in the design phase.

### [251] Polymorphic phase transition in liquid and supercritical carbon dioxide (board MO-191)

*Presenter: PIPICH, Vitaliy*

Thermal density fluctuations of supercritical CO$_{2}$ have been studied using small-angle neutron scattering (SANS), whose amplitude (susceptibility) and correlation length show the expected maximum at the Widom line. At low pressure, the susceptibility

is in excellent agreement with the values determined from the mass density. Surprisingly, droplets form between 20 and 60 bar above the Widom line, which we identified as the Frenkel boundary line separating liquid-like and gas-like states of supercritical fluids [1]. This observation is in contrast to the classical picture of supercritical fluids, where there are "no discernible differences between liquid-like and gas-like states" [2]. The droplets initially form spheres with a radius of ≈ 45 Å and transform into rods and globules at higher pressure, representing a liquid-liquid (polymorphic) phase transition with same composition but different density, the last one determining the order parameter [3]. The polymorphism in CO$_{2}$ is a new observation that will stimulate discussions about gas-like and liquid-like states in SC fluids, in particular as CO$_{2}$ represents a "simple" van der Waals fluid, unlike water, the most studied fluid showing polymorphism in its supercooled state. [1] V. Pipich, D. Schwahn, Phys. Rev. Lett. 120 (2018) 14570b1. [2] C. Cockrell, V.V. Brazhkin, K. Trachenko, Physics Reports 941 (2021) 1-27. [3] V. Pipich, D. Schwahn, Scientific reports (2020) 10:11861.

## [123] Dynamics of water molecules on the surface of iron oxide nanoparticles: A QENS study (board MO-193)

*Presenter: PLEKHANOV, Maksim*

In many applications like in biomedicine, ferrofluids, or heterogeneous catalysis, iron oxide nanoparticles (IONPs) feature a solid-liquid interface with the wetting water molecules. The interfacial properties including dynamics play an important role, yet have been barely addressed so far. Quasielastic neutron scattering (QENS) can access the dynamics of water molecules at the surface of TiO2, CuO, SnO2, and BaSO4 nanoparticles as shown in ref. 1-3. However, the water dynamics on the surface of magnetic IONPs are largely unknown. We will report on QENS experiments performed at IN16B at ILL on IONP samples synthesized according to Ref 4 and stabilized at 8 % (nominally water-free) and 75 % (about two layers of water molecules) relative humidity (RH). Based on fixed window scans and energy-resolved spectra in the temperature range of 2 – 334 K over a Q-range of 0.19 – 1.83 Å-1, we aim to identify possibly coexisting diffusional modes of water molecules and the stabilizing citrate molecules at the IONP surface by analyzing the Q-dependency of the quasielastic intensity when comparing the nominally dry (8 %RH) and wet (75 %RH) sample. Possible contributions of superparamagnetic relaxations will be considered in the data analysis process as well. References: [1] E. Mamontov, et al. J. Phys. Chem. C 2007, 111, 4328-41 [2] A. G. Stack, et al. Phys Chem Chem Phys 2016, 18, 28819-28 [3] J. R. Torres, et al. AIP Adv. 2022, 12, 065124 [4] S. L. J. Thomä, et al. Nat. Commun. 2019, 10, 995

## [165] Bulk crystal growth of materials with possible novel quantum states with RMX structure-type (board MO-195)

*Presenter: POMJAKUSHINA, Ekaterina*

First discovered in 1992, RAlGe (R –rare earth metal) was reported initially to crystallize in the so-called ThSi2 structure-type with a centrosymmetric space group I41/amd (No. 141) [1]. Later on, it has been realized instead that RAlGe crystallizes in the LaPtSi-type structure [2,3] with a body-centered space group I41md (No. 109). From recent first principle theoretical calculations, it has been predicted that the members of the RAlGe (R = Pr, Ce) system, which crystallize in the LaPtSi-type structure, are new magnetic Weyl semimetals [4]. This system offers remarkable tunability, since the number and location of Weyl nodes may be controlled by choice of the rare-earth metal, and the types of broken symmetry, via the Al/Ge content. In addition, in the presence of combined broken symmetries, the system offers a rich phase diagram that may be explored via self-doping or chemical substitution. Therefore, to enable a broad range of experimental studies on this class of material, there is a clear interest in establishing the details for the growth of sizable (mm3) single crystals and their basic physical characterization. Recently we have reported on the crystal growth by floating zone and a flux-growth techniques and basic characterization of RAlGe family (R = Ce, Pr) [5]. We investigated the macroscopic and microscopic physical properties of the solid solution of Ce1−xPrxAlGe [6] and reported the discovery of topological magnetism in the candidate magnetic Weyl semimetal CeAlGe [7]. [1] S. Dhar, S. Pattalwar, R. Vijayaraghavan, Journal of Magnetism and Magnetic Materials, 1992, 104-107, 1303. [2] S. Dhar and S. Pattalwar, Journal of Magnetism and Magnetic Materials, 1996, 152, 22. [3] E. Gladyshevskii N. Nakonechna, K. Cenzual, R. Gladyshevskii, J.-L. Jorda, Journal of Alloys and Compounds, 2000, 296, 265. [4] Guoqing Chang, Bahadur Singh, Su-Yang Xu, et al., Physical Review B, 2018, 97, 04114. [5] P. Puphal, C. Mielke, N. Kumar, Y. Soh, T. Shang, M. Medarde, J. S. White, E. Pomjakushina. Physical Review Materials, 2019, 3, 024204. [6] Pascal Puphal, Sarah Krebber, Emmanuelle Suard, Robert Cubitt, Chennan Wang, Tian Shang, Victor Ukleev, Jonathan S. White, and Ekaterina Pomjakushina, Physical Review B, 2020, 101, 214416. [7] Pascal Puphal, Vladimir Pomjakushin, Naoya Kanazawa, Victor Ukleev, Dariusz J. Gawryluk, Junzhang Ma, Muntaser Naamneh, Nicholas C. Plumb, Lukas Keller, Robert Cubitt, Ekaterina Pomjakushina, Jonathan S. White, Physical Review Letters, 2020, 101, 214416.

## [65] Thin film fabrication for users: Possibilities and perspectives (board MO-197)

*Presenter: PÜTTER, Sabine*

JCNS at MLZ offers the opportunity for thin film fabrication in combination with neutron investigation proposals utilizing a Molecular Beam Epitaxy (MBE) setup on site. The design of the MBE setup will be presented revealing its versatility with respect to the fabrication of different material compositions of thin films like “classical” magnetic thin films, transition metal oxide heterostructures or thin metal films for soft matter studies, acting as defined surfaces. Examples like SrCoO$_x$, Fe$_4$N or [Pt/Co/Ta] multilayers will be discussed. The focus lies on stoichiometry, morphology and thickness precision and detailed

information about the possibilities and constraints in sample fabrication for users will be given. For quasi in-situ neutron reflectometry of thin films, which are sensitive to ambient air, a small versatile transfer chamber is may be used for sample transfer from the MBE setup to the neutron reflectometer MARIA and measurement under UHV conditions. [1] Recently, we have utilized 50 nm thick niobium films fabricated at the JCNS lab to perform neutron reflectometry experiments during hydrogen loading. The momentum-space position of the prominent waveguide resonance allows tracking of the absolute hydrogen content with an accuracy of about one atomic percent on a timescale of less than a minute. [2] [1] A. Syed Mohd et al. Rev. Sci. Instrum., 87, (2016) 123909 [2] L. Guasco, et al. Nature Comm. 13 (2022) 1486

### [167] Upgrade of JCNS SANS instrument KWS-2 for improved performance and beam-time efficiency (board MO-199)

*Presenter: RADULESCU, Aurel*

KWS-2 is a classical small angle neutron diffractometer where the pinhole mode with different neutron-wavelengths and detector distances can be combined with focusing mode with MgF$_2$ lenses to reach a wide Q-range between 2x10$^{-4}$ and 1.0 Å$^{-1}$. Upgrades of the detection system and sample environment are currently in progress. A wide-angle detection option is currently being tested and optimized and will allow measurements over an extended Q-range up to 2 Å$^{-1}$, which will be beneficial for semi-crystalline materials and small biological morphologies. The high neutron flux provided by the FRMII reactor and transported by the optimized neutron guidance system required an adjustment of the measurement method for a more rational use of the beam time. A new versatile in-beam sample positioning system, including a multi-position thermostatted carousel, robotic elements and a pool of sample cuvettes, is currently being installed at the instrument's sample position. This enables the instrument to be continuously supplied with samples and the possibility to plan measurements on similar samples or effects in a common long experimental session. Finally, a new size exclusion chromatography setup with in-situ UV-Vis spectroscopy, is currently in construction for providing the instrument with samples of a desired quality, which will improve the performance of KWS-2 for studying aggregation prone proteins and will allow for highly individualized studies of biophysics and soft matter samples. The new upgrades in progress at the instrument will be presented in details.

### [260] Fine-Tuning the Swelling Behavior of PNIPMAM Thin Films – The Case of Salt Addition (board MO-201)

*Presenter: REITENBACH, Julija*

Stimuli responsive polymers have gained much attention due to their unique properties. If polymer thin films exhibit a reversible volume change upon exposure to external stimuli such as temperature, pH, or solvents, they become promising candidates for applications such as nanoswitches or sensors. Polymers like poly(N-isopropyl methacrylamide) (PNIPMAM), which are sensitive to two stimuli can be used as bisensitive devices. PNIPMAM is a LCST-type thermoresponsive polymer and absorbs water molecules when it is exposed to water rich atmospheres. Due to low swelling times and strong volume changes upon water incorporation PNIPMAM thin films are of special interest. In this work, the influence of two different magnesium salts on the swelling behavior of PNIPMAM thin films is explored. In situ time-of-flight neutron reflectometry (ToF-NR) measurements are performed to investigate the macroscopic swelling behavior of the salt containing polymer thin films. By fitting the obtained reflectivity patterns, information about the distribution of the compounds vertically through the thin films can be deduced. To gain further insights on a molecular level and to understand the underlying hydration mechanism, additional in situ Fourier-transform infrared spectroscopy (FTIR) measurements are performed. Our studies showed, that the addition of different salts highly influences the swelling behavior as well as the hydration mechanism of PNIPMAM thin films depending on the salt additive.

### [330] Virtual experiments at the KWS-1 instrument with VITESS to assist training of machine learning algorithms (board MO-203)

*Presenter: ROBLEDO, Jose*

VITESS [1] is a Monte Carlo based simulation package for neutron ray-tracing now hosted by the Forschungszentrum Jülich. We show the VITESS simulation results of the KWS-I Small Angle Neutron Scattering (SANS) instrument at the FRM-II research reactor and compare them with experimental measurements. With the instrument correctly simulated, it is possible to generate a synthetic database of enough size for machine learning algorithm training tasks, which would be difficult otherwise to obtain due to long measurement times in Small Angle Neutron Scattering experiments. In this work we show the potential of this approach and discuss its advantages and disadvantages. [1] C. Zendler, K. Lieutenant, D. Nekrassov, M. Fromme, Vitess 3 – Virtual Instrumentation Tool for the European Spallation, J. Phys. Conf. Ser. 528 (2014) 012036.

### [28] Nanoscale magnetization in lithiated iron oxide nanoparticles (board MO-205)

*Presenter: ROCHELS, Leonhard*

The search for renewable and sustainable electrical energy storage devices has become vital to meet current environmental challenges [1]. Iron oxides represent a promising,environmentally friendly material [2,3] which can be converted into a lithium intercalating material via chemical lithiation [4]. Owing to their high surface area and thus potential high electrochemical surface activity, nanostructured iron oxides are ideally suitable for use as electrode materials. A continuous lithiation process starting at

the materials surface is expected to proceed through different phases. A detailed understanding of the lithiation progress is therefore crucial for the optimization of chemical lithiation processing. In this contribution, we apply magnetic small-angle neutron scattering to gain detailed insight into the lithiation progress from the particle surface to the core. We observe the formation of a core-shell nanoparticle morphology, which we attribute to a lithiated shell that grows in thickness upon lithiation. By correlating chemical and magnetic nanoparticle morphologies, we aim to link the magnetic properties with the degree of lithiation. **References:** [1] D. Larcher, J.-M. Tarascon, *Nat. Chem.* **7**, 19-29 (2015). [2] L. Zhang, H. B. Wu, X. Wen, *Adv. Energy Mater.* **4**, 1300958 (2014). [3] M. Valvo, A. Liivat, H. Eriksson *et al*, *ChemSusChem* **10**, 2431-2448 (2017). [4] P. G. Bruce *et al. Angew. Chem. Int. Ed.* **47**, 2930-2946 (2008).

### [395] Neutron scattering studies of phonon lifetime in SrTiO3 (board MO-207)

*Presenter: ROSHANINEJAD, Parisa*

$SrTiO_3$ is an incipient ferroelectric material with a large static dielectric response, which shows notable phonon anomalies and electrostrictive response (PRB 62, 13942). It is also a neutron triple-axis classic, with seminal work by Cowley, Shirane in which they show the application of available phonon theories and sixties neutron scattering methods. First principles calculations of classic perovskites like $SrTiO_3$ and benchmarking with experimental data have been helpful to figure out a wide range of fundamental characteristics like the electronic origins of ferroelectricity, soft phonon modes and their role in the structural phase transition (PRB 77, 134111). However, the large deviation between phonon lifetime calculations and experimental data remains unanswered. In this work, we try to resolve it by implementing unified methods, diagrammatic approaches and self-consistent phonon theory which include anharmonic effects (PRB 92, 054301). These calculations are compared to the neutron scattering measurements of the phonon line width in the cubic phase of $SrTiO_3$ at various temperatures. For these measurements two types of neutron spectrometers were used, the time of flight spectrometer Merlin at ISIS and the multiplexing spectrometer CAMEA at PSI. Data analysis has been done considering the instrumental resolution effects in the signal lineshape. Additionally, we will discuss the relevance and state of the art of neutron methods for the analysis of excitations lifetimes.

### [26] Evolution of Magnetization in Sequentially Grown Ferrite Nanoparticles (board MO-209)

*Presenter: ROUZBEH, Nahal*

Magnetic nanoparticles (NPs) are technologically relevant for catalysis, high density magnetic data storage, ferrofluids and medical applications. A drastically reduced magnetization compared to the bulk material is commonly attributed to spin disorder in magnetic NPs. Such spin disorder has recently been suggested to be beneficial for magnetic heating, e.g. in intracellular magnetic hyperthermia [1] and is typically considered confined to the NP surface but has also been observed in the NP interior [2]. A key challenge in magnetic NP research lies therefore in the quantitative description and control of the nanoscale distribution of magnetization and spin disorder. Magnetic SANS provides the nanoscale spatial sensitivity to monitor the intraparticle magnetization distribution [3, 4]. In this contribution, we will present our approach of using sequential growth for a systematic variation of spin disorder in ferrite NPs. Our aim is to follow the surface near spin disorder in NPs when the initial surface becomes the interior of the grown particle. Structural and magnetic characterization confirms a systematic particle growth that is accompanied by a significant evolution of the NP magnetization upon the first growth stages. **References:** [1] A. Lak, S. Disch *et al*., *Adv. Science* **2021**, *8*, 2002682. [2] S. Disch *et al*., *New J. Phys*. **2021**, *14*, 01302. [3] S. Mühlbauer, S. Disch *et al*., *Rev. Mod. Phys*. **2019**, *91*, 015004. [4] D. Zákutná, S. Disch *et al*., *Phys. Rev. X* **2020**, *10*, 031019.

### [293] The one-dimensional antiferromagnetic S=1/2 Heisenberg chain in an applied magnetic field (board MO-211)

*Presenter: SAFIULINA, Irina*

Almost a century ago, in 1931, Bethe provided an ansatz to find the exact eigenvalues and eigenvectors of the spin-1/2 Heisenberg Hamiltonian with antiferromagnetic nearest-neighbor interactions. In zero field, the ground state is a singlet, and the inelastic neutron spectrum is a continuum of pairs of topological excitations called spinons. In an applied magnetic field, longitudinal and transverse spin fluctuations are no longer equivalent. For intermediate magnetic fields, below the saturation field that overcomes the antiferromagnetic interaction, the spinon continuum splits into several continua associated with new types of quasi-particles. Here we present a very accurate quantitative study of such a system in applied magnetic field by means of time-of-flight neutron spectroscopy. Additional polarized triple-axis experiments allowed to distinguish longitudinal and various transverse contributions to the spectra.

### [173] Considering Instrumentation for a High Intensity Moderator at the European Spallation Source (board MO-213)

*Presenter: SAMOTHRAKITIS, Stavros*

The European Spallation Source, currently under construction in Lund, Sweden, will originally make available a suite of 15 state-of-the-art neutron scattering instruments, which will be served by a high-brightness moderator placed above the spallation target. The current infrastructure of ESS, however, allows for a second, alternative moderator to be constructed and positioned

below the spallation target. The second moderator is currently considered to have a larger viewable area, offering higher intensities at longer wavelengths, potentially spanning a range from Cold (4 – 10 Å) to Ultra Cold (> 100 Å) neutrons. It is assumed that several areas of condensed matter research profit from such second moderator concept, including small-angle neutron scattering, spin-echo spectroscopy, and neutron imaging. Here, we present the conceptual designs of potential instruments, mainly giving focus to small-angle neutron scattering.

### [452] EasyDiffraction: Making diffraction data analysis and modelling easier (board MO-215)

*Presenter: SAZONOV, Andrew*

Diffraction is a key tool for structure analysis. However, currently available software for modelling and analysis of diffraction data may be, on the one hand, difficult for new users looking to apply diffraction to their field of expertise and, on the other hand, not flexible enough for domain experts. EasyDiffraction [1] aims to lower the barrier of entry to diffraction data analysis by providing an intuitive and user-friendly graphical interface allowing for the simulation of diffraction patterns based on structural models and refinement against experimental data. It is distributed as an all-in-one package that includes all dependencies and can be installed with just a few clicks on different operating systems. For more complex problems and increased flexibility the Python library behind EasyDiffraction can be used through Jupyter notebooks and scripting. Simple interface of EasyDiffraction can help improve the user experience and thereby make it easier to train users and students, as well as be better prepared for experiments. We plan to integrate EasyDiffraction into the full data processing workflow to increase experiment automation and make better use of beam time. EasyDiffraction is built on the EasyScience framework [2], a platform aimed at unifying neutron scattering analysis software. In addition to diffraction, this framework has been successfully applied to reflectometry. Quasielastic neutron scattering will also be targeted in the future. EasyDiffraction relies on existing crystallographic libraries as calculation engines to cover the necessary functionality. It is still in beta and has only some basic features of the CrysPy [3] and CrysFML [4] libraries, such as support for one-dimensional constant wavelength and time-of-flight powder neutron diffraction data. We are collaborating with LLB and ILL regarding the CrysPy and CrysFML, respectively, and more functionality will become available as the project matures. EasyDiffraction is being developed free and open source and we hope to attract interested people to jointly contribute to this project and help us, for the benefit of everyone, in making diffraction data analysis and modelling easier. [1] https://easydiffraction.org [2] https://easyscience.software [3] https://github.com/ikibalin/cryspy [4] https://code.ill.fr/scientific-software/crysfml

### [270] The cold neutron three-axis spectrometer IN12 at the ILL (board MO-217)

*Presenter: SCHMALZL, Karin*

The cold neutron three-axis spectrometer IN12 is operated by the Juelich Centre for Neutron Science (JCNS) in collaboration with the CEA-Grenoble as a CRG-B instrument at the Institut Laue-Langevin (ILL) in Grenoble, France. With an upgrade accomplished in 2012 the instrument has been relocated to an end position of a new guide and the whole primary spectrometer has been upgraded. With a virtual source concept and a new double focussing PG monochromator IN12 has gained a factor of 10 in flux at the sample position with a peak flux of about 10$^8$ n/sec/cm$^2$ around k$_i$ = 2 Å$^{-1}$. An extended wavelength range far into the warmish region (max. k$_i$ $\approx$ 5.1 Å$^{-1}$) is now available. A velocity selector in the guide ensures a clean beam, and a vertical guide changing system with a transmission polarizing cavity guarantees an easy-to-use polarization set-up. IN12 is one of the rare spectrometers that can use polarisation analysis in combination with high magnetic fields. The multi-analyser multi-detector option IN12-UFO is interchangeable with the standard secondary spectrometer and allows to program simultaneous scans in Q-$\omega$ space. We plan the installation of a second monochromator using perfectly bent Si(111) crystals. For lowest accessible wavevector range and energy transfer, it will provide a cleaner signal-to-noise ratio, clean tails of the elastic line and better energy resolution. Its sharper focussing is advantageous when using high field magnets.

### [420] FLASH-NT - A proposal for a complementary neutron imaging instrument on a cold guide at MLZ (board MO-219)

*Presenter: SCHULZ, Michael*

MLZ successfully operates the two neutron imaging beam lines NECTAR and ANTARES. NECTAR provides fast fission neutrons, thermal neutrons and gammas, which can be combined for multi-modal characterization of larger samples with spatial resolution down to ~100 µm. ANTARES offers a spectrum with a thermal maximum, extended towards cold neutrons, providing higher sensitivity and spatial resolutions down to ~20 µm. Many applications such as studying the water management within membranes of fuel cells of only a few µm thickness or lithium transport phenomena and dendrite growth in batteries require highest possible spatial resolution for small samples, combined with a true cold neutron spectrum for highest contrast and high flux. Moreover, many scientific questions requiring modern and advanced imaging techniques (e.g. nGI, Bragg edge imaging) would strongly benefit from a broader spectral range and a colder spectrum. We propose to build a complementary neutron imaging instrument at a neutron guide end position providing a small beam cross section and a cold neutron spectrum, combined with an extremely low background. The instrument should be optimized for applications requiring highest possible spatial resolution down to the single µm range and applications using advanced imaging techniques that will benefit most from the broad spectral range and the low background at a neutron guide, thus adding new possibilities to the portfolio of neutron imaging applications at MLZ.

### [361] Diffraction computed tomography and its applications (board MO-221)

*Presenter: SENYSHYN, Anatoliy*

Attenuation-based radiography and tomography (CT) are well-established experimental techniques for non-destructive visualisation of the object interior, where X-/gamma-rays and neutrons are most commonly used types of the incident radiation, but also protons or heavy particles (e.g. ions) can be used as a source. Different radiation sources are used along with phase-contrast, Bragg and/or energy-selective imaging for gathering complementary information enabling the enhancement of contrast and sensitivity beyond the limitations of X-rays. Alternative way to increase sensitivity to density variations and chemical composition as well as to improve the discrimination of chemically and morphologically similar, but structurally distinct phases is the accounting for scattering effects in the radiography and tomography. This pawed the way to diffraction CT – an experimental technique combining diffraction with Computed Tomography in the form of either XRD-CT or ND-CT, where similar to traditional CT, the sample is scanned by a pencil-beam, but the diffraction picture is collected instead of the attenuation pattern in the transmitted beam. Prominent progress has been achieved during the last decades in increasing spatial and temporal resolution especially for studies of energy materials, biological samples, catalysts, fuel cells etc. In the current contribution we report the applications of diffraction-CT to studies of lithium distribution in commercial cylinder-type Li-ion batteries as well as the implementation and first results of ND-CT (Neutron Diffraction with Computed Tomography) experiments using monochromatic thermal neutrons.

### [58] Micromagnetic simulation of neutron scattering from spherical nanoparticles: Effect of pore-type defects (board MO-223)

*Presenter: SINAGA, Evelyn*

It is well known that beyond a certain size magnetic nanoparticles exhibit a nonuniform internal spin structure. This feature, which is of relevance for many problems of practical interest (e.g., biomedical imaging and drug delivery), is commonly ignored when it comes to the analysis of magnetic neutron scattering data on nanoparticle ensembles. By means of numerical micromagnetic computations we study the transition from single-domain to multi-domain behavior in nanoparticles and its implications for the ensuing elastic magnetic small-angle neutron scattering (SANS) cross section. Furthermore, we model the effect of pore-type microstructural defects on the magnetic SANS cross section and the related pair-distance distribution function of spherical magnetic nanoparticles. Our expression for the magnetic energy considers the isotropic exchange interaction, the magneto-crystalline anisotropy, the dipolar interaction, and an externally applied magnetic field. The signatures of the defects and the role of the dipolar energy are highlighted, and the effect of a particle-size distribution is studied. We are also interested in the signature of the Dzyaloshinskii-Moriya interaction on the SANS observables.

### [374] Relocation of the cold triple axis spectrometer FLEXX to MLZ, Munich: Larmor diffraction and inelastic scattering (board MO-225)

*Presenter: SKOULATOS, Markos*

The cold triple-axis spectrometer (TAS) FLEXX at HZB is a well-designed and upgraded instrument [1-4]. There is a strong wish that this excellent instrument should be preserved for the community after the shutdown of the HZB neutron source. One attractive gap in the present instrumentation suite of MLZ, is the Larmor-diffraction technique [5-6] (LD) and, as a natural extension, cold neutron resonant spin echo (NRSE). LD permits the exact measurement of lattice constants and their distribution (internal strains, structural distortions or magnetostriction). In addition, spin correlation lengths in antiferromagnets and antiferromagnetic domain sizes of up to 1 μm can be determined. For looking at time-dependent processes one needs the NRSE mode. TAS comes at no extra cost, as is the main backbone of such an instrument. The instrument will be placed on a cold neutron source. This will allow for a x4 increase in Q resolution, as well as most importantly access to the low Q region, as compared to the existing TRISP@MLZ. Further, new developments are under way to allow for application of magnetic fields at the sample, hitherto not possible [7-9]. This opens up new vistas in the exploration of materials. A last attractive option is the possibility to combine high magnetic fields together with cold TAS. [1] M. Skoulatos et al., NIMA 647, 100 (2011). [2] M.D. Le et al., Nucl. Instr. Meth. Phys. Res. A 729, 220 (2013). [3] F. Groitl et al., Rev. Sci. Instrum. 86 025110 (2015). [4] K. Habicht et al., EPJ Web of Conferences 83, 03007 (2015). [5] M.T. Rekveldt, Jour. Appl. Phys. 84, 31 (1998). [6] M.T. Rekveldt et al., Europhys. Lett. 54, 342 (2001). [7] Neutron Spin Echo - Proceedings of a Laue-Langevin Institut Workshop, Grenoble, Springer- Verlag, Ed: F. Mezei (1980). [8] M.T Rekveldt et al., Jour. Appl. Cryst. 47, 436 (2014). [9] K. Habicht, “Neutron-Resonance Spin-Echo Spectroscopy: A High Resolution Look at Dispersive Excitations”, Habilitation, University of Potsdam (2016).

### [211] Variation of Structural and Dynamical Flexibility of Myelin Basic Protein in Response to Guanidinium Chloride (board MO-227)

*Presenter: STADLER, Andreas*

Myelin basic protein (MBP) is intrinsically disordered in solution and is considered as a conformationally flexible biomacromolecule. Here, we present a study on perturbation of MBP structure and dynamics by the denaturant guanidinium

chloride (GndCl) using small-angle scattering and neutron spin–echo spectroscopy (NSE). A concentration of 0.2 M GndCl causes charge screening in MBP resulting in a compact, but still disordered protein conformation, while GndCl concentrations above 1 M lead to structural expansion and swelling of MBP. NSE data of MBP were analyzed using the Zimm model with internal friction (ZIF) and normal mode (NM) analysis. A significant contribution of internal friction was found in compact states of MBP that approaches a non-vanishing internal friction relaxation time of approximately 40 ns at high GndCl concentrations. NM analysis demonstrates that the relaxation rates of internal modes of MBP remain unaffected by GndCl, while structural expansion due to GndCl results in increased amplitudes of internal motions. Within the model of the Brownian oscillator our observations can be rationalized by a loss of friction within the protein due to structural expansion. Our study highlights the intimate coupling of structural and dynamical plasticity of MBP, and its fundamental difference to the behavior of ideal polymers in solution.

### [303] Neutron scattering of the easy-plane magnet ErB$_2$ (board MO-229)

*Presenter: STEKIEL, Michal*

We present neutron scattering data on the hexagonal rare-earth diboride ErB$_2$. ErB$_2$ orders magnetically below $T_c$ = 14 K, where the magnetocrystalline anisotropy exhibits strong easy-plane characteristics, as established from measurements of the specific heat, ac susceptibility, magnetisation, and electrical transport. In order to investigate the magnetic structure we performed neutron Laue diffraction, as well as single crystal neutron diffraction in zero and finite field as a function of temperature.

### [348] Neutron polarimetry study on the phonon-crystal field coupling in CeAuAl3 (board MO-231)

*Presenter: STEKIEL, Michal*

The magnetoelastic coupling between phonons and f-electron transitions in crystal electric field (CEF) has been of interest for long time already but still lacks a systematic understanding. It was first recognized in 1980s in CeAl2 that showed an unexpected excitation spectrum. It was explained by a qualitative theory developed by Thalmaier and Fulde [2] but limited to this case. Such phonon-CEF coupling in CeAuAl3 seems to be exceptionally interesting. Just as CeAl2 it hosts a coupled phonon-CEF excitation that manifests in the measured spectra as an additional non-dispersive excitation at 8 meV. However, it also shows an anti-crossing of the CEF excitation at 5 meV and an acoustic phonon [3]. We have performed polarized inelastic neutron scattering measurements on CeAuAl3 to elucidate on the polarization of the coupled excitation as well as on the phonon-CEF anti-crossing. We have observed a transfer of the spectral weight between the magnetic and nuclear channels in the anti-crossing region. Most importantly we have adapted and extended the Thalmaier-Fulde model and performed calculations with McPhase software [4] that allow to quantitatively reproduce the measured spectra and the spectral weight transfer. [1] M. Loewenhaupt et al, Phys. Rev. Lett, 42, 1709, (1979). [2] P. Thalmeier and P. Fulde, Phys. Rev. Lett., 49, 1588, (1982). [3] P. Cermak et al, PNAS, 116, 6695-6700, (2019). [4] M. Rotter et al, J. Phys.: Condens. Matter, 24, 213201, (2012).

### [323] Chemical Analysis with Neutrons for Cultural Heritage Research (board MO-233)

*Presenter: STIEGHORST, Christian*

Elemental analysis based on neutron activation provides a number of advantages for the study of ancient objects. It is non-destructive, the sample preparation is simple, and most elements can be analyzed with low detection limits. The most commonly used methods are prompt gamma activation analysis (PGAA) and instrumental neutron activation analysis (INAA), which enable a panoramic bulk analysis. Since PGAA and INAA are complementary for some elements, a combination of both methods is possible to further increase the number of detectable elements. One of the main tasks in archaeology is provenance analysis. Multivariate statistics can be applied to chemical fingerprints, which can be used to find out the origin of ancient building materials, everyday objects or works of art. This makes it possible to reconstruct old transport and trade routes. Activation analysis can also be used to solve conservation and restoration issues, e.g. to find out which treatment methods can minimize corrosion. Another PGAA-related method used in cultural heritage research is prompt gamma-ray activation imaging combined with neutron tomography (PGAI-NT), which provides spatial resolution of the elemental composition. This technique can be used to "look inside" objects non-destructively to reveal ancient manufacturing processes or their previous usage. We will provide an overview of the methods and their applications at the MLZ.

### [220] Concept study of an indirect spectrometer of mushroom type at the reactor source FRM II (board MO-235)

*Presenter: TANG, Ran*

Mushroom is a concept of an indirect neutron spectrometer with a secondary spectrometer based on a super flat-cone analyser made of highly oriented pyrolytic graphite with an array of position-sensitive detectors (PSD) below it. This combination of the analyser and PSD gives the complete information of the outgoing wave vectors from each detected point on the PSDs. The idea has been first presented by R. Bewley for a new spectrometer at the spallation source ISIS in the UK. We aim to adapt the Mushroom concept to the reactor source at FRM II, such that a much higher count rate can be reached than at a traditional triple-axis spectrometer (TAS). This is possible thanks to the special analyser in Mushroom covering a solid angle up to 2π steradian. This allows for obtaining an overview of the dispersion relation and/or diffuse scattering with only a few scans. We report on the theoretical calculations of matching the resolution function of the secondary to the primary spectrometer using

monochromatized neutrons from one of the neutrons guides of FRM II. Besides this McStas simulations are presented showing predictions on the instrument performance.

### [209] magnetic structure of Mn2GaC thin film by neutron diffraction (board MO-237)

*Presenter: TAO, Quanzheng*

Mn2GaC (space group P63/mmc) is a laminated material consisting of Mn2C layers interleaved with Ga layers. The competition between antiferromagnetic and ferromagnetic interactions within the Mn2C planes gives rise to complex magnetic behaviors. It orders magnetically below TN = 507 K and shows another magnetic transition at TC = 220 K. We employed neutron diffraction to study the nature of the magnetic order with single crystal neutron diffractometer D10 at ILL and WISH at ISIS. We identified two sets of reflections that are consistent with two propagation vectors, q1= (0 ,0, 2/3) and q2=(0, 0, 0.54) at both 300 K and 1.5 K, where q1 is predominant at 300 K while q2 is stronger at 1.5 K. By fitting the integrated intensity of the magnetic reflections and by considering the presence and absence of certain peaks, we proposed a transverse spiral structure along c axis.

### [352] Magnetic structure and spin flip transition of MnSb4Te7 (board MO-239)

*Presenter: TOBIN, Siobhan*

The family of materials (Mn(Sb,Bi)$_2$Te$_4$)((Sb,Bi)$_2$Te$_3$)$_m$ offer a smörgåsbord of topological electronic states and magnetic phenomena [1-3]. The hexagonal MnSb$_4$Te$_7$ is one such van der Waals material. The unit cell can be described by the $P\bar{3}m1$ space group, where the Sb$_2$Te$_3$ topological layers are sandwiched between magnetic MnSb$_2$Te$_4$ septuple layers. Theoretical calculations indicate that different spin arrangements of the Mn magnetic sublattice can strongly influence the topology of the charge carriers in the Sb2Te3 quintuple layers [1]. Symmetry analysis and theoretical calculations indicate that the axion insulator state usually associated with A-type AFM order will in fact persist even when the material becomes FM ordered in the presence of an external magnetic field along the c axis [1]. We have conduct-ed neutron diffraction on a single crystal of MnSb$_4$Te$_7$ at the D10 instrument at the ILL. Our zero field measurements are consistent with A-type AFM order as seen in the Bi equivalent compound [2,3]. With increasing field along the c axis, we find evidence for a spin flip transition occurring at $\sim$0.15 T. The magnetic structure as a function of both temperature and external field will be discussed. We also comment on implications for the dimensionality of the magnetism. Finally we compare the magnitude and site mixing of Mn$^{2+}$ moments to those of the Bi analogue compound. References [1] Huan, S. et al. Physical Review Letters 126, 246601 (2021). [2] Ding, L. et al. Journal of Physics D: Applied Physics 54, 174003 (2021) [3] Ding, L. et al. Physical Review B 101, 020412 (2020)

### [475] Polydispersity analysis based on a unified exponential/power-law approach to small-angle neutron scattering (board MO-241)

*Presenter: TOMCHUK, Oleksandr*

Small-angle neutron scattering in the comprehensive analysis of particulate systems brings a number of benefits in a deeper understanding of physicochemical processes. The method is capable of providing a detailed structural description at the mesoscale level. Such a description must contain information about polydispersity. There are many approaches to determining the size distribution function. Nevertheless, they all include certain integral equations, which can introduce additional mathematical artifacts. Beaucage *et al.* proposed an alternative approach [1]. They took into account that each of the parameters of the Guinier and Porod equations is proportional to some moment of the size distribution function. This is the basis for an approach that makes it possible to analytically calculate the parameters of a lognormal distribution based on a dimensionless combination of parameters, designated as PDI. We consider the possibility of using additional scattering invariants, such as the Porod integral or the correlation length (weight-averaged chord length), to construct an additional polydispersity index containing lower distribution moments compared to the PDI from [1]. This makes it possible to determine the parameters of polydispersity functions other than lognormal analytically. The cases of normal, Boltzmann, uniform, triangular, Schultz and exponential distributions are considered in detail. [1] Beaucage G. *et al.*, *J. Appl. Cryst.* **37** (2004) 523.

### [242] Investigation of temperature distribution and phase of InBi eutectic alloy through energy resolved neutron imaging (board MO-243)

*Presenter: TREMSIN, Anton*

The possibility to measure neutron transmission spectra in each pixel of imaging dataset enables various studies of microstructure within solid materials. Among these studies there is a possibility to map the temperature distribution within materials without direct access to them, e.g. enclosed within other structures. Variation of both Bragg edge wavelength and the width of neutron resonance absorption with temperature can be utilized for such temperature mapping, providing the neutron transmission spectrum can be measured in a wide energy range. Neutron spallation sources provide the opportunity to measure neutron transmission in a wide range of energies, all in one measurement [1-5]. In this paper we demonstrate how temperature distribution maps can be reconstructed for an InBi eutectic alloy sealed within a brass container. We also demonstrate that transition from liquid to solid phase can be studied within a closed container with sub-mm spatial resolution through the analysis of neutron

resonance absorption spectra. Such analysis can be beneficial for non-destructive testing of various solid materials and for in-situ studies where materials are enclosed within structures opaque to other conventional techniques. 1. T. Kai, et al., Physics Procedia 43 (2013) 111. 2. A.S. Tremsin, et al., Nucl, Instr. Meth. A 746 (2014) 47. 3. A. S. Tremsin, et al., Nucl, Instr. Meth. A 803 (2015) 15. 4. A.S. Tremsin, et al., AIP Advances 7 (2017) 015315. 5. A. S. Losko, S. C. Vogel, Scientific Reports 12 (2022) 6648.

### [77] Phonon confinement gap in CeO$_2$ nanocrystals (board MO-245)

*Presenter: TYMOSHENKO, Yuliia*

The phonon density of states (PDOS), which plays an important role in the mechanisms that determine the unique physical properties of nanocrystals (NCs), strongly depends on the reduced size of the NC. While these confinement effects are often invoked to explain surprising results, the direct study of lattice dynamics in NCs is difficult. Theoretically, it is shown that as the NC size decreases, the gapless and continuous PDOS observed in the bulk becomes discrete and is characterized by a cutoff in the low-frequency part of the spectrum -- the so called phonon confinement gap. Here we present our measurements of the PDOS of both nanocrystalline and bulklike microcrystalline samples of CeO$_2$ with high resolution cold TOF neutron spectrometer LET. The data obtained allow us to investigate the size effects on PDOS and extract the phonon confinement energy gap.

### [205] The Topology of Polymer Brushes Determines Their Nanoscale Hydration (board MO-247)

*Presenter: VAGIAS, Apostolos*

By utilizing time-of-flight neutron reflectometry (ToF-NR) under different relative humidities, we demonstrate that grafted polymer brushes constituted by hydrophilic cyclic macromolecules exhibit more compact conformation with lower roughness compared to linear brush analogues, due to the absence of dangling chain ends extending at the interface. [1] In addition, due to increased interchain steric repulsions, cyclic brushes feature larger swelling ratio and increased solvent uptake with respect to their linear counterparts presenting the same composition and comparable molar mass. Moreover, the two topologies exhibit differences in ageing, upon repetitive runs of swelling/drying trials. To correlate the equilibrium swelling ratios as a function of relative humidity for different topologies a new form of the Flory-like expression for equilibrium thicknesses is proposed. The relative humidity represents the chemical potential balance between brush and surrounding environment. The Flory-like expression, which has been successfully utilized so far for thin polymer films, breaks down for the cyclic brush. Additional topological contributions need to be taken into account in this expression, in order to rationalize differences reflected in swelling ratios and solvent content between the linear and cyclic polymer brush topologies. [1] A. Vagias et al., in preparation

### [376] The SAPHiR instrument for neutron diffraction and radiography at high pressure and temperature (board MO-249)

*Presenter: WALTE, Nicolas*

SAPHiR is an instrument-under-construction designed for neutron diffraction and radiography under extreme pressure and temperature conditions at the FRM II neutron source. A multianvil press with six independently controlled rams subjects powder, fluid, and melt samples with volumes of 10–50 mm3 to a current maximum pressure of 15 GPa and temperatures up to ca. 2300 K. An additional cryo-system can also cool samples below room temperature to ~80 K. Neutrons are focussed on the sample position by a double-elliptic neutron guide system with a super-mirror coating m = 1.5-4. Due to geometrical restrictions by the press, neutron diffraction measurements will use the time-of-flight method with a thermal neutron wavelength of 1-2.4 Å and a flux of ~10^7 n/s/cm2 at the sample position. For diffraction, SAPHiR will use three detector banks with 640 position sensitive helium-3 detectors that are arranged at both 90° from the primary beam and in the forward scattering direction, and a wavelength-shifting-fibre scintillator system in the backscatter direction. Future applications of SAPHiR include in situ crystallography and phase relations of light-element-bearing phases, equations of state, reaction kinetics, high-resolution radiography, and rheological studies. The SAPHiR press is currently operating for offline studies whilst other components are installed. This instrument will be ready for final commissioning and neutron measurements when the reactor is restarted in early 2024.

### [210] Lithium-ion Batteries: a microscopic view! -- of Lithium-ion transportation in 4-arm star PEO (board MO-251)

*Presenter: WANG, Hui*

Lithium-ion batteries (LIBs) play an important role in our daily life with a variety of important applicants. To this day, significant resources have been dedicated to the development of high-performance LIBs, particularly the research necessary to identify the optimum electrolyte materials to solve the safety issue. Up to this point polymer electrolytes are widely investigated for their potential to improve batteries' safety. Given the relative high ionic conductivity, around 10-3 S/cm, poly-ethylene oxide (PEO) is frequently utilized as the polymer matrix in this scenario. But compared to the commercial liquid electrolyte, the ionic conductivity of polymer electrolytes need to be improved dramatically. It is widely acknowledged that the transportation of Li+ is directly related to the segmental and backbone motions of the polymer. This contribution aims at developing a microscopic picture of the Li–ion transportation process to instruct the polymer tailoring for optimized ionic conductivity and hence fastest charging and discharging

of the battery. Based on our previous studies, the structure optimization is performed on the PEO 4-arm star (4-arm-PEO). First, the microscopic picture of the Li+ transportation mechanism in the 4-arm-PEO is investigated through molecular dynamics (MD) simulation. Then the polymer dynamics are clarified with Quasi-elastic Neutron Scattering (QENS). By comparing the polymer dynamics from MD simulation and QENS, the microscopic view of Li+ transportation is firmly validated through Neutron scattering experiment. The microscopic view clearly shows that Li+ is easily trapped by the O atoms near the core of the 4-arm-PEO (the cross point of the 4 PEO arms) resulting in the relative low ionic conductivity. We replace the O atoms near the core with –CH2. This structure optimization improves the dynamics of the 4-arm-PEO and increases its ionic conductivity. This contribution improves the ionic conductivity of the polymer electrolyte of LIBs by tailoring the polymer structure. Moreover, the microscopic mechanism will further offer scientific instructions for the ionic conductivity enhancement of the polymer electrolytes.

### [213] A hitchhiker’s guide to the EasyScience galaxy (board MO-253)

*Presenter: WARD, Simon*

easyScience[1] is an initiative from the European Spallation Neutron Source (ESS) to unify simulation software across neutron scattering. DON’T PANIC! While this goal seems an unsurmountable challenge, it is achievable as demonstrated by our current releases. The easyScience project has the following aims; Provide a unified method to interact the most popular technique specific simulation software/libraries, a professional and welcoming graphical interface for new users, JuPyter notebooks for experienced users, unified data structures and workflows across multiple techniques. As an opening to this project, diffraction and reflectometry techniques were chosen to demonstrate the easy philosophy. These techniques have multiple complex calculation engines available, which it is unrealistic to expect users to master. easyReflectometry and easyDiffraction unifies these calculation engines for their respective techniques and provides a complete, feature rich and easy to use interface. In the future QENS and spectroscopy will also be targeted. As a bonus, the technologies behind the easyScience programs allow for advanced modelling and statistical analysis techniques with the ability to scale for large datasets. Behind these programs is easyCore, a unified simulation, optimisation and analysis package. easyCore is built on the latest techniques and libraries including scipp (developed at ESS) for dataset handling, jax for machine learning and PyMC for Bayesian analysis. Hence all these features are available for all easyScience software. We present the main features of easyScience, where it came from, where it’s going and how it will be used to enhance the analysis workflow with the latest analysis techniques. [1] https://github.com/easyScience

### [16] Unconventional magnetic phase transitions and non-trivial spin structures in the DMI-magnet Ba2CuGe2O7 (board MO-255)

*Presenter: WILD, Peter*

Incommensurate spiral magnets have raised tremendous interest in recent years, mainly motivated by their wealth of spin structures with potential non-trivial topology, such as skyrmions. A second field of interest is multiferroicity: Helical spin structures are in general ferroelectric, enabling the coupling of the electric and magnetic properties. Both fields present enormous potential for future devices, where spin and charge degrees of freedom are coupled. Ba2CuGe2O7, characterised by a quasi-2D structure with Dzyaloshinskii-Moriya interactions (DMI), is a material that is interesting in both of these regards and combines them with a third one: a variety of unconventional magnetic phase transitions. Neutron diffraction is used for a careful examination of the distribution of critical fluctuations in reciprocal space, associated with the paramagnetic to helimagnetic transition of Ba2CuGe2O7. Caused by the reduced dimensionality of Ba2CuGe2O7, a crossover from incommensurate antiferromagnetic fluctuations to 2D antiferromagnetic Heisenberg fluctuations is observed, highlighting the rich cornucopia of magnetic phase transitions in spiral magnetic textures.

### [140] News from the McStas instrument simulation package (board MO-257)

*Presenter: WILLENDRUP, Peter*

The McStas[1] Monte Carlo ray-tracing package is a well known and widely adapted tool for the design and optimisation of neutron instrumentation world wide. The contribution presents an overview of the project in its current state with highlight on new features in the 3.2 and 2.7.2 releases from the fall of 2022. Further the contribution demonstrates how to easily port an existing 2.x instrument to the 3.x range which has support for NVIDIA GPU processors. [1] Willendrup and Lefmann, Journal of Neutron Research 22, 1 (2020) and 23, 7 (2021).

### [76] The direct geometry cold chopper spectrometer TOFTOF (board MO-259)

*Presenter: WOLF, Marcell*

TOFTOF is a direct geometry disc-chopper time-of-flight spectrometer. A cascade of seven fast rotating disc choppers is used to prepare a monochromatic pulsed beam which is focussed onto the sample by a converging super-mirror section. The scattered neutrons are detected by 1000 $_3$He detector tubes with a time resolution up to 50 ns. The detectors are mounted at a distance of 4 m and cover 12 m$^2$ (or 0.75 sr). The high rotation speed of the chopper system together with a high neutron flux in the wavelength range of 1.4 -14 Å allows free tuning of the energy resolution between 3 meV and 2 µeV. The fast neutron background is suppressed by the s-shaped primary neutron guide. This enables the investigation of weak signals. The existing linearly tapered neutron guide yields a beam spot size of 23x47 mm$^2$. As alternative option a focussing guide can be used. This leads to an

intensity gain up to a factor of 3 (wavelength dependent) on a sample area of 10 x 10 mm$^2$. TOFTOF represents a versatile instrument combining high energy resolution, high neutron flux (also at short wavelengths), and an excellent signal-to-background ratio. It is perfectly suited for inelastic and quasielastic neutron scattering for a broad range of scientific topics.

### [422] Event Mode Neutron Imaging with ns Temporal and µm Spatial Resolution (board MO-261)

*Presenter: WOLFERTZ, Alexander*

Recent developments in event driven camera systems allow the construction of a new type of scintillator-based event mode imaging devices. A neutron imaging device employing this new technology to reach high spatial and temporal resolution is currently under development at the NECTAR instrument at FRMII. The goal is for the detector to have a spatial resolution better than 100 µm and a timing resolution of 10 ns. At the same time, the individual neutron detection approach should improve the signal to noise ratio. With high temporal and spatial resolution, the detector can be used in applications where timing and location are critical, such as high-resolution time of flight imaging and modulation of intensity with zero effort (MIEZE). The structure of the detector consists of a scintillator screen, an image intensifier and a photo-sensitive sensor with single photon readout. A lens is used to collect the light from the scintillating screen on the image intensifier. The setup is flexible and allows an easy change of the scintillator screen and the field of view. A working prototype has already been built and successfully tested. The current development is focused on determining the properties of different scintillating screens and categorize them with respect to their usefulness in achieving the targeted detector parameters. First results from different scintillators will be presented at the ECNS. This project is funded by the BMBF under the grant number 05K22WO5.

### [108] KWS-X: The new SAXS/WAXS Laboratory Beamline at JCNS-MLZ (board MO-263)

*Presenter: WU, Baohu*

The new customized SAXS/WAXS instrument from XENOCS have be installed in the JCNS X-ray laboratory from the end of 2021. As a young member of our small angle scattering instrument by using x ray as beam, the new instrument is equipped with a high flux metal-jet source and a moveable Eiger 2R4M SAXS detector. With additional 4-axis motorized WAXS detector and Bonse-Hart USAXS the scattering vector q can cover a wide area from 0.0002 to 7 Å-1. Compared to other instruments, it also comprises a large sample environment station that can be used with ambient pressure conditions. A large number of sample environmental accessories make it possible to perform experiments at temperatures from -150oC to 1000oC, under shear, tensile, RheoSAXS, SEC-SAXS, GISAXS/GIWAXS etc. As a very powerful complementary instrument to SANS and other neutron-related instruments, it will strongly support our users' work in the MLZ.

### [267] New options on the polarized neutron single crystal diffractometer POLI at MLZ (board MO-265)

*Presenter: XU, Jianhui*

Polarized neutron diffraction is a powerful tool for studying condensed matter physics and to probe the spin and orbital properties of unpaired electrons. POLI is a polarized neutron single crystal diffractometer built on the hot neutron source at MLZ. Currently three standard setups are implemented on POLI: 1) zero-field spherical neutron polarimetry using CRYOPAD; 2) polarized neutron diffraction in magnetic fields; 3) non-polarized diffraction under various conditions. We recently implemented a new actively shielded asymmetric split-coil superconducting magnet with a maximal field of 8T. The magnet is designed to facilitate polarized neutron diffraction with low stray fields, a large opening (30° vertical) and a large sample space suitable for e.g., piezo goniometers and pressure cells. We also built a compact-size solid-state supermirror bender polarizer optimized for short neutron wavelengths to provide high neutron polarization in the vicinity of the magnet. An in-situ SEOP polarizer and analyzer will be available in 2022 which maintains high levels of neutron polarization and intensity over long periods of time. The SEOP polarizer are well shielded magnetically and can be used with the large magnet. Transferring the BIDIM26 area detector of size 26cm by 26cm from LLB to MLZ is in progress [3]. [1] V. Hutanu, J. Large-Scale Res. Facil. 1, A16 (2015). [2] V. Hutanu et al., IEEE Trans. Magn. 58, no. 2, pp. 1-5, (2022). [3] A. Gukasov et al., Physica B 397, 131 (2007).

