Neutron Science

This session has been organised in collaboration with the Swiss Neutron Science Society.

Tuesday, 10.09.2024, Room ETF E 1

Time	ID	**Neutron Science I** *Chair: Fanni Juranyi, PSI Villigen*
14:00	**701**	**Quantitative imaging and understanding of water dynamics and flow in soil and roots** *Andrea Carminati [1], Sara Di Bert, Pascal Benard, Pavel Trtik [2], Anders Kaestner* *[1] ETH Zürich, [2] Paul Scherrer Institut* Roots have long been considered the “hidden half” of plants. Due to the opaqueness of soils, root research has focussed on roots growing in artificial growth media, such as agar or hydroponics. Recent advances in imaging methods has led to unprecedented progresses in studying root functions in soils. Neutron imaging, thanks to the high sensitivity of neutrons to water, has been particularly useful for revealing root water uptake patterns and for identifying new mechanisms of how plants take up water from the soil. This talk will show examples of neutron imaging of water dynamics in soils, roots, and at their interface.
	~~702~~	*cancelled*
14:30	**703**	**Exploring Microfluidic-Small Angle Neutron Scattering for Soft Matter Physics** *Viviane Lütz Bueno, Paul Scherrer Institut* Our contribution to non-equilibrium soft matter physics involves developing an in situ method for studying structural changes under flow, impacting materials properties and processing. Our research spans various model systems, from wormlike micelles to 3D printing ink. We tackle challenges in flow studies with microfluidic-small-angle neutron scattering (microfluidic-SANS), enhancing visibility and control. Using selective laser-induced etching (SLE), we create neutron-transparent fused silica microchannels in parallel, increasing sample volume exposure while maintaining the resolution. We explore techniques to reduce reflection signals and present in situ contrast matching and flow mapping experiments. This work advances understanding of soft matter structures under flow, with applications in pharmaceuticals, cosmetics, and 3D printing.
	~~704~~	*cancelled*
14:45	**705**	**Texture analysis capabilities at the neutron strain diffractometer POLDI at PSI** *Florencia Malamud, Steve Gaudez, Ezequiel Fogliatto, Markus Strobl, Paul Scherrer Institut* Neutron strain scanners have been proven to be a key tool for non-destructively determining the crystallographic texture at selected locations within a macroscopic object. Here we will present the implementation of a novel data analysis methodology to perform spatially resolved texture analyses in bulk specimens at POLDI, the Pulse Frame Overlap diffractometer at Paul Scherrer Institute. The method is based on the determination of several incomplete pole figures after splitting POLDI’s diffraction detector, with an angular range of 30°, into several units of smaller angular coverage. We will present demonstration experiments on additive manufacturing specimens and Zr-based components of nuclear power plants.

15:00 | **706**

AMPLIFY - A Novel Neutron Instrument for Surface Scattering

Artur Gregor Glavic, Jochen Stahn, Paul Scherrer Institut

Grazing incidence small angle neutron scattering is a powerful techniqu to investigate surface-near lateral structures on the nanometer scale.
We develop a novel instrument concept as part of an investigation into a new guide hall at the PSI SINQ neutron source. The Adjustable Monochromator to Perform Liquid grazing Incidence, Focused or magnetic Yoneda scattering (AMPLIFY) makes use of two parabolic multilayer monochromators to provide a tunable wavelength resolution between 2 % and 10 %.
We have compared the expectec instrument performance with a SANS-like configuration. For collimations in the range of 5 m to 20 m AMPLIFY can reach similar or better angular resolution with slightly higher intensity and more homogenous beam profile.