### [317] Monte-Carlo simulations of cold neutron transmission measurements of clathrate hydrates and graphite compounds (board MO-267)

*Presenter: XU, Shuqi*

The European Spallation Source (ESS), which is currently under construction in Lund, Sweden, will be the most powerful pulsed neutron source in the world. A design study project named HighNESS is dedicated to develop a second neutron source at ESS that compared to the first source, located above the spallation target and designed for high cold and thermal brightness, provides higher intensity cold neutrons, very cold neutrons (VCN) and ultra cold neutrons (UCN) [1]. This work carried out within the HighNESS project presents the Monte-Carlo simulations of cold neutron transmission measurements of clathrate hydrates as potential moderator candidates [2] and graphite compounds as reflector materials. The Monte-Carlo simulations are performed by using the neutron transport codes OpenMC [3] and McStas [4], with the neutron scattering kernels prepared by the toolkit NCrystal [5, 6, 7] developed in the project. The scattering kernels of clathrate hydrates and graphite compounds are generated thanks to the phonon density of states obtained by density functional theory (DFT) calculations. The simulated results including neutron scattering cross sections, scattering kernels and diffraction patterns are further validated by comparing with the transmission

measurements performed at Institut Laue-Langevin (ILL) and Paul Scherrer Institute (PSI). References [1] V Santoro, KH Andersen, M Bernasconi, M Bertelsen, Y Beßler, D Campi, V Czamler, DD Di Julio, E Diane, K Dunne, et al. Development of a high intensity neutron source at the european spallation source: The highness project. arXiv preprint arXiv:2204.04051, 2022. [2] Oliver Zimmer. Neutron conversion and cascaded cooling in paramagnetic systems for a high-flux source of very cold neutrons. Phys. Rev. C, 93:035503, Mar 2016. [3] Paul K. Romano, Nicholas E. Horelik, Bryan R. Herman, Adam G. Nelson, Benoit Forget, and Kord Smith. Openmc: A state-of-the-art monte carlo code for research and development. Annals of Nuclear Energy, 82:90–97, 2015. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013, SNA + MC 2013. Pluri- and Trans-disciplinarity, Towards New Modeling and Numerical Simulation Paradigms. [4] P. K. Willendrup and K. Lefmann. Mcstas (i): Introduction, use, and basic principles for ray-tracing simulations. 2020. [5] X.-X. Cai, T. Kittelmann, E. Klinkby, and J.I. M´arquez Dami´an. Rejection-based sampling of inelastic neutron scattering. Journal of Computational Physics, 380:400–407, 2019. [6] X.-X. Cai and T. Kittelmann. Ncrystal: A library for thermal neutron transport. Computer Physics Communications, 246:106851, 2020. [7] T. Kittelmann and X.-X. Cai. Elastic neutron scattering models for ncrystal. Computer Physics Com- munications, 267:108082, 2021.

### [502] Multi-Incident-angle Neutron Reflectometer with Focusing Optics at SOFIA (J-PARC) (board MO-269)

*Presenter: YAMADA, Masako*

SOFIA is the horizontal-type neutron reflectometer at Beamline 16 (BL16) of the Materials and Life Science Experimental Facility (MLF) of the Japan Proton Accelerator Research Complex (J-PARC). Allowing users to keep the sample horizontal while measuring the whole q-range, SOFIA is advantageous for observing liquid-vapor and liquid-liquid free interfaces. Thus, SOFIA is, by and large, utilized for investigating soft matters. The required data acquisition time for sufficient statistics at SOFIA is relatively short, owning to the highest intensity of the beam in the world from J-PARC (as of today), and to the efficient measurement with the pulsed beam and Time-of-Flight method. On the other hand, its accessible Qz range is limited by the wavelength band. The current setup of SOFIA requires three to four points of angle scan to cover the dynamic range of reflectivity from 1 to 10<sup>-6</sup>-10<sup>-7</sup>, which corresponds to the Qz range from a little less than 0.1 nm<sup>-1</sup> to 1.5-4 nm<sup>-1</sup>. To enhance the performance of SOFIA, especially for time-slicing measurements, we are upgrading to a Multi-Incident-angle Neutron Reflectometer (MI-NR) with a combination of focusing optics. With this setup, we could cover the range of 0.09 ≤ Qz [nm<sup>-1</sup>] ≤ 3.3 with a single shot with an enhanced beam intensity. In the presentation, the details of the upgrade concept and the progress status of commissioning will be presented.

### [240] The High Brilliance Neutron Source Target Stations (board MO-271)

*Presenter: ZAKALEK, Paul*

The advent of high-current accelerator systems launched the development of high-current accelerator-driven neutron sources (HiCANS) utilizing low energy nuclear reactions. This development can counteract the increasing shutdown of existing fission-based neutron sources and a resulting decline in available neutron beam days as well as establishing HiCANS as a next generation national neutron source. A main component of a HiCANS is the target station used to release neutrons, to moderate the neutrons to the required energy in the keV or meV range, to extract the neutrons to the instruments with the proper phase space volume as well as to shield the surrounding equipment. Within the High-Brilliance neutron Source (HBS) project, three target stations will be operated simultaneously with one long pulse, and two medium pulse proton beams. The target stations have target / moderator / reflector geometries optimized to the specific proton beam structure resulting in tailored neutron beams for different groups of neutron instruments. At the ECNS conference, we will present the general design ideas of such HiCANS target stations, show the flexibility they offer and present the resulting TMR assemblies for the HBS project. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [297] Residual stresses in the bronze matrix composite surface deposits after laser melting injection (board MO-273)

*Presenter: ZHANG, Xingxing*

Wear causes a loss of 2% to 7% of the gross national product in industrialized countries [1]. Therefore, developing wear-resistant coatings and optimizing their manufacturing processes are essential. A novel metal matrix composite (MMC) coating has been developed via laser melting injection (LMI) technique over the last few years, which consists of a bronze matrix and tungsten fused carbides. Tribological tests have shown that this MMC coating has the potential to reduce wear by ~80% [2]. However, macro and micro residual stresses exist in the MMC coatings, which significantly affect the performance of the MMC coatings, such as causing dimensional distortion, reducing the fatigue strength and service life [3]. Therefore, it is critical to characterize the residual stresses in the MMC coatings. In this research, the residual stresses in the LMI bronze matrix composite surface deposits were measured via neutron diffraction experiments. The residual stresses along the depth direction from the surface of the deposit to the center of the sample were determined nondestructively due to the large penetration depth of neutrons. A thermo-mechanical finite element model was developed. This combined experiment and simulation study provides a detailed insight into the residual stress state in the LMI MMC coatings. The results will be helpful in optimizing the laser processing and tailoring the residual stress. References [1] GfT (Gemeinschaft für Tribologie e.V.), https://www.gft-ev.de/en/what-is-tribology/, accessed on 28.01.2021. [2] H. Freiße, A. Langebeck, H. Köhler, T. Seefeld, Dry Metal Forming Open Access Journal 2 (2016) 001-006. [3]

G.A. Webster, A.N. Ezeilo, International Journal of Fatigue 23 (2001) S375-S383.

### [229] Polarizing neutron optics with higher reflectivity, polarization and no magnetic coercivity (board MO-275)

*Presenter: ZUBAYER, Anton*

Neutron supermirrors are the bedrock of all modern neutron beamlines both polarized and unpolarized. However, while the technology has improved remarkably over the last 20 years there are still areas where significant improvements can be made regarding interface roughness reduction, better polarization and elimination of magnetic stray fields when polarizing the neutrons. Adding 11B4C to Fe/Si supermirrors has potential to alleviate some of these issues. Boron has been shown to form metal-boron bonds which restricts metal diffusion which, in turn, inhibits metal crystallite formation during DC magnetron sputter deposition. Element-pure Fe/Si multilayers inherently exhibit large interface widths due to crystallization of Fe layers and Fe-silicides at the interfaces. It has been shown that incorporation of 11B4C helps reducing the interface width as it promotes amorphization in Fe layers due to Fe-B bonding and reduces diffusion at the interfaces to suppress Fe-silicide crystallization. In this work, isotope enriched 11B is used since; (a) 10B is a widely known neutron absorber and (b) a high scattering length density (SLD) of 11B4C can be used to maximize polarization by maximizing the SLD contrast for one spin state while minimizing it for the other spin state by compositional variation of 11B4C in the Fe and Si layers. Through X-ray and neutron scattering-, magnetometry-, microscopy- and spectroscopy techniques we prove our case that Fe/Si + 11B4C would be of preference.

### [495] A 3T compatible in-situ 3He analyser for KWS1 (board MO-277)

*Presenter: SALHI, zahir*

We present a compact 3He polariser to be used as polarisation analyser for KWS1.The 38 cm long magic box magnetic cavity with angled plates on the entrance side provides a 3He magnetic lifetime of 300 hours with the cell centred in the device, up to 7 cm diameter cell is used and polarization is performed with one laser, a relatively large angular coverage providing up to ±0.07 ˚A−1 at 4.5 ˚A is possible due to its close proximity to the sample and sample magnet .When used with the HTS-110, New Zealand sample magnet and a 3T horizontal (towards the 3He cell) field this magnetic lifetime was reduced to 163 hours , This level of performance is more than adequate, especially for an in-situ polarized system where spin- exchange rates on the order of 10 hours or less can be obtained . The system was recently used in tests at TU Delft and ISIS and 3He polarisation of 65 % was obtained.

# Tuesday, 21 March 2023

## Plenary - MW 2 001 - Lecture hall (21 Mar 2023, 09:00 - 10:30)

**-Chairs: Stephan Förster**

### [518] Harnessing the power of neutron to quantify softness (09:00)

*Presenter: SCOTTI, Andrea*

Although softness is a concept used in everyday life, its precise quantification is still far to be achieved. This is a fundamental step to build bridges between model systems which are largely studied and bio-relevant materials. The softness of a building block in solution plays a key role in determining the macroscopic properties of the material, such as viscosity or apparent yield stress. Controlling these properties is fundamental for application in the pharmaceutical field, for paint and health-care product, and for the stabilization of Pickering emulsions or foams. All these properties depend on the nature, interaction, and microstructures formed by the nanoparticle suspended in the material under flow. Small-angle neutron scattering, and neutron reflectivity are fundamental tools to probe softness for soft compressible colloids. In this talk, I will show examples of the use of these techniques to quantify and investigate the softness of micro- and nanogels, compressible crosslinked polymeric network swollen in a good solvent that are widely used as model system for soft spheres but also useful in application as emulsion stabilizer, nano-reactors, nanocarrier for targeted drug delivery, and disposable scaffold for 3D printing.

### [529] Advances in Neutron Imaging (09:45)

*Presenter: STROBL, Markus*

Neutron imaging has seen a remarkable transformation from a non-destructive testing tool spotting cracks on millimetre length scales in industrial components to a diverse research tool in material science and beyond. Direct spatial resolutions of a few micrometers are state of the art today, but also structural features down to the Angstrom regime can be probed through modalities sensitive to scattering. In contrast to conventional attenuation contrast, today neutron imaging techniques are capable of considering and quantifying signals from small angle scattering, diffraction, magnetic interaction and quasi/inelastic scattering. This has paved the way to a wide range of contributions in numerous fields of research and unique insights into materials and processes that are of significant relevance in academia, industry and eventually society. An overview of advanced neutron imaging and the respective contrast modalities and techniques shall be provided alongside a few selected science cases of neutron imaging today.

## Data Evaluation & Software 1 - SCC/0-002 - Taurus 1&2 (21 Mar 2023, 11:00 - 12:30)

**-Chairs: Sebastian Busch**

### [417] Classification of Small-Angle Scattering Patterns Using Machine Learning on Transformed 2D-Data (11:00)

*Presenter: GANEVA, Marina*

X-ray and neutron scattering are widely used powerful techniques for probing the physical structure of materials at the molecular and supramolecular scale. With the simultaneous advent of high-speed detectors, previously unimaginable time-resolved in situ and high throughput photon and neutron experiments have become possible, with the subsequent explosion of data volumes. Data analysis is becoming the most serious bottleneck on the way from experiment to scientific insight and final publication. We aim to provide rapid machine learning-based data classification to (i) guide decisions during the course of an experiment and to (ii) guide users as to which models are most appropriate for subsequent data analysis. We developed a methodology where the small-angle scattering patterns or 2D detector data are first transformed from (qx,qy) into (r,phi)-coordinates to become independent of the specific beam position on the detector and the specific detector pixel array format. The subsequent Fourier transform transforms the data from (r,phi)- to a real-space representation in Carthesian (x,y) coordinates. This makes use of Friedel's law and the Fourier shift theorem for a reduced presentation of the data. It is thus possible to operate with one training set for different instruments and different detectors. We used a broad range of experimental and simulated 2D-scattering data for spheres, ellipsoids, isotropic and oriented cylinders, as well as ordered lattice structures consisting of spheres, cylinders or lamellae of different degree of positional and orientational order and polydispersity. In the present work we compare performance of various classifiers, including decision trees, random forest, as well as probabilistic classification using variational inference neural networks. We show, that the transformed data can be better classified compared to the original 2D-detector data, enabling a reliable fast classification of scattering patterns with the possibility for a subsequent automatized data analysis with the selected models.

### [121] Diffraction at the European Spallation Source: instrument simulation and data reduction (11:30)

*Presenter: DURNIAK, Celine*

The European Spallation Source (ESS) will operate a suite of diffractometers, with the DREAM diffractometer [1] among the first instruments to be commissioned with neutrons. In order to take full advantage of this powerful source and to ensure smooth operation even for first-time users, the ESS Data Management and Software Centre is developing an integrated data pipeline linking all the steps from data acquisition and live visualisation to data analysis. The software used in the data pipeline should be efficient enough to deal with large amounts of data and respond to requirements from the scientific community while providing an intuitive workflow at the same time. To test this pipeline during the construction phase of ESS and of its instruments, we use instrument simulations with McStas [2], which has to be combined with GEANT4 [3] due to the complex three-dimensional geometry of the new 10B detectors of the ESS diffractometers. Here we report on preliminary tests of the reduction of powder diffraction data using McStas and GEANT4 simulations of the DREAM instrument and Scipp [4] for the reduction. References: [1] Andersen et al., Nucl. Inst. and Methods in Physics Research A 957, 163402 (2020). [2] Willendrup and Lefmann, Journal of Neutron Research 22, 1 (2020) and 23, 7 (2021). [3] Allison et al., Nucl. Inst. and Methods in Physics Research Section A 835, 186 (2016). [4] Heybrock et al., Journal of Neutron Research 22, 169 (2020) and scipp.github.io

### [261] Single crystal neutron diffraction data reduction with OpenHKL (11:50)

*Presenter: RAZA, Zamaan*

Data reduction is a crucial prerequisite to data analysis in neutron scattering expermients; in the case of single crystal diffraction, it involves the reduction of a set of detector images at fixed sample rotation increments to a set of miller indices with integrated intensities. However, the only avaailable mature software solutions are either legacy codes, converted from X-ray diffraction, or are closed source. [OpenHKL][1] (formerly NSXTool) is a standalone programe with a modern graphical user interface that facilitates the data reduction workflow: locating detector spots on the images, indexing the resulting peaks, predicting an exhaustime set of peaks, refining the instrument states and unit cell to improve the predictions, integrating the peaks, and finally merging the peaks. It is written in C++ for excellent speed, is open source and well-documented, natively handles neutron diffraction experiments with different detector geometries, and has a convenient Python scripting interface. In this presentation, I will demonstrate the capabilities of OpenHKL, describe the progress of the project, and show the results structural refinment computations using data reduced with OpenHKL. [1]: http://openhkl.org "OpenHKL website"

### [207] Simulation of complex neutron detectors using new features in the McStas Union components (12:10)

*Presenter: BERTELSEN, Mads*

The field of Neutron Scattering relies heavily on computer simulations for design of our instruments. Simulations can however be used in a broader scope, including preparation of beamtimes, training and understanding of spurions. To realize this broader

scope, simulation packages must be able to include the details necessary to describe the experiment, run sufficiently fast and be easy to use. In recent years the McStas simulation package was expanded with the Union components, capable of simulating multiple scattering in complex samples and sample environments in a modular manner for both geometry and underlying scattering processes. These components increased the achievable fidelity to new levels and support logging of scattering during the simulation, providing important insight. In this presentation we introduce a new feature in the Union components that allow logging of neutron absorption, which enables simulation of advanced detector systems in McStas. Many modern detector systems have multiple layers of 3D voxels and can have a complex response due to scattering within the detector system. Several ESS instruments will use such detector systems. Writing the description of such detectors can be repetitive, but can be significantly simplified with McStasScript. With these exciting new possibilities, McStas and the McStas Union components cover a significantly broader scope and will hopefully find many more applications that help the neutron scattering community at large.

## Energy Materials - MW 0 001 - Lecture hall (21 Mar 2023, 11:00 - 12:30)

**-Chairs: Neelima Paul; Alois Kuhn**

### [389] Competitive interplay between long-range oxygen and electronic ordering to promote low-T oxygen mobility in La2CoO4+d (11:00)

*Presenter: PAULUS, Werner*

Non-stoichiometric oxides with Ruddlesden-Popper structure type and the chemical formula A2BO4 (A = rare earth, B = transition metal) can uptake extra O-atoms on interstitial lattice sites (Oint). Due to their high mobility even at room temperature, long-range O-ordering up to the sub-mesoscale is observed in several A2BO4+d phases, which, together with charge and spin ordering, results into a competitive degree of freedom between structural and electronic ordering. Oxygen ordering thus adds an additional degree of freedom that may affect charge and spin ordering schemes, which is not present in the Sr-doped counterpart A2-xSrxBO4. In this regard, La2CoO4+d shows extremely high oxygen diffusion coefficients already at room temperature attaining diffusion coefficients of D = 1 x 10-9 cm2s-1. Combining neutron and synchrotron diffraction data, we evidenced for La2CoO4.25 a 3D modulated oxygen ordering setting in below 600°C, involving translational periodicities of more than 100 Å. Further on, a checkerboard charge ordering between Co2+/Co3+ occurs below 350°C, stabilizing a reconstructive rearrangement of the entire Oint-sublattice, showing a lock-in transition to a formal 4a x 4b x 4c ordered Ruddlesden-Popper type unit cell. The strong structural correlations induced by the sub-mesoscopic oxygen ordering are discussed to explain the unusually high oxygen mobility in terms of phonon softening.

### [366] Investigation of sodium-ion diffusion in NASICON solid state electrolyte materials (11:30)

*Presenter: PIVARNÍKOVÁ, Ivana*

The sodium superionic conductor materials, also known as NASICON, have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries due to their high conductivity and facile synthesis conditions. The aim of this work is to clarify the reason for extremely high conductivity exhibited by some compositions, specifically by Na1+xZr2SixP3-xO12 ($0 \leq x \leq 3$), and to explain the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which occurs at around 170°C, on the Na+-ion occupancy. We also investigate the role of Al/Y and Sc substitution and the overall temperature dependence of the ionic conductivity in the temperature range of 297-640K. The quasi-elastic neutron scattering (QENS) is used to measure the spatial and temporal dynamic properties of diffusion of Na+ ions in the crystal structure. The measurements were performed at the BASIS spectrometer at the SNS, Oak Ridge National Laboratory in Tennessee, USA. The Na+ ion diffusion mechanism can be described by the right choice of the diffusion model. Important parameters, such as diffusion coefficients, activation energies, jump distances between the occupation sites and residence times are extracted from the measured and modelled QENS data. Additionally, temperature dependent X-ray diffraction data have been obtained and analysed. Information about interatomic distances have been extracted in order to confirm the results obtained from the QENS data.

### [8] Behaviour of the Jahn-Teller effect in NaNiO2 with changing temperature and pressure (11:50)

*Presenter: NAGLE-COCCO, Liam*

The structural chemistry of NaNiO2 is driven by the Jahn-Teller distortion. NaNiO2 consists of alternating layers of edge-sharing NiO6 and NaO6 octahedra. The high-temperature phase has a rhombohedral symmetry, but with cooling there is a monoclinic distortion, as a result of a cooperative Jahn-Teller-driven elongation of the NiO6 octahedra, with the axis of elongation parallel for all octahedra. This JT effect is common in battery materials such as LiNiO2 and its Co-, Mn-, and Al-doped solid solutions, however, these exhibits non-cooperative behaviour, with no JT effect seen by diffraction, although the JT distortion can be observed with local probes such as PDF. The resulting ambiguity has led to various differing interpretations of the experimental data for these lithium nickelates. We present a study of NaNiO2 using neutron total scattering and EXAFS as a function of temperature, along with neutron diffraction at elevated pressures, with the hope that a better understanding of NaNiO2 may aid the understanding of the LiNiO2-based cathode materials. Additionally, we show advanced statistical analysis of the total scattering data using Rietveld analysis of a supercell. Our results differ from prior works on LaMnO3, with differences in part attributed to the reduced degrees of freedom in NaNiO2 due to the edge-sharing octahedra. We contextualise our findings in terms of theoretical and computational works, and make predictions for the lithium nickelates based on our results.

### [308] Exploring The Structure of MAPbI3 Across its Phase Diagram Using Neutron Spectroscopy, Thermophysical Properties and First-Principles Simulations – A Closer Look at High Pressures (12:10)

*Presenter: MARÍN VILLA, Pelayo*

Hybrid Organic-Inorganic Perovskites (HOIPs) have attracted an unprecedented attention as promising candidates for the next-generation of photovoltaic materials due to their exceptional energy conversion rates. Moreover, a better understanding of their remarkably soft atomic structures and their stabilization mechanisms is still necessary [1,2]. In this contribution we present an extensive study on the structure of the prime example of HOIPs methylammonium lead iodide (MAPbI$_3$) using a wide variety of radiation-scattering techniques validated by first-principles simulations across the temperature and pressure axes. We shall first introduce a model-selection protocol using inelastic-neutron scattering, thermophysical properties like the heat capacity, and

density-functional theory simulations [3]. This protocol was successfully implemented for MAPbI$_3$, showing that an alternative *P1* structure is statistically sounder than the crystallographic *Pnma* model. Furthermore, we present the first results of high-pressure radiation-scattering experiments performed on MAPbI$_3$ together with a new set of extensive ab initio molecular dynamics simulations. These findings will pave the way towards a better understanding of the fundamental yet scarcely explored role played by pressure in the stability of MAPbI$_3$. [1] K. Druzbicki et al. J. Phys. Chem. Lett., 7(22), 2016 [2] J. Breternitz et al. Angew. Chem. Int. Ed. 59(1), 2019 [3] P. Marín-Villa et al. J. Phys. Chem. Lett., 13(36), 2022

## From Polymers to Thermodynamics - SCC/0-001 - Lecture hall (21 Mar 2023, 11:00 - 12:30)

**-Chairs: Stéphane Longeville; Aurel Radulescu**

### [269] Kinetics of mesoglobules formation and disintegration in solutions of thermoresponsive polymers after fast pressure jumps (11:00)

*Presenter: PAPADAKIS, Christine*

The formation and disintegration pathways of polymeric nanoparticles are of key importance for their use for the transport and release of substances. Poly(*N*-isopropylacrylamide) in aqueous solution forms nanoparticles (“mesoglobules”) above its cloud point, which depends on pressure. In the temperature-pressure frame, the coexistence line is an ellipse with a maximum at ~60 MPa and 35 °C. Isothermal pressure jumps across this line allow for time-resolved small-angle neutron scattering investigations of the formation and disintegration of mesoglobules from the solution with a time-resolution of 50 ms and in a large range of length scales [1]. In the low-pressure regime, we find that the growth of the mesoglobules proceeds via diffusion-limited coalescence and, later, via hindered growth, which is due to the rigidification of the mesoglobules. In contrast, in the high-pressure regime, the chains stay hydrated and mobile, and the diffusion-limited coalescence proceeds without hindrance. The disintegration of the mesoglobules proceeds via the release of single polymers from the mesoglobules’ surface or via swelling, depending on the target pressure and thus on the osmotic pressure of water. Thus, pressure jumps allow the identification of a number of kinetic processes that are relevant for the efficient formation or cargo release. 1. B.-J. Niebuur, L. Chiappisi, F. A. Jung, X. Zhang, A. Schulte, C. M. Papadakis, ACS Macro Lett. 7, 1155 (2018), Macromolecules 52, 6416 (2019) and RSC Nanoscale 13, 13421 (2021)

### [114] Pressure-induced phase transition in polymer brushes: structural studies and thermodynamic predictions (11:30)

*Presenter: CHIAPPISI, Leonardo*

Polymers are key elements in modern material science, and, since the first polymer synthesis in 1907, tremendous progress in polymer chemistry were made. Today, an endless assortment of polymers – whose properties are adapted to specific needs – is available. In many cases, a thin polymer film, the coating, is sufficient to impart desired properties to the material. One of the most employed stimuli to tune phase transition in polymer coatings is temperature. Since the first reports of the thermo-responsive behaviour of poly(N-isopropylacrylamide) (PNIPAM) in an aqueous environment in the late sixties, PNIPAM has become the most studied model for non-ionic polymer systems. However, temperature is not the only physical parameter to tune the phase behaviour of polymeric systems. Pressure can be similarly used to control the phase behaviour of polymer solutions and thin films. Herein, we provide an extensive overview of the phase behaviour of end-grafted PNIPAM brushes as a function of pressure and temperature. The phase behaviour, extracted from the neutron reflectometry curves, is compared with the phase behaviour of semi-dilute solutions. Further, we show that the coexistence line as a function of pressure and temperature can be predicted assuming a two-state model – swollen and collapsed – knowing the different derivatives of the free energy of collapse as a function of pressure and temperature. These quantities can be precisely accessed using calorimetric and densitometric measurements. The results evidenced that the pressure-temperature phase behaviour of polymer solutions and coatings can be predicted from simple, laboratory-scale experiments, paving the way for the rational design of smart coatings with pressure and thermo-responsive behaviour.

### [152] Integration of molecular machines and motors into supramolecular polymeric materials: structural properties studied by small-angle neutron scattering (11:50)

*Presenter: BUHLER, Eric*

Switchable functional molecules capable of producing mechanical work constitute an active focus in nanotechnologies as they can be a source of components for molecular-based devices and materials. In particular, the dynamic nature of mechanically interlocked molecules allows their components to undergo relative internal movements, which can be exploited in translation and circumrotation. When it comes to using molecular machines to facilitate the creation of materials on the macro-scale, the primary concern is whether the nano-sized machines will be able to amplify their mechanical behavior to create a response in the bulk material. Hence, one of the most fundamental and challenging objectives associated to nano-machines rests on their coupling (in space and time) in order to transfer controlled motions from the molecular arena to the supramolecular and macroscopic scale. In the present work, we have developed two kinds of responsive contractile polymeric materials, which can behave as artificial muscles: i) The first one concerns nano-machines linked into a supramolecular polymer in which we produced micrometric motions (contraction/extension) by the integration of thousands of single contractile nano-switches by altering the pH of the solution; just like myofibrils do when packed in bundles in muscles. ii) The second one is based on the connection of light-driven rotary motors acting as reticulation units in an entangled polymer network. Small-angle neutron scattering (coupled with light and X-ray scattering) has been used to investigate the structure of the supramolecular self-assemblies of nano-machines before and after the induced structural changes as well as the dynamics of the contraction process at different length and time scales. We discuss here the relation between the local and overall structure of the self□assemblies and the properties of the materials. These findings open up new possibilities of using molecular machines in smart responsive materials.

### [84] The role liquid-liquid phase separation in biological process; a study with small angle neutron scattering and neutron reflectometry (12:10)

*Presenter: BUCHANAN, Claire*

The role of Liquid-liquid phase separation (LLPS) in biology is increasingly recognised. Here we study two different cases in which LLPS occurs. First, actin remodelling has been found to involve LLPS, which likely acts to upregulate critical proteins and adjust their activity. Preliminary data indicates that cell membrane stiffness is a key factor in coacervation at the cell membrane. The relationship between membrane stiffness, coacervation, and actin remodelling will be investigated by creating a neutron reflectometry (NR) and Atomic Force Microscopy (AFM) data set of the effect of protein XopR on supported lipid bilayers (SLB). AFM will allow for effect of XopR on the SLB to be monitored in real-time, while NR with selective deuteration will allow the detailed analysis of structural change in the SLB due to XopR, as well as providing information on the nature and origins of the coacervation (i.e. is coacervation 2D or 3D, and is it seeded at the membrane?). Second, re-engineered beak squid peptides that undergo LLPS have been proposed as a gene and drug delivery carrier. We use small angle neutron and X-ray scattering (SANS/SAXS) to show that the structure of the cargo protein in the coacervate phase remains unchanged as compared to the dilute phase. In summary, we hope to show the strength of SANS and NR to study LLPS in biology. This project results from a new collaboration between Nanyang Technological University, Malmo University and Institute Biofisika.

## Frustrated Magnets 2 - SCC/3-Venus - Venus (21 Mar 2023, 11:00 - 12:30)

**-Chairs: Sebastian Muehlbauer; Dmytro Inosov**

### [358] Bound states and triplet excitations at very high magnetic fields in the Shastry-Sutherland compound, SrCu$_2$(BO$_3$)$_2$ (11:00)

*Presenter: FOGH, Ellen*

Chasing new states of quantum matter is a central element in condensed matter physics, motivated both by fundamental curiosity but also by the need for a better understanding of many-body quantum effects for future technologies. Of particular interest are frustrated systems such as the Shastry-Sutherland (SS) model consisting of spin pairs (dimers) embedded in a square lattice. The model has an exact dimer product ground state when the ratio, $J'/J$, between the inter-dimer coupling, $J$, and intra-dimer coupling, $J'$, is less than 0.675 [1]. The network of Cu$^{2+}$ ions in SrCu$_2$(BO$_3$)$_2$ (SCBO) is topologically equivalent to the SS lattice and with $J'/J \sim 0.6$ close to the critical point, this compound presents unique experimental testing grounds for the model. Upon applying a magnetic field, SCBO exhibits a series of phase transitions [3,4] and we study the magnetic excitations upon approaching the first transition at 27T to the 1/8 magnetization plateau using inelastic neutron scattering. At field values much below the transition a novel and unexpected mode shows up. We use state-of-the-art model calculations to identify the nature of this mode: Is it a bound state or a triplet excitation? And why does it appear before the transition? [1] B. S. Shastry and B. Sutherland, Physica 108B, 1069-1070 (1981) [2] S. Miyahara and K. Ueda, Phys. Rev. Lett. 82, 3701 (1999) [3] M. Takigawa et al., Phys. Rev. Lett. 110, 067210 (2013) [4] P. Corboz and F. Mila, Phys. Rev. Lett. 112, 147203 (2014)

### [397] Neutron diffraction study of S = $1\over2$ triangular lattice Heisenberg antiferromagnet Ba$_3$CoSb$_2$O$_9$ in high magnetic fields (11:30)

*Presenter: PROKHNENKO, Oleksandr*

A S = $1\over2$ triangular lattice Heisenberg antiferromagnet (TLHAF) is its typical example, where combined effects of geometrical frustration and quantum fluctuations lead to stabilization of novel spin structures as function of external magnetic field. Hexagonal Ba$_3$CoSb$_2$O$_9$ (BCSO) compound exhibits magnetic properties typical of an ideal S = $1\over2$ TLHAF, making it a perfect model system for testing theoretical predictions [1-2]. In this contribution we present the results of neutron scattering experiments on BCSO single crystal with a magnetic field applied both in-plane and out-of-plane [3-4]. A sequence of magnetic phase transitions, including the magnetization plateau phase and the new high-field phase at 22.5 T reported recently [1-2] has been followed at low temperatures as a function of field and modeled using the large-size cluster mean-field plus scaling method [5]. While our results show good agreement with the theoretical model for the field applied in-plane, for the out-of-plane field the model reproduces the experiment only qualitatively. The discrepancies between theory and experiment are discussed, suggesting further efforts are necessary to fully understand the TLHAF system in magnetic fields. References: [1] Y. Shirata et al, Phys. Rev. Lett, 108, 057205 (2012) [2] K. Okada et al, Phys. Rev. B 106, 104415 (2022) [3] X. Z. Liu et al, Phys. Rev. B 100, 094436 (2019) [4] X. Z. Liu et al, Phys. Rev. B 105, 214433 (2022) [5] D. Yamamoto et al, Phys. Rev. Lett. 114, 027201 (2015)

### [402] Chiral Spin Liquid Ground State in YBaCo3FeO7 (11:50)

*Presenter: SCHWEIKA, Werner*

A chiral spin liquid state is discovered in the highly frustrated, layered kagome system YBaCo3FeO7 by polarized diffuse neutron scattering [1]. From the antisymmetric part of scattering, related to vector chirality, we determine the chiral correlation function by Fourier analysis. The chiral short-range order indicates the emergence of chiral lumps. It can be described by cycloidal waves, which originate from the trigonal sites and extend into the kagome layers. The observed vector chirality agrees with the underlying antisymmetric Dzialoshinsky-Moriya exchanges arising from broken spatial parity. This chiral spin liquid state is stable down to lowest temperatures despite of strong antiferromagnetic spin exchange. The observation of a possible short-range ordered ground state raises a fundamental challenge. However, based on the classical theory of magnetic order, we show that such a ground state may arise from the antisymmetric exchange acting as a frustrating gauge background stabilizing local spin lumps. This scenario may appear in many highly frustrated magnetic systems in non-centrosymmetric compounds and has similarities to the avoided phase transition in coupled gauge- and matter-fields for subnuclear particles. [1] W. Schweika, M. Valldor, J. D. Reim, and U. K. Rößler, Chiral Spin Liquid Ground State in YBaCo3FeO7, Phys. Rev. X 12, 021029 (2022).

### [36] Deducing multi-k magnetic structures via spin-waves in Gd-pyrochlores (12:10)

*Presenter: STEWART, Ross*

Pyrochlore Heisenberg antiferromagnets (HAFs) are commonly studied as an archetypal example of three- dimensional geometrical magnetic frustration. The study of these so-called “highly frustrated magnets” provides a route to access a large variety of fascinating emergent low-temperature magnetic states including spin-liquids, spin-glasses, spin-ices, and fragmented spin-structures. Gd-pyrochlores should, in principle, be rather simple examples of pyrochlore HAFs due to the spin-only ground state of Gd$^{3+}$. However, dipolar interactions, and admixed orbital states, result in a variety of magnetic ground states ranging from the co-planar *Palmer--Chalker* (PC) state, to fascinating partially ordered multi-k structures. We will present spin-wave

studies on 3 examples of Gd-pyrochlore HAFs, Gd$_2$Ti$_2$O$_7$ (GTO) [1], Gd$_2$Sn$_2$O$_7$ (GSO) [2] and Gd$_2$Pt$_2$O$_7$ (GPO) [3]. GSO and GPO are uncontroversial PC magnets, where powder TOF-INS measurements on isotopically substituted samples elucidate the leading magnetic interactions. In the case of GTO, analysis of the spin-wave spectra, even in a powder sample, is found to solve the multi-k problem - where (even single crystal) diffraction cannot decide between mutli-k variants, but the ground state excitations are decisive in this regard. [1] J A M Paddison, *et al.*, Suppressed-moment 2-k order in the canonical frustrated antiferromagnet Gd2Ti2O7. npj Quantum Materials, 6(1), 99 (2021). https://doi.org/10.1038/s41535-021-00391-w [2] J R Stewart, *et al.*. Collective dynamics in the Heisenberg pyrochlore antiferromagnet Gd 2Sn2O7. Physical Review B, 78(13), 3–6 (2008). https://doi.org/10.1103/PhysRevB.78.132410 [3] P G Welch, *et al.*, Magnetic structure and exchange interactions in the Heisenberg pyrochlore antiferromagnet Gd2Pt2O7. Phys. Rev. B, 105(9), 094402. (2022) https://doi.org/10.1103/PhysRevB.105.094402

## Functional Materials 1 - MW 2 001 - Lecture hall (21 Mar 2023, 11:00 - 12:30)

**-Chairs: Ralph Gilles; Pavel Strunz**

### [432] Neutron diffraction and imaging of degradation and sodium storage process in sodium-ion batteries. (11:00)

*Presenter: BATTAGLIA, Domenico*

A way to reduce the world's reliance on conventional fuels is to obtain cost-competitive alternatives to convert and store energy. This could be done by implementing cheap storage devices, such as Na-Ion batteries [1], which are the focus of our investigations. During the first part of the project, major attention was dedicated to the fabrication of Prussian blue analog-based batteries, which are considered a good choice for stationary energy storage devices. However, there are still many unknowns related to this technology [2]. Neutron scattering and imaging allow performing operando experiments during charge-discharge without any repercussions on the battery's functional properties. Neutrons are well suited to measure light elements making them a viable probe to study morphology and composition changes as well as ionic transport processes in Na-ion batteries. We have performed operando tomographic studies of the degradation processes, hereby imaging the dendrite growth process, to investigate the effect of cycling on the morphology and long-term stability of the cell. Dendrite formation and electrolyte degradations are two of the most predominant failure mechanisms in these devices [3]. Thus our studies are highly relevant for getting an insight into the key processes the technology is based on. [1] A. Mauger, et al., Materials 2020, 13, 3453. [2] Bingxing Xie, et al., Coordination Chemistry Reviews 2022, 460, 214478. [3] Huan Shi, et al., Chem. Rec. 2022, 22, e202200112.

### [106] Hydrogen motion in Li$_4$(BH$_4$)(NH$_2$)$_3$ investigated by Quasielastic Neutron Scattering (QENS) (11:30)

*Presenter: LOHSTROH, Wiebke*

Fast and efficient hydrogen storage is one of the key components for the use of hydrogen in a sustainable energy economy. Reactive Hydride composites have been considered for some time as potential solid state storage systems, among others also the amide based mixture Mg(NH$_2$)$_2$ + 2 LiH. The kinetic performance of the hydrogen exchange reaction in this system is significantly enhanced by the addition of LiBH$_4$ [Gizer et al. Inter. J. Hydrogen Energy 44, 11920-11929 (2019)] and the subsequent formation of the amide-borohydride compound Li$_4$(BH$_4$)(NH$_2$)$_3$. Here, we present a study of the structure and of the anion motion of in Li$_4$(BH$_4$)(NH$_2$)$_3$ investigated with synchrotron radiation powder X-ray diffraction (SR-PXD) and quasielastic neutron scattering (QENS) at temperatures close to operating condition. SR-PXD confirms the recrystallization of Li$_4$(BH$_4$)(NH$_2$)$_3$ into the $\alpha$-phase during cooling from the melt. The QENS measurements prove a long-range diffusive motion of hydrogen containing species at 514 K with the diffusion coefficient $D \sim 10^{-6}\,\frac{\mathrm{cm}^2}{\mathrm{s}}$. At temperatures below 514 K, localized rotational motions were observed which have been attributed to (BH$_4^-$ tetrahedra units undergoing rotations mainly around $C_3$ axes. The results will be discussed in the context of the improved hydrogen exchange reaction that is observed in Mg(NH$_2$)$_2$ + 2 LiH with LiBH$_4$ additions.

### [109] Hydrogen storage in high-entropy alloys studied by neutron scattering methods (11:50)

*Presenter: HAUBACK, Bjørn*

High-entropy alloys (HEAs) receive attention due to their diverse and often extraordinary properties. They are solid solutions where minimum four different elements randomly occu-py a single crystallographic site in structures such bcc and fcc. Because of the random distri-bution of metals, there is a large variety of different nearest-neighborhood environments surrounding the interstitial sites occupied by hydrogen. Local lattice distortions enable hy-drogen to occupy both the tetrahedral and octahedral interstices. Here hydrogen storage properties of several bcc HEAs with compositions related to TiVNb have been investigated. In particular, the local structure of alloys and the corresponding deuterides in the series TiVNb, TiVCrNb, TiVZrNb and TiVZrNbHf have been investigated with combined X-ray and neutron total scattering and Reverse Monte Carlo (RMC) modelling. Inelastic neutron scattering was used to determine the vibrational density of states in one system. The combination of probes is essential to obtain sufficient contrast between the dif-ferent elements. Pair-distribution functions obtained from the RMC structure models were used to evaluate the local lattice distortion in the HEAs. The local lattice distortion is much lower in the deuterides, but the trend observed for the alloys is still present. Furthermore, for the valence-electron concentration (VEC) >5 the hydrogen content is reduced, and it is also shown that the metal hydrides are destabilized with increasing VEC.

### [104] Investigating the Formation and Lithiation of Silicon-based Anodes by Neutron Depth Profiling (12:10)

*Presenter: GROSSMANN, Lukas*

Silicon anodes are prominent candidates to enhance the capacity of Lithium Ion Batteries. However, the volumetric changes of silicon upon (de-)lithiation regularly lead to a low life time of such electrodes. Our strategy to prolong the life time is based on a partial lithiation of silicon to ~30%, which significantly increases the cycling stability while maintaining a three times higher gravimetric capacity compared to common graphite anodes. In our study, we use Neutron Depth Profiling (NDP) on extracted silicon-based anodes to acquire quantitative lithium depth distributions after different formation and lithiation steps. This can help to understand the performance of the electrodes and to identify lithium-containing side reactions which are invisible for

electrochemical methods. We investigated three states of charge (SOC) and the formation with and without LiNO$_3$ as electrolyte additive, which was found to increase the cycling stability of silicon. Our results show that lithium is evenly distributed in depth across all studied anodes. The formation already leads to a moderate lithium concentration, which originates from irreversibly bound lithium in the as-formed solid-electrolyte-interface (SEI). With rising SOC (15%, 30%) the lithium concentration consistently increases and a sizable swelling of the electrodes is observed. Notably, the LiNO$_3$ electrolyte additive elevates the lithium content in the SEI, which indicates additional reactions in the formation process.

## European Neutron Sources: Status and Upgrades - MW 2 001 - Lecture hall (21 Mar 2023, 14:00 - 16:00)

**-Chairs: Martin Müller**

### [532] The European Spallation Source: a Project Update (14:00)

*Presenter: SCHOBER, Helmut*

The European Spallation Source (ESS) is Europe's answer in the continuous strive for the production of neutron beams of ever higher brilliance. The scientific instruments exploiting these beams are an indispensable tool for studying matter and material properties, which will unlock new discoveries from the very fundamental to the highly applicable. The concept underlying the ESS combines a powerful linear accelerator using a 62 mA proton beam that in its final stage will be delivering a 5 MW long-pulse proton beam to a highly innovative spallation solid tungsten target and a low-dimensional moderator assembly. A suite of initially 15 instruments is designed to exploit the full potential of the long-pulse nature of the neutron beam. In my talk, I will present the fundamental design of the accelerator and neutron source followed by an overview of the beam shaping and detection concepts retained to match the instruments optimally to the source characteristics. I will then concentrate on giving an update on the current project status going through accelerator, target, and instruments, and lay out the path forward to meet the goal of opening the ESS up for the user programme at the end of 2027.

### [512] The research neutron source Heinz Maier-Leibnitz (FRM II) (14:30)

*Presenter: MÜLLER-BUSCHBAUM, Peter*

The research neutron source Heinz Maier-Leibnitz (FRM II) is a central scientific institute of the Technical University of Munich (TUM) located at the Research Campus in Garching. The FRM II came into user operation in April 29, 2005 and provides neutrons for science, industry and medicine in up to four cycles of 60 days a year. The Heinz Maier-Leibnitz Zentrum (MLZ), a cooperation TUM and research centers of the Helmholtz Association, Forschungszentrum Jülich and Helmholtz-Zentrum Hereon, organizes the scientific use of FRM II. By offering a unique suite of high-performance neutron scattering instruments, scientists are enabled to pursue state-of-the-art research in diverse fields as physics, chemistry, biology, earth sciences, engineering or material science. News about the development of the instrument suite and FRM II operations will be presented.

### [81] Endurance – Modernisation of the instrumentation suite at the Institut Laue-Langevin (15:00)

*Presenter: MEYER, Andreas*

Endurance encompasses more than 30 new or upgraded instrument and infrastructure projects, rolled out over 8 years between 2016 and 2023 and with a financial envelope of nearly 60 M€. Many new or upgraded instruments have already been deployed and in user-operation including: the fission-fragment gamma ray spectrometer, FIPPS; the upgraded cold-neutron TOF spectrometer IN5; new thermal TOF spectrometer PANTHER; and a second protein crystallography station, DALI. The D3 hot-neutron diffractometer and thermal IN20 triple-axis spectrometer have been upgraded while new and additional detectors for the SANS instruments D11 and D22 have been installed. A fully modernised D16 cold-neutron diffractometer and new cold-neutron imaging instrument NeXT will be completed by the end of 2022. Delivering a full suite of modernised instrumentation is critically dependent on the renewed in-pile beam extraction, H1-H2 and the H24 (thermal) and H15 (cold) neutron guides. H24 will bring dedicated guides to the upgraded D10+ single crystal diffractometer, IN13 backscattering instrument and the new XtremeD powder and single-crystal diffractometer. H15 will accommodate a substantially upgraded D(00)7 polarised diffuse scattering and spectroscopy instrument while D11 will be rebuilt and relocated with an optically cleaner collimation. Two additional end-of-guide positions are available for new instrumentation: The SHARP+ cold TOF spectrometer and a 4th SANS instrument, SAM.

### [169] The Endeavour project at ISIS (15:30)

*Presenter: BEWLEY, Robert*

ISIS is continually updating and developing its suite of neutron and muon instrumentation in order to respond to the needs of the science community and to ensure ISIS remains a world-leading facility. Currently ISIS is embarking on a large programme called ‘Endeavour’ which aims to deliver 9 major instrumentation projects over a ten year time scale to meet current and future challenges in areas such as Materials for the Future, Clean Energy Technologies, Biosciences and Healthcare. This programme has been allocated funds from the UKRI’s Infrastructure fund, with an anticipated funding release in early 2023. The project contains 4 new instruments; Mushroom: a new concept for inelastic neutron scattering. eMAP: engineering diffractometer. LMX: large molecule systems single crystal diffractometer. Wish-II: single crystal diffractometer optimised for small crystals. In addition there are 5 major instrument upgrades; HRPD-X: a significant upgrade to the current HRPD. Super-MuSR: enhanced flux and time resolution for next-generation muon studies. Tosca+: an order of magnitude more flux for vibrational spectroscopy. Sandals-II: upgrade of Sandals secondary for amorphous and liquid samples. Osiris+: 5 fold rate increase over Osiris for high resolution spectroscopy. The presentation will give more details on the Endeavour programme and the instrument projects contained within.

## Neutron Sources: Developments and Foresight - MW 0 001 - Lecture hall (21 Mar 2023, 14:00 - 16:00)

**-Chairs: Mirijam Zobel**

### [204] ISIS-II: the future development of the ISIS Neutron and Muon Source (14:00)

*Presenter: LANGRIDGE, Sean*

ISIS-II is a project to explore and advance a successor facility to the ISIS Neutron and Muon Source. ISIS-II is expected to complement the international neutron landscape foreseen for the second half of the 21$^{\textrm{st}}$ Century. It will be a short pulse neutron and muon source covering a wide range of science areas consistent with ISIS user community's interests. The facility requirements will be optimised around delivering the most impactful science in an efficient manner. This requires not only a reliable, sustainable source but also state-of-the-art supporting instrumentation, computing and infrastructure. ISIS-II has received preliminary research and development (R&D) funding from the UKRI Infrastructure fund. In its early phases the focus is on understanding the key design drivers, choices and constraints. The key design drivers include both science and engineering considerations, such as background reduction, energy efficiency and lifetime carbon footprint. Key design considerations include the optimal match of accelerator, target and moderator technologies to meet the science requirements. The project is also identifying the areas where long term R&D and prototyping is needed to achieve the project aims. We present initial concepts and the outline time scale for the different project phases.

### [192] The future of ESS is bright (14:30)

*Presenter: SCHWEIKA, Werner*

Aiming for highest neutron peak brightness, limits are set by the capabilities of heat removal and for pulsed sources even more by the instantaneous power impact. In this respect, the long pulse ESS is still below its limits and has a high potential to boost its performance. Considering the current ESS, the goal should be a compression of proton pulses near to 50 to 100 µs, comparable to the moderation time of thermal neutrons. It will increase the peak brightness for thermal neutrons up to about a factor 50 and for thermal instruments, sufficiently high resolution can be achieved even without pulse shaping choppers. Including cold instruments, on average there is an order of magnitude increase in performance with some appealing options for the instrument suite. The upgrade of the ESS linac with a compressor ring is part of the neutrino physics proposal of the ESS, ESSnuSB. Its use for neutron production with 1.2 µs proton-pulses at 5MW will cause likely unacceptable thermomechanical shocks in the spallation target. Alternative proposals for slow extraction from the accumulator ring are less challenging for the target but more so for the accumulator extraction zone for which too high irradiation must be avoided. Clearly, the design of such options to generate compressed proton pulses of medium duration is strongly motivated by gaining the ultimate possible neutron peak brightness to tap the full high potential of the ESS.

### [219] Reactor Institute Delft 2.0 (15:00)

*Presenter: PLOMP, Jeroen*

The Reactor Institute Delft (RID) is the only research facility in the Netherlands that uses neutron- and positron beam line instruments for academic research. The 2.3 MW research reactor not only facilitates beam-line instruments that offer the unique opportunities of this special radiation but operates irradiation facilities where isotopes can be produced for heath research or element analyses as well. The field of application is very broad and varies from Energy to Health and even cultural heritage. New instruments and the implementation of a cold source (end 2023) and user program will broaden the scientific footprint of the reactor. Instruments available are: Neutron Imaging (thermal and in future cold), Neutron Powder Diffraction, Small Angle Neutron Scattering, Neutron reflectometry, Neutron Depth profiling, Posh-Pals, Posh-2D ACAR, Irradiation facilities, Instrument Neutron Activation Analysis We would like to present an overview of the latest developments and discuss the strengths and weaknesses of a, relatively small, university facility.

### [239] The Australian Centre for Neutron Scattering Operations (15:20)

*Presenter: IMPERIA, Paolo*

With 250 days per year of user operations and a suite of 15 neutron beam instruments, the Australian Centre for Neutron Scattering (ACNS) is considered one of the most convenient user facilities worldwide to perform neutron beam experiments. ACNS operations relies on the 300 days per year at power by OPAL reactor, one of the youngest and reliable reactors. This presentation will discuss the successful operations of ACNS suite of instruments, their scientific highlights, the current improvement projects, and will give an overview of future plans. Particular emphasis will be given to the challenges presented by the facility continuous operations with short reactor shutdowns, typically 5 days every 30 to 35 days of operations. The presentation will discuss user access and management program and will review the systems integration within the different ACNS function groups. A discussion of relevant past and future projects and the related regulatory and safety framework will be briefly exposed.

### [440] Neutron Physics Laboratory Řež (CZ) and its instrumentation for investigation of structure and microstructure of advanced materials (15:40)

*Presenter: STRUNZ, Pavel*

Neutron Physics Laboratory (NPL) of CANAM infrastructure (operated by Nuclear Physics Institute Řež), canam.ujf.cas.cz/npl, and its instrumentation for investigation of structure and microstructure of advanced materials will be presented. NPL consist of five neutron diffractometers (residual stress scanning, powder diffraction, small-angle neutron scattering, in-situ thermomechanical tests and neutron-optics testing diffractometers) and of three nuclear analytical techniques (Neutron Depth Profiling, Prompt Gamma Activation Analysis, Neutron Activation Analysis). The laboratory provides open access to academic users on the basis of proposals continuously evaluated by the international Scientific selection panel. Recently, several instruments were upgraded by new neutron-optics components, by new sample environment, as well as by sample preparation and auxiliary facilities. The strain scanner was equipped by radial neutron collimator, SANS diffractometer by a new bending holder with long analyzer crystal. New portable neutron camera facilitates sample adjustment within sample environment. A system for concurrent in situ neutron diffraction, mechanical testing and acoustic emission detection was obtained. Nuclear analytical techniques were improved by supermirror neutronguide, by electrochemical impedance analyzer, by cryogenic mill and by electrical fusion furnace. Selected examples from the studies with help of neutron physics facilities carried out at NPL will be presented.

**Poster session TUESDAY: Poster Session TUESDAY - Yards 4 - 6 (21 Mar 2023, 16:00 - 18:00)**

### [218] Atomistic Simulations of the Magnetic Neutron Scattering from Nanoparticles (board TU-002)

*Presenter: ADAMS, Michael*

We consider a dilute ensemble of randomly-oriented noninteracting spherical nanomagnets and investigate its magnetization structure and ensuing neutron-scattering response by numerically solving the Landau-Lifshitz equation. Taking into account the isotropic exchange interaction, an external magnetic field, a uniaxial magnetic anisotropy for the particle core, and in particular the Neel surface anisotropy, we compute the magnetic small-angle neutron scattering cross section and pair-distance distribution function from the obtained equilibrium spin structures. The numerical results are compared to the well-known analytical expressions for uniformly magnetized particles and provide guidance to the experimentalist. Moreover, the effect of a particle-size distribution function is modeled. Michael Adams and Andreas Michels thank the National Research Fund of Luxembourg for financial support (AFR grant No. 15639149).

### [504] Hydrogen bonding and local structure of imidazolium-based ionic liquids in the water-rich domain (board TU-004)

*Presenter: ALMASY, Laszlo*

Since water has a high impact on the chemical-physical characteristics of Ionic Liquids (IL), both as a contaminant or as cosolvent, the detailed knowledge of the intermolecular interactions in IL/water solutions is a crucial step for understanding and predicting the range of properties of these non-conventional solvents for applications in many fields including electrochemistry, biochemistry, and synthesis. In this work, aqueous solutions of a prototypical set of methyl-imidazolium (MIM) - based ionic liquids is investigated by UV Raman spectroscopy and Small-Angle Neutron Scattering in the water-rich domain. Selected Raman signals in different wavenumber ranges provide insights into the local organization of cation-anion pairs as a function of the increasing amount of water in a wide range of concentrations. The high-frequency range of Raman spectra is analyzed by a differential method to extract from the OH stretching profile of water the solute-correlate (SC) spectra, which emphasize the molecular structuring of the interfacial water present in the hydration shells around the selected anions. The neutron scattering data show the water – IL segregation at nanoscale. Peculiar solvation behavior is observed for the different MIM-based mixtures in connection with the hydrogen bonding features of the hydrating water molecules. Interestingly, the ionic liquid [MIM][Cl] seems more sensitive to hydration than [MIM][TfO] even in an extremely hydrated regime.

### [243] Investigation of the vortex lattice in NbS2 – a potential FFLO candidate (board TU-006)

*Presenter: ALSHEMI, Ahmed*

To date, several materials have been proposed as hosts for the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) spatially modulated superconducting state [1], but direct experimental proof has been challenging, with only the organic superconductors providing uncontested evidence for the state [2]. The FFLO state is expected to develop at high fields and low temperatures in materials with strong Pauli paramagnetic effects, an anisotropic Fermi surface, and clean superconductivity. 2H-NbS2 has recently been proposed as a potential candidate material based on torque magnetometry, specific heat and thermal expansion measurements as a function of orientation in magnetic field. Transition metal dichalcogenides (TMDs) are strongly anisotropic layered superconductors in which the two-dimensional planes are weakly coupled by van der Waals forces. The upper critical field of superconducting TMDs in the basal plane is shown to be dramatically enhanced by a special form of Ising spin orbit coupling [3]. When the field is applied exactly in the plane, the upper critical field increases dramatically above 16 T, beyond the limit expected from the Pauli paramagnetic effect. This behaviour is reminiscent of the organic superconductors where the FFLO state is seen. Using small angle neutron scattering, we have observed the vortex lattice in this material to test if this material is a good candidate to look for a direct FFLO diffraction signal. We have observed a strong intrinsic superconducting anisotropy between the c axis and the basal plane. Furthermore, we plan to go to higher magnetic fields and measure closer to 90° and try to get into the FFLO phase to look for direct diffraction signal. [1] J. Wosnitza, Annalen der Physik 530, 1700282 (2017). [2] C. Agosta, Crystals 8, 285 (2018). [3] C.-W. Cho et al., Nature Comm. 12,3676 (2021).

### [115] Coherent and Incoherent Scattering of Tetrahydrofuran from Meso- to Inter-molecular Scales by Neutron Spectroscopy with Polarization Analysis and Spin Echo (board TU-008)

*Presenter: ARBE, Arantxa*

We have extended our previous investigations on self- and collective dynamics of liquid water [1,2] to the case of tetrahydrofuran (THF). Neutron polarization analysis on a wide-angle time-of-flight spectrometer (PLET @ ISIS) has allowed measuring separately coherent and incoherent dynamic structure factor of deuterated THF with sub-meV resolution in a wide scattering vector (Q) range. The combination with Neutron Spin Echo (WASP @ ILL) experiments on deuterated and protonated THF with higher resolution has allowed to fully characterize the contributions to self- and collective dynamic structure factors also at low temperature. Interestingly, a low-Q mode (independent of Q), as that discerned in the collective dynamics of water and attributed to the reorganization of the HB-network, is also found in THF. The activation energy is however much lower, suggesting van der Waals interactions at the nature of the underlying process in this low-Q mode for the case of THF. References [1] A. Arbe, P. Malo

de Molina, F. Alvarez, B. Frick, and J. Colmenero, Physical Review Letters **117**, 185501 (2016). [2] A. Arbe, G. Nilsen, J. R. Stewart, F. Alvarez, V. García-Sakai and J. Colmenero, Physical Review Research **2**, 022015 (2020).

### [446] ORSO- The Open Reflectometry Standards Organisation (board TU-010)

*Presenters: ARNOLD, Tom, STAHN, Jochen*

ORSO is a group of reflectometry scientists from across the globe that are interested in im-proving neutron and X-ray reflectometry through collaboration. The aims and focus of our working groups are arranged as follows: • The education and outreach working group aims to develop understanding of reflec-tivity techniques and disseminate information about reflectivity analysis. • The File formats working group has recently developed specifications for a standard file format for use across X-ray and neutron reflectivity. This is an important step to-wards interoperability across facilities. The architecture of this .ort format will be pre-sented together with the python libraries (orsopy) to read and write it. • The analysis working group is focused on cross-facility collaboration on standardized data analysis “best practices” and shared resources to make it easier to build and use reflectometry analysis software • The reproducibility working group aims to improve measurement reproducibility through the creation of informative documentation regarding experimental set-up and standardisation of instrumentation, generate general guidelines on data reduc-tion, to ensure accurate and reproducible data and engage others in reproducible analysis, including help documentation and guides. ORSO is open to everyone, meaning its working groups are open to all, to join a working group please just contact one to the authors or go to our web page www.reflectometry.org. Together we can do better science.

### [511] Performing an accurate measurement of \Delta b_i of $^3$He using NSE (board TU-012)

*Presenter: BABCOCK, Earl*

We recently performed measurements of the neutron incoherent scattering lengths for $^{129}$Xe and $^{131}$Xe. As a part of those measurements the $\Delta b_i$ of $^3$He was also measured for a short time, only 6 hours, as a calibration. The results of this measurement indicate a very precise value could be obtained for a typical length experiment on NSE. Theories which take the data from measurements in three-body nuclear systems and predict what should be seen in a 4-body system like $^4$He or n-$^3$He, which is an essential step needed to check the internal consistency of the three-body force extraction from systems with only three bodies, do not quite agree with the data by amounts too large to be explained only by 4-body forces. Furthermore, in the specific case of the n-$^3$He system, the two best measurements of the n-$^3$He incoherent scattering length differ by 3$\sigma$. During the course of our test measurement we found several important experimental and theoretical factors relevant to a measurement with precision beyond the error of the current measurements. We estimate that we could obtain a 1% measurement for $b_i$ of $^3$He in one week.

### [174] FRAPPY a Python Implementation of SECoP (board TU-014)

*Presenter: BARTKOWIAK, Marek*

The development of the Sample Environment Communication Standard and its relase is a huge achievement. Since a standard is only good if it is applied, at SINQ/PSI we are in the process to implement SECoP into the data acquisition process. Together with the Maier-Leibnitz-Zentrum Garching/Germany we developed Frappy. Frappy is a python framework to implement a device communication and abstraction layer for complex sample environment equipment such as cyostats, cryomagnets, furnaces, humidity chambers and for the integration of measurement devices. We will present the current status of the project as well as the deployment efforts at SINQ.

### [507] Status and Perspective of the FRM II Conversion Project (board TU-016)

*Presenter: BAUMEISTER, Bruno*

Technical University of Munich (TUM) is committed to convert its research neutron source Heinz Maier Leibnitz (FRM II) to a lower enriched fuel. Since 2004, TUM together with its European and International partners develops new high-density fuels and tools for reactor core modelling for the conversion of FRM II. As today, three fuel options are on the way to be qualified for conversion: high-density uranium silicide (U3Si2, with a uranium density of 4.8 - 5.6 gU/cm³), disperse uranium molybdenum (U-Mo, with a uranium density of 8.0 gU/cm³) and monolithic U-Mo with a uranium density of 15.5 gU/cm³. Extensive irradiation experiments have shown that all three options are suitable for the demanding conditions of high-performance research reactors like the FRM II, but have strongly different potential for decreasing the fuel enrichment. Due to its highest achievable uranium density, TUM is focusing its efforts on the monolithic U-Mo fuel, which allows the lowest enrichment of all options. In parallel, modern computational methods were developed to simulate neutronics and thermal-hydraulics of a conversion core model. In this talk, we will present the most recent results of fuel irradiation experiments, fabrication technologies and core modelling studies, together with a tentative time schedule for the conversion of FRM II.

### [332] Short time diffusive properties in polydisperse solutions (board TU-018)

*Presenter: BECK, Christian*

In biological environments, proteins are exposed to polydisperse surrounding. The interaction of this environment is essential for a correct function of the cell and disfunctions may lead to diseases. To understand the diffusive properties of proteins in polydisperse environments, we performed several quasi-elastic neutron scattering (QENS) experiments. Changes in the probed short-time self-diffusion are important to understand, since they influence the long time diffusion, which is essential e.g. for transport mechanisms. By using different proteins in the presence of deuterated lysate, we systematically investigated the influence of volume fraction, tracer size as well as mixing ratio on the protein diffusive properties in a polydisperse surrounding. The previously investigated volume fraction dependence is not valid anymore but an additional influence of the radius is observed. While large particles are slowed down compared to a monodisperse solution with the same volume fraction, smaller proteins are accelerated. In case the protein radius is comparable with the averaged radius, no significant effects of the polydispersity on the diffusion are observed [1]. A further quantitative understanding on the polydispersity has been obtained from QENS spectra of solutions containing two proteins. With advanced analysis methods, the different diffusive contributions can be separated [2]. [1] J. Phys. Chem. Lett. 10 (2019) 1709 [2] J. Phys. Chem. B 126 (2022) 7400

### [408] Characterization of the low-dimensional antiferromagnet [Cu(H2O)2(pyz)2]Cr2O7 (board TU-020)

*Presenter: BEDDRICH, Lukas*

Metal organic magnets (MOM) have enormous potential to host a variety of electronic and magnetic phases that originate from a strong interplay between the spin, orbital, and lattice degrees of freedom. Due to the unique possibility of controlling interatomic distances and magnetic exchange pathways by coordination chemistry, a plethora of MOM have been reported. This way, 0D to 3D magnetic structures can be realized. In [Cu(H$_2$O)$_2$(pyz)$_2$]Cr$_2$O$_7$ (Cu-pyz), the magnetically active Cu$^{2+}$ ions exhibit a nearest-neighbour exchange coupling in a 2D square lattice, with no out-of-plane coupling. We have used static susceptibility, magnetization and neutron scattering (NS) measurements to characterize Cu-pyz single crystals. Our data supports the proposed model of a 2D isotropic quantum Heisenberg antiferromagnet (2D QHAF) model. Thus, magnetization curves show the characteristic upward bending with increasing external field. Likewise, the susceptibility displays a broad maximum at $T \approx 4.5\, \mathrm{K}$, which corresponds to the emergence of long range spin correlations within the individual planes. Usually, the spin wave excitations are mapped out from within the ordered state, however, neither in bulk measurements down to $T=2\,\mathrm{K}$ nor in elastic NS down to $T=38\,\mathrm{mK}$ a transition to 3D long range order was observed. Nevertheless, we were able to measure the in-plane spin wave dispersion of the 2D correlations above $T_\mathrm{N}$ and determine the exchange coupling $J_\mathrm{2D} = 5.2(3)\,\mathrm{meV}$.

### [289] Hydrogen bonding in the active site of a triosephosphate isomerase E97Q variant studied by quantum refinement (board TU-022)

*Presenter: BERGMANN, Justin*

We have studied room-temperature neutron and X-ray crystal structures of the triosephosphate isomerase Glu97Gln variant in complex with the inhibitor 2-phosphoglycolate (PGA) that mimics a reaction intermediate. The results clearly show that Glu-167 is protonated and hydrogen bonded to the carboxylate group of the inhibitor. The other carboxylate atom of PGA forms a hydrogen bond to Lys-13, but in this case the location of the hydrogen atom is less clear. The best fit to the data is obtained for a mixture with the proton 70% on Lys-13 and 30% on PGA. We have tried different ways to model this structure with quantum refinement, i.e. crystallographic refinement, in which the empirical restraints (normally used to supplement the experimental data and ensure that the structure makes chemical sense) are replaced by more accurate quantum mechanical (QM) calculations. With a typical QM system, involving models of PGA, Asn-11, Lys-13, Glu-167 and His-95, significant difference densities are observed in the electron-density maps, owing to the large negative charge of the system coming from the phosphate group of PGA). These can be improved by performing the QM calculations in a continuum solvent with a high dielectric constant or by using a point-charge model of the surroundings. Another way is to use a larger QM system, involving all groups that form hydrogen bonds to the phosphate group. Alternatively, a smaller QM system can be used, excluding the phosphate group (which gives a neutral QM system), but the results are then still improved by performing the QM calculations in a continuum solvent.

### [464] Measurement of the Fierz interference term with PERKEO III (board TU-024)

*Presenter: BERNERT, Karina*

Measurements of the free neutron decay enable a variety of tests of the Standard Model of particle physics. Observables of the decay are, among others, the beta asymmetry $A$, the proton asymmetry $C$, and the Fierz interference term $b$. From precision measurements of $A$ the CKM matrix element $V_{ud}$ may be determined, whereas measurements of $C$ provide limits on right handed currents. A non-zero Fierz term $b$ would signal the existence of scalar and tensor interactions beyond the Standard Model. Determinations of these neutron decay parameters were pursued by the PERKEO III experiment by measurements of the electron and/or proton energy spectrum, during multiple runs at the ILL PF1b facility. For these measurements we used a pulsed beam of cold neutrons to control major systematic effects. This beam is guided into the decay volume of the experiment, in which some of the neutrons decay. The charged particles from the decay are then guided by a magnetic field towards one of two detectors, depending on towards which hemisphere they were directed to. The detectors are identical scintillation detectors with a PMT readout. With this measurement technique PERKEO III delivers the currently most precise values for $A$ and $b$ with a polarized neutron beam. We present experimental details of the 2019/2020 campaign to

measure the electron spectrum of unpolarized neutrons to extract an improved limit for the Fierz interference term $b$ and the ongoing analysis.

### [150] Similarities between unfolded protein dynamics and polyelectrolyte dynamics (board TU-026)

*Presenter: BIEHL, Ralf*

Proteins are biological macromolecules built from a sequence of amino acids with varying characteristics as hydrophobicity, charge and side-group that determine their biological and physical properties. Unfolded proteins, like intrinsically disordered proteins (IDPs), share similarities with polymers in structure and dynamics. For thermal unfolded Ribonuclease A or the IDP myelin basic protein we showed already similarities to polymer dynamics reflected by Zimm-like dynamics with internal friction [1-3]. Also normal mode analysis based on explicit configurations resulted in improved description of the dynamics. Here we explore the dynamics of polystyrene sulfonic acid (PSS-H) and salt (PSS-Na) as a well-known polyelectrolyte well below the overlap concentration to examine the single chain conformation and dynamics. The aim is to observe the influence of the large charged sidechain onto the chain dynamics and to find similarities to the molecular dynamics of IDP that deviates from standard polymer dynamic models. The structure of PSS-H can be described by a wormlike chain model with a finite thickness. A disclike cross-section indicating the extended side chains can be observed by SAXS due to the specific contrast conditions. Neutron Spin Echo, observing the molecular dynamics, clearly indicate a change of chain dynamics as a function of salt concentration and temperature. The dynamics shows a crossover between rigid body like behavior (stiff chains) to Zimm-like dynamics as expected for flexible polymer chains.

### [368] Frustration-induced diffuse magnetic scattering in metallic HoInCu4 (board TU-028)

*Presenter: BORALEY, Xavier*

Materials with geometrically frustrated lattice structures are highly interesting as they often exhibit unconventional phases of matter. While most research on frustrated materials has been performed on insulating spin systems, only little work has been done on magnetically frustrated metallic systems. Notably, one of the pressing question in the field is how frustrated interactions can affect the ground state in itinerant systems. HoInCu4 is a metal with a face-centered cubic crystal structure that makes it prone to geometrical frustration. Its minuscule ordering temperature indicates a high level of frustration. This has been confirmed by recent experiments showing that the material features partial magnetic order where only half of the Holmium atoms exhibit long-range magnetic order, while the other half remain short-range ordered [1]. The behavior of the moments not participating in the long range order is, however, not yet understood. I will present our recent neutron scattering results on HoInCu4 that were obtained using thermal and cold neutrons. In detail, I will present diffuse magnetic scattering data as function of temperature, and discuss how they can be related to a model with nearest and next nearest neighbor magnetic interactions. [1] O. Stockert et al., Phys. Rev. Research 2, 013183 (2020)

### [112] Current-induced Self-organisation of Vortex Matter Studied by SANS (board TU-030)

*Presenter: BREMS, Xaver Simon*

In the superconductor Niobium the vortex-vortex interaction shows in addition to the purely repulsive also an attractive term. This leads to the formation of the intermediate mixed state (IMS) where flux-free Meissner state domains and vortex clusters coexist. Besides being a prominent example of exotic vortex matter this two-domain structure can also act as a highly tunable model system for universal domain physics [1]. Vortices in a superconductor can be depinned using transport currents resulting in the flux flow state: For currents higher than the depinning current $I_{c}$ vortices move orthogonal to the direction of the applied current. In contrast to the pure mixed state non-trivial ordering phenomena are expected in the flux flow state of the IMS due to its highly heterogeneous domain structure. Small-angle neutron scattering (SANS) is the perfect technique to study such a system as we can analyse Bragg peaks from the local vortex lattice and in parallel the very small angle scattering (VSAS) from the larger micron scale domain structure. We verified [2] the existence of the IMS in the flux flow state in a Nb single crystal sample. Our main result is the transition from isotropic to anisotropic VSAS indicating that the IMS rearranges into a stripe superstructure in the flux flow state. The stripe pattern is aligned perpendicular to the current direction. [1] M. Seul and D. Andelman 1995 Science 267(5197):476–483 [2] Xaver S Brems et al 2022 Supercond. Sci. Technol. 35 035003

### [180] Model cellular membranes: From flat to strongly curved structures (board TU-034)

*Presenter: CARDENAS, Marite*

Cellular membranes are essential components of cells that compartmentalize cellular events, control communication between compartments and with the exterior, enable the formation of gradients of ions and other solutes, and provide a proper environment for the large percentage of proteins that are membrane bound or associated to it1. The ability to carry out this diverse array of essential functions requires a high degree of dynamic organization at the nanoscale. It is proposed that the different functions are compartmentalized into different domains by lipid-lipid and/or lipid-protein interactions, but studying these systems have proved difficult due to the nature of cellular membranes and the requirement of sophisticated techniques to analyze them at the molecular level. The current state of the art on membrane organizations heavily focusses on planar membranes2 despite these membranes often being highly curved as in dynamic processes such as invagination and vesiculation, but also in organelles such as the

endoplasmic reticulum and the mitochondria. Neutron scattering combined with deuteration is an ideal technique to study the structure and dynamics of multicomponent systems where different parts of the system can be highlighted individually3–5. For example, Neutron Reflection (NR) allows to extract depth profiles of rather complex biointerfaces2 and revealed the overall structure of lipid bilayers as a function of composition6,7, the dependency of the core thickness on acyl chain type7, and the position of cholesterol in the bilayer 8,9, the flip/flop 10, and the ability of membranes to exchange lipids across bilayers3, among other parameters such as fluctuations on floating bilayers11. Similar depth profile information can be extracted for lipid vesicles from small angle neutron scattering (SANS) but the accuracy is lower as compared to NR due to the smearing by the inherent orientational averaging and lower dQ/Q. For example, using SANS the membrane thickness of photolipid vesicles was shown to be tuned in response to illumination by UV and blue light12. Both NR and SANS lack the possibility to extract lateral correlations, which is accessible to GISANS, such as local adhesion points, clustering of adhesion anchors13 as well as lipid rafts14. In this talk I will present a range of examples that demonstrate the power of neutron scattering and selective deuteration for studying the structure and composition of model cellular membranes. I will then finally present a new approach based on diffracting scaffolds to study membrane structure as a function of curvature suited for a range of surface sensitive techniques. I will also show fluorescence microscopy data for lipid diffusion on curved membranes among others. References: 1. Pomorski, T. G., Nylander, T. & Cárdenas, M. Model cell membranes: discerning lipid and protein contributions in shaping the cell. Adv. Colloid Interface Sci. 205, 207–220 (2014). 2. Clifton, L. A. et al. Design and use of model membranes to study biomolecular interactions using complementary surface-sensitive techniques. Adv. Colloid Interface Sci. 277, 102118 (2020). 3. Browning, K. L. et al. Human Lipoproteins at Model Cell Membranes: Effect of Lipoprotein Class on Lipid Exchange. Scientific Reports vol. 7 (2017). 4. Maric, S. et al. Time-resolved small-angle neutron scattering as a probe for the dynamics of lipid exchange between human lipoproteins and naturally derived membranes. Sci. Rep. 9, 7591 (2019). 5. Wadsäter, M. et al. Monitoring shifts in the conformation equilibrium of the membrane protein cytochrome P450 reductase (POR) in nanodiscs. J. Biol. Chem. 287, 34596–34603 (2012). 6. Luchini, A. et al. Peptide discs as precursors of biologically relevant supported lipid bilayers. J. Colloid Interface Sci. 585, 376–385 (2021). 7. Åkesson, A. et al. Composition and structure of mixed phospholipid supported bilayers formed by POPC and DPPC. Soft Matter 8, 5658–5665 (2012). 8. Waldie, S. et al. Localization of Cholesterol within Supported Lipid Bilayers Made of a Natural Extract of Tailor-Deuterated Phosphatidylcholine. Langmuir 34, 472–479 (2018). 9. Waldie, S. et al. The Production of Matchout-Deuterated Cholesterol and the Study of Bilayer-Cholesterol Interactions. Sci. Rep. 9, 5118 (2019). 10. Gerelli, Y., Porcar, L., Lombardi, L. & Fragneto, G. Lipid exchange and flip-flop in solid supported bilayers. Langmuir 29, 12762–12769 (2013). 11. Rondelli, V., Fragneto, G., Motta, S., Favero, E. D. & Cantù, L. Reflectivity from floating bilayers: can we keep the structural asymmetry? J. Phys. Conf. Ser. 340, 012083 (2012). 12. Urban, P. et al. A lipid photoswitch controls fluidity in supported bilayer membranes. Langmuir 36, 2629–2634 (2020). 13. Röttgermann, P. J. F. et al. Cell motility on polyethylene glycol block copolymers correlates to fibronectin surface adsorption. Macromol. Biosci. 14, 1755–1763 (2014). 14. Levental, I., Levental, K. R. & Heberle, F. A. Lipid Rafts: Controversies Resolved, Mysteries Remain. Trends Cell Biol. 30, 341–353 (2020).

### [288] Thermal moderator-reflector design of the 24Hz target station for the High Brilliance Neutron Source (board TU-036)

*Presenter: CHEN, Junyang*

The High Brilliance Neutron Source (HBS) is expected to be the next-generation neutron facility, which uses low proton energy (70MeV) to achieve high neutron brilliance. As the moderator-reflector unit is correlated to the neutron moderation, reflection, and transportation, designing a suitable moderator-reflector unit is one of the important issues for achieving the “high brilliance” of the thermal neutron cloud. In this research, the optimization of the thermal moderator-reflector of the 24Hz target station will be conducted to optimize pulse shape and intensity. The Monte Carlo simulation is applied to the design. PHITS and Diffmod are used. In this presentation, at first, the proof-of-principle simulation to reduce the absorption of hydrogenous moderator material is introduced. The time and energy characteristic of candidate material and structure are simulated and analyzed. Then, according to the neutron transportation simulation of different moderator-reflector unit, the specific design is presented. And we will show the result of thermal behavior and neutronic characteristics of this moderator-reflector unit. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [113] The soft matter and chemistry support facilities at the Institut Laue-Langevin (board TU-038)

*Presenter: CHIAPPISI, Leonardo*

The Institut Laue-Langevin has been performing experiments at the cutting edge of research for more than 40 years now, in fields as varied as molecular biology, chemistry, fundamental physics, materials science and the environment. The ILL provides the scientific community with 40 high-performance instruments constantly maintained at the highest state of the art. To exploit the full potential of the high-performance instruments, a number of support facilities are available at the ILL, i.e., the deuteration laboratory, sample environment or the computing for science groups. In this contribution, we aim at presenting the support given by the chemistry laboratories and the partnership for soft condensed matter (PSCM). The chemistry facility at the ILL manages several wet chemistry labs, as well as chemistry laboratories fully equipped to handle nano-powders. The PSCM laboratories provide approx. 30 laboratory scale equipment aimed at the characterization and preparation of samples in the domain of soft condensed matter.

### [149] Neutron investigations of high coercivity hexaferrite (board TU-040)

*Presenter: CHRISTENSEN, Mogens*

The syntheses of aluminum substituted strontium hexaferrite nanoparticles, SrFe<sub>12-x</sub>Al<sub>x</sub>O<sub>19</sub> with x=0-3, via three different preparation methods were investigated: hydrothermal autoclave synthesis (AC), a citrate sol-gel synthesis (SG) and a solid-salt-matrix (SSM). Evaluation of macroscopic magnetic properties revealed that for the SG sample with x=3, the saturation magnetizationm was reduce by 68% to 22.6Am<sup>2</sup>/kg, while the coercivity was increased by 73% to 830kA/m (10.4kOe), when compared with the x=0 sample. This very high coercivity for hexaferrites is comparable with the coercivity seen in rare earth magnets. Powder neutron diffraction (PND) patterns for all samples were collected at the powder diffraction instrument Echidna, ANSTO, Australia. Combined powder X-ray diffraction (PXRD) and PND Rietveld confirm that effective substitution of the Al only happens for the SG sample and reveal that the substitution occurs on the (2a)<sub>Oh</sub> and (12k)<sub>Oh</sub> sites at low substitution levels (*x*=1), as well as (4e)<sub>BP</sub> and (4f)<sub>Oh</sub> sites at higher substitution levels. The intrinsic magnetizations according to the refined moments and Al site occupancies from the NPD data are in remarkable agreement with the observed macroscopic magnetic data, confirming the robustness and accuracy of the model. The results reveal that Al only substituted into the structure in the SG sample. The Al site occupation fractions are also in excellent agreement with the previously reported theoretical calculations.

### [356] Best Practices for Management of the Construction Phase of Research Infrastructures: A Preliminary Case Study (board TU-042)

*Presenter: CLAUDIO WEBER, Tania*

The standard project management methodologies were developed to serve a world where the business objectives are focused on financial benefit. Such methodologies with emphasis on delivering programmes and projects within the triple constrain need to be strongly adapted to the unique environment of research infrastructures (RIs). Even the definition of project, programme and portfolio needs to be adapted to this environment. The “business case” of RIs are far from the profit-oriented culture, and the stakeholders range from several international funding authorities to society in general (depending on the type of RI). The word “business” itself also needs to be revisited since the main output of RIs are scientific achievements (such as articles, patents, spin-offs, etc.), as well as collaborations and political gain. The boundary conditions to obtain the funding for a large-scale RI such as ESS e.g., are based on political interests which results on overly optimistic schedules and budgets. This leads to the commonly known issue of RI construction repeatedly being delayed and presenting increasingly overrunning costs. One way to contribute to solving this issue, is to have a standard lean methodology to manage the construction phase of such facilities. A proposal for a new approach for project, programme and portfolio management during the construction phase of RI’s based on best practices with the construction of large-scale neutron facilities will be presented.

### [468] Magnetic order in the archetypical 2D van der Waals magnet CrI3 (board TU-044)

*Presenter: DALAL, KAMALDEEP*

Two-dimensional van der Waals materials host a diverse landscape of optical, electronic and topologically non-trivial states in the monolayer limit and have therefore fuelled a search for the next candidate materials that may enable novel information technologies. The magnetic features can be controlled by different processes including thickness, doping and other tuning parameters. CrI3 specifically shows a changing magnetic order and strong pressure dependence between ferromagnetic and antiferromagnetic in the limit of a few monolayers. However, it has recently become clear that even the bulk material hosts a much richer behaviour than initially assumed caused by the coexistence of different crystal structures. In a recent muSR study some of us revealed that bulk CrI3 shows several magnetic phases with distinct transitions below the established TC. Remarkably, the traditionally defined TC does not correspond to long range magnetic order in the full volume of the crystal but rather to a partial transition where less than 25% of the crystal is spin-ordered. In total three distinct magnetic phases were identified with specific amount of crystal structures (monoclinic and rhombohedral). Here we present a small angle neutron scattering study of the magnetic correlations in bulk CrI3. We find a complex behaviour in this inhomogeneous ferromagnet below TC, with several temperature regimes which are dominated by very distinct correlation lengths, including a regime of phase coexistence.

### [410] Research and development towards novel spin-selective neutron detectors for fundamental science (board TU-046)

*Presenter: DEGENKOLB, Skyler*

We present developments towards spin-selective *in-situ* detection of ultracold neutrons, motivated by the search for a permanent electric dipole moment. Magnetic fields generated by microstructured superconductors will produce a spin-dependent shift of the neutron-optical potential at a reflecting surface layer. Low-field-seeking neutrons then penetrate to an underlying absorber with increased probability, while high-field-seeking neutrons are more likely to be reflected without absorption. This concept is being tested via polarized cold neutron reflectometry; it could also open further applications as an alternative means of neutron depth profiling.

### [151] Silver Jubilee for the OSIRIS spectrometer: Achievements and Outlook (board TU-048)

*Presenter: DEMMEL, Franz*

In December 1997 the OSIRIS beamline at the ISIS Facility, UK, recorded its first neutron spectrum. The instrument enjoyed a first stint as a cold neutron diffractometer before the spectroscopic capabilities were fully commissioned. OSIRIS soon became a workhorse QENS spectrometer as well a highly successful cold neutron excitations spectrometer. The status of the instrument is recognized by the user community with high-impact publications ranging from energy materials over life science to quantum matter. Just now a new silicon analyser is under construction to extend the resolution capabilities. Within the Endeavour programme the primary spectrometer will be upgraded with an up to an order of magnitude increased flux. Beyond these developments further improvements of the energy resolution with a combination of a fast pulse shaping chopper and using a direct backscattering geometry are being investigated.

### [327] The ILL Deuteration Laboratory (ILL D-Lab) (board TU-050)

*Presenter: DEVOS, Juliette*

The ILL Deuteration Laboratory is a platform dedicated to isotope labelling of biological molecules. More specifically, the D-Lab team members are experts in the deuteration of biomolecules for neutron applications, such as neutron scattering, protein crystallography, dynamics and reflectometry. The D-Lab is part of the ILL Life Sciences Group within the Partnership for Structural Biology (PSB) located in Grenoble, France. It is run as a user platform available to all neutron users. Access to the platform is by a rapid electronic peer-review system, available at any time. In neutron experiments in biology, the replacement of the common hydrogen isotope protium (1H) by its stable isotope deuterium (2H) is of crucial importance for biomolecules [a]. Depending on the neutron experiment, various levels of deuteration of these molecules are necessary [b]. Microorganisms such as bacteria and yeasts have been successfully adapted to growth in deuterated minimal media. Large-scale protein deuteration by recombinant expression in high-cell density cultures was initially developed in the ILL D-Lab. The production of various labelled biomolecules required for the study of proteins, protein-nucleic acid complexes, protein-lipid complexes, glycoproteins, membrane proteins and stealth lipid nanodiscs will be presented. The in vivo deuteration of small biomolecules of major functional importance will also be highlighted, as well as recent advances and method developments for the deuteration of biomolecules *in vivo* and *in vitro*. For further information, you can consult the webpage on the ILL website (https://www.ill.eu/users/support-labs-infrastructure/deuteration-laboratory) dedicated to the platform. The ILL D-Lab team can be contacted at any time (dlab-proposals@ill.fr) and is fully available to assist neutron users in biology with their sample preparation.
REFERENCES: a. Haertlein M., Moulin M., Devos J.M., Laux V., Dunne O., Forsyth V.T. Biomolecular Deuteration for Neutron Structural Biology and Dynamics Methods Enzymol., 566, 113-157 (2016). b. Dunne O., Weidenhaupt M., Callow P., Martel A., Moulin M., Perkins S. J., Haertlein M., Forsyth V.T. Matchout deuterium labelling of proteins for small□angle neutron scattering studies using prokaryotic and eukaryotic expression systems and high cell□density cultures Eur. Biophys. J., 46, 425–432 (2017).

### [470] Understoichiometric CrBx/TiBy superlattices as novel materials for neutron mirrors (board TU-052)

*Presenter: DORRI, Samira*

The reflected neutron flux from state-of-the-art neutron multilayer mirrors is hampered primarily by insufficient layer definitions. To achieve the ultimate flat and abrupt interfaces (±½ atomic layer), the mirror should be made as a single crystal, artificially layered, heteroepitaxial structure (superlattice, SL). Here we explore CrBx/TiBy (0001)/Al2O3 (0001) SL mirrors, grown by magnetron sputter epitaxy. We study the effect of composition on the interface quality and neutron reflectivity of CrBx/TiBy SLs with periodicities Λ ≈ 6 nm and TiB2 thickness-to-Λ ratios, Γ ≈ 0.3, 0.5, and 0.7, grown from two set of target composition. Elastic recoil detection analysis shows overstoichiometric (B/TM > 2) SLs for one set of target materials and understoichiometric (B/TM < 2) for another set of targets. X-ray diffraction, X-ray reflectivity, and high resolution scanning transmission electron microscopy show that understoichiometric SLs exhibit significantly higher structural quality and smaller interface widths compared to overstoichiometric ones. Neutron reflectivity simulations using the GenX code show that small changes in B composition affect the neutron scattering length density of the SLs so that understoichiometric SLs exhibit higher neutron reflectivity with a different low intensity variation. Such structures have the potential to be used as novel materials for the compact slit package (~20×30 mm2) that is required for supermirror Fermi choppers.

### [427] Calcium(II)-containing borosilicate aerogels as promising materials for application in regenerative medicine (board TU-054)

*Presenter: DUDÁS, Zoltán*

Hybrid aerogels in general are promising scaffolds for bone regeneration owing to the high porosity, nanostructured surface and versatile functionalization of this family of sol-gel materials. Our study focuses on the design, synthesis, in-depth structural characterization and in vitro biological testing of calcium(II)-containing hybrid borosilicate aerogels. Little is known about the behavior of nanostructured porous borosilicate materials in biological media (changing micro- and nanostructure, altered physical and chemical properties, reaction to environmental influences, etc.). Understanding the structure-property-function relationships in relation to biological systems is the most important objective of the present research. Hybrid borosilicate aerogels were prepared

by sol-gel synthesis using various molecular weight PVAs and different calcium sources (CaCl2, Ca3(PO4)2, hydroxyapatite) as bioactive ingredients. The structural characterizations were done employing various techniques in terms of composition (FTIR, solid-state NMR), texture and morphological properties (N2–sorption porosimetry, small angle neutron scattering, electron microscopy). These studies reveal the interconnected mesoporous structure of the scaffolds with pore diameters of 20-45 nm and apparent surface areas of 540-1038 m2/g. The synthetized materials were characterized employing various techniques in terms of composition, texture and morphological properties. Contrast-variated SANS has been used to describe the mesoporous structure of the scaffolds and their behaviour in aqueous environment. The suspensions of the aerogels were studied by dynamic light scattering and Zeta potentials were measured. Selected materials were submitted to in vitro experiments to determine their biocompatibility and bioactivity. Viability assays and time lapse video microscopy imaging of cell proliferation and scratch closure were performed using human mesenchymal stem cells. These experiments revealed the high affinity of the cells towards the hybrid borosilicate aerogels.

### [48] Magnetic, electric and toroidal polarisation modes describing the physical properties of crystals - the NdFeO3 case (board TU-056)

*Presenter: FABRYKIEWICZ, Piotr*

We present a general classification [1, 2] to answer the question: which groups allow to describe a given magnetic, electric and toroidal polarisation mode? These three classifications are based on magnetic point groups used in two contexts: (i) the magnetic point group of the magnetic crystal class and (ii) the magnetic site symmetry point group of the Wyckoff position of interest. The following statements are true for magnetic, electric and toroidal modes: (i) there are 64 unique modes: 3 pure ferro-, 13 mixed ferro- with antiferro- and 48 pure antiferro-, (ii) a continuous reorientation of any moment is possible only in triclinic or monoclinic symmetry [3], (iii) canted antiferro- ordering is possible only in monoclinic or orthorhombic symmetry. To visualise the similarities of magnetic, electric and toroidal modes, we propose a new Rotation-Inversion (RI) notation [1] of magnetic point groups which does not prioritise or distinguish any of three generalised inversions: space inversion -1, time inversion 1’ and the space-and-time inversion -1’. In RI notation each operation is presented as a product of one proper rotation and one generalised inversion. The general classifications of modes are presented for the case of NdFeO3. **References** [1] P. Fabrykiewicz, R. Przeniosło and I. Sosnowska, Acta Cryst. A (in press) [2] P. Fabrykiewicz, R. Przeniosło and I. Sosnowska, Acta Cryst. A77 (2021) 327 [3] R. Przeniosło, P. Fabrykiewicz and I. Sosnowska, Acta Cryst. A74 (2018) 705

### [137] On the magnetization reduction in iron oxide nanoparticles (board TU-058)

*Presenter: FEOKTYSTOV, Artem*

Iron oxide nanoparticles are presently considered as promising objects for various medical applications including targeted drug delivery and magnetic hyperthermia. The nanoparticle solution in water has to posses large enough saturation magnetization to react on external magnetic field. However, there remains several unsolved questions regarding the e□ect of size onto nanoparticle overall magnetic behavior. One aspect is the reduction of magnetization as compared to bulk samples. A detailed understanding of the underlying mechanisms of this reduction will improve the particle performance in the applications. There are several proposed models for the spatial distribution of the magnetization, which include the presence of a magnetic core-shell structure, spin disorder around defects and a reduced magnetization in the core due to reversed moments and frustration. In this work we combine neutron and synchrotron X-ray scattering techniques with magnetometry, transmission electron microscopy (TEM), elemental analysis and Mössbauer spectroscopy to study nanoparticles of various sizes and to obtain as complete as possible picture of their properties. We find that the nanoparticles possess a macroscopically reduced saturation magnetization, mostly due to the presence of antiphase boundaries as observed with high-resolution TEM (HRTEM) and X-ray scattering and to a lesser extent due to a small magnetically depleted surface layer and cation vacancies.

### [148] Exploring the world of biological lipids – deuteration, purification and characterisation of yeast lipids for native-like cell membrane models at ESS (board TU-060)

*Presenter: FISHER, Zoe*

Neutron scattering is well-suited to the study of biological membrane lipids and has the potential to contribute unique view into the role membranes play in both health and disease, as well as medical treatments, by employing deuterium labeling. However, modeling the lipid environment in living cells poses a challenge due to their complex and tightly-controlled composition. By extracting and purifying biological lipid mixtures from cell cultures it is possible to reconstitute model membranes that capture the lipid complexity found in cells and to re-create specific membrane environments, e.g. those found in human mitochondria. We present here recent results on the large-scale deuteration, purification and characterization of yeast membrane lipids at the ESS DEMAX platform and illustrate some of their properties and interactions studied by neutron scattering.

### [490] The bispectral chopper spectrometer T-REX (board TU-062)

*Presenter: FRANZ, Christian*

T-REX is a bispectral direct geomentry neutron chopper spectrometer, currently being constructed at the ESS. The instrument is a collaboration between Forschungszentrum Jülich and Consiglio Nazionale delle Ricerche (CNR). T-REX 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 be supported in two modes, using polarized and non-polarized neutrons. Neutron polarisation is available for 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 is specifically designed to make an efficient use of the flux provided by the source, by means of poly-chromatic illumination of the sample. It enables variable acquisition time frames, by means of a specially developed chopper (the FAN chopper) that suppresses selectively the sub-pulses generated by the resolution-defining choppers. The secondary spectrometer features a vacuum path of 3 m 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.

### [63] The Source for Ultra-Cold Neutrons at the FRM II (board TU-064)

*Presenter: FREI, Andreas*

At the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) of the Technical University of Munich (TUM) a new source for ultra-cold neutrons (UCN) with a solid deuterium converter is currently under construction. The source is designed to deliver UCN to four different experiments simultaneously, located in the experiment hall and neutron guide hall east of FRM II. This poster shall give an overview of the project and its current status.

### [318] The GISANS instrument at the HBS (board TU-066)

*Presenter: FRIELINGHAUS, Henrich*

We present a concept of a GISANS instrument for the High Brilliance Source (HBS), a High Current Accelerator-based Neutron Source (HiCANS) using a moderate energy proton accelerator which allows very compact moderators and shielding, and flexible pulse repetition rates. The general layout resembles a classical SANS instrument with 10 m collimation and 10 m detector distance. In the beam preparation, there is a deflector, two choppers and a changeable polarizer. For reflectivity measurements, enlarged vertical divergence is transported to the entrance aperture at 4m. Then 2(3) mirrors and the direct beam transport 3(4) beams of different incident angles to the sample in order to have a simultaneous wider $Q_z$ range. In the GISANS mode, the vertical divergence is reduced and only one direct beam is used to hit a horizontal sample. Two detectors collect the scattered intensity simultaneously in order to have a large range of scattering angles. The simulated intensities at the sample are highly promising and are comparable to reactor-based instruments such as those at the FRM-2.

### [34] Fast Calculation of Scattering Patterns Using Hypergeometric Function Algorithms (board TU-068)

*Presenter: FÖRSTER, Stephan*

The scattering of light, X-rays, electrons or neutrons by matter is used widespread for structural characterization from atomic to macroscopic length scales. With the advent of high-brilliance beam sources and the development fast, large area pixelated detectors, scattering patterns are now acquired at unprecedented frame rates and frame sizes. The slow analysis of these scattering patterns has evolved into a severe bottleneck retarding scientific insight. Here, we present an algorithm that is based on the use of hypergeometric functions to rapidly compute 1D- and 2D-scattering data. Hypergeometric functions provide a simple mathematical description of geometrical objects, have analytical Fourier transforms, and can be rapidly computed via series and asymptotic expansions with recursive coefficients. Compared to numerical integration schemes we observe gains in computation speed of > 10^5. The algorithms can be efficiently implemented in GPUs for further acceleration. The algorithm provides the necessary computational speed to calculate scattering patterns on timescales required for real-time experiment feedback, the analysis of large volumes of scattering data, and for the generation of training data sets for machine learning. It enables the computation of 2D scattering patterns at > 1 fps even for current 4k pixel detectors.

### [291] Bulk texture and microstructure evolution of γ-TiAl alloy during hot compression (board TU-070)

*Presenter: GAN, Weimin*

Owing to low density (3.8-4.0 g/cm3), high specific strength and stiffness, excellent creep resistance and good corrosion resistance, the β-solidifying γ-titanium aluminide with properly aligned (α2+γ) lamellar-structure have been considered as excellent candidates for modern turbine blades. Recently, it has been evidenced that when the γ lamellae are oriented to the load direction the mechanical properties of the alloys can be greatly increased. Thus, lamella orientation control has become an interesting topic for property optimization. It has been shown that the microstructure of TNM alloys (Ti-43Al-4Nb-1Mo-0.1B(at%)) at the initial state was composed of multiple grains from three different phases. After uniaxial compressive hot-deformation at 1280°C for different deformations and strain rates, first results showed that (1) the microstructure changed and become mainly composed of the alpha phase and (2) the material can be texturized. Different type of characterization such as the neutron and synchrotron radiation to obtain texture bulk information at our study. For a better understanding of the formation and transformation of microstructure EBSD measurements were conducted and analyzed with respect to orientation relationships and microstructure stability. Bulk

texture evolution will be presented in detailed. Results has indicated that texturization of TNM alloy seems to be possible thanks to hot compression, which leads to different type of microstructure depending on the deformation speed and strains as well as the imposed temperature. Keywords : TNM TiAl alloys, texturization, microstructure, bulk texture

### [131] Lamellar diffraction from lipid bilayers on MIRA, a triple axis spectrometer at the MLZ (board TU-072)

*Presenter: GARVEY, Christopher*

Diffraction used in conjunction with molecular deuteration provides a model independent means to examine detailed structural and compositional information of model and real biological membranes in the lamellar phase. The technique provides specific information of localization of molecules and smaller units with respect to the unit cell. Deuteration is used to provide specific labelling and to provide phasing for the crystallographic reconstruction. Typical data sets consist of a series of lamellar diffraction peaks, usually collected under conditions of 3 contrasts of a water. Accurately integrated the diffraction peaks can be used for a Fourier reconstruction of the composition of the lamellar unit cell in real space. Each diffraction peak which can be integrated for 3 contrasts contributes to an additional Fourier term in the reconstruction and optimization of the number of peaks enhances the spatial resolution of the crystallographic reconstruction. Here we report on the use of the flexibly configurable cold triple-axis spectrometer, MIRA, at the Heinz Maier-Leibnitz Zentrum (Garching, Germany) for investigations of different lamellar systems using this approach. The data sets are acquired from lamellar stacks in an sample environment with humidity and temperature control with exceptionally low background. We discuss further enhancements of the instrument and sample environment which will provide information on the composition and equilibration of the sample.

### [197] SANS-LLB, the new small-angle instrument at SINQ, PSI (board TU-074)

*Presenter: GASSER, Urs*

In 2023, the user program at SINQ, Paul Scherrer Institut (PSI), will again offer two small-angle instruments, the new SANS-LLB and as before SANS-I. SANS-LLB is the adapted and optimised PA20 SANS instrument from the Laboratoire Léon-Brillouin (LLB) that was transferred to PSI after the shutdown of the Orphée reactor in 2019 and will be operated by LLB and PSI. SANS-LLB is a general-purpose SANS instrument with a flight path of up to 18 meters, a wavelength range from 3 to 20 Angstroms, with option for polarized neutrons, a versatile collimation section, and two 3He detectors - the central main detector and an L-shaped detector at a lower distance to increase the q-range covered with a single setting of the instrument. As SINQ obtained a neutron-guide upgrade in 2019-2020, SANS-LLB will become available with a new 45 mm x 45 mm guide system that is optimized from the SINQ source to the sample position. Various sample environments covering soft and hard matter research are available and are mostly shared with SANS-I. A novel semi-transparent beamstop will allow to take transmission data continuously without dedicated transmission measurements, thus shortening measurement times and increasing sample throughput. A new detector electronics developed at PSI will be installed in 2023 and will allow for time-resolved measurements. The neutron flux on SANS-LLB is expected to be comparable although somewhat lower than on SANS-I due to the smaller cross section of the guide and the larger distance from the source. With SANS-LLB, the number of SANS beam days offered at SINQ will be doubled.

### [309] Accurate determination of bound coherent neutron scattering lengths using Bragg diffraction (board TU-076)

*Presenter: GEHLHAAR, Florian*

Bound coherent scattering lengths b(coh) are one of the basic properties of any isotope, and many experimental neutron techniques in condensed matter as well as in nuclear physics rely on these values, determined by many different scientists over decades and collected in various tables. But many of the values listed in these respectable references have large experimental uncertainties, including possible systematic errors, due largely to having been measured decades ago with neutron instrumentation that has since greatly improved. Therefore, we use the advantages of modern neutron powder diffraction (NPD), like very good counting statistics even on sub-gram samples, for a redetermination of b(coh) of important isotopes. The measurement of integrated Bragg peak intensities I(hkl) using NPD has the huge advantage that only the *relative* peak intensities are affected by a change in one of the sample’s b(coh), such that there is no need to normalize the data to an absolute intensity scale, being therefore much less prone to systematic errors than are other techniques used for b(coh) determination. Rietveld refinement then provides the structure factor F(hkl), and in the case of fixed atomic positions, F(hkl) depends only on b(coh) which thus can be determined directly. The strategy for an accurate determination of b(coh) is therefore to use binary or ternary compounds with well-known crystal structures and ideally with a small number of free positional parameters.

### [367] Spin wave dispersion of the antiferromagnet CuMnSb (board TU-078)

*Presenter: GEORGII, Robert*

CuMnSb is a half Heusler alloy which orders type-II antiferromagnetically and is, thus, unique among the 3d transitional metal heusler alloys. Theoretical calculations suggested that type-II antiferromagmetism is not the energetically favored state and is only stabilized by structural defects. Further, a high quality CuMnSb single crystal exhibits a additional phase transition within the magnetic phase where the spins cant slighty away from the initial direction. Additionally, characterisitics of different interactions have been observed, namely itinerant, local moment and spin orbit coupling. This shows that the magnetic ground state is a more

complex nature than other typical type-II antifermagnets. We studied CuMnSb with inelastic neutron scattering and measured among others the spin wave dispersion. By that, we were able to quantize the interaction between neighbouring spins and answer some questions of the magnetic interaction in CuMnSb.

### [111] In-situ neutron diffraction and electron microscopy to study deformation mechanisms in Ni-based superalloys (board TU-080)

*Presenter: GILLES, Ralph*

The polycrystalline Ni-based superalloy VDM Alloy 780 is a further development of the Alloy 718, which is limited to around 650 °C in the operation temperature of gas turbines. The main differences between these two alloys are essentially the replacement of Fe by Co and a higher Al content in combination with a lower Ti content in VDM Alloy 780. Tensile loading and unloading experiments were carried out with a newly developed testing machine on the STRESS-SPEC instrument of MLZ to examine the deformation behavior at 25 and 500 °C. In addition, a detailed microstructural study using electron microscopy was performed before and after the test to correlate the macroscopic mechanical properties with micromechanical deformation behavior in various oriented grains. The deformation behavior, which is mainly dislocation motion and shearing of the Gamma Prime precipitates, does not change at this temperature range. The deformation is strongly anisotropic and depends on the grain orientation.

### [46] KOMPASS – the polarized cold neutron triple-axis spectrometer at the FRM II (board TU-082)

*Presenter: GORKOV, Dmitry*

KOMPASS is a polarized cold-neutron three axes spectrometer (TAS) currently undergoing its final construction phase at the MLZ in Garching. The instrument is designed to exclusively work with polarized neutrons and optimized for zero-field spherical neutron polarization analysis for measuring all elements of the polarization matrix. In contrast to other TASs, KOMPASS is equipped with a unique polarizing guide system. The static part of the guide system hosts a series of three polarizing V-cavities providing a highly polarized beam. The exchangeable straight and parabolic front-end sections of the guide system allow adapting the instrument resolution for any particular experiment and provide superior energy- and Q-resolution values when compared with the existing conventional guide and instrument concepts [1, 2]. In combination with the end position of cold neutron guide, the large doubly focusing HOPG monochromator and analyzer, the V-cavity for analysis of polarization of scattering beam, the KOMPASS TAS will be very well suited to study various types of weak magnetic order and excitations in variety of complex magnetic structures and indeed first successful experiments on chiral magnets or very small crystals could already be performed. [1] M. Janoschek et al., Nucl. Instr. and Meth. A 613 (2010) 119. [2] A. C. Komarek et al., Nucl. Instr. and Meth. A 647 (2011) 63. The construction of KOMPASS is funded by the BMBF through the Verbundforschungsprojekt 05K19PK1.