15:15 | **707**

Effect of Softness and Charges on the Volume Phase Transition of Colloidal Microgels and Macrogels studied via SANS

Boyang Zhou, PSI Villigen

Microgels and macrogels, due to their stimuli-sensitive nature and tunability, are of great interest in both applications and fundamental research. However, their softness increases the number of degrees of freedom compared to hard colloidal particles and gives rise to a more complex behavior. So far, there is no generally accepted model to describe microgel interactions, especially for concentrated microgel suspensions. In this project, we delve into the study of the effect of counterions on the microgel periphery resulting from the use of ionic initiators in the synthesis. Using small-angle neutron scattering (SANS), we confirm the presence of counterion clouds at the particle periphery. More importantly, we observe that counterions can delocalize and control the swelling of the microgel. Using confocal microscopy, we show that delocalized counterions lead to noncentral many-body forces between microgels, controlling the elasticity of the crystals—a behavior also observed in metals and crystals of charged, hard colloids. Our results not only contribute valuable insights for developing a model to describe microgel interactions but also showcase the capability of SANS in studying soft matter. Furthermore, we explore the thermodynamic instability of macrogels using SANS, neutron imaging, and rheology. We conduct a detailed examination of the characteristics of the polymer-dense skin that forms on the gel surface upon rapid heating and arrests the gel in a metastable coexistence of swollen and deswollen phases. These results are valuable for developing hydrogels that exploit thermodynamic instabilities for shape actuation in various applications.

15:45

16:00 | ***Coffee Break***

Neutron Science II

Chair: Romain Franck Sibille, PSI Villigen

16:30 | **711**

Determination of skyrmion-hosting transition metal-oxide Hamiltonian with predictive guidance from ab-initio quantum chemistry

Daniel Mazzone [1], L. Yu, R. Yadav, Priya Ranjan Baral [2], Romain Sibille [1], J. Lass [1], Christoph Niedermayer [1], Victor Ukleev, A. Magrez, J.-R. Soh, I. Živković, Henrik M. Rønnow [2], Bruce Normand [1], Oleg V. Yazyev [2], Jonathan. S. White [1]
[1] Paul Scherrer Institut, [2] EPFL

The remarkable tunability and inherent functionality of many quantum materials stem from intricate many-body states in which several degrees of freedom are entangled. These microscopic complexities manifest in collective excitations, forming the basis of their distinct properties. Inelastic neutron scattering is pivotal in testing theoretical predictions to unravel emergent quantum effects. However, in many cases it is challenging to find appropriate microscopic Hamiltonian candidates that can be refined against experimental observations. In this talk I will show that ab-initio quantum chemistry is a promising tool that can guide us in determining the microscopic interactions in transition metal-oxides.