### [6] Neutron Scattering Kernels for Methane I & II and Ethane III (board TU-084)

*Presenter: GRANADA, Rolando*

We present new scattering kernels for two materials of interest as cold and very cold neutron moderators: solid Methane in phases I &II and solid Ethane in phase III, based on simple models that include the main dynamical features of those three systems and the effect of spin correlations. Inelastic neutron scattering experiments were performed using the TOSCA spectrometer at the ISIS pulsed neutron source (Experiment Number: 2000128) on samples of solid CH4 and C2H6 and mixtures of them over a range of temperatures down to 13 K. From the measured INS spectra we derived preliminary Density of State (DOS) for Methane I & II and Ethane III, over the range of energy transfers where the translational and rotational degrees of freedom control de molecular dynamics. In addition, proton spin correlations as a function of temperature were also accounted for, involving all four protons in the methane molecule, and the three protons in each methyl group of the ethane molecule. In the case of methane, the model predictions of the total cross sections are in good agreement with a quantum mechanical calculation over the limited range where the latter was formulated, and with available experimental information over the complete thermal energy range.

### [13] Probing topological interactions in polymers under shear (board TU-086)

*Presenter: GVARAMIA, Manuchar*

Wormlike micelles may serve as a model system for linear polymers and are studied extensively. Micelles, unlike polymers, can break and reform. Their self-assembled structure makes them unique in applications where high shear rates may be encountered, such as drag reduction, and as a templates for materials synthesis. The rheological properties of viscoelastic materials can be described by the Maxwellian model. In this presentation we will present the influence of CTAB-NaSal solutions composition on the rheology of wormlike micelle and pave the road for microscopic investigation by neutron scattering. Fig. 1 shows the linear viscoelastic rheology of cationic wormlike micellar solution which has been shown to be Maxwellian, exhibiting a single dominant relaxation time. To study the microscopic dynamics of wormlike micelles, they can be measured by neutron spin echo spectroscopy (NSE). However, such measurements under shear are challenging as Doppler scattering may depolarize the beam. In this presentation we will present a new dedicated sample cell to allow Rheo-NSE studies. We show resolution measurements and compare them to theoretical predictions of Doppler scattering. We show that our shear cell allows to address Fourier times up to 140ns at Q values of 0.157 Å-1 and shear rates of up to 166 s-1.

### [411] Multi-time scale functional protein dynamics probed by quasielastic neutron scattering (board TU-088)

*Presenter: HASSANI, Abir Nesrine*

Proteins are complex molecular systems whose internal dynamics is characterized by a vast spectrum of time scales, ranging from sub-picoseconds for vibrations of chemical bonds to seconds and beyond for large conformational rearrangements. Using a "minimalistic" multi-time scale model for the relaxation dynamics of proteins~[1,2], we show here that even small changes due to external stress, such as temperature, solvent modification or ligand binding, can be elucidated by quasi-elastic neutron scattering (QENS). The neutron intermediate scattering function is here written in the form $F(q,t)=EISF(q)+(1-EISF(q))\phi(q,t)$, where $EISF(q)$ is the elastic incoherent structure factor which gives information about the motional amplitudes of the hydrogen-atoms in hydrogen-rich systems, and $\phi(q,t)$ is a relaxation function which is chosen to be the "stretched" Mittag-Leffler function, $\phi(q,t)=E_\alpha(-(t/\tau)^\alpha)$ in order to account for the asymptotically self-similar relaxation dynamics of proteins. An important technical point is the estimation of the EISF on the basis of its measured counterpart and the model parameters of the relaxation function, which are the $q$-dependent form parameter $\alpha $ and the time scale parameter $\tau$ [3]. Our first example concerns the intrinsically disordered protein Myelin Basic Protein (MBP) in solution, which is studied in pure D$_2$O-buffer and in a mixture of D$_2$O-buffer with 30\%\, deuterated Trifluoroethanol at different temperatures, in order to evaluate the impact of formation of secondary structure elements on the internal dynamics [4]. The second example concerns the change of the internal dynamics of myoglobin in solution in presence of denaturing agents, and the third example is devoted to understanding the functional dynamics of the enzyme Phosphoglycerate kinase. Here the model allows for determining unambiguously the amplitude of the inter-domain fluctuations which are important for its catalytic function. References: [1] G. R. Kneller. PNAS USA, vol. 115, no. 38, pp. 9450-9455, 2018 [2] M. Saouessi, J. Peters, and G. R. Kneller. J. Chem. Phys., vol. 150, p. 161104, 2019. [3] A. N. Hassani, A. M. Stadler, and G. R. Kneller. J. Chem. Phys. vol. 157, p. 134103, 2022. [4] A. N. Hassani, L. Haris, M. Appel, T. Seydel, A. M. Stadler, and G. R. Kneller. J. Chem. Phys. vol. 156, p. 025102, 2022.

### [467] Multi scale structural insight into cheese by scattering techniques (board TU-090)

*Presenter: HEIDEN-HECHT, Theresia*

Products derived from milk or plant based emulsions by gelation like cheese or yoghurt have a large range of structural features from atomic to macroscopic length scales. Scattering techniques with neutrons and x-rays provide an unique view into this fascinating world of interfaces and networks provided by proteins and lipids. Combining these ensemble averaging scattering techniques with a microscopic view into the gels with environmental scanning electron microscopy (ESEM) and cryo transmission electron microscopy helps in a thorough understanding of such gel systems and the emulsion stabilization and gel formation mechanisms. In this contribution, different milk based products, emulsions and different sorts of cheese and yoghourt, are characterized in terms of their structure on length scales from nm to µm. Information is gathered on the structure of the oil-water interfaces and the gelation process, providing valuable insight for further optimization, especially in view of the design of plant based gelated emulsions.

### [105] Elastic constants and deformation mechanisms in titanium alloys determined through diffraction under mechanical load (board TU-092)

*Presenter: HOELZEL, Markus*

In this contribution, we report on neutron and synchrotron diffraction studies under mechanical stress in titanium alloys Ti-64 (near α-alloy), Ti-6246 (α+β alloy), Ti-5553 (near β-alloy) and Ti-38644 (β-alloy) to investigate the deformation mechanisms. In particular, the determination of single-crystalline elastic constants derived from the measured lattice strains in the polycrystalline specimens will be presented. These results have been used further to quantify the load partitioning in the elastic regime between the softer β phase and stiffer α phase. In addition, diffraction data were collected along the entire elastic and plastic regime to determine the evolution of lattice strains, texture and phase compositions [1,2]. References: [1] A. Heldmann, M. Hoelzel, M. Hofmann, W.M. Gan, W.W. Schmahl, E. Griesshaber, Th. Hansen, N. Schell, W. Petry, J. Appl. Cryst. (2019). 52, 1144–1156. [2] A. Heldmann, M. Hofmann, M. Hoelzel, J. Appl. Cryst. (2022). 55, 656–662.

### [296] A wide aperture high field asymmetric magnet for diffraction at ESS (board TU-094)

*Presenter: HOLMES, Alexander*

We present a new cryomagnet development for ESS, principally for use on the MAGiC instrument, but also suitable for other diffraction instruments in the ESS suite. In order to take advantage of the large detector area and polarised beam, a very large, asymmetric, aperture has been prioritised, with a maximum field of 8 T. The bore size is 50 mm, to allow for ULT inserts and bulky samples such as pressure cells or low temperature rotation stages. Since all ESS instruments have the detectors on the left, the coils can be supported in bulk on the opposite side. The system will include motion stages for z- and omega axes. To help with rapid alignment on the instruments the magnet will be adapted to the ESS kinematic mounting system. The mounting will allow for in-situ magnetic force measurement at the exactly intended position before being put into regular service. As ESS will have a site-wide helium recovery network a wet system has been chosen.

### [59] Gluten versus gluten-free pasta: a structural analysis (board TU-096)

*Presenter: HOUSTON, Judith*

High quality gluten-free food alternatives are increasingly sort after as supplements for people requiring diets with low glycaemic indexes. The challenge to produce alternatives with high enough quality to meet consumer demands. Structure at the nanoscale is highly related to the texture, quality, mouthfeel of the final product. Here, we perform for the first time a structural characterisation of commercially-available gluten-free pasta combining small-angle x-ray and neutron scattering, and compare to the analogous regular gluten-containing pasta variety. We show how the pasta structure depends on cooking times, salt content in the cooking water, and mechanical processing. This study is the first step for a structural characterization of commercially-available pasta, moving forward the classic *in vitro* model system used so far to achieve information on the relation between pasta microstructure and its digestibility.

### [236] Activation energy of diffusion determined from a single in-situ neutron reflectometry experiment (board TU-098)

*Presenter: HÜGER, Erwin*

A new methodology for the determination of self-diffusivities in solids and the corresponding activation energy of diffusion using in-situ Neutron Reflectometry is presented. In contrast to the classical ex-situ approach based on a sequence of isothermal measurements at different temperatures, the in-situ method allows one to work with a single experiment based on ramping the temperature with a constant rate. Our experiment demonstrates the success of the method for the model system of amorphous germanium. The activation energy of 2.2 eV and the absolute values of diffusivities achieved by the new method are in good agreement with the results of the classical approach, while a significantly lower amount of experimental time and samples are necessary. The presented method allows for an all-in-one type of experiment which can provide clearer and quicker results than similar methods using isothermal annealing procedures.

### [415] From IN8 to THERMES – a thermal three-axis spectrometer at ILL (board TU-100)

*Presenter: IVANOV, Alexandre*

The three-axis spectrometer IN8 offers to ILL users advanced conditions for studies of thermal excitations in single crystals and liquids. The instrument performance and flexibility are ensured by the use of large double-focusing monochromators and analysers with independently variable and remotely controlled horizontal and vertical focusing (bending) of the crystal reflecting planes providing high counting rate even for small and low-scattering samples. The new monochromator unit consists of 4 different exchangeable crystal planes. The two planes are built from mosaic crystals of pyrolytic graphite and copper with the principal reflections PG002 and Cu200 chosen to provide a broad range of monochromatic neutron wave vectors and energy resolution of the incident beam. The other two planes are assembled with elastically bent perfect silicon crystals set to make use of the reflections Si111 and Si311 with prohibited second-order diffraction harmonics. The mosaic crystal planes are used in experiments requesting maximum monochromatic intensity at the sample position and variable resolution. The silicon crystal planes, with similar to mosaic crystals available resolution range, provide particularly “clean” conditions for experiments with multi-analyser configurations (such as FlatCone) at the expense of marginally lower monochromatic flux. The further step in renovation of the spectrometer is a classical single-detector secondary spectrometer set-up called THERMES (THERMal Excitations Spectrometer) now commissioned at IN8. The new instrument benefits from a compact design that permits a larger accessible dynamic range (wider available angular ranges in the existing experimental zone) with particular attention paid to neutron shielding including special construction of the detector diaphragm. The user experiments have been routinely performed over the last few reactor cycles. Further development of specific sample environment for this spectrometer is under way.

### [4] Incommensurate and multi-q magnetic misfit structure in the frustrated quantum spin ladder material antlerite, Cu3SO4(OH)4 (board TU-102)

*Presenter: INOSOV, Dmytro*

In frustrated magnetic systems, the competition amongst interactions can introduce extremely high degeneracy and prevent the system from readily selecting a unique ground state. In such cases, the magnetic order is often exquisitely sensitive to the balance among the interactions, allowing tuning among novel magnetically ordered phases. We present antlerite, Cu$_3$SO$_4$(OH)$_4$, as a potential platform for tuning frustration. In this naturally occurring mineral, Cu$^{2+}$ ($S = 1/2$) quantum spins populate three-leg zigzag ladders in a highly frustrated quasi-one-dimensional structural motif with coupled ferro- and antiferromagnetic spin chains. Contrary to previous reports, the low-temperature magnetic state of its three-leg zigzag ladders is a quasi-one-dimensional analog of the magnetic state recently proposed to exhibit spinon-magnon mixing in botallackite. Density functional theory calculations indicate that antlerite’s magnetic ground state is exquisitely sensitive to fine details of the atomic positions, with each chain independently on the cusp of a phase transition, indicating an excellent potential for tunability [1]. In addition to its low-temperature commensurate phase with ferro- and antiferromagnetic order on the outer and inner legs of the ladders, this mineral also hosts an incommensurate helical+cycloidal state, an idle-spin state, and a multiple-$\mathbf{q}$ phase

which is the magnetic analog of misfit crystal structures [2]. The antiferromagnetic order on the central leg is reentrant. The high tunability of the magnetism in antlerite makes it a particularly promising platform for pursuing exotic magnetic order and spin excitations. [1] A. A. Kulbakov *et al.*, Phys. Rev. B **106**, L020405 (2022). [2] A. A. Kulbakov *et al.*, arXiv:2207.05606 (submitted).

### [349] Small-Angle Scattering at HBS (board TU-104)

*Presenter: JAKSCH, Sebastian*

Small-angle neutron scattering is a very versatile technique which can be applied in virtually any field of neutron science, be it soft matter, biological or medical sciences, material science, hard matter or magnetic materials. In all those fields, SANS helps investigate structure on the nano-scale from a few nanometers up to several hundred nanometers. In order to achieve this, SANS has very specific requirements concerning the collimation of the beam, selection of the wavelength band at time-of-flight sources, detector setup and beam extraction, all of which heavily impact instrumental resolution, background and available neutron flux at the sample. Several SANS instruments at the High Brilliance Neutron Source (HBS) optimized for high resolution and GISANS have been outlined [1]. In this contribution we will describe the considerations which went into the design of a SANS at the HBS to optimize instrument length, chopper positions and pulse shaping as well as the detector requirements. Special emphasis will be put on how to obtain a state of the art instrument by using the full potential of the high brilliance neutron beams from dedicated moderators at the HBS to allow for low background measurements that can achieve a competitive Q-range and measurement time-scale compared to instruments at high flux neutron sources. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. [1] Gutberlet, T. (2020). Conceptual Design Report-Jülich High Brilliance Neutron Source (HBS). T. Brückel (Ed.). Forschungszentrum Jülich GmbH.

### [418] Effect of solvent on the ps dynamics in PNIPAM microgel (board TU-106)

*Presenter: JURANYI, Fanni*

Microgels are stimuli responsive polymers with possible applications e.g. for drug delivery. A key feature of them is the sudden shrinkage, induced by temperature or other external parameters, called Volume Phase Transition (VPT). The VPT is intrinsically connected to the water-polymer, or more generally to the solvent-polymer interaction. PNIPAM in ethanol, e.g. remains swollen also at higher temperatures. We used Quasielastic Neutron Scattering (QENS) at the Time-of-Flight Spectrometer FOCUS at PSI to study the differences in atomic level water-polymer and alcohol-polymer interactions through their dynamics. In order to avoid the presence of bulk-like solvents, but preserve the network structure, re-hydrated freeze-dried powders were used. Ab initio molecular dynamics (AIMD) simulations delivered inputs for choice of model, fit parameter restrictions and interpretation.

### [208] Simulations of background scattering from a 15 T magnet (board TU-108)

*Presenter: KARAKOSTA, Petroula*

Neutron scattering allows for quite complicated sample environments with control over the sample conditions, such as controlled temperature, as well as the presence of strong magnetic fields. The presence of magnets in scattering experiments necessitates a significant amount of materials in the structure. The coils of the magnets, which are not in the direct beam, add more material into the structure and could influence the experiments, since neutrons would scatter multiple times before reaching the detector. Additionally, they exert large forces on the structure that need to be withstood, requiring more material to safeguard the structural integrity of the system. In an attempt to investigate the effect of the sample environment on the resulting background scattering, simulations of inelastic neutron scattering data in the presence of multiple scattering from the sample environment are carried out with the Union tool in McStas, a neutron ray-trace simulation package. A model of the 15 T magnet for the BIFROST spectrometer at ESS is constructed and incorporated into models of existing spectrometers, such as triple-axis, direct TOF and indirect TOF. Optimisation of the sample environment is pursued in such a way as to minimize background scattering within a variety of particular instruments and structures.

### [365] Radiation Shielding Calculations for the PERC Magnet (board TU-110)

*Presenter: KLENKE, Jens*

The free neutron decay offers an extensive test field for the Standard Model of Particle Physics. Several measurable correlation coefficients between the neutron and its main decay particles, protons and electrons, can be tested against the Standard Model description of this decay. The PERC experiment, currently being assembled at the white neutron beam line MEPHISTO at the FRM II in Garching, is capable to measure these correlation coefficients with a high precision. The experiment is a 12 m long superconducting magnet which separates the electrical charged particles of the decay from the incoming neutron beam with a tunable magnetic field. The charged particles are measured outside of the magnet, the neutrons have to be stopped inside the magnet. The neutron beam stop together with the decay volume are sources of unwanted radiation outside of the experiment. This radiation must be minimized by design of the beam stop or additional shielding. The Author presents the status of the shielding calculation based on these conditions.

### [465] Updates in SASfit for fitting analytical expressions and numerical models to small angle scattering patterns (board TU-112)

*Presenter: KOHLBRECHER, Joachim*

Small-angle scattering is an increasingly common method for characterizing particle ensembles in a wide variety of sample types and for diverse areas of application. SASfit has been one of the most comprehensive and flexible curve fitting programs for decades, with many specialized tools for various fields. Here, a selection of enhancements and additions to the SASfit program are presented that may be of great benefit to interested and advanced users alike: (a) further development of the technical basis of the program, such as new numerical algorithms currently in use, a continuous integration practice for automated building and packaging of the software, and upgrades on the plug-in system for easier adoption by third-party developers; (b) a selection of new form factors for anisotropic scattering patterns and updates to existing form factors to account for multiple scattering effects; (c) a new type of a very flexible distribution called metalog, and regularization techniques such as the expectation-maximization method, which is compared with fits of analytical size distributions via the non-linear least-squares method; and (d) new structure factors, especially for ordered nano- and meso-scaled material systems, as well as the Ornstein–Zernike solver for numerical determination of particle interactions and the resulting structure factor when no analytical solution is available, with the aim of incorporating its effects into the small-angle scattering intensity model used for fitting with SASfit.

### [199] Order and disorder in a new potential quantum spin liquid (board TU-114)

*Presenter: KORSHUNOV, Artem*

The idea of quantum spin liquid (QSL) on the triangular lattice was proposed by P. Anderson in 1973. Since his work, a lot of theoretical and experimental efforts have been made to explore deeper this state. Here we present the results for the combined study of structural and dynamic properties in application to the polycrystalline CuSb$_2$O$_6$ sample. The diffraction experiments using both synchrotron x-ray (ESRF) and neutron (ILL) scattering techniques showed the main motive of metastable rosiaite-type phase with the presence of microstructural defects. This system likely hosts the QSL state since the magnetic cations Cu$^{2+}$ with $S$ = ½ were found to be trigonally arranged within the distinguished magnetic layers and no long-range order is observed down to 46 mK. Indeed, the antiferromagnetic spin-spin correlations tend to appear below ~50K in a presence of a strong geometrical frustration without any sign of spin freezing. Low-temperature inelastic neutron scattering showed gapless dispersive-like magnetic excitations, which are believed to be associated with the fractionalized quasiparticles, spinons, that are expected for the QSL state. Reverse Monte Carlo simulations conclude the fully frustrated, most probably 3D AFM interaction scheme. We examine the observed results as a potential quantum spin liquid behavior in CuSb$_2$O$_6$.

### [398] Simplifying elaborate model building and refinement for neutron reflectivity data (board TU-116)

*Presenter: KOUTSIOUMPAS, Alexandros*

Neutron reflectometry is used by a wide community of scientific groups addressing questions in many different fields, including materials science, magnetism, polymer physics and biophysics. The analysis of reflectivity data from instruments around the world is traditionally performed either with computer programs that use a graphical user interface for building simple slab models of the interface, or with more sophisticated packages that require the writing of code for the description of models with higher complexity that incorporate functional dependencies and constraints in the model's parametrisation. In the present contribution we discuss the advantages of a newly introduced software package (anaklasis) [1] that attempts to simplify the definition of elaborate interfacial models by permitting the definition of constraints and layer features (sld, thickness, roughness etc.) directly as symbolic mathematical expressions involving parameters. Through a set of representative examples that include polarised and multi-contrast data, we showcase the abilities of the package for the generation of reproducible, easily readable and statistically accurate analyses. [1] A. Koutsioubas, J. Appl. Cryst. (2021). 54, 1857–1866

### [60] An engineering diffractometer for the High Brilliance neutron Source (HBS) (board TU-118)

*Presenters: KRASNOV, Igor, FENSKE, Jochen*

The HBS is a high brilliance accelerator driven neutron source currently in the design process. It provides different target stations that follow the same duty cycle but offer different frequencies and pulse length. Cold and thermal moderators are used to adjust the neutron spectrum. The target stations with its moderators thus allow choosing the parameters best fitting to an instrument or instrument class. We here present the design and expected performance of an engineering diffractometer for one of the target stations at the HBS. While optimized for straining scanning measurements the design of the instrument will allow further the analysis of textures and the investigations of phase transitions. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. It has been funded in part by BMBF, GNeuS, CSC.

### [499] Influence of Nonmagnetic Cation Substitution on Magnetic Order Temperature in Y type hexaferrite: Ba0.5Sr1.5Zn2Fe12O22 and Ba0.5Sr1.5Zn2Al0.08Fe11.92O22 (board TU-120)

*Presenter: KREZHOV, Kiril*

The sol-gel auto-combustion method and the sonochemical co-precipitation method were used to prepare Ba0.5Sr1.5Zn2Fe12O22 (S1) and partially Al substituted Ba0.5Sr1.5Zn2Al0.08Fe11.92O22 (S2) powders. The XRD analyses show that the samples are single-phase Y-type hexaferrite. SEM images of the S1 sample obtained by auto-combustion revealed particles of a very non-uniform shape and well-agglomerated to form clusters of different sizes and shapes. in contrast, the particles of the samples obtained by sonochemical co-precipitation had the perfect hexagonal shape typical for Y-hexaferrite of an estimated size of 1.2 µm and an average thickness of 168 nm. We report magnetic structure determination from patterns of the samples at 5 K and 300 K and the magnetic order evolution by temperature-dependent diffraction taken on SPODI (MLZ) between 10-350 K in the heating and cooling runs using a cryostat with a closed cycle refrigerator.

### [134] Exploring the lithium intercalation mechanism and critical role of structural water in layered H2V3O8 high-capacity cathode material for lithium-ion batteries (board TU-122)

*Presenter: KUHN, Alois*

H2V3O8 (HVO) is a promising high-capacity cathode material for lithium-ion batteries (LIB). It allows reversible two-electron transfer during electrochemical lithium cycling processes, yielding a very attractive theoretical capacity of 378 mAh g–1. Aimed at providing insights into the lithium storage behavior of HVO, we employed a combination of high-resolution synchrotron X-ray and neutron diffraction to accurately describe the crystal structures of both pristine and lithiated H2V3O8. The role of water in network stabilization was examined using density functional theory (DFT) calculations. Furthermore, magic-angle spinning (MAS) NMR spectroscopy allowed to follow the influence of structural water on the intercalated lithium in the crystal host. and related . The hydrogen bonds mitigate the volume expansion/contraction of vanadium layers during Li intercalation/deintercalation, resulting in improved long-term structural stability, explaining the excellent performance in rate capability and cycle life reported for HVO in LIBs. This study suggests that many hydrated materials can be good candidates for electrode materials in not only implemented Li technology but also emerging rechargeable metal-ion batteries.

### [362] Printing parameter optimisation of additively manufactured ER120S-G steel using neutron tomography (board TU-124)

*Presenter: KUMAR, Richi*

Additive Manufacturing (AM) has become a viable manufacturing technique, because of its remarkable ability to manufacture parts with intricate shapes and superior mechanical properties. Wire laser additive manufacturing (WLAM) is a kind of Direct Energy Deposition (DED) technology where a wire is fed through a nozzle and deposited onto a substrate or an existing part and is melted by focussing one or more laser beams onto it. This technique is especially advantageous for local repair as well as printing large and complex 3D parts. This has driven the commercial development of both technology and steel wires for automotive applications among others. Like most AM techniques, this involves rapid heating and cooling of samples, leading to specific microstructures and defects, which are influenced by both: the type of technique and the process parameters used. A proper characterization of these defects is imperative for optimal manufacturing process development. In this work neutron tomography -performed at the NEUTRA instrument of SINQ (PSI, Switzerland) has been used to image the pores and defects in approximately cm-sized ER120S-G steel samples manufactured via Wire DED using three different printing strategies. These results have been linked with the assessment of the mechanical properties to arrive at suitable printing conditions. Additionally, different build strategies for the formation of complex shapes for this alloy have also been similarly characterized. The results from thermal neutron tomography will be duly presented.

### [154] SAGA - a dedicated GISANS instrument for the ESS (board TU-126)

*Presenter: KÖHLER, Sebastian*

In the evaluation of capability gaps in the initial instrument suite, the European Spallation Source (ESS) has identified a dedicated surface scattering beamline as a high priority for the next phase of instruments. Therefore, a wide consortium, building on the strength in surface and interface science in Sweden, has formed to push for a project to design and construct such an instrument at ESS. The SAGA project is a collaboration with partners from different Swedish universities and aims to deliver a conceptual and technical design for a TOF GISANS (time of flight grazing-incidence small-angle neutron scattering) instrument for the ESS. Currently, GISANS experiments are strongly limited by the neutron flux that is available at existing neutron sources, which leads to measurement times of multiple hours up to days. Using the high source brightness of ESS, these measurement times could be decreased significantly, and thus make GISANS feasible as a mainstream technique. None of the currently planned ESS instruments are well-optimised for grazing incidence measurements, which makes a dedicated GISANS instrument necessary. The output of the SAGA project will be a competitive instrument construction proposal for the next ESS call and a detailed plan for the implementation of such a leading instrument. The current status of the project will be presented, together with first design concepts which were simulated and refined using the Monte-Carlo ray-tracing simulation package McStas.

### [255] Effect of the polymer conformation on the structure of protein single-chain nanoparticles. (board TU-128)

*Presenter: LE, Thu Phuong*

Single chain nanoparticles (SCNPs) are unimolecular polymer chains folded or collapsed via intra-molecular cross-linking under high dilution, leading to sparse conformations and a topological polydispersity similar to that of intrinsically disordered proteins (IDPs). Currently, there is great interest in expanding this technology to biodegradable and biocompatible polymers, including proteins. Recently, we fabricated BSA-SCNPs via intramolecular cross-linking of denatured bovine serum albumin (BSA) using disuccinimidyl suberate (DSS) that mainly reacts with lysine moieties in a polypeptide. SANS measurements demonstrated that the denatured protein progressively shrinks along with a lowering of the scaling exponent by cross-linking, thus allowing for size control of the BSA-SCNPs. To extend SCNPs to polypeptides, it is important to understand the role of the chain conformation of the precursor on the resulting SCNP morphology. For this, we have systematically varied the solvent conditions (pH, salt and denaturant concentrations) of BSA solutions as well as the cross-linker concentration and studied the resulting SCNPs by dynamic and static light scattering as well as small angle X-ray scattering. Our results indicate that the precursor conformation has an effect on the SCNP morphology as well as on the balance between intra- and inter-molecular binding. We will now probe the microstructure in an upcoming SANS beamtime.

### [67] Modelling and design of the new engineering diffractometer eMAP at ISIS (board TU-130)

*Presenter: LEE, Tung Lik*

ISIS Neutron and Muon Source is now seeking its next phase of new instruments and significant upgrades to existing instruments: a portfolio of projects that has been called the Endeavour Programme. Endeavour will increase both capacity and capability of the facility to address 21st century challenges and enable research in areas such as advanced materials and manufacturing, clean energy technologies, and biosciences and healthcare. Starting in the 2023/24 financial year, the Endeavour Programme will construct 4 new experimental instruments and 5 significant upgrades to existing instruments over a 10-year period. Here we report on the modelling and design of the new engineering diffractometer, eMAP, at ISIS. eMAP is a new instrument providing greater depth penetration capability to enable measurements on real size engineering components, and represents a step change in our ability to study real world engineering components. The flux and resolution characteristics of eMAP will allow: 3D residual stress mapping; high spatial resolution; large, thick, heavy and complex shaped components; near-to-surface measurements; process measurement (e.g. in□situ welding); in-situ loading and special environments; long□term tests (e.g. creep). eMAP is designed with a performance complementary to the diffraction capabilities offered by the existing ISIS engineering instruments. ENGIN-X, the current “workhorse” instrument is oversubscribed, especially for industrial partnership access. eMAP will bring extra capacity with new capabilities for stress measurement of full size engineering components, enabling engineering manufacturers and emerging technology SMEs to design the next generation of complex machines with improved performance, durability and capability.

### [128] Magnetically frustrated dynamics on the Cairo pentagonal lattice (board TU-132)

*Presenter: LENANDER, Emma Ynill*

The octahedrally and tetrahedrally coordinated Fe3+ (S=5/2) ions in Bi2Fe4O9 form a quasi two-dimensional Cairo pentagonal lattice (*Pbam*). Combined with predominantly antiferromagnetic interactions, this leads to a strong frustration with Tn=245 K while θCW=1670 K in a fairly unexplored geometry. The magnetic structure for T < Tn can be indexed with k=(½, ½, ½) with a noncollinear magnetic structure of Fe1 and Fe2 moments, 2 different sites, and an interpenetrating pattern of fourfold spin rotations, a very novel magnetic state. Previous measurements studying the low-lying excitations, 0–30 meV, in the ordered phase were measured on small single crystals (< 0.6 g). Beauvois et al. (PRL2020) argues that no anisotropy is required while Duc Le et al. (PRL2021) indicates an easy-plane single-ion anisotropy. Accordingly, Beauvois find the acoustic AF mode is not gapped while it is for Duc Le. We have synthesized a 2.35 g, high quality single crystal of Bi2Fe4O9 and are re-examining the magnetic excitations. Already at energy transfers below 10 meV we see distinct discrepancies between our data and previous data in the ordered phase using CAMEA and EIGER (PSI). Our data show a clear double spin gap, that allows us to differentiate axial and planar anisotropy scenarios. This will enable us to establish the microscopic model and perform quantitative analysis of the frustrated state above Tn.

### [335] The Thermal Powder Diffractometer of the HiCANS source HBS (board TU-134)

*Presenter: LIEUTENANT, Klaus*

Apart from fission and spallation, neutrons can also be generated by nuclear reactions induced by protons in the MeV range. This is now applied in High-Current Accelerator-driven Neutron Sources (HiCANS), which are able to reach performances like medium sized reactor or spallation sources. One of these projects is the High Brilliance neutron Source (HBS) at Forschungszentrum Jülich, which is planned to operate a complete instrument suite enabling large scale structure investigations, diffraction, spectroscopy, imaging and analytics. Six diffractometers are under discussion for different kinds of diffraction experiments. As the pulses of the HBS source are not very short and the instrument length is limited, high resolution can only be reached by pulse shaping. This is foreseen for the Thermal Powder Diffractometer, which shall be installed at the 24 Hz long pulse target station and, as DREAM at ESS, use wavelength frame multiplication to reach a sufficient band width. Like POWTEX at FRM-II, it will be equipped with a large detector covering nearly 3$\pi$ solid angle thus enabling also single crystal measurements. It can also be operated in high-intensity option, where the whole pulse is used, to offer time-resolved measurements. Here we present the

results of Monte-Carlo simulations of this diffractometer using the program VITESS to compare its performance to existing powder diffractometers. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [428] New Perspectives for Neutron Imaging through Advanced Event-Mode Data Acquisition (board TU-136)

*Presenter: LOSKO, Adrian*

With the transformative development of event-based detectors, new perspectives for detection systems for various types of radiation were opened up. A recently developed event-driven imaging system based on Timepix3 sensor technology is capable of observing and time-stamping the optical signal induced by particle interactions in scintillator materials with nanosecond temporal and micrometer spatial resolution, providing a pathway to fuse the benefits of integrating camera type with counting type detectors. In this approach, the reconstruction of the interaction position of a neutron with the scintillator with sub-pixel accuracy can provide a precise determination in location, as well as in time-of-arrival of the individual neutrons. Utilizing such a principle, it was shown that spatial and temporal resolution can be improved beyond the classical limits of “regular” neutron imaging. Additionally, a significant increase of signal-to-noise ratio was achieved using the unique potential of event-mode detection to discriminate gamma background from neutron signal based on the spatiotemporal signature of single neutron events produced in the scintillator. Here, we present the most recent results in utilizing this concept for imaging applications and scintillator characterization measurements. It is considered that this novel concept will replace regular cameras in neutron imaging detectors as it provides superior detection capabilities compared to conventional camera systems.

### [212] A macromolecular diffractometer for the High Brilliance Neutron Source (HBS) (board TU-138)

*Presenter: MA, Zhanwen*

The HBS project for a High Current Accelerator-based Neutron Source (HiCANS) uses a pulsed proton beam of 70 MeV energy and 100 kW of time-averaged power for each target station. With the benefit of the time structure, a low background, and flexible, high brilliance moderator set-ups, the instruments at the HBS are expected to be very competitive to existing state-of-the-art scattering instruments [1]. The low dimensional moderators of the HBS are well suited for instruments studying small samples. A prototypical example is neutron macromolecular diffractometers, where typical sample volumes reach from 0.01 mm3 to 1 mm3. In this work, the design progress of a macromolecular diffractometer for the HBS will be presented. SELENE neutron guides will be used in this instrument. The neutron optics have been optimized with VITESS Monte Carlo simulations. With the optimized neutron optics, we can obtain a low background, and a very bright, tunable neutron beam spot at the sample with a cross-section as small as 1 mm2, thus promising a very competitive instrument for the life science community. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. It has been funded in part by BMBF, GNeuS, and CSC. [1] Gutberlet T. Conceptual Design Report-Jülich High Brilliance Neutron Source (HBS). Brückel T, editor. Forschungszentrum Jülich GmbH, Zentralbibliothek, Verlag; 2020. E-mail of the corresponding author: zh.ma@fz-juelich.de

### [91] INS study of spin stripe fluctuations in antiferromagnetic Pr2−xSrxNiO4+δ (board TU-140)

*Presenter: MAITY, Avishek*

Spin and charge stripe correlations and their dynamics have been well explored in the ordered state of La-based 214-nickelates for last 3 decades. Recently, we have also explored magnetic excitations in the ordered spin-stipes phases of hole-doped Pr-based nickelates Pr$_{2-x}$NiSrO$_{4+\delta}$ [1-3]. In this regards, what remains less explored is the fluctuating state of the spin stripes from which the long-range spin stripes develop on cooling. In this talk, we present our recent inelastic neutron scattering study of the low energy spin stripe fluctuations in Pr$_{2−x}$Sr$_{x}$NiO$_{4+\delta}$ with magnetic incommensurability ϵ= 0.33 above the spin stripe ordering temperature T$_{so}$ = 190 K [4]. The spin stripe fluctuations measured at the incommensurate wave vector show a non-dispersive character with no detectable anisotropy persisting up to a maximum energy 10 meV, and strongly suppressed already below the charge stripe ordering temperature T$_{co}$ = 255 K. Our results clearly indicate that the presence of static charge stripe order is essential for the spin stripe fluctuations in 214-type nickealtes. References: [1] A. Maity et al., Physical Review Letters 124, 147202 (2020). [2] R. Dutta et al., Physical Review B 102, 165130 (2020). [3] A. Maity et al., Physical Review B (Letter) 103, L100401 (2021). [4] A. Maity et al., Physical Review B 106, 024414 (2022).

### [416] Computation of the X-ray and neutron diffraction patterns of mesoscopic continuum simulations (board TU-142)

*Presenter: MAJUMDAR, Arnab*

Neutron and X-ray scattering are well-established techniques to understand the material structure and different phenomena within the systems. However, the structure can not be uniquely determined from the scattering experiments due to the phase problem, i.e. two different structures can yield the same scattering curve. Also, it is important to explain the reasons behind the phenomena observed in the experiments. Simulations can bridge this gap as they are governed by physical laws and therefore reach a unique final state given some initial state and subjected to certain conditions. By mimicking the conditions of experiments, we can reproduce the experimental results. Although simulations are bound by their own approximations and assumptions in order to simplify computational effort, they can still reproduce the actual situation with reasonable accuracy. In this work, we develop a

workflow to calculate the scattering pattern from continuum simulations,e.g. phase field simulations. This extends the already established workflow of calculating scattering patterns from atomistic simulations and accommodates the analysis of much larger, mesoscopic systems. This work applies the proposed method to simple structures, such as a sphere in a parallelepiped in order to validate the results against analytical expressions and applies it to continuum simulations. Our final goal is to describe hydrogen storage materials at a mesoscopic scale and validate them using scattering experiments.

### [294] Polarised neutron inelastic scattering on Tb3Fe5O12: Investigating the role of chiral magnons in a spin Seebeck prototype. (board TU-144)

*Presenter: MANNIX, Dan*

Spin caloritronic materials are currently in the spotlight due to their potential exploitation in the next generation of spintronics applications. Composite systems, consisting of magnetic-insulator (MI) and heavy-metal (HM) bilayers, combine both spintronic and thermoelectric functionalities by interconversion of charge-, spin-, and heat-currents. 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. The development of emerging technologies based on spin caloritronic phenomena therefore requires a microscopic understanding of their magnetic structure and dynamics. To this end, polarised neutrons can provide direct measurement of the magnon chirality of the MI layer. In this presentation, we discuss recent polarised neutron inelastic scattering results on the prototype compound Tb3Fe5O12. Our analysis, based on microscopic description of the rare-earth's magnetic moments, unveils the origin of their anisotropies and accounts for the hybridisation between crystal-field and magnon modes [1], with the chiral effects crucial for the SSE signal generation in this class of compounds. [1] Origin and dynamics of double umbrella states in rare-earth iron Garnets B. Tomasello, D. Mannix, S. Geprägs, T. Ziman Annals of Physics, p169117 (2022).

### [215] Conceptual design of supermirror polarizers at the European Spallation Source (board TU-146)

*Presenter: MARTIN RODRIGUEZ, Damian*

The use of polarized neutrons is very important to cover new science cases and polarized neutrons. Polarized neutrons will be made available on many European Spallation Source (ESS) instruments. There are a number of technologies available for polarizers and polarization analyzers, among them polarizing supermirror and polarized 3He, which will both be used at the ESS. The selection of the technology for an instrument is based on the performance and the constraints of the instrument. Supermirror polarizer has been selected as the polarizer for instruments BIFROST (indirect geometry spectrometer), MIRACLES (backscattering spectrometer) and ODIN (imaging). BIFROST AND MIRACLES are long baseline instruments where the polarizer is placed in the neutron guide system upstream from the instrument cave. In ODIN, the polarizer needs to be placed after the guide system, imposing a stricter constraint. Careful design studies need to be done for the polarizer. At ESS, Monte Carlo ray-tracing simulation of neutron trajectories is an integral part of instrument design process. To search for the appropriate parameters for the polarizer, we have developed the module for simulating multi-channel v-cavity polarizer and incorporated it into the respective instrument model. Subsequently systematic simulation studies of the polarizer parameters have been carried out. In all these three cases we will analyze how the polarizers can be designed to obtain an outstanding performance.

### [52] Neutron diffraction study of the 1/2 quantum magnetization plateau compound Ni$_2$V$_2$O$_7$ (board TU-148)

*Presenters: MATSUO, Masashi, MATSUO, Yukari*

We report on the results of powder neutron diffraction of Ni$_2$V$_2$O$_7$. Two crystallographic Ni$^{2+}$-ion sites carrying spin-1 exist. Magnetic phase transitions occur at $T_{\rm N1} = 6.7$ and $T_{\rm N2} = 5.7$ K. A 1/2 quantum magnetization plateau appears between 8 and 30 T at 2 K. We carried out neutron diffraction experiments at 0 T using the HRPT diffractometer at PSI. The wavelength of the neutrons was 2.450 □. We observed magnetic reflections at 2.3 and 6.0 K. We can index the magnetic reflections with the propagation vector $(k_x \sim 0.46, 0, 0)$, indicating an incommensurate magnetic structure. We are analyzing the data to determine the magnetic structure. We conducted neutron diffraction experiments at zero and finite magnetic fields using the WOMBAT diffractometer at ANSTO. The wavelength of the neutrons was 2.412 □. We observed magnetic reflections at 10 T and 1.9 K where the 1/2 quantum magnetization plateau appears. Indices of the magnetic reflections except for those at $Q = 1.06$ and $1.02$ □$^{-1}$ are integers and nuclear reflections exist at the positions of the magnetic reflections with the integer indices. The magnetic reflections remain at 10 T and 15 K that is much higher than $T_{\rm N1}=6.7$ K, indicating that the magnetic reflections are generated by field-induced magnetic moments. The sum of $m_1$ and $m_2$ at 10 T and 1.9 K should be 2.2 because of the 1/2 quantum magnetization plateau phase and $g=2.2$. Here, $m_1$ and $m_2$ are magnitudes of field-induced magnetic moments on Ni1 and Ni2 sites, respectively. We calculated the integrated intensities of the magnetic reflections under the condition that $ m_1 + m_2 = 2.2$. The calculated and experimental intensities agree with each other in the vicinity of $m_1 = 0.2$. The magnetic reflections at $Q = 1.06$ and $1.02$ □$^{-1}$ exist below 10 T at 1.9 K, whereas they do not exist at 10 T and 10 K. Therefore, the origin of the magnetic reflections seems to be magnetic order. Although the 1/2 quantum magnetization plateau phase at 10 T and 1.9 K is paramagnetic, the magnetic order phase may coexist.

### [492] Magnetic Wollaston Prisms for spatial intensity modulations of polarized neutron beams at FRM II (board TU-150)

*Presenter: METTUS, Denis*

The MIEZE (Modulated IntEnsity with Zero Effort) resonant spin-echo technique at the RESEDA instrument at FRM II has its optimum resolution at small scattering angles, i.e. SANS type geometries. Recent upgrades (MIASANS) have further increased the resolution in the small angle regime. Going forward, there is the possibility [1] to extend the optimum MIEZE resolution to wide angles by incorporating superconducting magnetic Wollaston prisms (MWPs) into the beamline. These MWPs will produce controlled spatially intensity modulations in addition to the intensity modulations in time inherent to MIEZE. The resultant capability to make corrections to the neutron time of flight allows for the systematic spatial focusing of the MIEZE resolution function to any desired scattering angle. Additionally, MWPs will be useful in the context of intra-particle mode-entangled neutron beams for potential use in probing many-body quantum entanglement in materials [2]. Finally, the compact and modular nature of the MWPs will allow them to be used to measure diffraction peaks with enhanced resolution at several polarized beam instruments such as MIRA, KOMPASS, LaDiff, and in general at small angle neutron scattering instruments [3]. We present the plans for the construction of these superconducting MWPs for use at FRM II, and describe the details of their operation and the various possibilities they offer. [1] F. Li., J. Appl. Cryst. 55, 90-97 (2022). [2] S. Kuhn et al., Phys. Rev. B 3, 023227 (2021). [3] F. Li et al., Sci. Rep. 7, 865 (2017)

### [343] Combining Neutron Spin Echo and Polarization Analysis (board TU-152)

*Presenter: MEZEI, Ferenc*

Neutron Spin Echo (NSE) spectroscopy uses polarized neutrons; however, it was never used for performing polarization analysis at the same time, which can offer a very promising extension. In NSE experiments one requires a polarizer for preparing the precessing polarization of the incoming neutron beam and a polarization analyzer for observing the precessing polarization of the scattered beam. For a mixture of coherent and nuclear spin incoherent scattering in conventional NSE analysis the directly measured signal S(q,t) is the difference of the intermediate scattering function of the coherent scattering minus 1/3 of the same for the incoherent scattering, We have used the inherent polarization analysis capability of NSE spectrometers to identify the individual magnitudes of the coherent and incoherent scattering intensities within the energy transfer window of the NSE set-up with effective FWHM width in energy E, as primarily determined by the energy transmission function of the NSE polarization analyzer. This information can be very efficiently made use of as powerful evidence and constraint for the models used in the interpretation of a mix of coherent and incoherent scattering. These intensities can be considered as the S(q,t=T) points of the NSE spectra at the NSE time value T about h/E. The method has been successfully used for the first time in the study of quasielastic scattering processes in ordinary and heavy water on the WASP multiangle NSE spectrometer at ILL.

### [375] Made2Reflect, a python package for evaluating the neutron or X-Ray reflectivity of systems simulated by Atomistic Molecular Dynamics (board TU-154)

*Presenter: MOULIN, Jean-Francois*

Complementary use of scattering methods and molecular dynamics (MD) makes it possible to elucidate structural details of complex molecular systems such as biological or electrochemical interfaces. Although several softwares aiming at some of the tasks involved in the process have been described in the past, an easy to use, well documented and tested, fully FOSS, solution was lacking. In this work we present a *Python* software package aimed at evaluating the neutron or X-ray reflectivity of systems for which the structure has been simulated via atomistic MD. *Made2Reflect* was written to be a fully featured package with both a functional programming API and an Object Oriented interface. The low level API allows to write scripts, in which every single step, from reading the data, extracting the relevant atomic concentration profiles, conversion to SLD profiles, up to the actual reflectivity computation, is performed as an individual function call. The object oriented API, on the other hand, abstracts the overall process into an intuitive high level language formulation which mimics an actual measurement on a digital twin of the sample. Detailed analysis such as elemental or isotopic substitution, evaluation of instrumental effects and of the influence of substrate roughness over lengthscales which cannot be accessed by the MD simulation are easily performed. The package was built with the ultimate goal to lower the barrier to a routine use of the combination of scattering experiments and MD simulations. A special attention was given to the documentation aspects, numerous Jupyter notebooks describing in detail how to perform an analysis. Last but not least, in order to ensure the stability of the package during further development, a comprehensive test suite has been built.

### [501] Structural design of polyelectrolyte-protein nanocarriers for targeted drug delivery (board TU-156)

*Presenter: MURMILIUK, Anastasiia*

Co-assembly of oppositely charged polyelectrolytes with proteins is a well-studied approach for designing stimuli-responsive nanocarriers for targeted drug delivery. [1,2] However, the complexity of protein structure limits the ability to predict and tune properties of the formed nanoparticles. The ultimate goal of our research is to reveal the main triggers for the morphological

transition of protein/polyelectrolyte complexes, their encapsulation efficacy and particles stability by systematic study of complexes formed by block copolymers with proteins and encapsulated ionic drug. Using scattering and microscopy techniques, we showed that block copolymers consisting of a weak polyelectrolyte block and a neutral hydrophilic block co-assemble with proteins at pH close to protein isoelectric point and the morphology of the formed particles can be tuned by varying pH and nature of proteins. Moreover, we observed that formed protein/polyelectrolyte complexes with an excess of a charge can be used for encapsulation of an oppositely charged drug thus allowing us to use one carrier for both protein and drug delivery, and to design nanocapsules with such tunable properties as charge, stability and size. [1] C.L. Cooper et al. COCIS 2005, 10, 52 [2] A. Skandalis; A. Murmiliuk et al. Polymers 2020, 12(2), 309

### [179] Optimizing the microstructure of compositionally complex CoNiCr-base superalloys for enhanced high temperatures strength (board TU-158)

*Presenter: NAGEL, Oliver*

Superalloys are key materials of our modern society. They are not only used in harsh environments of power plants for energy conversion but also in aerospace or marine applications, as they combine excellent mechanical properties at high homologous temperatures with very good oxidation and corrosion resistance. To further improve the efficiency of engines, advanced superalloys with improved properties are needed that can operate at significantly higher temperatures. Newly developed Co-based superalloys seem to be interesting candidates for new high-temperature materials. In this work, Co-based superalloys are presented whose development and characterization was supported by neutron scattering methods. It will be shown how neutron diffraction on simple, coarse grained experimental Co/Ni-Al-W-X alloys helped to determine the temperature-dependent lattice misfit between the main constituent phases and how small angle neutron scattering investigations on compositionally complex polycrystalline CoNiCr-base superalloys could be used to adjust the heat treatments to optimize their mechanical properties. Various microstructures after different heat treatments were analyzed by scanning and transmission electron microscopy and especially in-situ small-angle neutron scattering during heat treatment experiments. The corresponding mechanical properties were determined by compression tests and hardness measurements. From this, an optimum precipitate size was determined that is adjusted mainly in the first precipitation heat treatment step. This is discussed on the basis of the theory of shearing of precipitates by weak and strong pair-couplings of dislocations. A second age hardening step leads to a further increase in the volume fraction above 60% and the formation of tertiary precipitates in the matrix channels, resulting in an increased hardness and yield strength. A comparison between two different three-step heat treatments revealed an significant increase in strength for the optimized heat treatment.

### [161] Four Dimensional Neutron Depth Profiling with the N4DP Instrument at MLZ (board TU-160)

*Presenter: NEAGU, Robert*

Neutron Depth Profiling (NDP) is a non-destructive, element-specific, high-resolution nuclear analytical technique, which is often used to probe concentration profiles of lithium, boron, nitrogen, helium and several other light elements in different host materials. The N4DP instrument is located at the Prompt Gamma Activation Analysis (PGAA) beam line of Heinz Maier-Leibnitz Zentrum (MLZ), which provides a cold neutron flux up to $5\times10^{10}\,$s$^{-1}$cm$^{-2}$. When a neutron is captured by a specific nuclide, ions with well-defined energies are emitted. The energy loss of the charged particles traveling through the host material is related to the depth of origin at a resolution level up to tens of nanometers. We applied NDP to study the lithium-ion concentration gradient in energy storage systems, e.g. Li-ion batteries. Here, NDP reveals the evolution of immobilized lithium, which is one of the main causes of battery lifetime limitation. Furthermore, the status of the ongoing development towards 4D profiling is presented, where not only the concentration gradient, but also the lateral position of probes as well as its time evolution will be measured. For this, a highly segmented Si-based detector with 32$\times$266 stripes, including integrated, self-triggering electronics, were successfully assessed. Using a camera-obscura geometry set-up, we aim for lateral scanning with a space resolutions down to 100\,$\mu$m $\times$ 100\,$\mu$m and highest time resolutions using a newly developed elliptical focusing neutron guide. This project is supported by the BMBF, Contract No. 05K16WO1, 05K19WO8.

### [142] Polarisation analysis of QENS on per-deuterated proteins. (board TU-162)

*Presenter: NIDRICHE, Agathe*

Deuterated samples are used in neutron scattering to investigate the dynamics of hydrogen atoms by contrast matching, due to the low incoherent and high coherent cross-sections of deuterium. The use of fully deuterated proteins has been restricted so far to the study of light hydration water or the collective dynamics of proteins in D_2 O. In order to study kinetic isotope effects of the internal dynamics of proteins, we produced two D_2 O hydrated powders : a protonated Green-Fluorescent Protein and its deuterated counterpart with 99% H→D labelling. We recently performed QENS experiments combined with polarisation analysis on LET, ISIS, on the usual space range probed with proteins (r □ [2.5Å^ ,20Å]) and at the pico-second time scale corresponding to structural relaxation. Polarisation analysis enables to separate the coherent and the incoherent parts of scattering. Unexpectedly, it shatters the usual assumption that neutrons probe mainly collective dynamics in fully-deuterated proteins. We came across the conclusion that in this space region, where the structural pattern is weakly dependent on the size or the secondary structure of the proteins, the magnitude of the coherent contribution of scattering is fairly lower than the incoherent one. It is verified at both very low (T=2K) and high (T=310K) temperatures and compared to non-polarized experiments on IN5, ILL.

### [185] Comparison of neutron and synchrotron diffraction methods in texture analysis of a cold rolled Cu-cube standard sample (board TU-164)

*Presenter: NOWAK, Gregor*

Texture analysis by means of non-destructive, diffraction methods offers the statistical access to the orientation space of crystalline building blocks on microstructural level in materials characterization. Depending on the combination of the investigated material and incident type of radiation, the necessary diffraction signal can be detected from different depth and volumes of a sample. Systematic neutron and synchrotron diffraction measurements on the same sample at different instruments can experimentally demonstrate the advantage and complementary of the respective methods and instruments and allow the performance benchmarking of new ones. A cold rolled Cu-cube of a size of 10 x 10 x 11 mm$^{3}$ had been investigated using, thermal, monochromatic neutrons at STRESS-SPEC (MLZ) and high-energy x-ray's at P07 (DESY). The choice fell on cold rolled Cu for the sample, since Cu was extensively investigated in the past [1,2]. The absorption effects in the Cu-cube of the above mention size are for the X-ray's significant compared to neutrons and were corrected for a very close agreement to the volume neutron data (without absorption correction). Additionally, the (111), (200) and (220) pole figures by ToF-neutron diffraction at HIPPO (LANCE) were recorded and compared with the monochromatic data. [1] T. Leffers, R.K. Ray, Progress in Materials Science, 54, 351-396, (2009) [2] N. Al-hamdany, H.-G. Brokmeier, C. Randau, W. M. Gan, and M. Völler, Cryst. Res. Technol., 49, p. 888, (2014)

### [384] Interfacial behaviour of sugar-based surfactants at the solid-liquid interface in relation to their structure and solution behaviour (board TU-166)

*Presenter: NYLANDER, Tommy*

Sugar-based surfactants offers an appealing and environmentally friendly alternative to traditional surfactants but can also offer new functionality in applications. The interfacial behaviour of sugar-based surfactants will be discussed in relation to their solution behaviour. Here, the adsorption behaviour of the α- and β-anomer of hexadecylmaltoside (α-C16G2 and β-C16G2) at the solid-liquid interface has been studied by means of ellipsometry and neutron reflectometry. Even this subtle difference in headgroup configuration affects the formed layer structure, where the adsorbed amount was higher for the β-anomer. This suggests that the β-anomer can be packed more efficiently. For both anomers the adsorbed layer structure on a hydrophobic surface cannot be assigned to a surfactant monolayer, reflecting the strong head group attractive interactions between these types of surfactants. Similar attractive intermolecular interactions also control the bulk solution behaviour where the two anomers form different types of aggregates, where the β-anomer form worm-like micelles, while the α-anomer form significantly shorter, more spherical micelles.

### [191] Suppression of segmental chain dynamics on particle's surface in attractive polymer nanocomposites (board TU-168)

*Presenter: OHL, Michael*

The Rouse dynamics of polymer chains in model nanocomposite PolyEthylene Oxide (PEO)/Silica NanoParticles (NPs) was investigated using QuasiElastic Neutron Scattering (QENS). The fraction of segments immobile on the picosecond/nanosecond timescale, as they are adsorbed on the NP surface, was identified. The Rouse rate of the remaining polymer chains decreases as the particle loading increases. This experimental result is analyzed in terms of modified Rouse models for the chains in the NP interphase region. Thus, two chain populations, one bulk like and the other characterized by a suppression of Rouse modes, are identified and the spatial extent of the interphase region is estimated to be`$\approx$2 nm. These findings provide a detailed description of the suppression of the chain dynamics on the surface of NPs. The results are relevant for the fundamental understanding of surface effects and confinement and provide a foundation for the understanding of the rheological properties of well dispersed Polymer NanoComposites (PNCs).

### [57] The Macromolecular Neutron Single Crystal Diffractometer BIODIFF for Proteins at the Heinz Maier-Leibnitz Zentrum MLZ (board TU-170)

*Presenter: OSTERMANN, Andreas*

Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules. At the FRM II neutron source the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is mainly dedicated to the structure determination of enzymes. Typical scientific questions address the determination of protonation states of amino acid side chains in the active center, the orientation of individual water molecules essential for the catalytic mechanism and the characterization of the hydrogen bonding network between the enzyme active center and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behavior of an enzyme. BIODIFF is designed as a monochromatic diffractometer and is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. This allows to adapt the wavelength to the size of the unit cell of the sample crystal.

Data collection at cryogenic temperatures is possible, allowing studies of cryo-trapped enzymatic intermediates. Recently a hexapod has been installed at BIODIFF which allows an easy online collimator alignment. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography. In addition, a potential detector upgrade for BIODIFF will be presented, which will expand the maximum unit cell limits.

### [406] Hierarchical polymer nanocomposite structures in SANS and SESANS (board TU-174)

*Presenter: PARNELL, Steven*

Carbon based polymer nanocomposites have many useful applications and the change in the physical properties of the modified composite from that of the raw polymer is of significant importance. In this presentation I will discuss a series of polymer-carbon composites (graphene oxide, carbon black, carbon nanoparticles) measured using both SANS and SESANS and apply a number of different approaches to quantify the structure of these hierarchical systems. In principle a combination of SANS and SESANS has the ability to probe from ~1nm to ~10 microns and this presents challenges in modelling. We discuss these approaches and present models for these various systems.

### [1] Neutrons and X-ray methods for investigation of Li-ion batteries at material, electrode and cell level (board TU-176)

*Presenter: PAUL, Dr. Neelima*

Neutrons are powerful and have unique characteristics, which make possible non-destructive and operando characterizations of cylindrical and prismatic Li-ion batteries. X-rays are an equally competent tool that can provide complementary information on pouch type Li-ion cells during cell operation. Expectedly, both are also capable of providing information at material and electrode level. This contribution will show with several examples how neutrons and x-rays methods such as diffraction, small and wide-angle scattering and neutron depth profiling were helpful in estimating electrochemically active Li losses, Li plating and Li diffusion kinetics at cell level, Li distribution profiles and pore morphologies at electrode level, interplay between mechanics and their molecular origins at material level. These insights are useful to understand the improvement in cell performance by (a) altering the graphite electrode morphology, (b) by preparing composite silicon-graphite electrodes, (c) by Si deposition on TiO2 nanotubes, (d) and by applying polymer coatings to Li metal anode surfaces.

### [97] The HERMES reflectometer at the JULIC neutron platform (board TU-178)

*Presenter: PAULIN, Mariano Andrés*

The Laboratoire Léon Brillouin is currently evaluating the use of High brilliance Compact Accelerator-driven Neutron Sources (HiCANS) to provide the French neutron scattering community with a suite of world-class instruments. For that purpose, the performances of neutron scattering instruments around this novel type of sources must be evaluated. HERMES is a time-of-flight horizontal reflectometer designed for soft-matter studies that operated at the Orphée reactor until 2019. Through a collaboration with the Jülich Centre for Neutron Science, HERMES is being installed at the HBS demonstrator neutron source at the JULIC accelerator of the Institute for Nuclear Physics (IKP) Forschungszentrum Jülich. This source is able to deliver a cold spectrum with pulses in the 100 µs-1 ms range and is very well suited to evaluate the feasibility of reflectivity experiments at a HiCANS. As the flux at the JULIC neutron platform is 5 orders of magnitude lower than the one expected for a HiCANS, our current goal is to perform reflectivity experiments with supermirrors as a proof of concept. Nevertheless, Monte-Carlo simulations showed that HERMES instrument's performances at a HiCANS could match that of reflectometry instruments operating at medium power research reactors. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. It has been funded by the "CANS Inflexion" program at the CEA and the "IPHI-Neutron" SESAME project of the Île de France region.

### [248] The new data infrastructure at MLZ (board TU-180)

*Presenter: PEDERSEN, Bjoern*

We will present how the data storage and processing landscape at MLZ will evolve in the of DAPHNE4NFDI and ERUM.

### [22] The TOSCA secondary spectrometer upgrade: design and simulations (board TU-182)

*Presenter: PERRICHON, Adrien*

TOSCA is a high-resolution, broad band, indirect geometry chemical spectrometer operated at the ISIS Neutron and Muon Source, UK. As a neutron analogue to optical spectroscopy, it is optimised for the study of molecular vibrations in fields such as catalysis, hydrogen storage materials, hydrogen bonded systems, or biological and organic compounds. We present the detailed design and performance of the proposed upgrade of the TOSCA secondary spectrometer. The entire secondary spectrometer will be replaced and new sets of large, curved pyrolytic graphite analysers, beryllium filters and position sensitive detectors will be installed. The design, dimensions and placement of each component has been optimised with neutron ray-tracing simulations. A gain factor in detected intensity of a least 10 is expected over the current instrument, independent of the neutron energy. This results from the increased solid angle coverage, increased transmission through the filter, and increased neutron detection

efficiency. The predicted spectral resolution remains close to 1% of the energy transfer at high energy transfer. Furthermore, the performance of the beryllium filter in eliminating high energy neutrons has been improved by a factor 10, which should improve the signal-to-noise ratio and thus the sensitivity and detection limit of the instrument. This upgrade will ensure that TOSCA remains highly competitive in years to come.

### [313] Development of a Time-of-Flight Grating Interferometer for the Measurement of the Neutron Electric Charge (board TU-184)

*Presenter: PERSOZ, Marc*

Neutron grating interferometers can be employed as powerful tools to perform high-precision measurements of deflection angles and scattering. A novel concept of a symmetric Talbot-Lau interferometer using three identical absorption gratings in a time-of-flight mode is under development at the University of Bern. The ultimate goal of this project is to conduct a sensitive measurement of the neutron electric charge and to improve the current best upper limit $(−0.4 ± 1.1) × 10^{-21}~e$ [Baumann et al., 1988]. A proof-of-principle apparatus has been characterized at the cold neutron beamline BOA at the Paul Scherrer Institute, Switzerland. A description of the experiment, alignment procedures and first results concerning beam deflections measurements and the setup stability will be presented.

### [321] Lithium Distribution in 18650-type Li-ion batteries over its lifetime (board TU-186)

*Presenter: PETZ, Dominik*

During electrochemical cycling of lithium-ion batteries, ionic and electron transfer occur simultaneous, i.e. lithium ions and electrons are exchanged between positive and negative electrodes. Besides the materials properties, such an exchange is influenced by cell characteristics, such as electrode dimensions and geometry, current density, temperature, pressure, reaction rate etc. In cell designs adopting high volumetric and gravimetric densities these parameters are neither uniformly distributed nor static in general and, therefore, serve as stabilizing factor of heterogeneous state in Li-ion batteries, which is typically reflected in the non-uniform distribution of the intercalated lithium in the electrodes [1, 2]. Previous studies revealed the modification of the distribution of the lithium-ions in the graphite anode of 18650-type lithium-ion batteries upon increasing cell aging [3]. In this contribution, this effect was investigated in detail on a set of quasi-identical commercial cells with different stabilized aging states applying spatially resolved neutron powder diffraction. Details of lithium distribution over the lifetime of a commercial 18650-type lithium-ion battery were determined. 1. Senyshyn, A., et al., Sci. Rep., 2015. 5(1): p. 18380. 2. Petz, D., et al., Batter. Supercaps, 2021. 4(2): p. 327-335. 3. Mühlbauer, M.J., et al., J. Power Sources, 2020. 475: p. 228690.

### [498] Solution structures of native photosystems revealed by small-angle neutron scattering (board TU-188)

*Presenter: PIEPER, Jörg*

Photosystems I (PSI) and II (PSII) are pigment-protein complexes capable of performing the light-induced charge separation necessary to convert solar energy into a biochemically storable form, an essential step in photosynthesis. Small-angle neutron scattering (SANS) is unique in providing structural information on PSI and PSII in solution under nearly physiological conditions without the need for crystallization or temperature decrease [1-4]. We show that the reliability of the solution structure critically depends on proper contrast matching of the detergent belt surrounding the protein. Especially, "invisible" specifically deuterated detergents are shown to be properly matched out in SANS experiments by a direct, quantitative comparison with conventional matching strategies. In contrast, protonated detergents necessarily exhibit incomplete matching, so that related SANS results systematically overestimate the size of the membrane protein under study. While the solution structures obtained are close to corresponding high-resolution structures, we show that temperature and solution state lead to individual structural differences compared with high-resolution structures. We attribute these differences to the presence of a manifold of conformational substates accessible by protein dynamics under physiological conditions. 1.) M. Golub et al., J. Phys. Chem. B 2022, 126, 2824–2833. 2.) A. Kölsch et al., Current Research in Structural Biology 2 (2020) 171–179. 3.) M. Golub et al., J. Phys. Chem. B 2022, 124, 8583−8592. 4.) M. Golub et al., Crystals 2021, 11, 203.

### [373] The SORGENTINA-RF project: fusion neutrons for medical radioisotopes and beyond (board TU-190)

*Presenter: PIETROPAOLO, Antonino*

The SORGENTINA-RF project is presented in terms of general structure and description of the main tasks and activities to be carried out. It is devoted to the design and development of a medium power 14 MeV fusion neutron source relying on a rotating target and a deuterium/tritium ion accelerator. The main focus of the neutron facility is the production of radiopharmaceutical precursors, in particular $^{99}$Mo as precursor of $^{99m}$Tc, a radio-tracer used in single photon emission computed tomography. The nuclear reaction involved in the production of $^{99}$Mo is the inelastic reaction $^{100}$Mo(n,2n)$^{99}$Mo. The facility will assess the chain that starts with the irradiation of the natural molybdenum (where $^{100}$Mo has an isotopic abundance of about 10\%) up to the production of the so-called mother solution, a liquid solution named sodium molybdate. The facility will also make available fast and thermal neutrons beams for studies on innovative medical radioisotopes as well as materials.

### [110] KWS-3 very small-angle neutron scattering focusing diffactometer at MLZ (board TU-192)

*Presenter: PIPICH, Vitaliy*

KWS-3 is a very small angle neutron scattering diffractometer operated by JCNS at Heinz Maier-Leibnitz Zentrum (MLZ) in Garching, Germany. The principle of this instrument is one-to-one imaging of an entrance aperture onto a 2D position sensitive detector by neutron reflection from a double-focusing toroidal mirror. In current state, KWS-3 is covering Q-range between 3·10-5 and 2·10-2 Å-1 and used for the analysis of structures between 30 nm and 20 µm for numerous materials from physics, chemistry, materials science and life science, such as alloys, diluted chemical solutions, hydrogels and membrane systems. Within the last few years we have finalized several big “evolutionary” projects; we have completely re-designed and commissioned the main components of the instrument: selector area, mirror positioning system, main sample station at 10m, beam-stop system; implemented new sample stations at 3.5 and 1.3m, second (very-high resolution) detector, polarization and polarization analysis systems; adapted the instrument to almost any existing/requested sample environment like 6-position Peltier furnace (-25°C to 140°C), high-temperature furnace (< 1600°C), cryostats/inserts (>20 mK), liquid pressure cell (<5 kBar/10-80°C), CO2/CD4 gas pressure cell (<0.5 kBar/10-80°C), humidity cell/generator (5-95%/10-90°C), magnets (horizontal < 3T, vertical < 2.2T), Bio-logic® multimixer stopped flow (5-80°C), rheometer Anton paar (tangential/radial) etc.

### [153] Competing magnetic phases in Dirac nodal line semimetals LnSbTe (board TU-194)

*Presenter: PLOKHIKH, Igor*

The introduction of the topology concept has revolutionized modern solid-state research by offering new materials with such key functionality as the topological Hall effect and high charge carrier mobility useful in quantum computing. $Ln$SbTe ($Ln$ – lanthanides) materials are one of the families extensively discussed as hosts of Dirac nodal lines, i.e., topological features in reciprocal space. These materials are an ideal platform for investigating the interplay between topological electronic structure, charge ordering instabilities, and localized magnetism stemming from $Ln^{3+}$ ions. Despite a significant number of works on their electronic structure, little is known about their microscopic magnetism. The magnetic aspect is of interest due to the suggested but elusive antiferromagnetic skyrmion in Te-doped GdSbTe and the possible influence of magnetic order on the electronic structure. We performed neutron powder and single-crystal diffraction study of $Ln$SbTe. The most striking results are on $Ln$SbTe (Ln = Ho, Tb, and Dy), where we observe the coexistence of several magnetically ordered phases below seemingly single transitions. Magnetic symmetry arguments hint at multi-$k$ magnetic order in the case TbSbTe, which is a prerequisite for forming long-period magnetic textures with non-trivial magnetic topology. These results and their possible relation to the electronic structure will be presented in detail at the conference.

### [21] Symmetry and anisotropic properties of β-PbO2 studied by DFT as well as SR and neutron diffraction (board TU-196)

*Presenter: PRZENIOSŁO, Radoslaw*

The structural and electronic properties of the rutile-type oxide beta-PbO2 (plattnerite) are studied by neutron and synchrotron radiation powder diffraction and first-principles density functional theory (DFT) calculations~[1]. The motivation to study the electronic properties of beta-PbO2 gained some additional impact related to the possible existence of topologically nontrivial [2,3] semimetallic states. Both diffraction measurements and DFT calculations show that beta-PbO2 has a CaCl2-type orthorhombic structure (space group Pnnm) instead of the widely accepted beta-PbO2 rutile-type tetragonal structure (space group P42/mnm). This symmetry lowering in beta-PbO2 is a robust effect observed at ambient pressure at temperatures between 100 and 400 K. The orthorhombic symmetry rules out the possibility of a semimetallic symmetry-protected state in beta-PbO2. Both diffraction measurements and DFT calculations show an anisotropy of thermal expansion, atomic vibrations and elastic constants of β-PbO2 along the [100] and [010] directions. [1] P. Fabrykiewicz, R. Przeniosło, N. Gonzalez Szwacki, I. Sosnowska, E. Suard and F. Fauth, Phys. Rev. B103, 064109 (2021). [2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010). [3] B. Peng, I. Bravic, J. L. MacManus-Driscoll, and B. Monserrat, Phys. Rev. B 100, 161101(R) (2019).

### [138] Hydrated paths and water dynamics in functionalized syndiotactic-polystyrene proton conductive membranes studied by extended Q-range SANS and multi-resolution QENS. (board TU-198)

*Presenter: RADULESCU, Aurel*

Using the selectivity of the crystalline $\delta$-form for hydrocarbon solvents, a controlled functionalization by sulfonation of the semi-crystalline syndiotactic polystyrene (sPS) films can be achieved when large sulfonation agents such as lauroyl sulfate in chloroform solution are used, which provides homogeneous sulfonation of only of the phenyl rings in the amorphous region without affecting the crystallinity of the material. Sulfonated sPS (s-sPS) is hydrophilic and shows a high proton conductivity comparable to Nafion, that is the benchmark in proton exchange membranes fuel cell technology. Thus, s-sPS membranes may be used in ion conducting applications since they are characterized by a nanoscale phase separation into hydrophilic domains and hydrophobic regions, which is a combination that enables a high ion conductivity and provides a good chemical and thermomechanical stability. The proton conduction in PEMs depends on water and is governed by the hydrated paths at nano-

and mesoscale and the water micro-dynamics at different time scales. Therefore, in order to understand the transport properties in different conditions one should first of all understand the membrane morphology over a wide length scale, between a few Å (crystal structure) and the mesoscopic scale (hundreds of nm), as a function of hydration level (relative humidity RH and water uptake) and temperature (T), and learn about the micro-dynamics in hydrated membranes under such conditions. We carried out a detailed microstructural characterization of uni-axially deformed s-sPS membranes by using the extended Q-range (10$^{-3}$ to 2 Å$^{-1}$) SANS method with the variation of the SLD achieved in the crystalline regions by using the guest-exchange phenomenon between H/D guest molecules in the $\delta$-form clathrates of sPS, and in the hydrated regions by using different H$_2$O/D$_2$O combinations. We also investigated the slow (100 ps) and fast (10 ps) water micro-dynamics in such membranes in a semi-free water hydration regime, at different temperatures (30°C, 50°C and 80°C) by multi-resolution QENS. Our experimental results concluded that the anomalous ionic conductivity behavior observed in the s-sPS membranes is an effect of structural features of the system: water accumulates in s-sPS in spherical clusters that grow in size and become interconnected in increasing the hydration level, ultimately giving rise to occurrence of water channels at very high humidity or in membranes equilibrated in liquid water; at limited RH, the water clusters lose interconnectivity with increasing temperature, what explains the observed drastic decrease in ionic conductivity for very little or no water desorption as delivered by SANS.

### [405] Improving a Molecular Dynamics Water Model by Comparing it to Neutron and X-ray Scattering Data (board TU-200)

*Presenter: REICH, Veronika*

The structure and dynamics of water in all its possible states has been investigated and simulated extensively in the past with multiple methods. Experiments have been conducted on a molecular level with neutron and X-ray scattering techniques; molecular dynamics (MD) computer simulations are also widely used for the study of water and solvated molecules. In our work we connect experimental data of water with MD simulations to further enhance the simulations and obtain forcefields that reproduce the data better. MD simulations were run of two well established water models, TIP3P and TIP4P/2005. X-ray and neutron scattering data were calculated from it with the program Sassena, and these structure and dynamics curves were compared to published experimental data of water at ambient conditions. The agreement between scattering curves and experimental data was improved by a multiple parameter fitting Monte Carlo scheme to obtain a set of parameters that reproduces the real nanoscopic structure and dynamics of water as probed by neutron and X-ray scattering experiments better. This scheme is highly adaptable to other substances.

### [85] Nuclear Analytical Facility at MLZ (board TU-202)

*Presenter: REVAY, Zsolt*

The Prompt Gamma Activation Analysis instrument is located at the strongest cold neutron beam at MLZ. The samples can be irradiated in vacuum, using the highest flux, their masses can be less than a milligram. The emitted prompt gamma radiation is detected using high-purity germanium detectors. PGAA is typically used for the determination of light elements, it is unique for H (also in deuterated materials), B, but it is also sensitive for a series of heavy elements like Cd, Hf, rare-earths etc. for which it can be used as a trace-element analytical technique. The method has successfully been used in the analyses of cultural heritage objects, geological and environmental samples, as well as in material science. Short-lived activation products can be analyzed in beam, too, thus further broadening the circle of high-sensitivity elements. A new setup is planned for short cyclic activation analysis. It will offer unprecedented sensitivity for such important elements as F, Ag, Pd. The instrument accommodates the Neutron Depth Profiling setup used for the determination of the concentration profiles of Li or B in thin layers. The method has successfully been used in operando investigations of lithium-ion batteries. The properties of the techniques, sensitivities, possibilities etc. will be presented in the poster.

### [363] Automated grouping of spatially distributed detectors in neutron time-of-flight experiments based on multivariate similarity (board TU-204)

*Presenter: ROBLEDO, Jose*

Nowadays, in neutron time of flight measurements, there are experimental setups in which many detectors record data during a single experiment. It is usually desirable to be able to sum several spectra in order to increase counting statistics, and therefore decrease uncertainties, for further analysis. A problem arises in time-of-flight experiments when the available spectra are acquired with a set of spatially distributed detectors, each forming a different source-sample-detector angle and at different sample-detector distances. Since these spectra record the neutron’s time of flight after scattering, and the neutron scattering depends on the Q vector, then these spectra are not arbitrarily summable. In this work, we propose an automated methodology for wisely adding spectra based on their multivariate similarity by means of machine learning techniques, such as k nearest neighbors combined with T-distributed Stochastic Neighbor Embedding (t-SNE). We exemplify it in the effective temperature determination of hydrogen in ethane and triphenylmethane samples by means of Deep Inelastic Neutron Scattering, measured at the VESUVIO spectrometer (ISIS facility, UK). The proposed methodology can be applied in other time-of-flight experiments, in which detectors located at different angles record complete spectra, and with this method their degree of compatibility can be determined.

### [390] Extracellular vesicles internalization mechanisms into cells (board TU-206)

*Presenter: RONDELLI, Valeria*

Extracellular vesicles (EV) are a potent intercellular communication system, delivering proteins and genetic material throughout the body, strongly influencing the fate of recipient cells. Due to their specific biological functions and to their peculiar molecular content they have been proposed as biomarkers for various diseases and as optimal candidates for therapeutic applications. Despite of their extreme biological relevance, their mechanisms of internalization into recipient cells are still hotly debated. We performed a multiscale investigation based on atomic force microscopy, small angle X-ray and neutron scattering, neutron reflectometry, infrared spectroscopy and scanning calorimetry to reveal the structural features of EV of different origin an to investigate their interaction with model membrane systems of variably complex composition, to spot the role of different membrane phases on the vesicles internalization routes. Our analysis reveals dependence of interaction mechanisms on EV nature. Our approach has clear implications on the modulation of EV internalization routes by targeting specific domains at the plasma cell membrane and, as a consequence, on EV-based therapies. [F. Perissinotto & V. Rondelli et al., Nanoscale, 2021] [M. Grava et al., Biomolecular Concepts, 2022] [V. Rondelli et al., ACS Omega, 2022] [M. Grava et al., Il Nuovo Cimento C, 2022]

### [364] Nanostructural changes in latex colloid-cellulose nanofibril hybrid films during humidity cycling (board TU-208)

*Presenter: ROTH, Stephan*

Cellulose nanofibrils (CNFs) are widely used due to their attractive properties such as low density, lightweight, thermal stability, and good mechanical properties. These prerequisites make cellulose nanofibrils a promising template material for the design of hybrid colloid-bio composites and bio-inspired functional coatings. Latex colloids are excellently suited to be incorporated in functional, e.g. amorphous photonic crystals, due to the tailored core-shell morphology. Hence, when combining such colloids and CNF, one needs to understand the nanoscale architecture of cellulose nanofibrils in networks and in the presence of other nanoparticles. Especially their reaction to external fields, e.g. humidity changes, is crucial in terms of stability and reversible/irreversible structural rearrangements. Here, we used depth sensitive grazing incidence small-angle neutron scattering (ToF-GISANS) to evaluate the humidity-induced latex colloid (of different sizes) and CNF rearrangements in situ during cyclic humidification. The measured kinetics help to resolve the time- and depth-dependence that particles of different sizes need to penetrate into the porous CNF network. We were able to resolve if the latex nanoparticles remain on the surface or penetrate the CNF matrix. After the first humidity cycle, a change in morphology on the scale of several 10 nm was observed, which is attributed to latex particles which diffused in the network and enlarged the pores of the network.

### [442] Microstructure of engineering materials studied by SANS (board TU-210)

*Presenter: RYUKHTIN, Vasyl*

Microstructure of engineering alloys is strongly connected with their mechanical properties such as hardness or ductility. Usually conventional methods of electronic microscopy are used for assessing morphological characteristics of the precipitates. However, in some cases the small-angle neutron scattering (SANS) technique can be more efficient due to unique properties of neutrons such as law absorption (it allows to study thick samples) and presence of magnetic moment (for better detection of magnetic microstructures). Here, we would like to show few examples of such cases. Medium carbon spring steel was studied by influence of copper on precipitations during aging. It was found that alloying by copper scientifically improves material characteristics (increases yield stress, better corrosion resistance, “self-healing” of ultrafine cracks). Magnetic SANS (MSANS) was used for accurate characterization of this nanosized copper particles nucleated by tempering at 400-500 °C. In this case MSANS was very effective and in perspective it can be used for in-situ study of Co precipitation kinetics in similar alloys. Another case – in-situ and ex-situ SANS study of sintering process in composite tungsten (W) grains in cobalt (Co) binder. In vanadium (V)-doped tungsten carbide (WC)-Co composite material system, both in-situ and ex-situ SANS and ultra-small-angle neutron scattering (USANS) experiments helped to explain how additions of V affect the nano- and microstructure during sintering and result in smaller WC grains. Whereas, SANS quantified the nano-scale interfacial layers responsible of grain coarsening inhibition, USANS was applied to study microstructural refinement.

### [68] Tuning of protein adsorption on nanoparticles using oppositely charged surfactant and multi-valent ions (board TU-212)

*Presenter: SAHA, Debasish*

The integration of the nanoparticles with proteins has a prime interest in the field of nanobiotechnology where these complexes are aimed to utilize for different applications such as targeted drug delivery, biosensing, etc [1]. The protein adsorption on nanoparticles is governed by several interactions such as hydrogen bonding, electrostatic complexion, hydrophobic attraction. Herein, the interaction of cationic lysozyme protein with the anionic Ludox HS40 silica nanoparticle has been tuned by anionic SDS surfactant and multi-valent $ZrCl_4$ ions in the multi-component soft matter system. The unique advantage of contrast matching SANS (bulk contrast, micelle contrast, and nanoparticle contrast) has been utilized to probe the role of individual components in the three-components system [2]. The results demonstrate that SDS induced preferential binding of the protein (lysozyme-SDS/lysozyme-HS40 nanoparticles) and the multivalent ion driven charge inversion of the nanoparticles/proteins can

be utilized to create switching between the protein adsorption and non-adsorption. These parameters can also enable the control over the undesired protein adsorption and nanoparticle aggregation in the nanoparticle-protein systems [3]. References 1. M. Hadjidemetriou et al. Nat. Nanotechnol. 12, 288 (2017). 2. D. Saha et al. Soft Matter 18, 434 (2022). 3. S. Kumar et al. Appl. Phys. Lett. 118, 153701 (2021).

### [436] STRESSFIT – software for analysis of residual stress distributions (board TU-214)

*Presenter: SAROUN, Jan*

Mapping of residual stresses in polycrystalline materials by neutron diffraction employs relatively large sampling volumes, which helps to smooth out stochastic noise due to limited number of contributing grains, but also causes a number of undesired effects commonly called as pseudo-strains. These include smearing of measured strain distributions, as well as false strains observed due to non-uniform sampling occurring at the sample surface or inner phase boundaries, and due to steep composition or texture gradients and variation of beam attenuation. STRESSFIT is a Python package developed with the aim to address this kind of problems. On the input, it employs a list of sampling events, which can be generated by neutron ray-tracing simulation of the instrument at given experimental geometry. STRESSFIT then provides tools for making convolution of this sampling distribution with the probed material properties, yielding “as measured” peak positions, widths and intensities suitable for evaluation of the pseudo-strains and for fitting of experimental data using free intrinsic strain and scattering intensity distributions as the model functions. As a result, the intrinsic (deconvoluted) strain distributions can be partially recovered. Apart of the package API, STRESSFIT also provides a user-friendly interface using Jupyter notebook widgets to facilitate usual workflow of neutron strain mapping data analysis. The package is available at https://github.com/NPLtools/stressfit.

### [24] FRM II neutron imaging exported to smaller reactors (board TU-216)

*Presenter: SCHILLINGER, Burkhard*

In the absence of available beam time at FRM II, we invested time to downscale detectors, computed tomography equipment and software used at the ANTARES neutron imaging facility to small, compact and portable versions that can be used at smaller low-power reactors where classic scattering experiments often cannot be performed due to lack of intensity. CT setups including experiment controls and 3D printed components were used and installed at reactors in Idaho Falls, in Prague, Santiago de Chile, Bariloche and Vienna. The International Atomic Energy Agency (IAEA) will endorse further installations. The talk will give an overview about external neutron imaging projects based on FRM II developments.

### [164] Conceptual design of neutron imaging instruments for the HBS (board TU-218)

*Presenter: SCHMIDT, Norberto*

The High Brilliance Neutron Source (HBS) project aims to develop a High-Current Accelerator-driven Neutron Source (HiCANS) for neutron scattering, analytics, and imaging. Amongst the instruments planned at HBS, there will be at least 5 different neutron imaging instruments to cover the different neutron energy ranges: cold, Bragg edge, thermal, resonance/epithermal, and fast. Each one of these imaging instruments will have different sample positions, which will be selected to optimize the flux, collimation, spatial, wavelength, and time resolutions. The selection of the positions will be best suited for studies considering the specific energy ranges to investigate hydrogen in metals, strain phase mapping studies, energy conversion processes, archeological characterization, aerospace applications, or battery processes. For the neutronic design, Monte Carlo simulations are used. The target and moderators are simulated with PHITS, while VITESS and McStas perform the ray transport through the instruments. Also, KDSource is used to estimate the source distribution at a given point in the beam trajectory, and then resample new particles that respect the correlations of the original source. The objective of this talk is to present to the neutron community the conceptual design of these instruments, the procedure for the simulations, the principal parameters, and the potential capabilities. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [292] Dynamics in polymer-fullerene blends and the influence of DIO as solvent additive studied with quasielastic neutron scattering (board TU-220)

*Presenter: SCHWAIGER, Dominik M.*

In the emerging field of organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active materials due to their superior performance compared to e.g. planar layered devices. In this optically active polymer layer, photons are absorbed and free charges are created. A frequently applied and well-studied system is the combination of PTB7 as electron donor and PCBM as electron acceptor. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited, even though molecular mobility plays a vital role in e.g. film formation and degradation processes. We investigated blend films of PTB7 and PCBM, prepared from chlorobenzene solution. The use of solvent additives such as DIO in the production process can significantly increase the power conversion efficiencies of resulting devices but also brings additional challenges in terms of stability. Quasielastic neutron scattering experiments at the cold neutron time-of-flight spectrometer TOFTOF (MLZ, Garching) were performed to determine hydrogen dynamics on a pico- to nanosecond timescale in both, pure PTB7:PCBM blend films and their variation, produced with DIO as solvent additive. The results indicate the presence of residual solvent in the latter samples, however, time resolved measurements during heat treatment reveal different kinetic

behavior for solvent removal and the underlying ‘aging’ of the polymer dynamics.

### [50] Neutron diffraction studies of crystal structure and orbital ordering in multiferroics, based on complex manganese oxides. (board TU-222)

*Presenter: SIKOLENKO, Vadim*

The great interest of researchers over the past years has been caused by multiferroics - materials in which magnetic and electric dipole ordering are simultaneously observed. One of the typical representatives of this class of compounds is the complex oxides of the manganese of the BiMnO3 with a structure of perovskite type. The magnetic properties of the compound are determined by positive exchange interactions between manganese ions, which are due to the orbital ordering of Mn3+ ions. Since the magnetic properties of compound are determined by the geometry of chemical bonds between Mn - Mn, it is possible to control the magnetic characteristics of the compositions based on BiMnO3 by chemical replacement or by changing the stoichiometric composition of the initial compound. Compounds with a nominal excess of oxygen ions are characterized by the presence of vacancies in A- and B- sublattice of the structure of perovskite, while in order to comply with the principle of electroneutrality, the deficiency of cations leads to the formation of Mn ions with an oxidation state of 4+. Bismuth and manganese cations vacancies, as well as the presence of Mn4+ ions, lead to a distortion of the crystalline structure, as well as to a significant change in the nature of the exchange interactions. Neutron diffraction and synchrotron data show that compounds with excessive oxygen content at room temperature are characterized by a monoclinic structure, with an increase in oxygen content - with a two -phase state with a dominant orthorhombic and monoclinic phases. An increase in temperature leads to a structural phase transition to a non -polar orthorhombic phase. At the same time, magnetization is reduced due to the destruction of the orbital ordering of Mn3+ ions, and the magnetic state changes from ferromagnetic to the spin glass state. During the chemical replacement of manganese ions into iron ions at room temperature, a structural transition occurs from the polar rhombohedra phase to the antipolar orthorhombic and then to the monoclinic phase through a two phase region. Accordingly, changes in the magnetic structure occur, in particular, the modulated antiferromagnetic phase passes into a noncollinear antiferromagnetic, and then into an orbital ordered ferromagnetic phase

### [214] Can Neutron Reflectometry help us observe the MscL ion channel in action? (board TU-224)

*Presenter: SKODA, Maximilian*

Neutron reflectometry (NR) is an ideal tool for studying biological membrane models, and many different models, mimicking bacterial and mammalian cells have been developed in recent years. Often, the focus of such NR studies is on the interaction of various molecules, e.g. proteins, polymers, peptides etc with the membrane model. Another interesting use of such models is the characterisation of membrane proteins under physiological conditions. This is in contrast to other techniques, such as NMR or cryo-EM, which often do not allow observation under physiological conditions. Here, we present a body of work dedicated to the characterisation of the pore-forming membrane protein MscL (Mechanosensitive Ion Channel of Large Conductance). Our interest in this protein is the fact that MscL is responsible for translating physical forces applied to cell membranes into electrophysiological activities. MscL has a relatively large conductance, 3 nS, making it permeable to ions, water, and small proteins when opened. MscL acts as stretch-activated osmotic release valve in response to osmotic shock. We discuss the benefits and limitation of two different membrane models, including a novel "suspended" one, with aim of not only determining the protein's location within the membrane, but also attempting to observe the actual opening (or gating) of MscL triggered by exposure of the membrane to the antimicrobial peptide (AMP) pexiganan (PXG). Our hypothesis is that MscL could serve as an Achilles heel that increases antimicrobial activity of AMPs.

### [38] Quenching and Deformation Dilatometer for In-Situ Materials’ Characterization by Neutron Diffraction (STRESS-SPEC) and Small Angle Neutron Scattering (SANS-1) at MLZ (board TU-226)

*Presenter: SOLIS, Cecilia*

A Quenching and Deformation Dilatometer (TA instruments DIL805A/D/T) operates at the MLZ for performing in-situ neutron diffraction (phase, texture, stress/strain) at STRESS-SPEC and small-angle neutron scattering (nanostructure) at SANS-1. Imaging applications are under preparation at ANTARES. With this setup, the evolution of the sample length during heating or quenching can be accurately monitored while scattering data are being acquired. Thanks to induction heating and gas cooling very high rates are accessible. Forces up to 20 and 8 kN can be applied in compression and tension, respectively. Besides, special sample holders for powders will soon extend the range of applications. The combination of the neutron scattering and dilatometry measurements yields a unique view on the microstructural evolution under thermomechanical treatment. In this work, we will show the parameters of the dilatometer and its possibilities to be used for in-situ scattering characterization. Besides we will present some results of different materials like TiAl alloy to investigate the mechanisms of hot compression and further to optimize the mechanical properties, and Cu-Ce<sub>0.8</sub>Gd<sub>0.2</sub>O<sub>2-$\delta$</sub> (CGO) composites to tune thermo-mechanical compatible electrodes for solid oxide fuel cells (electrolyzers).

### [354] Amor - an angle and energy dispersive reflectometer (board TU-228)

*Presenter: STAHN, Jochen*

In 2022, the neutron guide upgrade program at PSI was used to replace the old guide of the neutron reflectometer Amor by a full-scale *Selene* optics. In this context also a new polariser and a high-resolution detector were installed, and since then also the chopper and instrument electronics have been replaced. The *Selene* optics essentially consists of 2 subsequent elliptic reflectors (each 9 m long) which map the virtual source opening (down to 0.5 $\times$ 2 mm$^2$) to the sample position 30 m downstream. The resulting minimum beam spot there is 1 $\times$ 3 mm$^2$. A transmission polariser is placed behind the first mirror in the convergent beam. It has the shape of an equiangular spiral so that it provides the same angle of incidence across the full divergence of 1.6 deg. This high divergence (in both directions) enables high-intensity specular reflectometry, where the scattering angle is obtained from the spacial resolution of an area detector. We use technology developed at the ESS for their reflectometers Estia and Freia. The spatial resolution is 0.5 $\times$ 4 mm$^2$ and its count rate capability greatly exceeds the demands at Amor. All these components are installed, operational and tested. Sadly this can not be stated for the instrument electronics. The delay results from the prioritisation after the upgrade, followed by hardware shortages due to the pandemic and more recently the Russian war. The plan is that hot commissioning starts midyear and user operation in the second proposal cycle.

### [233] High-resolution neutron spectroscopy of zone-boundary magnons in Cu2OSeO3 under magnetic field (board TU-230)

*Presenter: STEKIEL, Michal*

We report a combined experimental and theoretical study of zone-boundary magnons in Cu2OSeO3 under magnetic field. High-resolution data were recorded at the triple-axis spectrometers Thales and IN8 at the ILL. As our main result we found a strong magnetic-field dependence of the zone-boundary magnons. We discuss our results in terms of theoretical modelling elucidating putative band-sticking [1] and topological nodal planes [2] expected for the non-symmorphic crystal structure of Cu2OSeO3. [1] C. Herring, Phys. Rev. 50, 361 (1937). [2] M. A. Wilde, et al., Nature 594, 374 (2021).

### [290] Polarized SANS & GISANS studies on condensed matter systems (board TU-232)

*Presenter: STELLHORN, Annika*

Small-Angle-Neutron-Scattering (SANS) and Grazing-Incidence-SANS (GISANS) techniques have seen a remarkable growth in their application in studies of magnetic materials. In combination with neutron polarization analysis, SANS and GISANS offer magnetic vector analysis on the micro- and mesoscopic length scale with high signal to noise ratio. However, in multiple sample environments like applied magnetic and electric field and at low temperatures, the experimental setup and data analysis procedures remain open issues. Two examples are presented here. Firstly, magnetic chiral domain walls in thin-film heterostructures of Nb/FePd [1] have been investigated using GISANS with polarization analysis in an applied magnetic field and at low temperature. Optimizing the neutron-spin transport for low magnetic guide fields and its impact on the data analysis using in-house developed tools will be discussed. Secondly, magnetic chiral phases occurring in the magnetoelectric single crystal Ba_{2-x}Sr_xMg_2Fe_12O_22 [2] are studied using SANS with polarization analysis in applied magnetic and electric fields at low temperatures. Considerations in the instrumental design and the SANS data analysis using the SasView software [3] will be reported. Polarization analysis has been incorporated as an integral part of the ESS instrument suite [4]. An introduction of its current scope will be provided. [1] A. Stellhorn *et al.*, New Journal of Physics 22, 093001 (2020). [2] K. Zhai *et al.*, Nature Communications 8, 519 (2017). [3] www.sasview.org [4] W. T. Lee *et. al.*, Report on ESS Polarisation Workshop, ESS-3549713 (2020).

### [357] BornAgain: Software for GISAS and Reflectometry (board TU-234)

*Presenter: SVECHNIKOV, Mikhail*

BornAgain is an open-source software package to model and fit SAS, GISAS, and reflectometry. It has been designed to fully reproduce the functionality of the standard software IsGISAXS, allow for hierarchical sample models of arbitrary complexity, in particular, support multilayers with arbitrary inclusions that may extend across layers, support neutron polarization and magnetic scattering, provide a graphical user interface for sample construction and fitting, give advanced users full control through Python scripting. After extension to reflectometry, BornAgain is currently undergoing thorough refactoring to facilitate future maintenance and prepare for the addition of new functionality. Among them SAS by crystalline 3D structures, fully generic slicing of cross-layer particles, source or detector below horizon, comprehensive handling of parameter distributions.

### [273] Ordered and disordered variants of the triangular lattice antiferromagnet Ca3NiNb2O9 (board TU-236)

*Presenter: TANG, Ran*

Single crystals of the triangular lattice antiferromagnet (TLAF) Ca$_3$NiNb$_2$O$_9$ and its non-magnetic analogue Ca$_3$MgNb$_2$O$_9$ are grown using the four-mirror optical float-zone furnace. During the growth of Ca$_3$NiNb$_2$O$_9$, the crystal boule tends to develop cracks upon cooling due to a high-temperature structural modification. Thus, depending on the growth conditions, the crystal boules contain varying amounts of high and low-temperature modifications, present in the form of mm-size grains distinguishable on the basis of their appearance: opaque, dark-green (AGO) and

translucent, light-green (AGT) for the high and low-temperature modifications, respectively. Furthermore, when the as-grown, AGO specimen is subject to air annealing at 1200°C, its appearance change from opaque to translucent green, without any noticeable change of weight. Low temperature specific heat and low-field magnetization measurements carried out on the AGO and AGT samples revealed contrasting ground state properties. While AGO exhibits a spin-glass-like ground state, the AGT sample exhibit a two-step, long-range antiferromagnetic ordering of the Ni spins with transitions at $T_{\mathrm{N}_{1}}$ $=$ 4.6 K and $T_{\mathrm{N}_{2}}$ $=$ 4.2 K. Detailed structural analysis shows that AGO and AGT crystals crystallize in *Pbnm* (orthorhombic) and $P12_1/c_1$ (monoclinic) space groups, respectively. The high-resolution TEM images confirms the 1:2 ordering of Ni and Nb in the AGT sample. The high-field magnetization up to 50 T in AGT reveals the presence of magnetization plateaus characteristic of TLAFs. The propagation vector in the ordered phase (2 K) is inferred to be $\vec{k} \approx (0, 1/3, 0)$ based on the magnetic neutron scattering.

### [409] Status update of ODIN, the neutron instrument for imaging at ESS (board TU-238)

*Presenter: TARTAGLIONE, Aureliano*

ODIN is the ESS state-of-the-art multipurpose neutron imaging instrument. Using wavelength-resolved imaging with tunable medium to high wavelength resolution, ODIN will provide significantly increased chemical and structural sensitivity compared to other traditional neutron imaging instruments, with fixed (or absent) wavelength resolutions. ODIN will view both the cold and the thermal moderators enhancing its spectral flexibility. Ten choppers, together with the neutron extraction and guide system, are the main instrument components behind ODIN´s flexible performance. Nine choppers are located inside the bunker, together with the heavy shutter, while the remaining frame overlap chopper is in the experimental hall D01. The cave is divided in the beam shaping area, with a variable pinhole and filter systems, and the experimental area with sample stages, flight tubes and detector systems; it will also provide ample space for sample environments, other equipment needed for specific imaging modalities (such as an x-ray source), as well as for future upgrades like a diffraction detector. ODIN is now in its installation phase, after two and a half years of detailed design, procurement and manufacturing of all the components. Here we will present some of the design highlights, how the challenging installation is accomplished in the framework of the ESS facility at Lund, Sweden, and what are the future perspectives towards the cold and hot commissioning phases.

### [353] Magnetic structure and spin waves of the doped cobalt oxide La2-xBaxCoO4 (board TU-240)

*Presenter: TOBIN, Siobhan*

The role of charge stripes in cuprate superconductors is not yet understood. The undoped cuprates are antiferromagnetic Mott insulators. A simple model is that doping disrupts the AFM order and the introduced holes form stripes, with the periodicity and values of charge stripes affected by dopant concentration $x$ [1,2]. There is competition between different forms of charge and magnetic order, manifesting in tension between the pseudogap and superconducting phases. Insights into the spin and charge stripes may be gleaned from studying isostructural compounds that share the same parent phase as the cuprates, but remain insulating at low temperatures and over a wide range of dopant concentrations, such as the cobalt oxides [3]. Stripes in superconducting La$_{2–x}$Ba$_x$CuO$_4$ have been shown to be more stable than those found in La$_{2–x}$Sr$_x$CuO$_4$; hence, we have investigated La$_{2-x}$Ba$_x$CoO$_4$ as a candidate striped insulator. We studied crystals of La$_{2-x}$Ba$_x$CoO$_4$ at two dopant concentrations $x$ = 1/2 and $x$ = 1/3 using neutron scattering. We will present single crystal diffraction data from ILL D10 highlighting magnetic and possible charge order. Neutron time-of-flight data from the ISIS MERLIN instrument displays strong spin wave dispersion and we will compare this to the characteristic hour-glass dispersion of other cobalt oxides [3]. Finally, we will discuss the connection between charge stripes and hour-glass spin wave spectra. References [1] Tranquada, J.M., Adv. Phys. 69 437 (2020) [2] Emery, V.J., Kivelson, S.A., and Tranquada, J.M., PNAS 96 8814 (1999) [3] Boothroyd, A.T. et al., Nature 471 341 (2011)

### [476] Development of isoscattering point approach in SANS contrast variation for polydisperse and anisotropic particles (board TU-242)

*Presenter: TOMCHUK, Oleksandr*

There are several approaches to the analysis of contrast variation data in small-angle neutron scattering (SANS) when the solvent scattering length density (SLD) is manipulated by H/D substitution. There are specific points at which the scattering intensity from the liquid system is independent of the SLD contrast between dispersed particles and dispersing media. These points, *q**, are referred to as ‘isoscattering points’ [1]. *q** is analytically related to particle size. Usually, the nature of the isoscattering point is associated with the high symmetry of the nanoparticle shape and low polydispersity. Here we discuss the conditions for observing an isoscattering point for non-spherical and non-monodispersed core-shell structures, as well as additional possibilities of structural characterization via SANS based on this effect. It seems that certain ratios of the SLDs of the components make it possible to detect an isoscattering point even for significantly polydisperse [2] or elongated [3] inhomogeneous particles. [1] Kawaguchi T., *Crystallogr. Rev.* **10** (2004) 233–246. [2] Tomchuk O.V., Bulavin L.A., Avdeev M.V., *Soft Materials* (2022) *in press*. [3] Tomchuk O.V., Bulavin L.A., Zabulonov Yu.L., *Phys. Part. Nucl. Lett.* **19** (2022) 536-538.

### [400] Tunable critical correlations in kagome ice (board TU-244)

*Presenter: TURRINI, Alexandra*

The kagome ice state is a two dimensional critical state of algebraic spin correlations formed by the application of a moderate magnetic field along the cubic [111] direction of a pyrochlore spin ice. Tilts of the field away from perfect alignment allow for tuning of these algebraic correlations by variations of tilt angles, field or temperature, leading to symmetry-sustaining Kasteleyn transitions. We present a detailed experimental/theoretical study of the kagome ice Coulomb phase, which explores the fine tuning of critical correlations by applied field, temperature and crystal orientation. We observe the continuous modification of algebraic correlations with polarized neutron scattering experiments, and they are found to be well described by numerical simulations of an idealized model. We further clarify the thermodynamics of field tuned Kasteleyn transitions and demonstrate some dramatic finite size scaling properties that depend on how topological string defects wind around the system boundaries. We conclude that kagome ice is a remarkable example of a critical and topological state in a real system that may be subject to fine experimental control realizable at easily accessible temperatures and fields.

## [462] Polyoxometalate-rich complex micelles for functional mesoporous materials (board TU-246)

*Presenter: UNNIKRISHNAN, Ananthapadmanabhan*

Poster Abstract The newly developed Polyion complex (PIC) micelles have unparalleled significance in the construction of functionalized and ordered mesoporous materials. MesoPIC micelles are fabricated through the electrostatic complexation between a charged double hydrophilic block copolymer (DHBC) and an oppositely charged polyelectrolyte. The formation and deformation of these micelles could be controlled by physico-chemical proceedings such as a pH change, a property of predominant importance in templeting agents employed for the preparation of ordered mesoporous materials. The immense study of PIC micelles has opened a new array of opportunities in front of us. We are currently working on two different protocols, employing the MesoPIC process. Protocol 1: In this procedure, functionalised Polyion complex (PIC) micelles, fabricated through the electrostatic complexation between a charged double hydrophilic block copolymer (DHBC) and an oppositely charged polyelectrolyte, functions as structuring agent for the construction of porous materials. Hence, the primary aim of the strategy would be to synthesise DHBCs, with well controlled degree of polymerisation. Secondly, the focus would be the functionalisation of the DHBC synthesised. The functional DHBC envisaged, PEO-b-POMs, will contain a poly(ethyleneoxide) block and a block grafted with polyoxometalates (POMs). POMs are metal anionic nanoclusters with promising properties, especially as catalysts or UV-absorbers. This method will permit the direct formation of porous organised materials, functionalised with POMs at the pore surface. Protocol 2: In the giant novel complex micelles (Complex PIC Micelles) developed through this novel means, inorganic clusters exhibiting various structural and functional properties, referred to as Polyoxometalates (POMs), functions as the core and the DHBC builds the periphery. POMs employed for the initial studies are Pospho- and Silicotungstic acid. Preliminary analysis of the Complex PIC Micelles through DLS/SLS, confirm them to be giant structures, with a radius of approx. 45 nm. SAS would be employed for understanding these micelles in more detail. Knowing the structure and shape of the micelles prepared would be key, for the efficient use of them in order to construct mesoporous materials, with potential application in catalysis and UV-Adsorption.