17:00	**712**	**Dipolar-octupolar correlations in $Ce_2Hf_2O_7$ quantum spin ice candidate** *Victor Alexis Porée [1], Romain Franck Sibille [1], Anish Bhardwaj [2], Hitesh Changlini [3], Elsa Lhotel [4], Andriy Nevidomskyy [5], Sylvain Petit [6], Han Yan [7]* *[1] Paul Scherrer Institut, [2] St. Bonaventure, [3] Florida State University, [4] CNRS, [5] Rice, [6] CEA, [7] The University of Tokyo* Pyrochlore oxides incorporating magnetic Ce^{3+} have been the subject of intense experimental and theoretical efforts over the past few years. Their rich physics is related to their dipole-octupole magnetic degrees of freedom and possibility to stabilise a quantum spin ice (QSI) ground state – the prototype three-dimensional quantum spin liquid. While all studied materials show continua of excitations attributed to the fractionalized spinon excitations of QSI, the nature of the underlying correlations has been subject to debates. Here we show using neutron scattering that $Ce_2Hf_2O_7$ develops hybrid dipolar-octupolar correlations. The large contrast between dipolar and octupolar form factors allows to determine the weak dipolar-octupolar exchange of the Hamiltonian.
17:15	**713**	**The spiral magnetic order in $YBaCuFeO_5$ single crystals** *Arnau Romaguera-Camps [1,2], Marisa Medarde [2], M. Ciomaga Hatnean [2,3], O. Fabelo [4], N. Qureshi [4], J. A. Rodríguez-Velamazán [4], José Luis García-Muñoz [5]* *[1] Lab. for Advanced Spectroscopy and X-ray sources, Paul Scherrer Institute, 5232 Villigen PSI* *[2] Laboratory for Multiscale Materials Experiments, Paul Scherrer Institute, 5232 Villigen PSI* *[3] Materials Discovery Laboratory, Department of Materials, ETH Zürich, 8093 Zürich* *[4] Institut Laue-Langevin, CS 20156, FR-38042 Grenoble Cedex 9* *[5] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), ES-08193 Bellaterra, Barcelona* The low ordering temperatures of most non-collinear cycloidal magnets (typically < 50 K) limit their use in ambient temperature devices. The layered perovskites $LnBaCuFeO_5$ are a rare case of frustrated oxides where a novel "spiral order by disorder" mechanism appears to account for the existence of a spiral order with extraordinary stability, but direct evidence of the chiral nature of this incommensurate phase is lacking. This presentation aims to fill this gap by providing proofs of the magnetic structures through spherical neutron polarimetry and crystal neutron diffraction, highlighting critical features relevant to the search for high temperature magnetoelectric response induced by the spiral phase.
17:30	**714**	**Extreme Quantum Fluctuations of the Heisenberg Antiferromagnet on the Honeycomb Lattice** *Jose Abraham Hernandez Sanchez, Bertrand Roessli, K. W. Krämer, M. Schüler, A. A. Eberharter, Bruce Normand, Andreas M. Läuchli, Michel Kenzelmann, Paul Scherrer Institut* Enhanced quantum fluctuations are believed to give rise to new ground states and magnetic excitations in electronic insulators. I will present the effect of strong quantum fluctuations in the honeycomb van der Waals antiferromagnet $YbBr_3$. Quantum fluctuations are believed to be enhanced in $YbBr_3$ due to the two-dimensional nature of the exchange interactions. The low-energy spin dynamics of the system measured with inelastic neutron scattering are excellently reproduced by the spin-½ Heisenberg model treated with the matrix-product states (MPS) numerical method. The coexistence of magnon-like and continuum excitations are spectacularly reproduced by the method.
	~~**715**~~	*cancelled*

17:45	716	**A High Visibility Grating Deflectometer for the Measurement of the Neutron Electric Charge** *Marc Persoz, Universität Bern* Neutron grating interferometers are powerful tools for high-precision measurements of deflection angles and scattering. A novel symmetric Talbot-Lau interferometer, utilizing three identical absorption gratings in a time-of-flight mode, is currently 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 improve the current upper limit: $Q_n < (-0.4 \pm 1.1) \cdot 10^{-21}$ e [Baumann, 1988]. A proof-of-principle apparatus has been characterized at the cold neutron beamline PF1b at the Laue-Langevin Institute in Grenoble, France. A general description of the setup, alignment procedures and initial findings regarding the setup stability and neutron electric charge measurements will be presented.
18:00		***END***
18:30		***CERN 70***
19:45		***Postersession with Apéro***

ID	Neutron Science Poster
731	**Characterisation of high-energy neutron fields at the Swiss spallation neutron source (SINQ) using a Bonner sphere spectrometer** *Daniel Zeitz [1,2], Uwe Filges [1], Eike Hohmann [1], Marc Janoschek [1,2], Sabine Mayer [1]* *[1] PSI, [2] Uni Zürich* At the BOA beamline at SINQ, neutron imaging and scattering experiments are conducted using cold polarised neutrons, which are obtained via moderation of spallation neutrons in a cold D_2 moderator. Nevertheless, fast scattered neutrons can penetrate the beamline shielding, resulting in undesired noise for experiments. The presence of fast neutrons in the BOA cave is demonstrated using an experimental technique based on a Bonner sphere spectrometer in combination with a shadow cylinder. Identifying the high-energy neutron flux at key locations while blocking out the beam allows for an estimation of the fast neutron background in the BOA cave and provides key information for future upgrades of the SINQ facility.