## [249] Evaluation of a method for time-of-flight, wavelength and distance calibration for neutron scattering instruments by means of a mini-chopper and standard neutron monitors (board TU-248)

*Presenter: VERGARA, Lisa*

Accurate conversion of neutron time-of-flight (TOF) to wavelength is of fundamental importance to neutron scattering measurements in order to ensure the accuracy of the instruments and the experimental results. Equally important in these measurements is the determination of uncertainties, and with the appropriate precision. Especially in cases where instruments are highly configurable, the determination of the absolute wavelength after any change must always be performed (e.g. change of detector position). Inspired by the manner with which neutron spectrometers determine the absolute wavelength, we evaluate for the first time, in the author's knowledge, a commonly used method for converting TOF to neutron wavelength, the distance of a monitor from the source of neutrons and we analytically calculate the uncertainty contributions that limit the precision of the conversion. The method was evaluated at the V20 test beamline at the Helmholtz Zentrum Berlin (HZB), emulating the ESS source with a long pulse of 2.86 ms length and 14 Hz repetition rate, by using a mini-chopper operated at 140 Hz and two portable beam monitors (BMs), as well as accompanied data acquisition infrastructure. The mini-chopper created well-defined neutron pulses and the BM was placed at two positions, enabling the average wavelength of each of the pulses created to be determined. The used experimental setup resulted in absolute wavelength determination at the monitor positions with a □□□□□□/□□□□□ of 1.8% for □ > 4 Å. With the use of a thinner monitor, a □□□□□□/□□□□□ of 1% can be reached and with a modest increase of the distance between the reference monitor positions a □□□□□□/□□□□□ of below 0.5% can be achieved. Further improvements are possible by using smaller chopper disc openings and a higher rotational speed chopper. The method requires only two neutron measurements and doesn't necessitate the use of crystals or complex fitting with sigmoid functions and multiple free variables, and could constitute a suitable addition to imaging, diffraction, reflectometers and small angle neutron scattering instruments, at spallation sources, that do not normally utilise fast choppers.

### [183] Expanding the Sr–B–N–H system with the compound Sr13(BN2)6H8 validated by X-ray and neutron powder diffraction (board TU-250)

*Presenter: WANDELT, Sophia Lena*

Multianionic compounds containing hydrides built a large variety of compounds, e. g. hydride fluorides, hydride oxides or hydride nitrides, which can act as functional materials such as hydride ionic conductors or host lattices for Eu2+ luminescence.[1] On the other hand, the compound class of nitridoborate hydrides is with only two known compounds, namely Ca2BN2H and Sr2BN2H, only little explored so far.[2,3] We hereby present a new member of this group, Sr13(BN2)6H8. The compound crystallizes in the hexagonal space group P63/m (no. 176) and reveals trigonal planar and distorted tetrahedrally coordinated hydride ions as well as slightly bent [N–B–N]3− units coordinated by strontium atoms. The structure was partially solved by X-ray powder diffraction and corroborated with neutron powder diffraction of the corresponding deuterated compound. Further analytics such as 1H and 11B MAS NMR, FTIR and Raman spectroscopy confirm the proposed structure model and the presence of anionic hydrogen. DFT calculations further validate the experimental outcome and reveal the electronic structure of Sr13(BN2)6H8. [1] H. Kageyama et al., *Nat. Commun.* **2018**, *9*, 772. [2] M. Somer et al., *Z. Allg. Anorg. Chem.* **2004**, *630*, 1068. [3] S. Wandelt et al., *Inorg. Chem.* **2022**, *61*, 12685.

### [101] KCl modulated D2O Hydration and Subsequent Thermoresponsive Behavior of Poly(sulfobetaine)-Based Diblock Copolymer Thin Films (board TU-252)

*Presenter: WANG, Peixi*

The modulation of thermoresponsive behavior of PNIPAM (or PNIPMAM) in aqueous solution has been widely studied by varying temperature, solvent composition, and salt concentration, which causes significant conformational changes between extended or collapsed chains via absorption or release of water. However, rare studies report on the salt effects on its block copolymer containing the zwitterionic poly(sulfobetaine)s (PSBs), especially in thin film geometry. In contrast, PSBs exhibit a UCST-type behavior in aqueous solution and are well-known as the closest structural analog to phospholipids and lipid membranes. To study the salt effect on D2O hydration and subsequent thermoresponsive behavior of PSBP-b-PNIPMAM thin films, we prepared thin films pre-loaded with KCl for the asymmetric DBC during film formation. The 'salting-in effect' of KCl on film composition and D2O distribution along with the film normal is studied by in situ spectral reflectance (SR) and time-of-flight neutron reflectivity (ToF-NR) in combination with isotope sensitivity, and the solvation-triggered phase transition upon D2O hydration and subsequent heating is probed in situ by Fourier transform infrared spectroscopy (FT-IR). Besides, the migration and/or aggregation of KCl domains inside the DBC thin films is also demonstrated by complementary methods, namely, X-ray reflectivity (XRR) and atomic force microscopy (AFM).

### [74] Electron-phonon coupling in Mn$_{1-x}$Fe$_x$Si (board TU-254)

*Presenter: WEBER, Frank*

The interplay of ferromagnetic exchange, Dzyaloshinsky-Moriya interaction and crystal potential results in the complex phase diagram of the chiral magnet MnSi ($T_C$ ≈ 30 K). In Mn$_{1-x}$Fe$_x$Si, long-range magnetic order is suppressed and helimagnetic correlations vanish at $x$ ≈ 0.2 along with a redistribution of d states at the Fermi energy. Here, we present a study of the lattice dynamical properties of Mn$_{1-x}$Fe$_x$Si with 0 ≤ $x$ ≤ 0.22. Employing time-of-flight neutron spectroscopy and high energy resolution inelastic x-ray scattering, we investigate the doping dependence of phonon energies, $E_{phon}$, and line widths, $\Gamma_{phon}$ ($\Gamma_{phon} \propto$ 1/life time). In contrast to the general trend of slightly increasing energies with doping because of the reduced lattice constant, we find a significant softening and broadening of a phonon mode propagating along the [111] direction, which is also the direction of the magnetic ordering wave vector in MnSi. Ab-initio lattice dynamical calculations based on density-function theory predict an increasingly strong electron-phonon coupling for this particular mode linked to changes of the Fermi surface geometry upon doping.

### [144] Impact of S addition on the dynamics and on the structure of glass forming Ti75Ni25-xSx melts (board TU-256)

*Presenter: WILDEN, Johanna*

S addition enables bulk metallic glass formation in Ti-based systems. To understand the role of S on glass formation, we analyzed the melt dynamics and the melt structure in Ti75Ni25-xSx (x = 0, 5, 8, 11). To process these reactive Ti-based melts, we applied containerless methods as electromagnetic and electrostatic levitation. The microscopic melt dynamics (self-diffusion) were studied by quasielastic neutron scattering, whereas the macroscopic melt dynamics (viscosity) were studied by the oscillation drop method. In both cases, S addition reduces the melt dynamics. However, the decrease in melt dynamics is accompanied by a decrease in melt packing, as derived from melt density measurements. Employing neutron diffraction experiments in combination with Ni isotope substitution, we were able to extract the full set of partial structure factors for Ti75Ni25 melts. Using this partial structure information, our analysis shows that the change in melt structure for Ti75Ni25 upon S addition cannot be simply explained by an isomorphous substitution of Ni by S. S atoms seem to occupy a larger space in melt structure than Ni atoms, which is in accordance with the previously reported decrease in melt packing. This indicates that the decrease in melt dynamics is

associated with chemical interactions between the S atoms and the transition metal atoms (Ti and Ni), rather than with a denser packing of the melt.

### [401] Interaction of Prohibitin peptides with membrane models (board TU-258)

*Presenter: WINTER, Anja*

Prohibitins (PHB1 and PHB2) are highly conserved heterodimeric proteins arranging into a large multimeric ring at the inner mitochondrial membrane. They play a crucial role in premature cellular aging, tumor suppression, cell cycle regulation, apoptosis and mitochondrial homeostasis via their interaction with AAA-proteases. We set out to (i) characterize the interaction between the N-terminal helices of PHB (NT-PHB) with the membrane and establish a possible synergy of the two PHB homologues, and (ii) understand the role of cardiolipin in this interaction using interface and bulk neutron techniques. NR and QCM-D experiments demonstrate that both peptides are able to remove lipid from the bilayer. In SANS, the addition of peptide disrupts the membrane, modifying its integrity by fusing membranes and removing lipids from the vesicles. The effect of the peptide on the membrane is concentration-dependent as well as dependent on the lipid membrane composition with CL and PE enhancing the effect of the peptides on the vesicles. We propose that both PHB peptides act in synergism to remodel the inner mitochondrial membrane in order to create raft-like areas that allow the support of large protein complexes such as the hexameric AAA-proteases. Future studies will investigate how the interaction between PHB and AAA-proteases is realized at a molecular level in order to understand PHB's role in mitochondrial homeostasis.

### [102] New sample environments at the cold neutron chopper spectrometer TOFTOF (board TU-260)

*Presenter: WOLF, Marcell*

We will discuss the different new sample environment at the cold neutron chopper spectromenter TOFTOF. For expample the combination of in-situ Raman and neutron spectroscopy is very powerful in order to investigate the molecular dynamics and chemical reactions inside a sampleat the same time. For this purpose we will introduce our new sample environments to combine quasi elastic (QENS) and inelastic (INS) neutron spectroscopy with Raman spectroscopy. Additional to the Raman setup we will introduce a humindity chamber which can also combined together with the Raman spectrometer. We will discuss also introduce also ideas for a laser pump-probe and a hydrogen gas dosing system.

### [328] Spectroscopic binning of event mode neutron data: Sub-second time resolution for the study of soft matter (board TU-262)

*Presenter: WOLFF, Maximilian*

Neutron scattering methods enable a broad range of material studies that are difficult to carry out with other experimental methods. One specific example is the study of soft condensed matter, which includes polymeric systems. Under certain temperatures and concentrations, these polymers may crystallize into crystalline structures. This results in interesting viscoelastic properties of the material, such as gelation or shear thinning. We use Large Amplitude Oscillatory Shear (LAOS) to exert strain on a polymeric sample with a rheometer. Small Angle Neutron Scattering (SANS) is used to probe the periodically assembling crystal structures in the bulk of the material and address unanswered questions about nonlinear effects, such as shear bands and stress-overshoots which could be linked to non-uniform structures. To access the time scales necessary for analyzing an excitation with e.g. a frequency of 1 Hz, we take the neutron data in event mode, capturing every neutron event with a precise time stamp. Via a time-of-flight measurement, the detector data can then be linked to the stress-strain curve of the rheometer at the same synchronized time. Developing a corresponding data reduction pipeline based on the ESS software scipp is a core component of the project. This method also enables improved post processing and rebinning of the data at a later stage.

### [120] The Structure Evolution in Thin Films of a Nearly Symmetric Polystyrene-block-Poly(methyl methacrylate) on a Layer of homopolystyrene chains (board TU-264)

*Presenter: WU, Chun-Ming*

The distributions of dPS in PLs // can be probed by grazing-incidence small-angle neutron scattering (GISANS) and time-of-flight neutron reflectivity (ToF-NR). In this work, by adjusting the composition (ϕPS+dPS = 63.8 vol%) of the total PS/dPS component and annealing temperature (230 and 270 °C), P(S-b-MMA)/dPS blend films mainly form perforated layers with parallel orientation (hereafter PLs //). Where basically follow up our previous studied segmental distributions of polymer chains in blend films of a weakly-segregated polystyrene-block-poly(methyl methacrylate) [P(S-b-MMA)] and deuterated polystyrene (dPS). The GISANS and ToF-NR results offer evidence that dPS chains are preferentially located at the free surface and within the PS layers for blend films that were annealed at 230 °C. Upon annealing at 270 °C, dPS chains distribute within PS layers and perforated PMMA layers. Nevertheless, dPS chains still retain a surface preference for thin films. In contrast, such surface segregation of dPS chains is prohibited for thick films when annealed at 270 °C.

### [271] Long-range order, re-entrant spin glass and spin liquid correlations in Anion disordered Gd2Hf2O7 (board TU-266)

*Presenter: XU, Jianhui*

Pyrochlore antiferromagnets (AFM) Gd2T2O7 (T: tetravalent metal elements) are prototypical materials for realizing classical spin liquid states. However, all of them have been observed to show long-range magnetic order [1-3]. Previous specific heat data of Gd2Hf2O7 show a tiny sharp peak on the top of a large broad maximum indicating a long-range AFM order [4]. However, our sample does not show that sharp peak in specific heat, but the ac susceptibility evidences an ordering transition followed by a spin-glass transition. Using neutron diffraction, we found that the sample has oxygen Frankel defects. The polarized neutron diffuse scattering pattern shows liquid-like scattering without any magnetic Bragg peaks. The subtle long-range order and re-entrant spin glass are attributed to bond disorder due to oxygen anion disorder. [1] J. S. Gardner, et al., Reviews of Modern Physics 82, 53 (2010). [2] X. Li et al., Phys. Rev. B 94, 214429 (2016). [3] A. M. Hallas et al., Phys. Rev. B 91, 104417 (2015). [4] M. D. Alice et al., J. Phys: Conden Matter 20, 235208 (2008).

### [157] Dipolar spin ice regime proximate to an all-in-all-out ground state in the dipolar-octupolar pyrochlore Ce2Sn2O7 (board TU-268)

*Presenter: YAHNE, Danielle*

We present neutron diffraction measurements on newly synthesized dipole-octupole pyrochlore Ce$_2$Sn$_2$O$_7$ powders grown by hydrothermal methods. We find a diffuse signal at low scattering vectors, reminiscent of a *dipolar* spin ice, in striking contrast to previous neutron diffraction on powder Ce$_2$Sn$_2$O$_7$ samples grown by solid-state synthesis, which found diffuse scattering at high scattering vectors associated with magnetic octupoles. While this raises the question about subtle crystalline structural differences between the samples, we detect no oxidation or other crystallographic disorder in the hydrothermally-grown powders through complementary neutron structure refinement and atomic PDF measurements. To understand the underlying interactions that result in the low-Q diffuse signal, we characterize the exchange interaction parameters in the near-neighbor XYZ model Hamiltonian by fitting quantum numerical linked cluster expansions to heat capacity and magnetic susceptibility measurements, as well as classical Monte-Carlo (MC) simulations of the powder averaged structure factor. This places Ce$_2$Sn$_2$O$_7$'s ground state within the ordered dipolar all-in-all-out (AIAO) Néel phase. Further, quantum MC calculations suggest that the transition to long-range order occurs at temperatures below those accessed experimentally. We conclude that new hydrothermally-grown Ce$_2$Sn$_2$O$_7$ samples host a finite-temperature proximate dipolar spin ice phase, above the expected transition to AIAO Néel order.

### [235] Novel idea of neutron polychromator and application for reflectometry and spectroscopy (board TU-270)

*Presenter: YAMADA, Norifumi*

Historically, two methods are used to determine the wavelength of neutrons: one is a time-of-flight method separating the velocity of pulsed neutrons by the flight time, and the other is a method utilizing Bragg reflection by a monochromator such as a single crystal and multilayer mirror. The former cannot be applied for electromagnetic waves because the light velocity is constant and independent of wavelength, while “polychromators”, such as a prism and grating, separating the wavelength utilizing chromatic dispersion are often used in the range from infrared to soft x-ray. Though the polychromators require collimated beams to separate the wavelength with the enough resolution, it does not matter especially for laser and synchrotron light because they are naturally collimated. On the other hand, collimating neutrons leads to the drastic decrease in the intensity because neutrons naturally diverge from the source. This is the reason why the use of polychromators for neutron scattering instruments are quite limited: the RAINBOWS reflectometer [R. Cubitt *et al.*, *J. Appl. Cryst.* **51** (2018) 257] is the only practical example as far as the author knows. Here, we will propose a novel idea of a neutron polychromator utilizing an elliptic multilayered mirror, which can be applied for a wide beam with a large beam divergence. In the presentation, the principle of the polychromator and application examples for reflectometer and spectrometer will be shown.

### [96] Inelastic neutron scattering study of thymol as potential neutron-moderating material (board TU-272)

*Presenter: ZEPPELIN, Lukas*

Neutron moderators come in many forms and sizes with water (H2O), methane (CH4) and molecular hydrogen (H2) being the most commonly used moderating materials. These materials have very good neutron moderating characteristics but serious disadvantages as well. As a result, the active search for a new types of moderator materials, and especially cryogenic moderator materials, is underway around the world [1]. This has led to the investigation of thymol (C10H14O). Inelastic neutron scattering (INS) spectra of thymol have been recorded with the help of TOSCA neutron spectrometer [2], and the derived experimental data were compared with the theoretical calculations of the molecule optimised geometry and associated vibrational frequencies calculated with the help of Gaussian 16 software package [3]. AbINS software [4] as implemented in Mantid [5] has been used to derive theoretical INS spectra from the Gaussian output. The goal is to use this theoretical and experimental data as a framework to further clarify the moderating capabilities of thymol as well as its possible application within neutron moderators. [1] G. Skoro et

al., EPJ Web of Conferences 239, 17008 (2020). [2] S.F. Parker et al., J. Phys.: Conference Series 554, 012003 (2014). [3] Gaussian 16, Revision B.01, M.J. Frisch et al., Gaussian, Inc. Wallingford CT, 2016. [4] K. Dymkowski et al., Physica B: Condensed Matter 551, 443 (2018). [5] O. Arnold et al., Nuclear Instruments and Methods in Physics Research A 764, 156 (2014).

### [201] Effect of architecture in thermoresponsive hydrogels from PEG-based terpolymers (board TU-274)

*Presenter: ZHENG, Feifei*

The lower critical solution temperature (LCST) polymers have attracted great interest in the biomedical sectors, as they are water-soluble at room temperature, while they can form a gel at body temperature. Under the appropriate conditions, thermoresponsive polymers may form a 3D network, namely a thermoresponsive gel [1] with the mechanical properties in the gel state strongly depending on the architecture of the polymer [2]. Here we address an ABC triblock terpolymer and a BABC tetrablock terpolymer consisting of the hydrophilic oligo(ethylene glycol) methyl ether methacrylate with an average Mn of 300 g mol–1 (OEGMA, A), hydrophobic n-butyl methacrylate (BuMA, B), and thermoresponsive di(ethylene glycol) methyl ether methacrylate (DEGMA, C). Visual observation shows that ABC has a wider gelation region compared to BABC. The results from dynamic light scattering (DLS) on dilute solutions show that the hydrodynamic radii Rh of the micelles formed by both, ABC and of BABC, increase strongly above 25 °C, and the solutions feature a cloud point, i.e. aggregation of the micelles sets in. By synchrotron small-angle X-ray scattering (SAXS), it was found that, ABC and BABC form elongated and spherical micelles, respectively. Forward scattering attributed to large aggregates is observed at temperatures above the cloud point for both terpolymers. References [1] A. P. Constantinou et al., Polym. J. 2016, 78, 366. [2] A. P. Constantinou, B. Zhan et al., Macromolecules, 2021, 54, 1943.

### [15] Focusing High-Resolution Three Axis Neutron Diffractometer for Microstructure Investigations of Polycrystalline Materials (board TU-276)

*Presenter: MIKULA, Pavol*

Presented three-axis neutron diffractometer setting documents the feasibility of using it in special cases high-resolution powder diffraction studies, namely, for thermomechanical (elastic and/or) plastic deformation studies of bulk polycrystalline samples when the whole powder diffraction spectrum is not required. Contrary to the conventional double-axis setting the suggested alternative providing a much higher resolution, consists of an unconventional three axis set-up employing a bent perfect crystal monochromator and analyzer with a polycrystalline sample in between. The analysis of the profile of the beam diffracted by a sample is carried out by rocking the BPC-analyser and the neutron signal is registered by a point detector. Then, the so-called analyzer rocking curve providing a sample diffraction profile can reflect the lattice or structural changes. Moreover, much larger widths (up to 10 mm) of the irradiated gauge volumes can be investigated when just slightly affecting the resolution of the experimental setting. Finally, a feasibility of the proposal of the three-axis alternative employing PSD for strain/stress studies which could substantially decrease a long measurement time when using the step-by-step rocking curve scanning will be documented.

### [194] Deuteration at ISIS. Contributions to DEUNET and LENS (board TU-278)

*Presenter: WEBSTER, john*

ISIS deutertion laboratory has made significant contributions to the DEUNET collaboration and will further develop it's capabilities in both chemical and biological deuteration. This will in turn help deliver a roadmap for deuteration within the LENS vision.

## Zeitreisen – wie Neutronen der Archäologie helfen. Öffentlicher Vortrag von Rupert Gebhard, Direktor der Archäologischen Staatssammlung München - MW 2 001 - Lecture hall (21 Mar 2023, 19:00 - 20:30)

**-Chairs: Wolfgang Schmahl**

### [533] Zeitreisen – wie Neutronen der Archäologie helfen (19:00)

*Presenter: GEBHARD, Rupert*

Woher stammt der Kopf eines lächelnden Engels im Metropolitan Museum, wurde das Gold von Bernstorf in der Bronzezeit gefertigt oder wie haben Steinzeitmenschen Messer hergestellt? Dies sind Fragen, die Professor Rupert Gebhard mit Hilfe von Neutronen aufklärt. In seinem öffentlichen Vortrag am Dienstag, 21.3., um 19 Uhr, nimmt der Leiter der Archäologischen Staatssammlung München die Zuhörenden im Rudolf-Diesel-Hörsaal des Maschinenwesens (MW 2001) auf dem Campus Garching mit auf eine spannende Zeitreise aus der Gegenwart über die Zeit der Kelten bis hin zu den Steinzeitmenschen und erklärt, wie Neutronen den Archäologen zerstörungsfrei Auskunft über ihre Fundstücke geben. Der Eintritt ist frei. Der populärwissenschaftliche Vortrag in deutscher Sprache findet im Rahmen der Europäischen Konferenz für Neutronenstreuung (#ECNS2023) statt, die vom 20. bis 23. März in Garching vom Heinz Maier-Leibnitz Zentrum organisiert wird. Mehr als 500 internationale Forschende tauschen sich dabei über aktuelle wissenschaftliche Ergebnisse und Methoden der Neutronenforschung aus.

# Wednesday, 22 March 2023

## Plenary - MW 2 001 - Lecture hall (22 Mar 2023, 09:00 - 10:30)

**-Chairs: Dieter Lott; Marc Janoschek**

### [530] Vortices in unconventional superconductors (09:00)

*Presenter: BLACKBURN, Elizabeth*

Over thirty years ago, the high-temperature cuprate superconductors were discovered, and although many of the phenomenological tools developed to describe superconductivity could still be applied, the Bardeen-Cooper-Schrieffer (BCS) theory for superconductors was found not to work. It became clear that a Cooper pair of electrons formed, but that the superconducting energy gap had become more complicated. At the same time, other families of so-called ‘unconventional’ superconducting states were being discovered, creating a complicated landscape where quantitative predictions have proved elusive. Many varied experimental techniques have been deployed on these materials. Most of these unconventional superconductors fall into the class known as Type-II, meaning that above a certain critical field, magnetic field can penetrate deep into the material, but only in the form of lines of magnetic flux, creating magnetic vortices. This creates a network of normal (non-superconducting) state in the vortex core. These vortices are very sensitive to the nature of the superconductivity and can tell us about properties like the London penetration depth (how far magnetic field extends into the pure superconducting state) and the coherence length (roughly the size of the Cooper pair). Using neutron diffraction, we can explore how these properties vary throughout the superconducting phase of a material, and then compare with other experimental and theoretical results. In some cases, we observe unexpected deviations, and in this talk I will explore what we can conclude from this [1-3]. **References** [1] E. Campillo et al., Phys. Rev. B 104, 184508 (2021). [2] E. Campillo et al., Phys. Rev. B 105, 184508 (2022). [3] A. Cameron & E. Campillo et al., arXiv:2208:06706 (2022).

### [516] Ultracold Neutrons as powerful probes in particle physics and cosmology (09:45)

*Presenter: JENKE, Tobias*

Experiments with very slow – so-called ultracold – neutrons are a powerful probe of models of the early universe at the precision frontier. Flagship experiments with ultra-cold neutrons measure the lifetime of the free neutron and search for its electric dipole moment. Ultracold neutrons are as well excellent objects to test gravity at short distances, as they are electrically neutral, only hardly polarizable, and offer large observation times. Today, flagship experiments apply spectroscopic techniques to investigate gravity at short distances. The results are used to test various Dark Energy and Dark Matter scenarios in the lab, and to study the interplay between gravity and quantum mechanics. In my talk, I will review the experiments, explain key technologies and summarize the results obtained.

## Data Evaluation & Software 2 - SCC/0-002 - Taurus 1&2 (22 Mar 2023, 11:00 - 12:30)

**-Chairs: Andreas Stadler; Mads Bertelsen**

### [94] Euphonic: efficient inelastic neutron scattering simulations and more from force constants (11:00)

*Presenter: PERRING, Toby*

Chopper spectrometers produce large 4-dimensional inelastic neutron scattering (INS) datasets, allowing investigations of vibrational and magnetic properties of materials over large regions of momentum-energy (**Q**-E) space. While software (e.g. Horace) exist to enable visualisation and analysis of such data, computational challenges remain for the simulation and fitting of vibrational spectra, which requires the calculation of phonon frequencies and displacements at millions of **Q**-points to simulate a single 2D slice of data. Here we present Euphonic, a Python package designed to efficiently interpolate phonons and calculate INS intensities directly from force constants. Currently supported are CASTEP and Phonopy force constants, with the potential for more to be added in the future. Euphonic has a focus on performance, with key components written in C and OpenMP. The performance scaling of Euphonic means that, for example, instrument resolution convolved simulations of phonon spectra are now tractable for the first time. Euphonic is also useful as a library to the wider scientific community - providing both a Python API and command line tools. Euphonic has been developed following software best practice, is open source and can be obtained via Github, PyPI and the conda-forge Conda channel. This talk will give an overview of: the main features and benefits of Euphonic; development following the 1.0 release in August 2022; and development priorities going forward.

### [396] From molecular dynamics simulations to diffuse scattering maps (11:30)

*Presenter: KULDA, Jiri*

Modern materials often exhibit a considerable portion of structural disorder, playing a key role in their functionalities. In order to characterise local atomic arrangements and short-range correlations one has to study the shape of Bragg lines and the distribution of diffuse scattering below and between them. To extract information from experimental data one has to compare model-based intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices by a variety of approaches ranging from ab initio DFT methods via molecular dynamics (MD) to phase-field models based on the Landau formalism. With this progress in place the bottleneck has shifted from producing supercell models to generating the corresponding diffuse scattering distributions in reciprocal space. The principal issue being the fact that scattering amplitudes from a distorted lattice cannot be summed up using fast Fourier transform algorithms (FFT) because of the displacement phase factor exp(-iQR) being Q-dependent. As a consequence, many efforts in recent years have been restricted to simple models on small supercells or to more involved pair distribution function (PDF) analysis, where the summation problem is reduced to a single dimension. To address this issue, we will present the results of a new approach based on recent developments of the non-uniform fast Fourier transform algorithm [1], implemented in the MP_tools program suite [2]. Diffracted intensities from model supercells containing millions of atoms as well as dynamic scattering functions S(Q,ω) based on time sequences of thousands of frames can be addressed in an interactive manner. [1] Barnett A.H. et al., J. Sci. Comput. 41 (2019) C479-C504, https://github.com/flatironinstitute/finufft [2] Kulda J., https://github.com/jkulda/MP_tools

### [404] Refining Molecular Dynamics Simulations to Neutron and X-ray Diffraction and Spectroscopy Data (11:50)

*Presenter: REICH, Veronika*

The structure and dynamics of materials can be studied on the atomic level with neutron and X-ray scattering experiments as well as molecular dynamics (MD) simulations. We connect experimental data with MD simulations to further enhance the simulations and obtain forcefields that are able to reproduce the measured structure and dynamics. On the example of water, we establish a workflow of running MD simulations in the program LAMMPS, calculating X-ray and neutron scattering data with the program Sassena, and comparing the diffractograms and incoherent intermediate scattering functions to already published experimental data. The agreement between computed scattering curves and experimental data was optimized and the parameter distributions characterized with a Bayesian approach to obtain a set of parameters that can simultaneously reproduce the real nanoscopic structure and dynamics of water probed by the neutron and X-ray scattering experiments. This scheme is highly adaptable to different MD simulations and will be adapted to crystalline materials in the future, in particular hydrogen storage materials.

### [372] AI-assisted neutron spectroscopy - Log-Gaussian processes for TAS (12:10)

*Presenter: TEIXEIRA PARENTE, Mario*

Three-axes spectroscopy (TAS) is a well-established method that has not substantially changed in the past decades of its use. Nowadays, with increasing demand and limited availability of TAS, application of AI methods is one option to increase their efficiency. From an AI perspective, TAS experiments collect noisy observations of a 2D intensity function to investigate a material of interest. If the intensity distribution is unknown, experimenters usually decide manually where to place measurements for a rapid overview. AI methods can assist this process by avoiding measurements in the background but preferring more informative

regions of signal while taking instrument costs into account. Our method for discovering regions of signal is based on Gaussian Process Regression as a technique for probabilistic approximations of log-intensity functions. It handles noise and background and respects weak as well as strong intensities to avoid loss of information. For example, for simple dispersions like intensity-modulated phonons, full information can be achieved only within a reasonably short amount of experimental time. The algorithm was tested on simulated intensity functions (e.g., CEF, phonon, SDW) and experimentally on EIGER/PSI. In order to quantify the benefit of our approach, we present results of a benchmarking procedure that we have developed as a cost-benefit analysis in a synthetic but still representative setting.

## Engineering 2 - SCC/0-001 - Lecture hall (22 Mar 2023, 11:00 - 12:30)

**-Chairs: Michael Schulz; Markus Strobl**

### [360] Investigation of hydrogen distribution in hybrid Ti-Mg implant materials using neutron tomography (11:00)

*Presenter: KUMAR, Richi*

Hybrid implant materials consisting of a permanent Ti-based part combined with a degradable Mg part, where the Ti is used for its high strength while the temporary part is used for bone stimulation or drug delivery, are promising solutions to improve biocompatibility and stability of current implants. As Mg degrades hydrogen gas is released which ingresses into the Ti part, leading to changes in its properties. The profile of hydrogen distribution is a critical parameter for the biocompatibility and mechanical stability of Ti parts, especially in long-term applications. Macroscopic measurements by gas fusion technique showed that the profile of hydrogen absorption is not constant, with a maxima at the region between Mg, Ti and solvent contact [1]. To investigate this phenomenon on microscopic scale, sintered hybrid samples prepared using metal injection molding were subjected to saline degradation for a period of 0 to 120 hours. These samples were then characterized using neutron tomography performed at the ICON and NEUTRA instruments of SINQ (PSI, Switzerland) to study the spatial distribution (pixel size ~ 33 µm and 14 µm) of hydrogen in the Ti-part. Neutron data are in agreement with gas fusion results and additionally characterize H penetration profile normal to Ti-Mg interface. 1. Garamus, V.M. et. al. Metals 2021, 11, 527. 10.3390/met11040527

### [147] In-situ Neutron Imaging Study on Ammonia Sorbents for Novel Ammonia Synthesis Routes (11:30)

*Presenter: KARABANOVA, Anastasiia*

In 2021, the global production of ammonia was estimated at around 200 megatons, which makes ammonia the second-most produced chemical in the world. Among different ammonia synthesis routes, the most prevalent one is the Haber-Bosch process, occurring over the iron catalyst at high pressures (more than 150 bar) and high temperatures (more than 400□C). However, it has been recently demonstrated that with new types of catalysts, ammonia can be synthesized at lower pressures and temperatures, leading to significant reduction in capital and operational expenditures. To unlock the potential of this mild-condition ammonia synthesis, it is necessary to find an alternative to ammonia condensation, which, in the conventional Haber-Bosch process, is used for the cleaning of unreacted hydrogen and nitrogen (recycle gas). The promising solution can be ammonia absorption by metal halides, as these materials can efficiently and selectively remove ammonia down to ppm level, even at elevated temperatures. Within the framework of the ARENHA project (Horizon 2020, No 862482), we develop manganese chloride - silica gel sorbents to promote novel ammonia production paths. In this work, the manganese chloride – silica gel sorbents were studied using in-situ neutron imaging at the NEUTRA beamline (SINQ, Paul Scherrer Institute, Villigen, Switzerland). Two-dimensional neutron radiography images of the sorbent bed were taken during breakthrough tests, during which a gaseous mixture of ammonia and nitrogen was passed through the bed at controlled flowrate. During the tests, we could observe ammonia uptake and release within the sorbents, thanks to the high neutron scattering cross section of hydrogen. The results of the image analysis are discussed with respect to the homogeneity of the ammonia sorption over the volume of the reactive bed and how it is affected by manganese chloride loading in the sorbents. Changes in the sorbent bed dimensions and sorbent morphology during cycling are also reported.

### [163] Polarization contrast neutron imaging of magnetic phases in additively manufacturing specimens (11:50)

*Presenter: BUSI, Matteo*

Martensitic phase transitions are of utmost importance for structural and smart materials such as for example steels and shape memory alloys, respectively. Apart from destructive, local or integral methods neutron imaging techniques have been explored to spatially map and quantify martensitic phase fractions in such materials. Such techniques include neutron Bragg edge and neutron dark field imaging. However, the latter methods require long exposures to achieve suitable signal to noise ratio and can suffer from significant bias e.g. in strongly textured materials. The depolarization of a polarized incident white neutron beam when interacting with the field of magnetic domains in a ferromagnetic material is a well-known effect. In this work, we show how polarization contrast neutron imaging can be used to map and quantify ferromagnetic phases in additively manufactured samples of iron-based alloys and Fe-Mn-Si shape memory alloys. The method provides spatial resolutions significantly beyond these of conventional neutron diffraction and is exceptionally sensitive to low ferritic phase fractions. Furthermore, the method requires exposure times of only a few tens of seconds to a few minutes, making it efficient in particular for time-resolved studies, e.g. to follow the evolution of the crystalline phase transformations in response to external loads, but also for tomographic measurements with many angular projections for correspondingly high spatial resolution.

### [238] Targeted use of residual stress in electrical steel to increase energy efficiency (12:10)

*Presenter: SEBOLD, Simon*

The magnetic flux guidance in an electric engine is achieved by introducing cutouts in the electrical steel (ES) sheets that make up its core. However, these cutouts create thin structures, reducing the mechanical strength of the ES sheets and limiting the

achievable rotational speed and therefore the energy efficiency of the engine. Residual stress in ES sheets reduces the mobility of magnetic-domain walls due to the magneto-elastic effect. This effect was used to create a novel type of magnetic flux barrier relying on the local decrease in magnetic permeability introduced by embossing of the ES sheet. Such barriers show similar flux guidance as traditional barriers while the mechanical strength is comparable to unworked ES. To prove the applicability of such magnetic flux barriers in future electric drives, the performance under different external parameters was probed using neutron grating interferometry (nGI). In nGI the dark field image (DFI) maps ultra-small-angle neutron scattering as resulting from the interaction of the magnetic moment of the neutron with the magnetic domain structure in the bulk of the sheet sample. Hence, enabling the visualization of the local distribution of magnetization. In this presentation, we will give a comprehensive overview of the influence of operational conditions, such as tensile load and alternating magnetic fields (time-resolved), in an electric motor on embossed magnetic flux barriers.

## Micro Symposium CANS 1 - SCC/3-Venus - Venus (22 Mar 2023, 11:00 - 12:30)

**-Chairs: Alain Menelle**

### [156] The European Low Energy accelerator-based Neutron facilities Association (ELENA) – Current Status and Perspectives (11:00)

*Presenter: PEREZ LOPEZ, MARIO*

The European Low Energy accelerator-based Neutron facilities Association (ELENA – www.ELENA-neutron.eu) is promoting the development of Compact Accelerator-driven Neutron Sources (CANS) and High Current Accelerator-driven Neutron Sources (HiCANS) in Europe. It represents 7 projects and 8 institutions from major European countries: Italy, Spain, France, Germany, Norway, Sweden, Hungary and Israel. HBS, SONATE and ARGITU are examples of HiCANS with an instrument performance equal to or exceeding that of medium size research reactors, while LvB is a CANS project serving industry. The projects, which we develop in collaboration, are aimed at rejuvenating the European neutron ecosystem after the shut-down of major older research-reactor based national neutron sources. To cite the recent LENS – BrightnESS - ENSA position paper “Neutron Science in Europe”: “Though ESS will provide enhanced capabilities, these can only be fully exploited if the supporting ecosystem has sufficient strength, depth and diversity.” … “The only route for entirely new facilities with significant capacity are High Current Accelerator-driven Neutron Sources …” The members of ELENA strongly believe that we have to act now if we don’t want to be limited with only four major sources (ESS, ISIS, SINQ and MLZ) in the future for about 5000 European neutron users – a situation which will not allow most of these users to maintain a strong research program with neutrons. The situation is even more serious if we consider the downtimes for maintenance, technical problems and upgrades as the last years have shown, where sometimes only one of the remaining major sources was in operation. Such a situation is prohibitive for doctoral projects, where students typically need at least a few days beam times per year for three years. Having only very few sources makes the ecosystem extremely vulnerable. In this paper, an overview of the ELENA association and on-going projects is given, presenting the potential of HiCANS as an opportunity to regain a strong, diverse, and healthy neutron landscape. At ECNS the community shall be informed first-hand about these prospects in order to gather support for a rejuvenated European neutron ecosystem. **This work is part of the collaboration within ELENA and LENS on the development of HiCANS.**

### [14] Towards a new neutron source in France for materials science and industry. (11:15)

*Presenter: OTT, Frédéric*

The European landscape of neutron facilities is evolving quickly with the closure of a number of aging research reactors: for example the reactor Orphée in France, BER in Berlin and Kjeller in Norway closed in 2019. While the European Spallation Source (ESS) should start later in this decade, its capacity will not be sufficient to replace the closed facilities. Hence, the Laboratoire Léon Brillouin (LLB), operated by the CEA and the CNRS in France, is developing the technologies necessary to build a new type of neutron source using low energy proton accelerators: High Current Compact Accelerator driven neutron sources (HiCANS). We will describe the ideas driving the design of HiCANS and present the potential capabilities of such sources. Since 2018, the CEA has been engaged in an experimental research program around the IPHI accelerator and has demonstrated a number of technologies on the IPHI – Neutrons platform [1]. We will report on the recent progress in the field of neutron producing targets, the first diffraction measurements on the DIoGENE instrument and the developments around cold moderators. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. It has been funded by the "CANS Inflexion" program at the CEA and the "IPHI-Neutron" SESAME project of the Ile de France region.

### [129] The High Brilliance Neutron Source (HBS) Project for a Next Generation Neutron Research Facility (11:30)

*Presenter: BRÜCKEL, Thomas*

With very few large-scale facilities left to serve a leading community of about 5000 European neutron users in the 2030s, the European neutron ecosystem will become extremely vulnerable and capacity-limited. Neutron research in Europe risks losing its strength and diversity if limited access to neutron beam time makes it extremely difficult to maintain a sustainable research program based on the use of neutrons. High Current Accelerator driven Neutron Sources (HiCANS) are a completely new type of neutron research facility based on an innovative concept. They have the potential to rejuvenate the European neutron ecosystem and provide complementary capabilities. The High Brilliance Neutron Source (HBS) project is a highly ambitious HiCANS project characterized by cost efficiency, sustainability, reliability, resilience, easy access and flexibility. We present the concept of the HBS, discuss the physical and technical solutions for challenging components such as the high-power target, report on simulations and experimental verifications, and prototyping for all major components of the facility. The HBS features a complete set of instruments for diffraction, large-scale structural research, inelastic scattering, and high-resolution spectroscopy, imaging, and neutron analytics with highly competitive instrument performance. The Technical Design Report (TDR) provides a blueprint for construction of the facility. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [246] The neutron source system proposal for the ARGITU project (11:45)

*Presenter: SORDO BALBÍN, Fernando*

High-current accelerator-driven neutron sources (HiCANS) [2] claim to cover the gap of neutron production in Europe created by the shutdown of research reactors. The ARGITU project is one of these initiatives to build a regional neutron source in the Basque Country area (Spain). In this work, a view of the proposed facility focused on accelerator and target will be given. The accelerator is based on ESS-Bilbao ion source facility that will be upgraded with the completion of the RFQ (already on manufacturing phase) and new DTL tanks to achieve 31.5 MeV of final energy. The proton beam will target a beryllium plate cooled with water. The relative low energy of the protons minimizes the shielding requirements and thus, it allows to reduce the size of the Target station up to 2 m in diameter. The relative compact dimensions of the as well as the use of low activation materials will minimize the requirements on services like remote handling, lifting devices, cooling supply etc. Finally, the ARGITU cold and thermal moderators will be based on HBS 1-D proposal/concept (la que prefieras) [3]. The 1-D moderator proposal optimizes the coupling between target, moderator, premoderator and reflector and thus increase the efficiency of the complete moderation process. This highly efficient coupling will partially compensate the reduced efficiency of the neutron production reaction (p,Be) giving a final moderator brightness comparable with mayor facilities in Europe. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. References [1] ARGITU, Compact Accelerator-Driven Neutron Source: A Unique Infrastructure Fostering our R&D Ecosystem. CFM / BC-Materials / Ineustar / ESS Bilbao. [2] LENS Report – Low Energy Accelerator-driven Neutron Sources (2020) https://www.lens-initiative.org/wp-content/uploads/2021/02/LENS-Report-on-Low-Energy-Accelerator-driven-Neutron-Sources.pdf. [3] Conceptual Design Report Jülich High Brilliance Neutron Source (HBS) Allgemeines / General Band / Volume 8, ISBN 978-3-95806-501-7

### [345] Hot commissioning of the accelerator driven compact neutron source "LvB" (12:00)

*Presenter: MEZEI, Ferenc*

After completion of assembling the hot commissioning of the compact neutron source CANS facility “LvB” in Martonvásár will start in January 2023. The system consists of a 35 keV proton ion source, a 2.5 MeV RFQ proton accelerator a thin Li layer target, Pb reflector and bi-spectral thermal-cold low dimensional moderator, that can serve up to 8 neutron scattering instruments. In addition, a fast neutron beam will be available in the direction of continuation of the incoming proton beam. The first results of the hot commissioning work will be presented in the talk, with main emphasis on the observed characteristics of the extracted neutron beams. The concepts developed for funded plans of building up a second Lithium target for the potential of controlled irradiation capabilities for biological studies. Experience in hot commissioning shall also focus on potentials of efficiently building further similar, custom designed turnkey CANS facilities for collaborating customers.

### [319] A compact accelerator driven neutron source for Sweden (12:15)

*Presenter: WOLFF, Maximilian*

Sweden is hosting the European Spallation Source (ESS), which will be the worlds most brilliant neutron source once it is commissioned. In order to take best benefit of the capabilities of high-end facilities an ecosystem of smaller sources is required but currently Sweden has no neutron source allowing materials research. As a consequence of that the number of experts in the field has stagnated or slightly decreased, despite of the fact that the total number of occasional Swedish neutron users has increased over the past years. Currently, two projects are ongoing, the conversion of a single end 3 MV accelerator in Lund and the procurement of a commercial D-T fusion source (NESSA) in Uppsala. Both sources may provide neutron production rates on the order of 10$^{10}$-10$^{11}$, which may be sufficient for nuclear physics and detector testing but do not provide the fluxes required to serve the material science user community. A low to medium power compact accelerator driven neutron source can overcome this challenge and the development of such a facility will build on the countries strength in accelerator and nuclear physics. It will enable and facilitate long term projects, industrial research, method and technological developments as well as training and straight forward and complementary, to ESS, experiments. We will provide a summary of the current stage of planning and outline potential funding lines.

## Soft Matter Interfaces - MW 0 001 - Lecture hall (22 Mar 2023, 11:00 - 12:30)

**-Chairs: Henrich Frielinghaus; Adrian Rennie**

### [168] Looking at Buried Layers and Interphases Using Neutron and X-ray Scattering (11:00)

*Presenter: MOEHL, Gilles*

Energy storage – with its fundamental: electrochemistry - has become a key element of society. The making of cheaper, lighter and safer batteries or the synthesis of novel functional materials relies on understanding dynamic processes. Many of those take place at so-called “buried-interphases”, which require advanced characterisation techniques with high penetration depth and sufficient sensitivity in order to be investigated. This is fulfilled for neutrons and high energy x-rays, which can be used to unravel reactions and mechanisms whilst ongoing inside devices and e.g., liquid environments. Small-angle scattering is sensitive to structural changes from a couple to a few hundreds of nanometers with high statistical relevance due to the high flux beam and relatively large sample area (compared to electron microscopy). The morphology of a single-ion polymer electrolyte during cycling at high temperature was revealed by Small Angle Neutron Scattering (SANS), proving the durability of the material when used with a lithium metal anode. In reflection geometry, the average structure of thin films can be determined by Grazing Incidence Small Angle X-ray Scattering (GISAXS). This was done during the electrodeposition of mesoporous silica films in aqueous solution, allowing for the monitoring of the self-assembly process both on the electrode surface as well as the bulk solution.

### [438] Progress in organic solar cells based on advanced neutron scattering methods (11:30)

*Presenter: MÜLLER-BUSCHBAUM, Peter*

Polymer-based organic solar cells receive a growing interest and achieve a substantial progress concerning device efficiency and lifetime during the last years. Moreover, the potential low fabrication costs, fast energy payback times and the use of lightweight materials make them very appealing. In terms of champion device efficiency, values above the 18% limit were reported recently. Mainly combinations of novel low bandgap polymers and non-fullerene acceptor materials have boosted the device efficiencies. Therefore, polymer-based organic solar cells are addressed in many research groups with a very high level of attention. However, basic understanding is still very limited due to the complexity of the systems. Typically, polymer-based organic solar cells have an active layer made out of a mixture of a positive charge carrier conducting polymer and a small molecule electron acceptor material. Light is absorbed in both components. Excitons are created and split into free charge carriers in case an interface between both components is reached by the exciton within its lifetime. Thus, the morphology of the active layer of an organic solar cell has a significant influence on the final device performance. To enable a high interfacial area between the components, so-called bulk heterojunction (BHJ) geometry is realized in a self-assembly process of the materials. This bulk heterojunction geometry is optimized for exciton splitting and charge carrier transport. Using advanced neutron scattering techniques such as grazing incidence small angle neutron scattering (GISANS) enables to probe the morphology of the active layers from the molecular to the mesoscopic scale. Typically, contrast conditions are favorable as compared with x-ray scattering and allow for the detection of the intermixed phase between donor and acceptor molecules. As a result, a structure function-relationship can be established, which provides insights into fundamentals of organic solar cells.

### [466] Insights from scattering into plant based dairy products (11:50)

*Presenter: HEIDEN-HECHT, Theresia*

The importance of sustainable human nutrition is growing with the increasing effects of the climate change. Usually, emulsions systems like milk are composed of unsustainable, animal derived milk proteins, phospholipids, oil and water. To increase the sustainability of emulsion systems, milk proteins are substituted with sustainable plant proteins, whereby the stabilization mechanisms, and the long-term stability of these sustainable emulsions are of interest. A central role within the stabilization mechanisms of emulsions play proteins and phospholipids, since they stabilize the oil/water interface as interfacial active components [1,2]. Proteins and phospholipids adsorb at the interface. In addition, these components may also interact with each other and may co-adsorb at the interface, depending on their molecular structure, origin, and the pH of the environment [3]. The interfacial stabilization undergoes with reorganization of the molecular structure of proteins. Small angle scattering experiments with neutrons and x-rays allowed to study the interfacial arrangement of -Lactoglobulin as a standard milk protein, and different plant based proteins like Cruciferin from rapeseed or Rubisco, and their interaction with phospholipids at the interface. The results are leading to a systematic understanding of the interfacial properties of protein and phospholipid stabilized o/w interfaces. This knowledge will guide to a tailored formulation of food-based emulsion systems. 1. T. Heiden-Hecht and S. Drusch, Food Biophys 17.2 171-180 (2022). 2. T. Heiden-Hecht, M. L. Taboada, M. Brückner-Gühmann, H. P. Karbstein, V. Gaukel, and S. Drusch, Int Dairy J 121, 105134 (2021). 3. P. Wilde, A. Mackie, F. Husband, P. Gunning, and V. Morris, Adv Colloid Interface Sci 108–109, 63 (2004).

### [338] Using Neutron Reflectometry to study atmospheric ageing of organic surfactant aerosol proxies (12:10)

*Presenter: SKODA, Maximilian*

Atmospheric aerosol particles can be coated with organic materials, impacting aerosol atmospheric lifetime and urban air quality. Coatings of organic materials are also found on indoor surfaces such as window glass. Oleic acid is a fatty acid surfactant that is abundant in cooking and marine aerosol emissions. Under ambient conditions it can self-assemble into lamellar bilayers (stacks)

with its sodium salt. We have used neutron reflectometry (NR) to characterise the morphology of oleic acid–sodium oleate mixed films spin-coated onto solid silicon substrates and found these to form a mixed-phase film containing lamellar stacks and amorphous parts. When subjected to simulated atmospheric ageing (ozonolysis and humidity changes), we observed significant changes in structure and properties of these films (orientation of lamellar stacks, increase in film hygroscopicity after oxidation etc). Lamellar stacks, consisting only of starting materials, persisted at the end of simulated atmospheric ageing. These findings for atmospherically relevant nano-scale films corroborate previous work on micrometre-scale layers, thus demonstrating that fatty acid self-assembly could significantly increase the atmospheric lifetime of these molecules. The persistence of such semi-solid surfactant arrangements in the atmosphere has implications for the climate as well as urban and indoor air pollution. [1] Milsom et al., Environ. Sci.: Atmos., 2022, 2, 964.

## Superconductors - MW 2 001 - Lecture hall (22 Mar 2023, 11:00 - 12:30)

**-Chairs: Jitae Park; Frank Weber**

### [383] Single-domain stripe order in a high-temperature superconductor (11:00)

*Presenters: MAZZONE, Daniel, SIMUTIS, Gediminas*

The coupling of spin, charge and lattice degrees of freedom results in the emergence of novel states of matter across many classes of strongly correlated electron materials, ranging from unconventional superconductivity to skyrmions, multiferroicity, materials with a giant magnetoresistance, or hidden order states. Although, the importance of coupled degrees of freedom is widely appreciated, how this coupling is realized microscopically remains a key issue in many materials. A model example is high-temperature superconductivity, which is widely believed to arise from the coupling of electrons via spin excitations. In cuprates the interplay of charge and spin degrees of freedom is also reflected in a zoo of charge and spin-density-wave orders that are intertwined with superconductivity. A key question is whether the different types of density waves merely coexist or are indeed directly coupled. Here I will present our latest result on the prototypical high-temperature superconductor La1.88Sr0.12CuO4, where we used neutron diffraction with superior beam-focusing that allows us to probe the subtle spin-density wave order under applied uniaxial pressure to demonstrate that the two density waves respond to the external tuning parameter in the same manner [1-3]. Our result shows that suitable models for high-temperature superconductivity must equally account for charge and spin degrees of freedom via uniaxial charge-spin stripe fluctuations. [1] G. Simutis et al. Comm. Physics and arXiv:2204.02304 [2] J. Choi et al., Phys. Rev. Lett. 128, 207002 (2022) [ 3] Q. Wang et al. Nat. Commun. 13, 1795 (2022)

### [31] Universal stripe order as a precursor of the superconducting phase in BaFe2Se3 Spin Ladder (11:30)

*Presenter: BALÉDENT, Victor*

In the last years, superconductivity has been observed in a couple of iron based one dimensional compounds, BaFe$_3$X$_3$ X=S,Se. Indeed, for both compounds, a pressure induced superconducting dome develops above 10 GPa and below 14 K. A significant difference between the two systems is their magnetic ground state at low pressure. The magnetic order of BaFe$_3$Se$_3$ takes the form of staggered ferromagnetic blocs along the ladder [6], while for BaFe$_3$Se$_3$ a conventional antiferromagnetic order is formed along the ladder. These different magnetic symmetries raise the question of the role of magnetism in the mechanism leading to superconductivity. One would indeed expect a similar magnetic order for both compounds allowing a common and universal mechanism. Our recent neutron scattering results on the compounds BaFe$_3$Se$_3$ revealed a new picture of the magnetic properties from ambient pressure up to the superconducting critical pressure [[1],2]. Using single crystal and powder neutron diffraction on BaFe$_3$Se$_3$, we refined the magnetic structure at ambient pressure and discovered a new magnetic order similar to the BaFe$_3$S$_3$ stripe phase near the superconducting dome. This magnetic phase thus appear to be universal for this family, giving a strong indication of its role in the origin of superconductivity. [[1]] W. Zheng, V. Balédent et al. [Nature Communication Physics 5, 183 (2022)][1] [2] W. G. Zheng, V. Balédent et al. Accepted in Physical Review B (2022) [1]: https://www.nature.com/articles/s42005-022-00955-7

### [443] Studying the effects of trapped magnetic fields on current flow in a multifilamentary YBCO superconductor using polarized neutron imaging. (11:50)

*Presenter: QVISTGAARD, Cédric*

This study aims to investigate the changes in superconducting current flow induced by a trapped magnetic field. This is done by using polarized neutrons to image both the trapped magnetic field and the screening field induced by the current flow. The experiment was conducted at the J-PARC RADEN facility on a multifilamentary YBCO superconductor [1] with a 1T field applied along the current flow path, trapped at 5K. Measurements were performed both with and without an applied current of 1Amp. Using polarized neutrons [2] the trapped field can be directly imaged, and by assuming a local unidirectional current flow, the current can be piece-wise reconstructed from the measured screening field. The presentation will give an overview of the experiment along with data analysis procedures. As a result, the effect of screening currents on the current flow behavior and its response to a trapped magnetic field inside the current path, can be directly investigated for a better understanding of internal current flow in superconductors. [1] Wulff, A. C., Abrahamsen, A. B., & Insinga, A. R. (2021). Multifilamentary coated conductors for ultra-high magnetic field applications. In Superconductor Science and Technology (34, 5). IOP Publishing Ltd. https://doi.org/10.1088/1361-6668/abee2b [2] Takenao Shinohara et al 2017 J. Phys.: Conf. Ser. 862 012025

### [481] Composition of magnetic interactions in the heavy-fermion system CeIn3 (12:10)

*Presenter: SIMETH, Wolfgang*

We report high-resolution neutron spectroscopy on the archetypal heavy fermion material CeIn3 that exhibits an antiferromagnetic (AFM) order below TN= 10.1 K. Increasing pressure suppresses the AFM state to zero temperature resulting in a quantum critical point, the critical fluctuations of which are believed to mediate unconventional superconductivity. Previous neutron results with moderate resolution reported a substantial spin gap of about 1 meV, which suggest a substantial magnetic anisotropy, in contrast to the observed bulk properties. Our results unambiguously demonstrate that CeIn3 does not exhibit a spin gap. Instead, we find that the spin waves disperse quasi-vertically up to almost 1 meV. We show that via ab-initio band structure calculations fed into

the multi-orbital periodic Anderson model can predict the magnetic excitation spectrum quantitatively. Our results show that this model can be renormalized to a simple Kondo lattice model decorated with short-range super exchange as well as long-range particle-particle interactions to account for the formation of magnetic order. This microscopically-derived modified Kondo lattice model quantitatively reproduces the low-energy magnetic soft modes in CeIn3, which are key to understanding unconventional superconductivity.

## Functional Materials 2 - MW 2 001 - Lecture hall (22 Mar 2023, 14:00 - 15:30)

**-Chairs: Bjørn Hauback; Ralph Gilles**

### [176] Laue and time-of-flight neutron diffractive imaging methods for 3D grain mapping of polycrystalline materials (14:00)

*Presenter: LARSEN, Camilla Buhl*

For polycrystalline materials, key material properties including strength, deformation behavior, magnetic susceptibility, weldability and stress corrosion cracking resistance depend significantly on the texture of the crystalline microstructure. Conventional assessment of texture is either limited to thin surface regions or it is destructive while only probing small fractions of a bulk specimen. Only high energy X-ray diffraction at synchrotron sources and neutrons enable quantitative studies of bulk texture. Here, we report how transformative progress in advanced Laue three-dimensional neutron diffraction tomography and six-dimensional X-ray and neutron diffraction enable to map several hundred grains and, thus, allows grain orientation assessment in the volume of centimeter-sized samples with statistical significance. Laue 3DNDT is performed with short exposure times and efficient experimental processes, utilizing a white thermal neutron beam, while the 6DXND method makes use of a wavelength-resolved beam, in a time-of-flight mode, to provide sub-grain levels of information. The non-destructive nature of both methods will support in-situ studies, while future improvements in spatial resolution shall provide with more accurate grain morphology in corresponding microstructure studies.

### [444] Chalcogenides for wearable thermoelectrics (14:30)

*Presenter: FEJERCAK, Milos*

Wearable renewable energy generators are an attractive alternative to battery-based systems and can generate power up to a few Watts for portable electronic equipment. Although the most inorganic semiconductor materials are brittle at room temperature (RT) the Ag2SeTeS)1 chalcogenides show exceptional plastic deformability and high thermoelectric performance making them suitable materials for wearable thermoelectrics. In this study, we investigate ternary and quaternary Ag2(SeTeS)1 solid solutions with Se/Te doping closer to Ag2S end. A series of samples was prepared by rapid casting: Ag2S1-xSex, Ag2S1-xTex and Ag2S0.5Te0.5-xSex (x = 0.1, 0.2, 0.3, 0.4) in to form of Ø = 3 mm, 12 mm long homogeneous ingots. Significantly high ZT = 0.47 at RT was observed for Ag2S0.7Se0.3 (so far measured by Harman method). Ag2(S/Se)1 and Ag2(Se/Te)1 ternary systems crystalize in an orthorhombic or monoclinic structure, depending on the detailed S/Se, Se/Te atomic ratio. Addition of Te into these systems is introducing favorable cubic phase, as well observed in Ag2(S/Te)1 ternary middle region. Well known monoclinic – cubic phase transformation of Ag2(S/Se)1 [1] is pulled down to lower temperatures (even under RT) where it stabilizes with rising Te concentration. Highly disordered Ag atoms stay present in the cubic phase mimicking amorphous structure examined by diffraction. In this contribution we present a systematic study of Ag2(SeTeS)1 chalcogenides. Temperature induced structural phase transformations are examined by differential scanning calorimetry and synchrotron in situ diffraction. Inelastic neutron scattering investigations shed light on the compounds' phonon properties showing a phonon renormalization and broadening with addition of Se/Te to Ag2S and temperature treatment. The results are backed up by density functional theory and molecular dynamics calculations. We present data from thermoelectric characterizations carried out from RT up to 200°C. [1] Bontschewa-Mladenowa, Z. and Zaneva, K. (1977), Untersuchung des Systems Ag2Se-Ag2S. Z. anorg. allg. Chem., 437: 253-262. https://doi.org/10.1002/zaac.19774370137

### [53] Neutron scattering study on the structure-property relationship of polymer electrolyte membranes (14:50)

*Presenter: ZHAO, Yue*

Polymer electrolyte membranes (PEMs) are of great interest as solid electrolytes for applications such as fuel cells, water treatment and electronic devices. Typically, PEMs are composed of the hydrophobic polymer matrix, hydrophilic polymer chains with ionic groups. Upon hydration, ionic groups absorb water resulting in the formation of ion channels that phase-separated from the hydrophobic polymer matrix. The properties of PEMs are controlled by not only the density of the ionic groups but also the morphology and connectivity of ion channels. In this talk, we quantitatively elucidate the structure-property relationships of radiation grafted PEMs using small-angle neutron scattering (SANS) technique. Particularly, we develop the partial scattering function (PSF) analysis through contrast variation SANS, which gives the concrete structure information of individual components with locations in the membrane. PSF was for the first time used to understand the detailed structure of the benchmark material Nafion and compared to that of radiation grafted PEMs. This work provides a mechanistic insight into membrane conductivity and structure correlations. In particular, the structural guidelines at the molecular level are significant and relevant for establishing superior design rules for fuel cell membranes. This work is currently published in Macromolecules 54, 4128 (2021) and 55, 7100 (2022).

## [496] Structural and Magnetic Domains in Ni2MnZ Heusler Alloys (15:10)

*Presenter: ZWECK, Ulrike*

NiMn-based Heusler compounds show a variety of interesting functional properties such as the ferromagnetic shape memory effect or the magnetocaloric effect. The room temperature ground state structure is L$2_1$ order, while at higher temperature a state of increased entropy is preferred, corresponding to B2 order. Quenching a crystal from the B2 stable regime preserves its disordered structure while going to low temperatures, where atomic diffusion is inactive. During subsequent annealing, L2$_1$-ordered domains nucleate independently and grow, leading to a division of the crystal into anti-phase domains (APDs) [1]. The magnetic moments are mainly carried by the Mn atoms, which interact ferromagnetically in the L2$_1$-ordered state. However, it has been found that at structural anti-phase domain boundaries the magnetization tends to reverse, leading to atomically sharp ferromagnetic domain walls [1]. To study this interplay of magnetic and structural order as well as the mechanism of coupling of ferromagnetic domains across APD boundaries, we have investigated Ni$_2$MnAl and Ni$_2$MnAl$_{0.5}$Ga$_{0.5}$ powder samples in distinct ordering states via temperature-dependent small-angle neutron scattering (SANS) as well as neutron powder diffraction, giving access to the magnetic and the structural microstructure. Further, we reproduce the correlation between structural and magnetic order by Monte Carlo simulations. [1] H. Ishikawa et al., Acta Mater. 56, 4789 (2008).

## Fundamental Physics - SCC/0-002 - Taurus 1&2 (22 Mar 2023, 14:00 - 15:30)

**-Chairs: Bastian Märkisch**

### [459] Fundamental physics possibilities at the European Spallation Source (14:00)

*Presenter: SANTORO, Valentina*

Despite the success of the Standard Model of particle physics long-standing open questions remain to be understood including the nature of dark matter, baryogenesis, and leptonic CP violation. Attention is being increasingly focused on the so-called intensity frontier at which small-scale experiments make high-precision measurements of a limited number of observables or search for rare or forbidden processes. Experiments can reveal evidence for hitherto unseen high mass-scale physics processes beyond that achievable at colliders or low-rate low energy etc. from phenomena such as sterile or right-handed neutrinos and light dark matter candidates. Presently under construction, the European Spallation Source (ESS) in Lund, Sweden, will be the world's brightest neutron source [1] , as part of its mandate, the ESS will deliver a program of fundamental physics at the intensity frontier. I will present a review of the physics potential of the wide variety of fundamental physics experiments which can be performed both with neutrons and neutrinos, the latter experiments benefit from the capability of the ESS to be a high-intensity neutrino factory. Several experiments are foreseen such as precision measurements of neutron decay parameters [2], gravitational spectroscopy, searches for a non-zero electric dipole moment of the neutron, and neutrons converting to anti-neutrons [3]. Research in the neutrino sector includes coherent elastic neutrino-nucleus scattering [4] as well as possible leptonic CP violation [5]. [1] S. Peggs. ESS Technical Design Report. 2013. [2] Torsten Soldner, Hartmut Abele, Gertrud Konrad, Bastian Märkisch, Florian M. Piegsa, Ulrich Schmidt, Camille Theroine, and Pablo Torres Sanchez. ANNI - A pulsed cold neutron beam facility for particle physics at the ESS. EPJ Web of Conferences, 219:10003, 2019. doi:10.1051/epjconf/201921910003. arXiv:1811.11692 [physics.ins-det]. [3] A. Addazi et al., “New high-sensitivity searches for neutrons converting into antineutrons and/or sterile neutrons at the HIBEAM/NNBAR experiment at the European Spallation Source” J. Phys. G: Nucl.Part. Phys. 48 070501 https://doi.org/10.1088/1361-6471/abf429 [4] D. Baxter et al. Coherent Elastic Neutrino-Nucleus Scattering at the European Spallation Source. JHEP, 02:123, 2020. doi:10.1007/JHEP02(2020)123. arXiv:1911.00762 [physics.ins-det]. [5] Elena Wildner et al. The Opportunity offered by the ESSnuSB Project to Exploit the Larger Leptonic CP Violation Signal at the Second Oscillation Maximum and the Requirements of This Project on the ESS Accelerator Complex. Adv. High Energy Phys., 2016:8640493, 2016. doi:10.1155/2016/8640493. arXiv:1510.00493 [physics.ins-det].

### [312] Beam EDM - A beam experiment to search for the neutron electric dipole moment (14:30)

*Presenter: FRATANGELO, Anastasio*

The neutron Electric Dipole Moment (EDM) has attracted interest as a promising channel for finding new physics for a long time. The existence of a neutron EDM would violate CP symmetry given CPT conservation. This new source of CP violation could explain the baryon asymmetry of the universe. The BeamEDM experiment aims to measure the neutron EDM using a novel technique which overcomes the previous systematic limitation of neutron beam experiments, the relativistic vxE effect. The experiment exploits the time-of-flight technique with a pulsed cold neutron beam which allows to distinguish between time dependent and time independent effects such as the EDM. A proof-of-principle apparatus has been developed to perform preliminary measurements for the future full-scale experiment intended for the European Spallation Source in Sweden. In this presentation the details of the experimental setup together with the latest results from a data taking campaign in August/September 2020 at the PF1b beamline at the Institut Laue-Langevin in France will be presented.

### [394] Reanalysis of the of $\beta$-$\bar{\nu_e}$ angular correlation measurement aSPECT with new constraints on Fierz interference (14:50)

*Presenter: SCHMIDT, Ulrich*

Ulrich Schmidt on behalf of the aSPECT collaboration The aSPECT collaboration published in 2020 the most precise value on the electron-antineutrino correlation coefficient $a=-0.10407(82)$ of neutron $\beta$-decay. The value of this correlation coefficient $a$ is directly linked to the $\lambda$ parameter of the Weak Interaction of the Standard Model. The value for $\lambda$ obtained in this way is in tension with the most precise determination of $\lambda$ via the measurement of the neutron spin verus electron momentum correlation $A$, measured by Perkeo III. Meanwhile we revised some systematic errors and reanalysed our data including parameters from physics beyond the Standard Model like the Fierz interference term $b$. We will present the status of our reanalysis and discuss out result in the context of today most precise result on $b$ from neutron $\beta$-decay published by the Perkeo III collaboration.

### [189] Weak and Which-Way Measurements in Neutron Interferometry (15:10)

*Presenter: SPONAR, Stephan*

Neutron interferometry [1], where an interference effects of matter waves passing through a perfect silicon-crystal interferometer is observed, has established a powerful tool for investigation of fundamental quantum mechanical concepts with massive particles [2]. In this talk I will give an overview of our recent work on weak measurements [3], a new type of quantum variable introduced by Yakir Aharonov in 1988. Our neutron optical approach is realized by utilizing neutron interferometry, where the spin of the neutron

is coupled weakly to its spatial degree of freedom [4] allowing to study a new counter-intuitive phenomenon, the so-called quantum Cheshire [5], or a direct experimental verification of the canonical commutation relation [6]. In a recent experiment, we experimentally demonstrate that an individual neutron moving through a two-path interferometer is actually physically distributed between the two paths where the weak value of the path projector and is not a statistical average but applies to every individual neutron [6]. [1] H. Rauch, W. Treimer, and U. Bonse, Phys. Lett. A 47, 369 – 371 (1974). [2] S. Sponar, *et al*., Nat. Rev. Phys. 3, 309 – 327 (2021). [3] Y. Aharonov, D. Z. Albert, and L. Vaidman, Phys. Rev. Lett. 60, 1351 – 1354 (1988). [4] S. Sponar, *et al.*, Phys. Rev. A 92, 062121 (2015). [5] T. Denkmayr, *et al.*, Nat. Commun. 5, 4492 (2014). 6] R. Wagner, *et al*., Phys. Rev. Research 3, 023243 (2021). [7] H. Lemmel, *et al*., Phys. Rev. Research 4, 023075 (2022).

## Micro Symposium DEUNET 1 - SCC/3-Venus - Venus (22 Mar 2023, 14:00 - 15:30)

### [388] Deuterated Molecules From Custom Synthesis Facilities- Opportunities and Challenges (14:00)

*Presenter: DARWISH, Tamim*

The molecular deuteration of organic compounds and biomolecules is an essential requirement in many neutron scattering and other characterization techniques. This need has been increasingly recognized by neutron facilities and research groups around the world. The custom synthesis of deuterated molecules can be laborious and costly to achieve optimum chemical as well as isotopic purity. Users of deuterated molecules can have different requirements for their deuterated molecules depending on the type of experiments they are performing. This becomes particularly challenging to commercial suppliers who are driven by market demand of specific and defined products. As such, custom synthesis of deuterated molecules tailored to the neutron users' need can produce more useful deuterated products. A better choice in deuteration decisions, made in consultation between the user-scientist, the deuteration scientist, and the neutron scattering scientist, can enable cost-effective experiments that are otherwise hindered by the elevated costs of the deuterated molecules and their limited supply and availability. The Deuteration Network (DeuNet) is an international network of deuteration facilities and laboratories which aims to facilitate access to deuteration services and customised deuterium labelling of molecules and biomolecules for use in neutron research and in other characterisation techniques. This presentation will detail the recent advances, challenges, the demand and supply, and the impact of the bespoke deuterated compounds produced.

### [20] Interface structure of epoxy adhesive studied by neutron reflectometry (14:30)

*Presenter: AOKI, Hiroyuki*

Epoxy resins have been widely used as adhesives in various fields. However, the fundamental factors to determine the adhesion performance have been still unclear although adhesion techniques are actively developed from the practical points of view. In this study, neutron reflectometry (NR) with deuterated materials was conducted to elucidate the relationship between the nanometric structure of the adhesion interface and the adhesive strength. For an expoxy adhesive made from bisphenol A diglycidyl ether (DGEBA) and 1,4-bis(aminomethyl) cyclohexane (CBMA), the neutron scattering length density (SLD) profile at the adhesion interface was characterized in a humid atmosphere of heavy water, showing a large increase in SLD between the epoxy resin and the substrate. This indicates the formation of a condensed layer of water at the adhesion interface. Whereas the fraction of the water absorbed in the bulk region was only 2-3 %, the fraction at the interface was as large as 40 %. In order to prevent the formation of the water layer at the interface, we developed a multi-step curing process of the epoxy adhesive on the substrate. The structure of the adhesion layer with this process was confirmed by NR measurements using a deuterated DGEBA. As a result, the formation of the water layer was prevented even in a humid environment and the improvement of the adhesion strength.

### [244] ANSTO's National Deuteration Facility: facility overview, diversity of capabilities, user program and impact. (14:50)

*Presenter: WILDE, Karyn*

Molecular deuteration of organic compounds and biomolecules significantly increases options available in characterisation and complex structure function investigations using neutron scattering and reflectometry, nuclear magnetic resonance (NMR), mass spectrometry (MS) and other techniques by providing contrast and improved data resolution and creates functional materials with superior properties in life sciences, pharmaceutical and advanced technology applications. The National Deuteration Facility (NDF) at the Australian Nuclear Science and Technology Organisation (ANSTO), the only facility of its type in the Southern Hemisphere, provides a broad range of deuterated molecules for research and industry through both chemical and *in vivo* biological deuteration techniques. Deuterated organic molecules produced using tailored deuteration approaches provides bespoke deuterated molecules generally unavailable commercially. These include a range of lipids, unsaturated phospholipids (e.g. POPC and DOPC), heterocyclics, aromatics, surfactants, ionic liquids, saturated and unsaturated fatty acids, sugars and detergents. Isotopically labelled proteins (variably deuterated, multiply-labelled - $^2$H, $^{13}$C, $^{15}$N) and cholesterol-*d45* are produced through bacterial recombinant expression and bio-engineered yeast growth respectively. An overview and update on the NDF will be provided including details on the NDF User Program and modes of access, capabilities and selected examples of research impact.

### [136] Tail-unsaturation Enables Fine-tuning on the Rheological Properties of Sugar-based Surfactants (15:10)

*Presenter: POON, Jia-Fei*

Sugar-based surfactants are recognized as green surfactants and widely used in various applications ranged from viscosity modifier to pharmaceutical applications. However, only a scarce number of examples were reported to exhibit non-Newtonian rheological behaviour, and equally underexplored is the strategy to fine-tune the rheological profile. Our recent study shed light on this area by showing how the headgroup anomeric configuration, axial (alpha) or equatorial (beta) of hexadecylmaltoside (C16G2) influences micelle formation and structure. Small-angle neutron and X-ray scattering revealed that alpha-C16G2 forms short cylindrical micelles (contour length ca. 1000 Å), whilst beta-C16G2 assembles into very long worm-like micelles (contour length ca. 10000 Å), which prompts a closer monomer-monomer packing of the head groups as induced by hydrophobic and hydrogen

bond interactions. Herein, we report on how tail-unsaturation influences the self-assembly and macroscopic response of the system, i.e. the rheology. Importantly, we showed how the configuration (cis vs trans), the position and the types (alkene vs alkyne) of the unsaturation can be utilized to fine-tune the rheological behaviour of sugar-based surfactants. Understanding the relationship between the physical properties and the chemical structure of these sugar-based surfactants would provide us the knowledge to design novel surfactants for different applications.

## Neutron Optics (and Polarization) - SCC/0-001 - Lecture hall (22 Mar 2023, 14:00 - 15:30)

**-Chairs: Robert Dalgliesh; Peter Link**

### [268] Nested Mirror Optics – Towards a New Generation of Neutron Transport Systems? (14:00)

*Presenter: HERB, Christoph*

The advent of compact high-brilliance neutron moderators has raised the question how to efficiently extract and transport neutrons from such sources while maximizing the brilliance transfer to an instrument. Nested mirror optics (NMO) offer a viable and flexible solution for this task by circumventing the under-illumination associated with long neutron guides. A basic version, consisting of an assembly of short elliptic mirrors, is able to image a well-defined volume of beam phase space from the moderator surface onto a target, e.g., a sample or a virtual source. In contrast to neutron guides, each of the NMO's individual mirrors reflects neutrons only within a narrow range of finite angles. Due to its geometrically well-defined reflection kinematics, one can tailor the divergence and spectrum of the transported beam to the needs of an experiment by design of the NMO. The device thus provides a clean beam without depending on optical elements close to the source or the target, which leads to a number of practical advantages. Besides a presentation of the concept, we will report on experimental results obtained at the multi-purpose instrument MIRA at FRM2 with an elliptic NMO prototype. We will further present results from recent experiments at the BOA beamline at PSI, which included, among others, the imaging of two-dimensional structures. Supported by McStas simulations, we will highlight various potential applications of NMO for neutron scattering and fundamental physics.

### [257] Realization of an advanced broadband supermirror solid-state neutron polarizer for fundamental physics applications (14:30)

*Presenter: BIGAULT, Thierry*

For many experiments performed at the cold-neutrons fundamental physics instrument PF1B at ILL, the polarizer is an essential component [1]. Placed after the guide exit, it should produce a large-area, intense and well polarized “white” beam spanning a broad wavelength range (from 0.2 to 2.0nm). Until recently, a “Schaërpf-type” bender based on Co/Ti supermirrors was used, showing 98.5% polarization efficiency and about 50% transmission of "good" spin component. For higher polarization, the "crossed configuration" [2] could be used, yielding 99.7% polarization and 25% transmission. After more than 15 years of successful exploitation, the polarizer showed significant Co activation and noticeable damage of the mirrors. The present project aims at replacing the polarizer with a new one, having less operational drawbacks. The concept [3] is a more compact solid-state “V-bender”, based on Fe/Si supermirrors deposited in-house on sapphire substrates. Special care was taken to limit depolarization effects [4] and to minimize angular misalignments when stacking the mirrors. Following the concept validation with the first prototypes and measurements [5], the realization of the record-breaking [6] final device [7] will be described, including fabrication, neutron characterization preceding final installation on PF1B, and possibilities to extend the concept to other cases. 1. E.g. D. Mund & al, Phys Rev Lett 110, 172502(2013) 2. M. Kreuz & al, Nucl Instr Meth A547, 583(2005) 3. A.K. Petukhov & al, Nucl Instr Meth A838, 33(2016) 4. C. Klauser & al, Nucl Instr Meth A840, 181(2016) 5. A. K. Petukhov & al, Rev Sci Instr 90, 085112(2019); presentation ECNS 2019 6. ILL Annual Report 2020, p.78 7. A. K. Petoukhov & al, ArXiv2208.14305(2022)

### [295] Wide-Angle Solid State Polarization Analysis for MAGiC (14:50)

*Presenter: KLAUSER, Christine*

We have developed the concept of a new type of a 120º wide-angle polarisation analyser and report first results of the prototype. The analyser is based on the principle of internal reflections of magnetic FeSi multilayers in straight, 150 µm thin Si channels. This internal reflection avoids the SLD step present between air. This technique yields high transmission and produces no blind spots on the detector in contrast to current supermirror-based wide-angle analysers. A first trial has been successfully performed at the AMOR reflectometer at SINQ for wavelengths between 3 AA and 8 AA. Particular care has been paid to the design of the holding field that provides a high field of minimum 0.1 T over the complete 120º with very high uniformity in the reflection plane. The analyser is being developed for the ESS instrument MAGIC, a permanently polarised diffractometer dedicated for magnetism studies using small single crystals, by the in-kind partners LLB, FZJ and PSI.

### [370] Considerations for achieving polarization analysis for high resolution QENS (15:10)

*Presenter: BABCOCK, Earl*

Polarization analysis provides profound additions in knowledge for the field of soft condensed matter research. The ability to study dynamics of incoherent and coherent scattering contributions separately gives unique information on the cooperative vs local dynamics of a system. The JCNS is interested in exploring new instrumentation ideas as a polarization analysis upgrade to our SHPERES backscattering instrument and new ideas for the proposed High-brilliance Source (HBS). We will discuss the current concepts and simulations on ways of achieving polarization analysis for the high resolution regime, i.e \DeltaE<1\mu eV on a traditional backscattering instrument such as SPHERES at MLZ.

## Polymers and Criticality - MW 0 001 - Lecture hall (22 Mar 2023, 14:00 - 15:30)

**-Chairs: Olaf Holderer; Fanni Juranyi**

### [264] Dynamic criticality of a 3d- and 2d-Ising system made of 3-picolin/D$_2$O and antagonistic salt (14:00)

*Presenter: FRIELINGHAUS, Henrich*

After the static criticality of 3-picolin/D$_2$O and 3-picolin/D$_2$O/sodium tetraphenylborate having been identified to be of the 3d-Ising and 2d-Ising type, respectively, we investigated the dynamic criticality of the two systems using dynamic light scattering and neutron spin-echo spectroscopy. The first method yields the hydrodynamic diffusivity, while the second method observes the dynamics of the critical fluctuations. The experimental data could be interpreted in terms of the crossover function of Kawasaki with slight modifications [1], yielding a dynamic critical exponent $z$ of $0.06$ for the first system and $z\approx 0$ for the second system. The result for the first system agrees with the measured critical exponent of the viscosity $x = 0.04$ and $z = x/\nu$ ($\nu = 0.63$). The result $z\approx 0$ for the second system appears consistent with the critical exponent of the heat capacity in two dimensions [2] being zero. The observation of rather undisturbed classical random walk diffusion in the 2d-Ising system contradicts the Pomeau divergence [3] that would predict a completely different diffusion behavior at larger times [4]. We believe that the wave fronts of the charge density waves of the antagonistic salt, that take place at very large wavelengths, confine the spatial extent of the 3-picolin/D$_2$O composition fluctuations. However, this is not a very strict confinement and so the system can enter the third dimension at a typical breakout time that we would connect to the charge density waves of the system (observed by DLS). We present this paper as a combination of SAXS, SANS, DLS, NSE and viscosity measurements. To our knowledge this is the first time that dynamic criticality in a 2d-Ising system has been observed experimentally. [1] Burstyn, H. C., Sengers, J. V., Bhattacharjee, J. K., and Ferrell, R. A. (1983). Dynamic scaling function for critical fluctuations in classical fluids. Physical Review A, 28(3), 1567. [2] Anisimov, M. A. (2011). Fifty years of breakthrough discoveries in fluid criticality. International Journal of Thermophysics, 32(10), 2001-2009. [3] Pomeau, Y. (1972). Low-frequency behavior of transport coefficients in fluids. Physical Review A, 5(6), 2569. [4] Liu, B., Goree, J., and Vaulina, O. S. (2006). Test of the Stokes-Einstein relation in a two-dimensional Yukawa liquid. Physical Review Letters, 96(1), 015005.

### [100] Chain confinement and anomalous diffusion in polymer melt. (14:30)

*Presenter: KRUTEVA, Margarita*

Dynamics of polymer melts is multiscale, extending from the local monomer motion to diffusion over the distances beyond the size of the whole chain. For relatively short chains (M<Mc, Me), where the inter-chain interactions are not pronounced, the Rouse model provides a good description with physically realistic parameters of the chain dynamics. Dynamics of long or strongly entangled chains can be successfully described by the reptation model. The intermediate range of polymer chain lengths is less understood. By neutron spin echo (NSE) and pulsed field gradient (PFG) NMR we study the dynamics of a polyethylene-oxide melt (PEO) with molecular weight in the transition regime between Rouse and reptation dynamics. We analyze the data with a Rouse mode analysis allowing for reduced long wavelength Rouse modes amplitudes including sub-diffusive center of mass motion . This approach captures the NSE data well and provides accurate information on the topological constraints in a chain length regime, where the tube model is inapplicable. As predicted by reptation for the polymer center of mass mean square displacement, we found a sub-diffusive regime with an exponent close to 0.5, which, however, crosses over to Fickian diffusion not at the Rouse time, but at a later time, when the mean squared displacement has covered a distance related to the tube diameter.

### [5] Cooperative tracer chain dynamics in highly entangled polymer melts (14:50)

*Presenter: ZAMPONI, Michaela*

Using neutron spin echo spectroscopy the dynamics of short unentangled tracer chains in the melt of a highly entangled polymer matrix has been investigated [1]. Independent of the tracer chain length the center of mass mean square displacement (MSD) is sub-diffusive at short times and crosses over to Fickian diffusion at longer times. The obtained diffusion coefficients on the nm scale agree very well 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 MSD, 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. [1] M.Zamponi et al., Phys.Rev.Lett. 126, 187801 (2021).

### [253] Structure of Neat Protein Single-Chain Nanoparticles from Partially Denatured BSA by SANS (15:10)

*Presenter: MALO DE MOLINA, Paula*

Protein nanoparticles can outperform polymer nanoparticles due to their versatility, biodegradability and low immunogenicity. We have exploited our previous experience in the preparation and characterization of synthetic unimolecular single-chain nanoparticles (SCNPs) to synthesize polypeptide SCNPs based on proteins. The conformational changes due to chain folding or collapse, i.e, an increase in compactness that goes along with size reduction, are best probed with small angle scattering and in particular small-angle neutron scattering (SANS), due to high contrast and no radiation damage. Here SCNPs were synthesized

with partially denatured BSA with succinimide type linkers containing three and six methylene spacer groups. The degree of internal cross-linking was followed simply and efficiently via 1H-NMR spectroscopy. Moreover, the associated structural changes —as probed by SANS— reveal that the denatured protein has a random-coil-like conformation, which progressively shrinks with the cross-linker addition. The longer cross-linker exhibits slightly more efficiency in chain compaction, with similar reactivity at a given cross-linker concentration but a somewhat stronger size reduction. This simple and effective method is applicable to a wide range of compact proteins, which denature in urea and have appropriate reactive amino acids, leading to the synthesis of biodegradable polypeptide SCNPs for a range of applications.

## Bio-inspired Soft Matter Systems - MW 0 001 - Lecture hall (22 Mar 2023, 16:00 - 18:00)

**-Chairs: Tobias Schrader; Valeria Rondelli**

### [382] Moisture dependent phonon transport and scattering in nanocellulose (16:00)

*Presenter: ÅHL, Agnes*

Heat transport properties in solid materials are driven by the accumulative contributions of phonons spanning a wide range of mean free paths. Porous, hygroscopic, nanocellulose foams exhibit super-insulating properties, highly dependent on their moisture content, and through theoretical estimations and simulations, it has been shown that the heat transfer in such materials is dominated by phonon scattering [1], [2]. Inelastic neutron scattering (INS) is one of the most powerful tools to investigate the vibrational excitation landscape in condensed matter. This work presents an INS study, in which the phonon density of states (DOS) has been extracted for nanocellulose as a function of moisture content and alignment. Through freeze casting, particles have been aligned along the Z-axis and in the XY-plane to carry out direction-dependent measurements in order to detect possible isotropic and anisotropic character of the phonon DOS. We also investigated the effect that particle size and crystallinity have on the phonon DOS; with the longer, thinner, and less crystalline cellulose nanofibrils (CNF) being more prone to moisture sorption than the shorter and more crystalline cellulose nanocrystals (CNC). The preliminary results show that the phonon DOS increases with the moisture content for CNC and CNF aligned along the Z-axis, and a decreasing phonon DOS was observed with increasing moisture content for the particles aligned in the XY plane. [1] V. Apostolopoulou-Kalkavoura, P. Munier, L. Dlugozima, V.-L. Heuthe, and L. Bergström, ‘Effect of density, phonon scattering and nanoporosity on the thermal conductivity of anisotropic cellulose nanocrystal foams’, Sci Rep, vol. 11, no. 1, p. 18685, Dec. 2021, doi: 10.1038/s41598-021-98048-y. [2] V. Apostolopoulou-Kalkavoura et al., ‘Humidity-Dependent Thermal Boundary Conductance Controls Heat Transport of Super-Insulating Nanofibrillar Foams’, Matter, vol. 4, no. 1, pp. 276–289, Jan. 2021, doi: 10.1016/j.matt.2020.11.007.

### [471] Self-Assembly and Electrostatic interactions in Deep Eutectic Solvents (16:30)

*Presenter: JACKSON, Andrew*

In recent years many studies into green solvents have been undertaken and deep eutectic solvents (DES) have emerged as environmentally friendly alternatives in many fields, such as separation processes, metal processing, biocatalysis and electrochemistry.[1] DES are solvents obtained through the complexation of organic compounds, where the interaction between the precursors promotes a depression in the melting point that allows the mixture to remain liquid at room temperature. Moreover, through different combinations of precursors the physicochemical properties of the solvent can be tuned for particular applications. Research into DES has dramatically increased in volume and variety, especially in the last few years, as the advantages of DES in multiple processes becomes clear. Our recent studies have been focused on the ability of DES to sustain self-assembly of amphiphilic molecules. Such alternatives bring the possibility to develop new, sustainable alternatives for surfactant templating, drug delivery and preservation of bioactive molecules. Our results provide a novel approach for aggregate manipulation in the absence of water through specific and non-specific ion interactions.[4,5] Small-angle neutron and X-ray scattering, in combination with other techniques, have been used to explore the bulk behaviour of these systems. Aiming to understand the fundamentals of amphiphile behaviour in these solvents, we will present details of self-assembly with varied physicochemical properties of the solvent, amphiphile characteristics and the effects of ion-ion interaction. References [1] E. L. Smith, A. P. Abbott and K. S. Ryder, Chem. Rev., 2014, 114, 11060-11082. [2] T. Arnold, A. J. Jackson, A. Sanchez-Fernandez, D. Magnone, A. E. Terry and K. J. Edler, Langmuir, 2015, 31, 12894-12902. [3] A. Sanchez-Fernandez, K. J. Edler, T. Arnold, D. Alba Venero and A. J. Jackson, Phys. Chem. Chem. Phys., 2017, 19, 8667-8670. [4] A. Sanchez-Fernandez, T. Arnold, A. J. Jackson, S. L. Fussell, R. K. Heenan, R. A. Campbell and K. J. Edler, Phys. Chem. Chem. Phys., 2016, 18, 33240-33249. [5] A. Sanchez-Fernandez, O. S. Hammond, A. J. Jackson, T. Arnold, J. Doutch and K. J. Edler, Langmuir, 2017, 33, 14304-14314. [6] A. Sanchez-Fernandez, A. J. Jackson, S. F. Prévost, J. J. Doutch and K. J. Edler, J. Am. Chem. Soc, 2021, 143, 14158

### [19] Hydration water dynamics between DMPE (1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine) phospholipid bilayers by quasi-elastic neutron scattering (17:00)

*Presenter: RAHMAN, Md. Khalidur*

Terahertz time domain spectroscopy (THz-TDS) revealed that fast (rotational) water dynamics depend on phospholipid headgroup structure by comparing PC and PE [1], but the comparison between them for the loosely and tightly bound (translational) hydration water (HW) observed for DMPC by quasi-elastic neutron scattering (QENS) [2], is still not revealed. We have done QENS experiments on the d54-DMPE+10D2O, to observe DMPE headgroup modes. After separating the headgroup modes, we analyzed the QENS profiles of HW from the d54-DMPE+10H2O by the sum of three Lorentz functions corresponding to slow, middle speed, and fast modes. The relaxation time of the fast mode is approximately six times faster than that in DMPC estimated by THz-TDS [3]. The diffusion coefficient of the middle speed mode was the same order of magnitude as the free water, the slow mode was approximately the same as that of the loosely bound water observed in DMPC [2], while the tightly bound water was not identified because it may be embedded in the headgroup dynamics. We also found that activation energy estimated from the temperature dependence of the mean residence time of the free water in the vicinity of DMPE is significantly lower than that of

DMPC [2]. We will discuss the headgroup dynamics with Molecular Dynamics simulation results. References: [1] Hishida et al., J. Phys. Soc. Jpn. 2014, 83, 044801. [2] Yamada et al., J. Phys. Chem. B 2017, 121, 8322. [3] Choi et al., J. Chem. Phys. 2012, 137, 175101.

### [234] Understanding membrane damage during freezing using neutron scattering (17:20)

*Presenter: BRYANT, Gary*

The removal of water from biological tissue by desiccation or freezing is associated with dramatic changes to membrane structure, often leading to cellular (and organismal) death. We now understand that much of the damage to under these conditions is physical, rather than biochemical. The maintenance of membrane structure is vital for cellular function, but these structures can be affected by relatively small changes in temperature and/or hydration, leading to phase transitions, loss of semi-permeability and cell death. In nature, some organisms have evolved methods to reduce damage, including accumulation of small sugars which can reduce dehydration and encourage glass formation. By contrast, artificial cryopreservation relies on the addition of membrane penetrating cryoprotectants such as DMSO. Both types of molecules affect membrane structure, but the interactions, and therefore cryoprotective mechanisms, are different. Over the past two decades we have applied a range of scattering techniques, including SAXS, SANS and neutron membrane diffraction, to understand the interactions between cryoprotective molecules and lipid membranes. In this paper we present an overview of this research and use this to contrast the different modes of action of the two classes of cryoprotective molecules. The wider implications for our understanding of cryopreservation will be discussed.

### [480] New insights in stability of protein-based and lipid nanoparticles solutions using SANS/WANS techniques. (17:40)

*Presenter: CRISTIGLIO, Viviana*

Many pharmaceuticals products are stored as frozen solutions or in amorphous solid (lyophilized) phases to minimize chemical and physical degradation during their shelf life. However, freezing and drying per se could also destabilize proteins. There are multiple protein degradation pathways, including, e.g., oxidation, deamidation, and aggregation. Protein aggregation, in particular, can lead to undesirable immunogenic reactions, and it often represents the main destabilization pathway. In order to stabilize pharmaceutical proteins against aggregation and chemical degradation during freezing, drying, and storage, cryoprotectors and lyoprotectors are usually used, with polyhydroxycompounds (PHC) (including sugars and sugar alcohols) being the most common choice. Despite its importance for pharmaceutical applications, there is only limited information on the freezing and thawing-dependent protein/protein separation and aggregation property of therapeutic proteins. In this presentation, we will show the impact of various polyhydroxycompounds (PHCs) on the structural arrangement and on protein-protein interaction in the dried state using small/wide angle neutron scattering (SANS/WANS ) technique at D16 instrument at ILL. Similarly, we will show first SANS/WANS results of structural characterization of lipid nanoparticles (LNPs) solutions. LPNs represent a novel and promising drug delivery system and rose to prominence recently with the remarkable success of Covid-19 vaccines from BioNTech/Pfizer and Moderna. The LNP-based vaccines are stored in a frozen state (at -20 or -70 °C) and cannot be re-frozen due to a potential disruption of the PL making up the LNPs. This can be caused by freeze-induced dehydration, high local pressure as the result of volume expansion during water-to-ice transformation, and pH changes. In this study, we have studied 4-component lipid system to elucidate LNP phase transitions during freezing and thawing using SANS and WANS reproducing the same storage conditions that are used nowadays for the vaccines. These studies can give new insights in proteins and LNPs solutions stability in different pH solutions, temperature conditions, and under both aqueous and lyophilized conditions. After the recent upgrade with the new large detector on D16 instrument, the larger detection solid angle and dynamical q-range, combined with the high flux, will open new perspectives to improve our knowledge of the stability and the effect of storage conditions of pharmaceuticals following in real-time the kinetics during the freezing process. Some improvement of these kinds of measurements now possible on D16 will be shown as well.

## Bulk Magnetism 1 - MW 2 001 - Lecture hall (22 Mar 2023, 16:00 - 18:00)

**-Chairs: Astrid Schneidewind; Chris Stock**

### [222] Exploring the fluctuation-induced first-order phase transition in MnSi using neutron scattering (16:00)

*Presenter: JOCHUM, Johanna K.*

Interactions of critical fluctuations in combination with an increased phase space may drive a second order phase transition first order. Using small angle neutron scattering (SANS) and modulation of intensity with zero effort (MIEZE) spectroscopy in combination with measurements of the magnetic, thermodynamic, and transport properties, we have investigated the fluctuation-induced first-order phase transition in MnSi and Mn$_{1-x}$Fe$_x$Si and its evolution as a function of field, temperature, and iron concentration x. Combining the results of the neutron scattering data with measurements of the magnetic, thermodynamic, and transport properties, we have investigated the existence of a putative tricritical point and have established the presence of fluctuating magnetic textures with nontrivial topology at temperatures above the onset of static magnetic order.

### [447] Field-induced phase transitions in Yb$_3$Fe$_5$O$_{12}$ (16:30)

*Presenter: PEÇANHA-ANTONIO, Viviane*

Yttrium iron garnet (Y$_3$Fe$_5$O$_{12}$) has, since its discovery in 1957, fundamentally contributed to the development of important research fields such as spintronics, magnonics and hybrid quantum information systems. Iron garnets incorporating magnetic rare-earth ions are relatively less well-known, but have also been studied for their interesting spin transport phenomena, magnetoelectric properties and magneto-optical effects. Following our zero-field work on the complete spectrum of Yb$_3$Fe$_5$O$_{12}$ [1] we extend our study to understand the effect of magnetic fields on the low energy magnetic excitations of the compound. A notable observation is a magnetic phase transition that takes place when the field is applied along the <111> crystallographic directions relative to the cubic unit cell. Using new, extensive inelastic neutron scattering data, we show how magnetic fields up to 7 T influence the hybridised 4f–3d magnetic excitations of the compound, and describe how the new experimental findings may be described within the magnetic model we recently developed for Yb$_3$Fe$_5$O$_{12}$ [1]. [1] V. Peçanha Antonio et al. Phys. Rev. B **105**, 104422 (2022)

### [479] Small-angle neutron scattering of kinetically driven skyrmion lattice motion (17:00)

*Presenter: METTUS, Denis*

Skyrmions are topologically non-trivial spin textures that exhibit an exceptionally efficient coupling to spin currents, notably spin-polarized charge currents and magnon currents as observed in MnSi, FeGe, and Cu2OSeO3 [1, 2, 3]. This raises the question for the microscopic mechanisms that control the pinning of the skyrmion lattice, and how they depend on the topology, electronic structure, and disorder. We report neutron scattering measurements of kinetically driven skyrmion lattice unpinning and motion by means of Time-Involved Small Angle Neutron scattering Experiment (TISANE) [4]. By interlocking the phases of neutron pulse, sample modulation, and detector signal, the technique allows to record data without major sacrifice in intensity at time-scales down to micro-seconds and provides a direct insight on the skyrmion lattice motion. In our study we examined the unpinning process under changing field orientation for different materials including the metallic systems Mn1−□Fe□Si and the insulator Cu2OSeO3. We discuss our results in the light of methodological aspects of the TISANE technique [5] and recent theoretical predictions of walking skyrmions. [1] T. Schulz et al., Nat. Phys. 8, 301-304 (2012). [2] K. Everschor et al., PRB 86, 054432 (2012). [3] S. Zang et al., Nat. Comm. 9, 2115 (2018). [4] S. Mühlbauer et al., New J. Phys. 18, 075017 (2016) [5] D. Mettus et al., J. Appl. Cryst. (in press).

### [55] Chiral Magnons in Multiferroic Ni3TeO6 (17:20)

*Presenter: LASS, Jakob*

The search for novel materials exhibiting non-trivial properties is the main task of solid state research. Ranging from high temperature superconductivity over quantum computers, novel batteries to spintronics and multi-functional materials, this field spans a wide range of disciplines and material types. One specific field of interest within magnetism is multiferroicity where especially materials experiencing strong couplings are promising. One such material is the multiferroic Ni$_3$TeO$_6$ which undergoes a hysteresis-free first order spin-flop transition from an antiferromagnetic collinear order to an incommensurate helical structure at 8.6 T along c, sporting one of the larges magnetoelectric responses measured. This transition is controllable through both magnetic and electric field. The ordering vector jumps from (0, 0, 1.5) to (0, 0, 1.5$\pm\delta$) with $\delta\sim$ 0.18. This position is mirrored in the minima of the low field spin-wave gap and in magnetic field the gaps move linearly but in opposite directions, with a cross over around the known phase transition field of 8.6 T. We hypothesize that these magnons condense at the phase transition establishing the high field ground state and have opposite chirality. Due the crystal symmetry (R3) the three distinct magnetic Ni ions are allowed to move along c relative to each other coupling the lattice, electric and magnetic degrees of freedom. In this talk I will present our resent polarized inelastic results.

### [435] Helimagnets by disorder: its role in the high-T$_S$ spiral magnet YBaCuFeO$_5$ (17:40)

*Presenter: ROMAGUERA, Arnau*

Most of the spiral magnetoelectric multiferroics investigated in recent years are geometrically or exchange frustrated magnets with low magnetic transition temperatures. The exceptional stability of the spiral magnetic order (at T$_S$) in the layered structure of YBaCuFeO$_5$ [1,2] involves a non-conventional mechanism (“spiral order by disorder”) theoretically developed by Scaramucci et al. [3]. Using neutrons we have investigated the impact of tuning frustration through B-site disorder (n$_d$) on the magnetic spiral phase in the reference compound YBaCuFeO$_5$ [4] The influence of disorder (and only disorder) on the magnetic phase diagram is studied on a quantitative basis. The interplay between disorder, stability and the detailed features of the incommensurate spiral magnetic orders has been investigated in samples of identical composition, spanning a wide range of n$_d$ values. Three different regimes are distinguished in the YBaCuFeO$_5$ phase diagram versus disorder, which set limits to T$_S$ and the cycloidal component of the helicoidal order [4,5]. This layered structure appears as a very efficient realization of the new avenue to supply functional helimagnets at normal working temperatures. [1] M. Morin et al. Nat. Commun. 7, 13758 (2016). [2] T. Shang et al., Sci. Adv. 4, eaau6386 (2018). [3] A. Scaramucci et al., Phys. Rev. Research. 2, 013273 (2020); Phys. Rev. X 8, 011005 (2018). [4] A. Romaguera et al., Phys. Rev. Research (2022) (accepted, in press). [5] X. Zhang et al., Acta Mater. 206, 116608 (2021); J. Magn. Magn. Mater. 551, 169165 (2022).

## Imaging & Neutron Detection - SCC/0-001 - Lecture hall (22 Mar 2023, 16:00 - 18:00)

**-Chairs: Adrian Losko; anton Tremsin**

### [275] A new generation of 3He curved detectors based on the trench-MWPC design (16:00)

*Presenter: GUERARD, bruno*

Curved 3He detectors used on single crystal and powder diffractometers are among the most advanced detectors in neutron scattering science. They provide high detection efficiency, low gamma background, and high position resolution, with no parallax error in the plane perpendicular to the detector axis. 6 of these detectors are currently in operation worldwide: D19, D20, and D1B at ILL, HRPT at PSI, WAND at HFIR, and Wombat at ANSTO. Those used at the ILL have been developed in-house, while the 3 others have been developed by BNL and CERCA, which are not active anymore in this field. A new generation of curved 3He detectors is being developed by FRM-II and ILL for upgrading several instruments (D20 and D16 at ILL; DMC at PSI), and to equip new ones (XtremeD at ILL, ERWIN at FRM-II). The XtremeD and D16 detectors will be mounted on the instruments at the end of 2022, and the D20 detector in 2024. They are based on the trench-MWPC, which provides better uniformity and higher counting rate capability compared to a standard MWPC. Furthermore, the absence of cathode wires makes them easier to assemble, in particular for replacing an anode wire, as it is sometimes needed during the fabrication phase. Some results obtained on the CT2 test beam line, as well as with an AmBe neutron source, will be presented. The local counting rate measured on CT2 with the XtremeD detector is 4 kHz/mm2 (@ 10% pile-up rejection); this is 3 times better than what we measured with an equivalent MWPC.

### [454] Status and perspectives of neutron imaging at MLZ (16:30)

*Presenter: SCHULZ, Michael*

MLZ successfully operates the two neutron imaging beam lines NECTAR and ANTARES. NECTAR provides fast fission neutrons, thermal neutrons and gammas, which can be combined for multi-modal characterization of larger samples with spatial resolution down to ~100 µm. ANTARES offers a spectrum with a thermal maximum, extended towards cold neutrons, providing higher sensitivity and spatial resolutions down to ~20 µm. Together, our instruments cover a broad range of different spectra from high energy fission neutrons to cold neutrons as well as gammas and x-rays, thereby providing users with excellent capabilities to adress a large number of scientific questions. In this presentation we will give an overview of the capabilities of the instruments illustrated by selected user experiments from different fields of applications. Moreover, the MLZ neutron imgaging group has a strong focus on the development of new and advanced neutron imaging methods. We will highlight our achievements in multimodal imaging, allowing to combine the different types of radiation and spectra provided by our instruments to obtain strongly improved material characterization capabilities. Additionally, we will demonstrate our activities in neutron grating interferometry, a spatially resolved SANS technique, as well as recent developments in event-mode detection systems, thereby overcoming classical limitations in neutron detection.

### [488] Material characterisation through neutron resonance absorption spectroscopy: advances in 2D quantitative isotopic mapping at the ISIS neutron and muon source (17:00)

*Presenter: SCHERILLO, antonella*

We present novel advances in the implementation of Neutron Resonance Transmission Imaging (NRTI), a non-destructive 2D quantitative elemental analysis technique, performed at the Italian Neutron Experimental Station (INES) beamline operating at the ISIS neutron and muon source, UK. Neutron spallation sources have high epithermal neutron fluxes, which is a profitable energy range for elemental and isotopic material characterisation thanks to the presence of intense resonance structures in the neutron-induced reaction cross-sections. The NRTI technique is based on the absorption in the sample of incident epithermal neutrons whose energy correspond to the one of absorption resonances, resulting in a transmitted neutron beam containing dips univocally related to the elemental composition. With a position sensitive neutron detector it is therefore possible to obtain 2D radiographies of the sample. However, in contrast with standard neutron radiography, through NRTI it is possible to obtain the distribution of elements and isotopes by selecting a resonance of interest, enhancing the contrast between elements with similar neutron attenuation coefficients. This striking features of NRTI make it suitable for the characterization of inhomogeneous samples, in particular but not limited to Cultural Heritage studies. Potential applications of NRTI will be presented with particular examples of archaeological sample characterisations.

### [399] Energy Resolved Time of Flight Imaging at the High Intensity Short Pulsed Neutron Instrument n_ToF at CERN (17:20)

*Presenter: BACAK, Michael*

Neutron radiography plays an important part in the diagnostic repertoire of nondestructive inspection techniques providing information of the inner part of an object often not accessible by any other means. Since the start-up of n_TOF's second experimental area (EAR2), the possibility of diversifying the capabilities of EAR2, profiting from a high instantaneous neutron flux, were exploited. First results with conventional neutron imaging have been published and showed a reasonable performance of the facility with respect to flux and resolution. The potential use of energy resolved neutron imaging was not exploited but the facility's

usefulness for imaging of highly radioactive objects proved valuable. The recent upgrade of the n TOF spallation target resulted in an increased neutron flux, which, combined with the rise of commercially available time-of-flight imaging detectors, opens the possibility to explore energy resolved neutron radiography at n_TOF EAR2. Here, we present recent results in utilizing a high spatial and temporal resolution time-of-flight imaging setup at EAR2, including absorption resonance imaging, Bragg-edge imaging and first data to compare experiments with simulations for a wide range of neutron energies at n_TOF.

### [256] Development of neutron detectors with solid converters and Timepix3 readout (17:40)

*Presenter: GÜRBÜZ, Saime*

Increasing demand for neutron detectors and the shortage (rise of the cost) of the Helium-3, opened a new era for using solid neutron converters. Our group at the University of Bonn is developing three different types of detectors by combining solid converters with high spatial and time resolution of a Timepix3-based readout. They are all thermal neutron sensitive. One of the detectors is based on a neutron-sensitive Micro Channel Plate (MCP). It is ideal for time-resolved imaging applications. The MCP, which also acts as an amplification stage, is Boron and Gadolinium enriched. Four Timepix3 ASICs are employed for reading out the signal. The other two detectors are gaseous detectors that aim for event-by-event high-precision measurements of space and time of the conversion point. Both detectors use boron-rich conversion layers. One is based on the Time Projection Chamber (TPC) principle with a GridPix readout for high-precision measurement, while the other is a multi-layer GEM-based detector, ideal for high rates. In this talk, the working principles and development stages of these three detectors with state-in-art readout electronics will be presented.

## Micro Symposium DEUNET 2 - SCC/3-Venus - Venus (22 Mar 2023, 16:00 - 18:00)

### [54] DEMAX: The Deuteration and Macromolecular Crystallization Support labs for the European Spallation Source. (16:00)

*Presenter: FISHER, Zoe*

For small angle neutron scattering (SANS), neutron reflectometry (NR), and neutron protein crystallography (NPX), using deuterated samples has numerous benefits. The molecules that are of most interest include proteins, lipids, fatty acids, small organic molecules, surfactants, and membranes. For SANS, NR deuteration is most commonly used to enable contrast variation, allowing scientist to selectively “match out” components of complexes. In NPX deuteration is used to boost weak signal-to-noise ratios, reduce the incoherent background due to hydrogen, improve neutron scattering length maps, and enable direct visualization of hydrogen bonds and solvent networks. DEMAX is the ESS Deuteration and Macromolecular Crystallography support lab for chemistry, soft matter, and life science users of the European Spallation Source (ESS). DEMAX support will be available to all users of ESS instruments and includes chemical deuteration, biological deuteration, and large protein crystal growth. We offer service for specific classes of deuterated inorganic or organic small molecules (e.g. pyruvate, trehalose, lactic acid), deuterated biomass/crude lipids/proteins, and access to our crystallization labs for large crystal growth. Access to DEMAX support is managed through a peer-reviewed, proposal-based system and is currently free of charge to user upon acceptance. For more details or information, researchers can contact us at demax@ess.eu.

### [12] Protein Production Sweden (PPS) and biological deuteration (16:15)

*Presenter: KNECHT, Wolfgang*

Protein Production Sweden (PPS; [www.gu.se/pps][1]) is a new national research infrastructure established in 2022 and focused on the production and purification of protein reagents for primarily Swedish researchers, both from academia and commercial entities. Well-established protein production platforms from five universities (the University of Gothenburg (host), Karolinska Institutet, KTH Royal Institute of Technology, Lund University, and Umeå University) collaborate to form the infrastructure and offer expert competence in 4 geographically distributed nodes (Gothenburg, Lund, Stockholm, Umeå). Researchers across Sweden can get access via a joint entry-point and have the possibility to get support based on their research needs throughout the whole process of protein production and purification, starting from project counselling and design to quality control, or for any single/multiple step(s) in the process. PPS does allow protein expression in 6 different expression systems (*E. coli*, *P. Pastoris*, Insect cells (BEVS), Plant cells, Mammalian Cells and Cell free expression). It also offers two Gateway modules, with one aiming at producing speciality reagents for use in X-ray crystallography. The other one aims at producing speciality reagents for and offer guidance to their use in neutron scattering experiments. (Per)deuteration of proteins is essential for neutron techniques such as neutron protein crystallography, neutron reflectometry and small angle neutron scattering. This module is thereby aiming to enable non-experts in protein production to get recombinant proteins fit for neutron scattering experiments. [1]: http://www.gu.se/pps

### [299] Deuteration Service for Users of the MLZ Neutron Scattering Instruments (16:30)

*Presenter: ALLGAIER, Jürgen*

In order to provide users of the neutron scattering instruments at the MLZ with the appropriate partially or fully deuterated materials, JCNS has started last year a deuteration service, primarily from our core competences of polymers, ethoxylation and organic synthesis. Based on our long standing expertise in synthesizing soft matter materials, we offer the deuteration of various polymers, surfactants and a variety of small molecules. In this presentation, some recent advances will be presented, which includes the synthesis of deuterated thermoresponsive polymers from the acrylate, methacrylate and vinyl families. In addition we have now implemented the technologies to produce the whole range of polyethylene glycols starting from very low molecular weight oligomers up to ultrahigh molecular weight polymers. Ethoxylation technologies also play the key role for the synthesis of many non-ionic surfactants. Recent advances include the synthesis of monodisperse alcohol ethoxylates, Span and Tween surfactants. In the latter case we implemented a completely new synthesis procedure, which allows to selectively deuterate all building blocks, the sugar moiety, the EO chains and the fatty acid units.

### [71] Recent highlights and perspectives on chemical deuteration activities in CROSS (17:00)

*Presenter: AKUTSU, Kazuhiro*

Since 2017, CROSS D-Lab has been developing and operating equipments for J-PARC users to perform chemical deuteration and analysis of D-labeled molecules. So far, aromatic compounds, ionic liquids, and other organic molecules have been deuterated using heterogeneous platinum-group catalysts under hydrogen gas-free conditions, and these molecules have been used in neutron experiments at J-PARC MLF. Additionally, physical and chemical analysis methods such as NMR and elemental analysis have been under development for the analysis of the chemical and isotopic purity of D-labeled molecules. Recently, research on heavy water recycling systems meeting the requirements of the economy and ecology has been carried out with a Japanese company. As a result, the cost of the deuterium labeling has been decreased by the recycling technique. In this presentation, we will show in detail recent highlights and perspectives of chemical deuteration activities in CROSS D-Lab.

### [478] Tuning the Nano Structures of Micellar Aggregates through a New Group of Surfactants, as Studied by SANS and SAX (17:20)

*Presenter: LI, Peixun*

Cationics are widely used for various applications, e.g. fabric softening, antimicrobial action, oilfield applications and pesticides, all of which involve the strong interaction of the cationic group with an oppositely charged surface. Their role would be considerably widened if the nonionic ethoxylate grouping could be reliably and accurately attached to the cationic group as it can for anionic surfactants. The incorporation of nonionic hydrophilic groups with anionic groups is particularly effective in that the nonionic groups improve solubilization, lower the Krafft point, and mitigate the effects of higher valence ions on aggregation or precipitation. Part of this pattern of behaviour seems to be that such surfactants show a tendency to form complex layers at the air water interface, e.g. multilayers, as formed by the alkyl ethoxy sulfonates. We have successfully synthesized a novel category of cationic surfactants, which incorporated a substantial fraction of nonionic ethylene oxide groups in a configuration where two ethylene oxide groups of nearly equal length and a single group are attached to the quaternary nitrogen The new method of making the ethoxylated cationics makes it possible to combine relatively precise amounts of EO as a pair of chains of close to equal length with a final single EO to create the cationic charge and hence to tune the amphiphilicity reasonably accurately. The self-assembly of this series cationic surfactants and its precursors, non-ionic surfactants has been investigated by small angle neutron and small angle X-ray, respectively. What we found is the micelle size of the cationic charged micelles has smaller size than the corresponding non-ionic micelles, and the size of their mixture is lower than non-ionic surfactant but is higher than cationic one. This may provide a simple and controllable methodology to tune the Nano structure of surfactant aggregates using a mixture of cationic and non-ionic surfactant ‘homologue’.

### [306] Deuterated Acryl- and Methacrylamides as Monomers for Thermoresponsive Polymers (17:40)

*Presenter: SCHWÄRZER, Kuno*

In order to provide users of the neutron scattering instruments at the MLZ with the appropriate partially or fully deuterated materials, JCNS has started last year a deuteration service, primarily from our core competences of polymers, ethoxylation and organic synthesis. Among the most requested building blocks for deuteration are monomers for the synthesis of thermoresponsive polymers from the acrylate and methacrylate families. In this presentation we will show our previously established route towards the synthesis of deuterated acryl- and methacrylamides. This procedure was utilized in the synthesis of fully deuterated N-isopropylmethacrylamide (NIPMAM), which was then employed by an MLZ-user for the preparation of partially deuterated microgels for SANS measurements. In addition, we established a new efficient synthetic route towards deuterated N-isopropylacrylamide (NIPAM) from relatively cheap commercial precursors in only two steps. This route combines a Ritter reaction with a ruthenium-catalyzed proton-deuterium exchange and can be used to selectively deuterate the isopropyl group, the double bond or the entire molecule.

## Source Materials - SCC/0-002 - Taurus 1&2 (22 Mar 2023, 16:00 - 18:00)

**-Chairs: Paul Zakalek; Jeroen Plomp**

### [510] A novel concept of staircase neutron moderator (16:00)

*Presenter: KONIK, Peter*

Cold neutron moderator design evolution has led to two main solutions. Flux-hungry instruments using large samples and limited angular resolution require a large bright surface and are better served by the LD2 moderators. Brilliance-hungry instruments using small samples and requiring a fine angular resolution are best served by L-pH2 moderators with sizes exactly matching the required. However, flux-hungry instruments do not enjoy high brilliance of L-pH2 flat moderators. Moreover, even brilliance-hungry instruments do not fully exploit potential of increased brilliance because for smaller moderator sizes beam intensity is significantly reduced. In the case of compact or spallation neutron source several cold moderators can be installed, each geometrically adapted to specific instrument needs. More issues arise when the neutron source has only one cold moderator, as it is typical for research reactors. Compromises required in such situation potentially reduce the overall performance of the whole instrument suite. In the present report we discuss in details a novel concept of a staircase pH2 moderator, which is made of a narrow elongated moderators having a high brightness (1), thus combining both high brilliance and high flux. This eliminates the need to compromise and paves the way to increased brightness (by factor 2-3) for the majority of cold neutron instruments. This approach can be potentially exploited for thermal moderators as well. [1] A.Ioffe, P.Konik, K.Batkov. "High-brilliance and high-flux neutron cold source based on elongated rectangular moderators", submitted to this conference.

### [449] Neutron experimental performance testing of low-dimensional cold moderators (16:30)

*Presenter: ROSTA, László*

A major milestone in cold neutron moderator developments has been the invention of low-dimensional geometries [1], such as the butterfly moderator of ESS. Monte-Carlo simulations have shown that if para-hydrogen is used as moderator material, these novel moderators can increase significantly the brightness, desired by most types of neutron instruments. Various designs were extensively studied by simulations, however, few experiments are available to validate them. Difficulties in experimental investigation of moderator properties can be overcome by the dedicated Test Facility installed at a radial channel of the 10 MW Budapest reactor [2]. This beamline is looking directly on the reactor core; thus an unusually hard neutron spectrum is available. The beam hits a Be plate installed in a Pb reflector placed close to the channel exit. Neutrons scattered by this Be are slowed-down in the cryogenic moderator cell tested, which is also installed in the Pb block. Cold neutrons leaving the moderator assembly (e.g. a tube-type vessel filled with liquid p-hydrogen) through a collimator are measured by a camera obscura system with time-of-flight option [3] using a chopper. This system enables to measure the spatial and spectral distribution of neutrons emerging from the moderator, thus its various features are characterized. [1] Mezei F et al, J.Neutron Research, 17, 101-105 (2014). [2] Rosta L, Applied Physics A 74, 52-54 (2002); [3] Füzi J et al, Physica B; 385-386, 1315-1317 (2006)

### [66] A new scattering kernel for superfluid helium (17:00)

*Presenter: GRANADA, Rolando*

We present the development of a model to describe the interactions of neutrons in normal and superfluid He-4 at temperatures below 2.17 K. The model was constructed based on the separation of the single-phonon and multi-phonon excitations at low temperatures. Below around 3.4 Å-1, the single-phonon excitations are described exactly by the dispersion relation, while the multi-phonon excitations and the single-phonon excitations above this limit, are included using the phonon expansion approach in the Gaussian approximation. A frequency spectrum, derived from the experimentally observed phonon-roton excitations, is used throughout the calculation, except of course in the single-phonon term over the momentum transfer range where the quasiparticle dispersion curve exists. The model can be used to calculate UCN production from down scattering processes, as the exact dispersion curve is included, and can also be used for the design of optimized target/moderator geometries at a neutron source as the first and second sum rules are well satisfied. We have modified the software NJOY to include this description, making it possible create thermal scattering libraries in the ACE format to be used in Monte-Carlo simulation of the production of ultra-cold neutrons from He-4.

### [51] Inelastic neutron scattering in pursuit of interesting neutron-moderating materials (17:20)

*Presenter: RUDIC, Svemir*

The way to identify and characterize potentially interesting neutron-moderating materials is to measure their neutronic properties: vibrational density of states (VDoS) and total cross-section. The idea behind the VDoS measurements is to look for low energy vibrational modes that can enable efficient moderation of neutrons in the so-called cold energy region. TOSCA instrument [1] at the ISIS is an indirect-geometry inelastic neutron spectrometer optimized for high resolution vibrational spectroscopy in the energy transfer region between -24 and 4000 cm-1 which makes it a perfect tool for the determination of VDoS of moderator material candidates in the cold region such as Triphenylmethane [2] or solid methane[3]. In this work, the measurements of VDoS of a number of hydrocarbons, which can be of interest for neutron moderation, will be described. The candidate materials have been chosen if they satisfy the following conditions: they have relatively high proton density (one of the main requirements for a good moderator); they have benzene ring(s) - this could imply that they are less prone to radiation damage; they are liquid at room

temperature and solid at the cryogenic temperatures (so relatively easy for operation). Using these criteria the following materials have been chosen: para-cymene (C10H14), thymol (C10H14O), mesitylene (C9H12) and toluene (C7H8). Mesitylene and toluene have been extensively studied in the moderator development work at JINR Dubna [4] but the idea here was to compare a mixture of mesitylene and para-cymene with a mixture of mesitylene and toluene under different cooling and annealing conditions for different fractions of the mixture constituents. [1] R. Pinna et al., Nuclear Inst. and Methods in Physics Research, A 896 (2018) 68–74. [2] G. Škoro et al., EPJ Web of Conferences 239, 17008 (2020). [3] R. Granada, Talk at the Workshop on Very Cold and Ultra Cold Neutron Sources at the ESS, Feb 2022. [4] I. Natkaniec et al., Physica B 350 (2004) e651–e653.

### [350] Clathrate Hydrates as Novel Moderator Material for Sources of Very Cold Neutrons (17:40)

*Presenter: CZAMLER, Valentin*

Clathrate hydrates [1] are water-based solids with large unit cells which show promise as moderators for use in the development of new and more intense sources of very cold neutrons (VCN). Such sources have the potential to enhance existing neutron scattering techniques as well as to increase the reach of particle physics experiments employing beams of slow neutrons The moderation potential of clathrate hydrates lies in their low energy modes, which are a consequence of the ability of these so-called inclusion compounds to host guest molecules in cages that are formed by networks of hydrogen-bonded water molecules. Of particular interest is a binary clathrate hosting oxygen and tetrahydrofuran (THF) as guest molecules. The molecular oxygen provides an additional path for neutron slowdown [2]. We present here, the results of an extensive experimental campaign with the aim of characterizing all relevant properties of deuterated clathrate hydrates for moderator applications. This includes, measurements of the temperature-dependent dynamical structure factor $S(q,\omega)$ in absolute units, neutron diffraction measurements and time-of-flight transmission experiments. These data serve as a baseline for NCrystal [4] scattering kernels, within the HighNESS project [5]. **References** [1] A. K. Sum et al., Ind. Eng. Chem. Res. 48 7457 (2009). [2] O. Zimmer, Phys. Rev. C 93, 035503 (2016). [4] X.-X. Cai, T. Kittelmann, Comput. Phys. Commun., 246, 106851 (2020) [5] V. Santoro et al., arXiv:2204.04051v1 (2022).

# Thursday, 23 March 2023

## Plenary - MW 2 001 - Lecture hall (23 Mar 2023, 09:00 - 10:30)

**-Chairs: Thomas Brückel; Jonathan White**

### [517] Spin-orbit excitons in transition metal oxides (09:00)

*Presenter: STOCK, Chris*

Transition metal ion compounds that have an orbital degree of freedom have recently been the focus of much attention owing to the importance that spin-orbit coupling plays in the creation of new phases and excitations. We will outline a series of scattering studies illustrating the role that neutrons have in characterizing spin-orbit physics in transition metal compounds. Particular focus will be given to third-row transition metal ions where spin-orbit coupling is of a similar energy scale to symmetric exchange coupling and distortion terms in the magnetic Hamiltonian. We will outline a formalism to understand these excitations based on single-ion physics which, due to the spatially diffuse nature of orbitals, we term spin-orbit excitons. This approach treats single-ion physics, exchange, and distortion terms equally and we will discuss examples applied to compounds containing V3+, Fe2+, and Co2+ containing materials. References:Phys. Rev. B 98, 024415 (2018); Phys. Rev. B 100, 075143 (2019); Phys. Rev. B 102, 245119 (2020); Phys. Rev. B 104, L020411 (2021); Phys. Rev. B 106, 054431 (2022)

### [519] Disclosing the unknown deep inside biomembranes (09:45)

*Presenter: RONDELLI, Valeria*

Cell membranes are complex objects made by several different molecular species. One of their most significant complexities is compositional asymmetry, key factor claimed to be associated to functional and structural roles. Nonetheless, membranes asymmetry is often hard to be reproduced in mimics. Experimental models, bearing forced membrane leaflets asymmetry in the form of dispersed aggregates in solution or of single supported bilayers, have been developed to be suitably investigated by complementary techniques such as scattering and reflectometry of neutrons and X-rays and calorimetry, to link their thermotropic behavior to their structuring on both the colloidal and the local scale in different environments. The possibility to create and study customized systems mimicking different cell membrane portions is indeed the way to the detailed structural investigation of a variety of specific molecule-membrane interactions, being also potentially predictive of the fate of extracellular bodies, macromolecules and nanodrugs intended to cross the extracellular medium and eventually enter cells.

## Bulk Magnetism 2 - MW 2 001 - Lecture hall (23 Mar 2023, 11:00 - 12:30)

**-Chairs: Denis Mettus; Kristiaan Temst**

### [314] Control of the emergent inductance in helimagnet YMn6Sn6 via Tb substitution (11:00)

*Presenter: WHITE, Jonathan*

The ac current-driven motion of spiral spin textures was shown to give rise to emergent electric fields that provide functionality as an electrical inductor - the so-called emergent inductance phenomenon [1-2]. Most recently, the first such system to display this phenomenon beyond room temperature was identified to be the helical magnet YMn6Sn6 [3]. To deepen the microscopic understanding of emergent inductance and optimise the materials conditions for its realisation, we report the investigation of the effect of partial substitution of Y by Tb. By both small angle neutron scattering and inductance measurements, we reveal that the pinning effect due to Tb doping selectively and largely suppresses the negative component of emergent inductance. In contrast, the positive component is left largely in tact. We find that the latter component can be hosted by both spin helical order, and even a spin-collinear antiferromagnetic structure in the presence of pronounced spin fluctuations. From our observations we extract empirical rules for the selection of either positive or negative emergent inductance effects in short period magnets. [1] N. Nagaosa, Jpn. J. Appl. Phys. 58, 12090 (2019). [2] T. Yokouchi et al. Nature 586, 232 (2020). [3] A. Kitaori et al. PNAS 118, e2105422118 (2021). [4] A. Kitaori, J.S. White et al., submitted (2022).

### [434] Complex magnetic orders and the emergent topological Hall effect in the kagome metal ErMn$_6$Sn$_6$ (11:30)

*Presenter: ZHOU, Yishui*

Following the discovery of a quantum-limit magnetic Chern phase in TbMn$_6$Sn$_6$ [1], and the observation of a large topological Hall effect (THE) related to the field-induced magnetic phases in YMn$_6$Sn$_6$ [2], the magnetic topological metal series RMn$_6$Sn$_6$ (R=Gd-Yb, and Y, Lu etc.) [3], that possess an ideal kagome lattice of Mn, have emerged as a new platform to explore exotic states and novel functionalities. We have recently carried out the growth of high-quality single crystals of the magnetic kagome metal ErMn$_6$Sn$_6$ via the flux method, and the physical properties characterizations via the magnetic susceptibility, heat capacity and Hall conductivity measurements. We have also undertaken comprehensive neutron diffraction experiments on both single-crystal and powder samples at the WISH diffractometer at ISIS. A number of distinct magnetic ordered phases, including the spiral, conical and *k* = 0 magnetic orders, have been identified in cooling to low temperatures. Furthermore, we have also observed a range of complex field-induced magnetic phases, including the multi-k non-coplanar magnetic orders, via field-dependent single-crystal neutron diffraction at WISH. We have found that these complex field-induced magnetic phases are directly associated to our observed THE over a wide phase space of field and temperature in this compound. Our study has clearly hinted a fascinating interplay between topologically non-trivial electronic band structures, magnetism and electronic correlations in ErMn$_6$Sn$_6$. [1] J. X. Yin, *et al*., Nature **583**, 533 (2020). [2] N. J. Ghimire, *et al*., Sci. Adv. **6**, eabe2680 (2020). [3] W. Ma, *et al*., Phys. Rev. Lett. **126**, 246602 (2021).

### [344] Neutron diffraction in MnSb2O6: Coupled chiralities in a polar magnet (11:50)

*Presenter: CHAN, Edmond*

Multiferroic materials have been intensively studied these last decades for their interesting physics and their promising magnetoelectric applications [1]. Materials having a crystallographic chirality are particularly interesting in the sense that their structure couples to magnetism and can display novel magnetoelectric coupling. This is the case of MnSb$_2$O$_6$ which crystallizes in *P* 321 space-group. The Mn atoms form a triangle in the unit cell, where the magnetic moments are dephased by 120° and follow a cycloidal modulation along the *c*-axis [2]. The sense of rotation of the spins are so-called magnetic chiralities and directly linked through Heisenberg interactions to the structural chirality, defined as the helical winding of super-super-exchange pathways along the *c*-axis. Due to the presence of 3-fold magnetic domains below T$_N$=12 K, this compound was predicted to have a unique switching mechanism, which was explained by an ambiguous magnetic ground state [3]. By a combination of unpolarized and polarized neutron diffraction techniques, we have extensively studied both the nuclear and magnetic structure of MnSb$_2$O$_6$ where we found a mixture of chiral structural and magnetic domains. We subsequently propose a mechanism leading to electric polarization based on coupled structural and magnetic chiralities. [1] S. W. Cheong et al. Nature Mater 6, 13 (2007) [2] R. D. Johnson et al. Phys. Rev. Lett. 111, 017202 (2013) [3] M. Kinoshita et al. Phys. Rev. Lett. 117, 047201 (2016)

### [282] Chemical Tailoring of Double Exchange in Mixed Valence Diiron Molecules (12:10)

*Presenter: CHRISTIANSEN, Rasmus Tang*

Molecules are promising building blocks for future generations of functional materials. A particularly interesting niche are molecules that contain metal-ions in different oxidation states, since double exchange can contribute to the molecular magnetic properties in addition to conventional Heisenberg exchange. The most promising prospect coming from competition between

these exchange mechanisms are molecules that switch from a low-spin to a high-spin ground state when an electric field is applied [1]. However, the mechanisms that govern double exchange in molecules are poorly understood and the full potential of mixed valence molecules is not realised. We have studied a series diiron Fe$^{II}$/Fe$^{III}$ molecules with S = 9/2 ground states using inelastic neutron scattering (INS) and high-field electron paramagnetic resonance (HF-EPR). These techniques probe the energies of spin excited states and the crystal field-induced splitting within the ground state manifold, respectively, giving complete information about the spin dynamics. Comparison of experiments with simulated INS and HF-EPR spectra, calculated from parametrised Hamiltonian models, allowed us to quantify the influence of bridge functionalisation and capping ligand chirality on the exchange and crystal field parameters. Thereby, we have shown the potential for INS and HF-EPR to collaboratively unveil the mechanisms governing double exchange in molecules. [1] C. S. Bosch-Serrano *et al.*, *ChemPhysChem.*, 13, 2662 (2012)

## Cultural Heritage - SCC/0-001 - Lecture hall (23 Mar 2023, 11:00 - 12:30)

**-Chairs: Christian Stieghorst; László ROSTA**

### [237] Neutron imaging applications in cultural heritage at ISIS (11:00)

*Presenter: SCHERILLO, antonella*

Scientific investigations and archaeometric studies have played a major role in the field of archaeology, especially with regard to materials that have been transformed through human activity, like metals. In this talk, I will give an overview of how neutron imaging can be useful to improve our knowledge of ancient manufacturing processes of metals, their technological evolution over the centuries, and how they degrade over time. Neutron imaging techniques are used to shed light on the inner structure of composite materials and their manufacturing techniques, but also can be used for elemental investigations. In addition, the combined use of X-rays and neutrons provides additional element-dependent information which is fundamental in case of multi-phase objects. The talk will give an overview of the imaging case studies carried out at the ISIS Neutron and Muon Source in the field of Heritage Science, spanning from Roman coins to Egyptian artefacts.

### [339] A non-destructive quantitative determination of the crystalline phase content in historical mosaic glasses through Time-Of-Flight Neutron Diffraction (11:30)

*Presenter: MARCUCCI, Giulia*

Time-Of-Flight Neutron Diffraction (TOF-ND) analysis was performed to obtain a quantitative identification of the mineralogical phase composition of historical mosaic glasses. The presented work is part of a multi-technique characterisation of such mosaic tesserae with the aim of obtaining a detailed quantitative description of the elemental and phase composition in a completely non-destructive way. In fact, in the Cultural Heritage research field, non-destructiveness is mandatory to prevent damage of unique archaeological objects during a scientific investigation. Neutron-based analyses are a profitable tool to study the bulk of specimens, especially when superficial or spot measurements on heterogeneous samples (such as the mosaic glasses) return position-dependent results. As neutrons can penetrate deep into the material, they can be exploited to determine and quantify the glass composition averaged over the bulk. However, no works related to the application of TOF-ND to historical mosaic glasses are currently in the literature. Therefore, an attempt to quantitatively extrapolate the crystalline phase content within the amorphous matrix from the neutron diffraction data using the Rietveld analysis method will be presented. TOF-ND results will be discussed and compared to the information obtained through a previous combination of Raman spectroscopy investigation, Ion Beam Analysis, Neutron Resonance Capture Analysis and Prompt Gamma Activation Analysis.

### [426] Application of small angle neutron scattering to investigate archaeological pottery production technologies (11:50)

*Presenter: LEN, Adél*

For the examination of the pottery forming techniques, two series of experimental vessels have been made with three different, historical forming techniques (coil-building, wheel-shaping, wheel-throwing). Cubical samples from each experimental vessel were measured by SANS in three perpendicular orientations, and the recorded anisotropic scattering maps were analysed in 2D. The measure of anisotropy and the direction of the elongation of the detected nano-inclusions indicate the preferential particle/void alignments. After examining the 2D scattering plots, correlation between forming techniques and the direction and magnitude of the alignment was detected. The differentiation of these techniques provides a significant new analytical tool for investigating the geographic and temporal dissemination of the potter’s wheel, contributing to ongoing debates regarding the spread of this technology. In order to examine the maximum firing temperature of archaeological ceramics, three different raw material series of control briquettes have been prepared and fired at temperatures from 500°C to 1000°C. These samples have been measured on a wide scattering vector range, and after the routine calibration process, the intensity versus scattering vector curves were obtained. The least square method fitting was used to obtain the fractal exponent which has been correlated to the firing temperature. This method was then applied to a series of Late Roman/Early Medieval archaeological pottery sherds from the fortification of Keszthely (Hungary) in order to better understand production technologies of the post Roman period. The measurements were performed at the YS-SANS and FSANS instruments at Budapest Neutron Centre.

### [439] Neutron/X-ray scattering studies of waterlogged archaeological wood (12:10)

*Presenter: PLAZA, Nayomi*

Conservators tasked with preserving waterlogged archaeological wood, such as artifacts found at the bottom of lakes or seas, must use reversible treatments that impart structural soundness on the often heavily decayed objects. They must also provide historical wood with appropriate resistance against further biodeterioration. Current treatments, while reversible, do not necessarily protect wood against decay organisms. Thus, there is a need to find new conservation agents and methods that can deliver all required protection. However, detailed knowledge about the wood structure and the degree of its degradation is necessary to develop effective treatments tailored to a waterlogged wooden artifact's needs. Wood, being a hierarchical material, benefits from multi-scale studies. The nanoscale length scales are often the most difficult to access due to the inherent low contrast between the wood polymers. Small angle scattering has proven particularly useful to measure changes in the nanoscale

features of wood as a function of moisture uptake or removal, chemical infiltration, and fungal exposure. Small angle neutron scattering (SANS), in particular, has revealed that water accessibility at the microfibril level plays a role in moisture durability, dimensional stability, and even the decay resistance of forest products. Wide-angle and small-angle X-ray scattering have been used to measure microfibril bundling sizes as well as microfibril alignment. Thus, here, we combine SAXS/SANS and WAXS to probe the nanostructure of archaeological wood samples in terms of microfibril aggregation/alignment and cellulose crystalline structure. These measurements have revealed that in heavily degraded samples, the characteristic microfibril alignment can be lost even when the characteristic diffraction peaks from cellulose are present. We expect these findings will help understand better the mechanisms of degradation and facilitate the development of new conservation treatments for waterlogged archaeological wood.

## Micro Symposium CANS 2 - SCC/3-Venus - Venus (23 Mar 2023, 11:00 - 12:30)

**-Chairs: Thomas Gutberlet**

### [92] Development of high intensity accelerators for CANS at CEA/Irfu (11:00)

*Presenter: SCHWINDLING, Jerome*

The Institute for Research into the Fundamental laws of the Universe (Irfu) at CEA, France, is developing and providing accelerator parts for various national and international projects. Our competences and realisations on high intensity light ion accelerators suitable for the development of Compact Accelerator-based Neutron Sources will be presented.

### [200] HBS High Power Density Neutron Target - An approach to meet the special requirements of HiCANS (11:15)

*Presenter: ZAKALEK, Paul*

Within the framework of the Jülich High Brilliance Neutron Source (HBS) project, a high current accelerator based neutron source (HiCANS) is developed. The main power-limiting factor is the target that releases neutrons via nuclear reactions from the impinging protons. The neutron yield of these nuclear reactions is quite small. This is compensated with a high proton current which leads to a strong heat release inside the target. At the same time the target has to be very compact. Overall, this leads to unique requirements of the HBS target given by a 70 MeV pulsed proton beam on a surface area of 100 cm² with a peak current of 100 mA and an average thermal power release of 100 kW inside the target. A solid tantalum target prototype with an innovative micro channel water cooling structure was developed, manufactured, and tested at 1 kW/cm² with an electron beam to match these requirements. Known challenges from low energy targets like blistering, joining, lifetime, and heat dissipation, as well as particular challenges of the HBS target design like coolant erosion, thermomechanical stresses, and critical heat flux have been consequently considered during the development. Here, we will present the HBS target design, explain various measures taken to solve the challenges mentioned, and show the successful high heat flux tests in the electron beam facility JUDITH 2. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [195] A proposal of the neutron instrument suite of ARGITU, the high-current accelerator-driven neutron source in the Basque Country (11:30)

*Presenter: J. VILLACORTA, Felix*

The ARGITU project is one of the initiatives framed within the joint European strategy to develop the next generation of high-current accelerator-driven neutron sources (HiCANS). In this envisioned facility, a high current proton beam (E=31.5 MeV) hits a beryllium target, producing neutrons by nuclear processes that can serve to run a suite of up to four neutron scattering instruments per target station. In this work, a proposal for a potential neutron scattering instrument suite for the ARGITU facility is presented. The long pulse delivered by ARGITU (t = 1.5 ms) can be fully exploited by not only the instruments with relaxed energy resolution, but also to the high-resolution instruments. Up-to-date neutron optical developments, dedicated moderators for each instrument, and other state-of-the-art compact devices will help to give shape to the conceptual design of the scientific instruments around the compact neutron source. The eventual selection of instruments will be done in close collaboration with the local scientific community, prioritizing the neutron scattering techniques that will provide more impact to the community, and exploring the different possibilities of this new infrastructure, to support high-level research and development, education, and as an integral part of wider experimental campaigns within long-term collaborations with large-scale European and international neutron facilities, such as ESS, ILL ISIS and MLZ. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [342] Thermal moderator-reflector assembly for HBS (11:45)

*Presenter: RÜCKER, Ulrich*

The thermal moderator is the key component in a research neutron source to convert the primary neutrons which typically have energies in the MeV regime into useful neutrons for investigations that shall have energies well below 1 eV. In the case of a HiCANS as HBS, the thermal moderator has to be optimized according to the compact target size and to the proton pulse lengths at the different target stations. Extraction channels in the thermal moderator are used to either place cold sources feeding instruments that need a cold neutron spectrum or to extract thermal neutron beams from the volume of highest thermal neutron flux density. Requirements of restricted space, neutron transparency of the main structural materials, the technically demanding flowing liquid thermal moderator material, the complex nature of intense thermal and induced mechanical loading, industry-standard requirements for operational safety, etc. impose important boundary conditions on the design of the thermal moderator. Here, we present the details of a thermal moderator design serving up to 12 instruments at a target station operated at 96 Hz. The thermal moderator consists of a combined welded complex-profiled Al vessel containing 12 thin-walled cast extraction channels arranged in 2 levels. The vessel is filled with H2O as moderator material which is pumped for cooling purposes. The entire system is surrounded by a lead reflector and arranged on top of the compact Ta target. We show the results of simulations concerning the neutronics and the thermal behaviour of this thermal moderator-reflector assembly. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

### [88] High temperature Be target for the French HiCANS (12:00)

*Presenter: MENELLE, Alain*

HiCANS are new neutron sources of a very high interest for the future. However some major technological issues remain; one the biggest one being the development of targets able to sustain the high intensity proton beam during a time long enough to have a smooth operation of the source. We will present the developments made in Saclay on high temperature Berylium targets. Two different targets have been tested with a 3 MeV proton beam during long runs; a small ones design to sustain a power up to 1 kW, and a big one design to sustain a power up to 50 kW. Results of 100 hours operations will be presented. This work is part of the collaboration within ELENA and LENS on the development of HiCANS. It has been funded by the "CANS Inflexion" program at the CEA and the "IPHI-Neutron" SESAME project of the Ile de France region.

### [304] Shielding design for the High Brilliance neutron Source (HBS) target station (12:15)

*Presenter: HANSLIK, Romuald*

In recent years, the development of high-current accelerator-based neutron sources (HiCANS) has gained in interest to propose a novel option for the next generation of neutron sources. In HiCANS high neutron yields are achieved by irradiating metal targets with proton beams with energies in the MeV range bellow the spallation threshold and currents of several tens of milliamps. Based on this concept, the High Brilliance neutron Source (HBS) project was developed at Forschungszentrum Jülich to deliver a high flux of neutrons to various scattering, analytics and imaging instruments. Relying on the experience and challenges of assembling the HBS shielding prototype at Forschungszentrum Jülich, the HBS target station shielding was developed from several layers of lead and borated polyethylene with a suitable stepped support structure. The aim of the shielding is to keep the dose rate in the monitored area well below the radiation protection criteria. The entire target station is modelled for particle transport simulation on the basis of the mechanical design. The dose rate distribution inside the target station as well as on the outside of the bunker walls is calculated during beam operation and also when the beam is switched off. The analysis of neutron and gamma flux and dose rate distribution in the target station from the radiation protection aspects will be presented. This work is part of the collaboration within ELENA and LENS on the development of HiCANS.

## Sample Environment - SCC/0-002 - Taurus 1&2 (23 Mar 2023, 11:00 - 12:30)

**-Chairs: Sebastian Jaksch; Alexander Holmes**

### [283] Recent developments in soft-matter related sample environments at the Institut Laue Langevin (11:00)

*Presenter: CHIAPPISI, Leonardo*

The neutron scattering facilities worldwide constantly replace or upgrade their instrumental suite to provide the scientific community with unprecedented capabilities. Progresses all-along a neutron scattering beamline, from the improved production and optics to more sensitive detectors, allow nowadays experiments which were unthinkable until some time ago. However, not less relevant are the strong progresses which have been made with sample environments, allowing samples to be probed under extreme conditions, with high throughput or under in-operando or in-vivo conditions. Herein, we provide an overview of some of the recent sample environment developments achieved at the ILL for soft condensed matter. By showcasing different experimental studies, we provide an overview of the following setups: - **High-pressure** equipment to probe colloidal systems in solution and at interfaces will be presented. Using the example of polymer-surfactant assembly, or polymer phase transitions, the use of high-pressure cells optimised for small-angle neutron scattering, neutron spin-echo and neutron reflectometry is described. The setup allows also to perform time-resolved SANS experiments with time resolution of few tens of milliseconds. - A recently developed **foam column**, entirely made in quartz and integrating optical prisms and electrodes, allows to probe liquid foams with small-angle neutron scattering, mesoscopic photography and electrical conductivity. The setup, associated with a fully consistent analysis, allows to characterize the relevant aspects of a liquid foam structure: liquid content, plateau border size and specific area, bubble size distribution, and thin film thickness and specific area. - Controlling the **humidity** in a system allows for a precise control of the water chemical potential in the system. Accordingly, it is an excellent tool to probe the role of water and the swelling behaviour of colloidal systems. A new setup has been developed, in which saturated vapours of D2O, H2O and an optional liquid are mixed with dry nitrogen or an additional gas. The setup precisely tunes the humid content in the system and allows to perform contrast variation experiments in humidity-controlled environments. The potential of the setup is showcased using the examples of time-resolved swelling of historic woods or of CO2-driven structural rearrangement in polymer coatings. In summary, recent development in sample environment allow to address challenging scientific questions in very different domains of soft condensed matter and to exploit to a maximum the neutron scattering instruments.

### [98] Using an industrial robot system at STRESS-SPEC for high accuracy neutron strain measurement (11:30)

*Presenter: HOFMANN, Michael*

The Heinz Maier-Leibnitz Zentrum (MLZ) operates at Germany’s sole neutron source FRM II the diffractometer STRESS-SPEC optimised for fast strain mapping and texture analyses. The STRESS-SPEC group was the first to pioneer sample handling and positioning via industrial robots at neutron diffractometers [1, 2]. However, the current robot is limited in its use due to insufficient absolute positioning accuracy of up to ± 0.5 mm in some cases. Usually, an absolute positioning accuracy of 10% of the smallest gauge volume size – which in case of modern neutron diffractometers is in the order of 1×1×1 mm3 – is necessary to allow accurate strain tensor determination and correct centering of local texture measurements. The original robot setup at the neutron diffractometer STRESS-SPEC has therefore been upgraded to a high accuracy positioning/metrology system. We will give a short introduction on the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50 µm or better during measurement of the full strain tensor, the sample position is tracked by an optical metrology system and actively corrected, which we will show in detail. Furthermore we will also present a custom fit sample environment and give an outlook what might be possible in current neutron strain scanners using such a system. [1] H.-G. Brokmeier et al., Mater. Sci. For. 652 (2010) pp. 197–201. [2] C. Randau et al., Nucl. Instr. Meth. A: 794 (2015) pp. 67–75.

### [451] Science 4.0 approach for sample preparation (11:50)

*Presenter: ČERMÁK, Petr*

The first industrial revolution enabled mass production by using steam power in the late 18th century. Progress continued by adding electricity and programmable logic controllers in the second and third industrial revolution, respectively. All this two-century progress was more-less irrelevant for science since progress there requires constant changes and our invention. We are now on the threshold of the fourth industrial revolution, which will bring smart factories by utilizing big data and artificial intelligence. Such techniques are, for the first time in mankind’s history, also beneficial for science. A persistent problem with inelastic neutron scattering is the need to use a sample with a minimum mass of hundreds of milligrams. For many samples it could be only achieved by co-aligning more single crystals. This process is very time-consuming and often not very precise (e.g. [1]). We will present you the newly constructed Automatic Laue Sample Aligner - **ALSA**, which will automatize the crystal co-alignment process by using a state-of-the-art X-Ray Laue diffractometer, robotized manipulators, real-time computer vision, and bespoke neural network software for crystal placing and Laue pattern solving. The device ALSA will be a true game-changer in the field of inelastic neutron scattering because it will drastically speed up sample preparation. [1] Duan, C. Et al. Nature 600, 636–640 (2021). [doi:10.1038/s41586-021-04151-5](https://www.nature.com/articles/s41586-021-04151-5)

## [125] High transmission, low-scattering neutron window material – a glass that is not fragile (12:10)

*Presenter: RENNIE, Adrian*

Glassy metals provide an attractive route to low-scattering window materials for neutron instruments and sample environments. These can improve significantly efficiency in use of neutrons. Studies with AMLOY-ZR01, a zirconium based bulk metallic glass from Heraeus have shown high transmission and low levels of small-angle scattering as well as the complete absence of Bragg diffraction peaks [1]. Additive manufacturing is very well suited to low-volume production of specialist components and fully retains the glassy structure. Samples 2.2 mm thick showed neutron transmission of 0.9 to 0.95 for wavelengths between 0.5 and 15 Å. Compared with alternative materials the mechanical properties are attractive: the Youngs modulus measured under compression is about 90 GPa and the stress at break is 1.5 to 1.7 GPa at ambient temperatures. The resilience of the material compared with other low scattering alternatives such as quartz glass, or single crystals of sapphire or silicon is much better. Glassy metals can now be used readily as large mechanical components: the additive manufacturing process retains the fully amorphous structure and keeps materials costs low for complex components. Potential applications for this material have been identified [2] as, for example, vacuum windows for neutron instruments and as components in complex sample environments such as shear cells. Efficiency benefits from high transmission and safety advantages make use of this new material worthwhile. The presentation will show scattering data and other results that identify a wide working range of applications. 1. A. Ericsson, V. Pacheco, J. J. Marattukalam, R. M. Dalgliesh, A. R. Rennie, M. Fisk, M. Sahlberg ‘Crystallization of a Zr-based metallic glass produced by laser powder bed fusion and suction casting’ J. Non-Crystal. Solids 571, (2021), 120891. https://doi.org/10.1016/j.jnoncrysol.2021.120891 2. Swedish Patent SE 574 674 C2

## Structure & Dynamics - MW 0 001 - Lecture hall (23 Mar 2023, 11:00 - 12:30)

**-Chairs: Karen Friese; Werner Schweika**

### [380] Neutron-driven exploration of the ice phase diagram (11:00)

*Presenter: DEL ROSSO, Leonardo*

Water and all its ice forms play a central role in everyday life and science and, as a consequence, the scientific community strives to deepen the knowledge about the polymorphism of ice. Beside this, the investigation of the phase diagram of the solid mixture of water and molecular hydrogen at high pressure has been particularly prolific and associated with exciting discoveries. Several solid stoichiometric and non-stoichiometric phases of the mixture have been characterized in the latest years, some of which, being metastable at ambient pressure and low temperature (77 K), can be recovered and handled in the laboratory. Among these, the so-called C$_{0}$ phase led to the discovery, by out-diffusion of hydrogen molecules at about 130 K, of a metastable phase of ice, named afterwards ice XVII. Surprisingly, this low-density solid is highly porous, and presents accessible spiraling channels where hydrogen molecules can be hosted in an essentially one-dimensional geometry. Moreover, by heating above 130 K, ice XVII transforms to metastable ice Ic, having an unprecedented structural purity. In this talk we show how neutron scattering has played an essential role to characterize both the structure and the dynamics of these two elusive forms of ice by reporting accurate studies of their crystal lattice and density of phonon states (DOPSs), as well as the quantum motion of confined H$_{2}$ molecules in the ice XVII framework.

### [206] Investigation of C2H4 and Ag exchanged Zeolites interaction by Inelastic Neutron Scattering and DFT calculations (11:30)

*Presenter: ALMEIDA, Gabrielli*

A fundamental step for the application of ethylene in derivatives is its separation/ purification from ethane after being obtained by naphta or ethane steam cracking. The state of art method for such task is cryogenic distillation, which lies as one of the most energy consuming industrial processes nowadays. A highly promising alternative method for this issue is the use of advanced porous adsorbents, among which Metal Organic Frameworks (MOFs) and zeolites stand out. While some MOFs may present a rather poor stability, zeolites have been standing the roughness of industrial applications since the 1950's. Another great advantage of zeolites is their tunability in terms of pore size, shape and surface functionality, allowing specific selective adsorption processes even at ambient temperatures. Due to the small differences of ethylene and ethane kinetic diameters, molecular sieving effect by itself is not effective for their separation. Thus, this process must rely also on a Lewis acid-base interaction between the alkene and a transition metal cation, specially Cu(I) and Ag(I), located in the adsorbent. However, the exact adsorption mechanism of ethylene on Ag(I) exchanged CHA, for example, is not completely understood yet. Here, we characterized this interaction between ethylene and silver aluminossilicate CHA at a microscopic level using a multidisciplinary approach involving Inelastic Neutron Scattering (INS), Nuclear Magnetic Resonance (NMR), UV-vis, Infrared (IR) and Density Functional Theory (DFT) calculations parting from a real system, as it has never been done before as far as we know. From UV-vis analysis, it was seen that the system under investigation contains not just cations but also charged Ag clusters. Both species interact with the ethylene, as confirmed by the comparison between the experimental INS spectrum and the DFT calculated INS spectra obtained for a cationic and a cluster models. 13C-Solid State NMR showed an upfield shift from 123 ppm to 110 ppm, suggesting a stronger proton shielding and electron transfer between the adsorbant/adsorbent. The downshield shift of 109Ag NMR, complimentarily, reveals a weaker proton shielding, also suggesting electron transfer after the sample's loading. These results were corroborated by DFT electron density difference calculations, proving the nature of this interaction, known as π-complexation. Finally, by analysing the red shift of C-C stretching frequency and C-C bond lengthening with information provided by IR and DFT, respectively, we could have a whole picture, not just confirming the interaction nature, but also evaluating the extension of it for each model. Although a higher preference of ethylene to cationic Ag species was noticed, the interaction does not change dramatically from one species to another. Considering ethylene's recovery, in fact, systems containing silver clusters would be preferable for the industry.

### [455] Adsorption and separations processes within metal-organic frameworks through neutron scattering (11:50)

*Presenter: BROWN, Craig*

Metal organic frameworks (MOFs) are crystalline materials that contain metal-ion nodes and organic ligands as linkers to form 1-, 2-, and 3-D structures. Their structural versatility and multifunctional properties have sparked much interest in advanced materials synthesis. Due to their modular nature, many of these materials can be constructed by design. Over the last decade there are several MOFs that reportedly have high surface areas allowing them to physically adsorb significant amounts of gas and/or exhibit significant separations performance. Adsorption of molecules in functionalized and high surface area microporous materials is of technological importance in a multitude of areas ranging from catalysis, drug delivery, chemical separations, and energy storage to personal care products. Through careful selection of the ligand and metal, which control pore size/shape and MOF-adsorbate interactions, their uptake properties can be tuned. Over the past several years we have focused our research efforts on understanding the properties of gas interactions within a variety of microporous materials with the goal of improving new optimal storage and separation materials.

### [217] Transport properties of H2 confined in carbide-derived carbons with different pore shapes and sizes (12:10)

*Presenter: HÄRMAS, Riinu*

Carbide-derived carbons (CDC) are porous carbon materials with widely different properties like pore size distribution or graphitization [1]. In this study, quasi-elastic neutron scattering method was used to investigate the hydrogen diffusion in the well-defined pores of three distinct CDC materials [2]. Namely, the predominant shape of pores of the studied CDCs had been shown to be different as well as the respective pore size distributions [2]. Two of the studied materials were mostly microporous, while the third mostly mesoporous. Using a combined approach of gas adsorption methods and in-situ quasi-elastic neutron scattering, some interesting insights were gained on the relation of local adsorbent structure and the molecular behaviour of confined hydrogen. It was shown that sub-nanometer pores of spherical and cylindrical shape strongly limit the diffusion of H$_2$. However, a much weaker adsorption was seen in mainly mesoporous CDC, resulting in higher H$_2$ mobility in that adsorbent. This demonstrates, that tailoring the pore structure of carbon materials can have a large effect on their H$_2$ storage capability. Refs. [1] Härmas, R.; Palm, R. et al. Carbon 2019, 155, 122–128, doi:10.1016/j.carbon.2019.08.041. [2] Härmas, R.; Palm, R.; et al. C 2021, 7, 29, doi:10.3390/c7010029. [3] Kurig, H.; Russina, et al. Carbon 2016, 100, 617–624, doi:10.1016/j.carbon.2016.01.061.

## Award ceremonies and closing - MW 2 001 - Lecture hall (23 Mar 2023, 14:00 - 15:45)

**-Chairs: Henrik Ronnow**