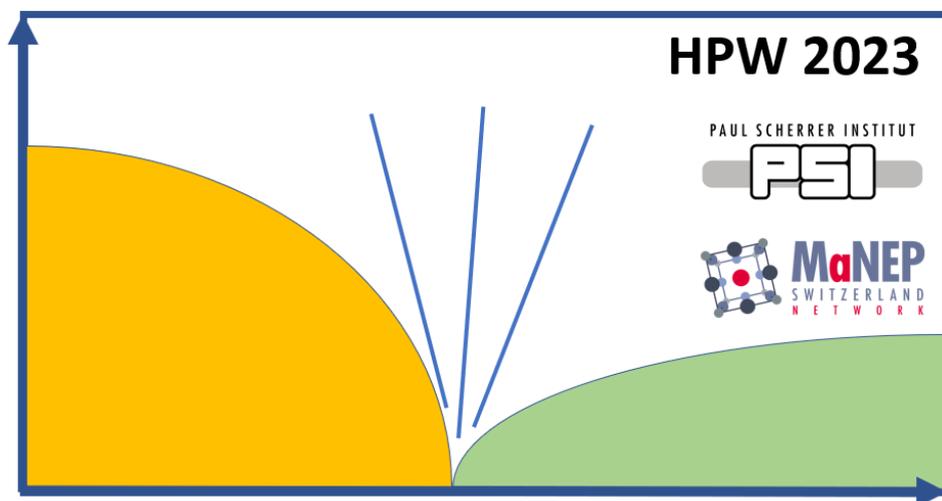


# High Pressure Workshop



## Report of Contributions

Contribution ID: 2

Type: **not specified**

## Opening remarks

*Wednesday 22 November 2023 09:45 (15 minutes)*

**Presenter:** SIMUTIS, Gediminas (PSI - Paul Scherrer Institut)

Contribution ID: 3

Type: **Talk**

## Squeezing charge stripe order unidirectionally

*Wednesday 22 November 2023 10:00 (30 minutes)*

This talk will present resonant and non-resonant x-ray diffraction experiments upon uniaxial pressure application to cuprate superconductors. Special attention is given to the symmetry properties of charge stripe ordering.

**Author:** CHANG, Johan

**Presenter:** CHANG, Johan

**Session Classification:** Morning Session

Contribution ID: 4

Type: **Talk**

## Probing material properties with neutrons under pressure

*Wednesday 22 November 2023 10:30 (30 minutes)*

Quantum magnets are physical realisations of many-body quantum systems which may host interesting phenomena such as entangled states or spin-nematic states and quantum phase transitions. There exists a number of experimental knobs for controlling the state of such system: Temperature, magnetic field, chemical doping and pressure. Of all these, the latter is the cleanest way of manipulating exchange paths in a system and therefore offers the possibility to dramatically manipulate the ground state. Inelastic neutron scattering is one of the most powerful tools to probe the finger print of non-ordered quantum entangled states: The spin dynamics. Therefore, in combination, pressure and inelastic neutron scattering are a super tool in experimental quantum magnetism. Using the archetypic quantum magnet, SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>, we present a number of high-pressure inelastic neutron scattering studies. SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> is the realisation [1] of what is known as the Shastry-Sutherland lattice [2] consisting of a network of spin dimers with exchange interaction  $J$  inside the dimer and  $J'$  between the dimers. For low ratios of  $J'/J$ , a product of dimer singlets is the ground state. Upon increasing  $J'/J$ , a singlet plaquette phase is encountered and finally an ordered antiferromagnetic state is established [3]. The phase diagram of SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> resembles the predicted one remarkably well with phase transitions around 1.8 GPa and 3.0 GPa to enter the plaquette and antiferromagnetic phases respectively [4]. We performed inelastic neutron scattering experiments with high pressures to investigate the nature of the predicted phases and in this way contribute with a piece in the puzzle for understanding many-body quantum physics.

[1] Kageyama et al., Phys. Rev. Lett. 82, 3168-3171 (1999)

[2] B. S. Shastry and B. Sutherland, Physica 108B, 1069-1070 (1981)

[3] P. Corboz and F. Mila, Phys. Rev. B 87, 115144 (2013)

[4] M. E. Zayed et al., Nature Physics 13, 962-966 (2017)

**Author:** NORMAND, Bruce (PSI)

**Co-authors:** PIOVANO, Andrea (ILL); MAZZONE, Daniel Gabriel (PSI - Paul Scherrer Institut); POM-JAKUSHINA, Ekaterina (Paul Scherrer Institute); FOGH, Ellen (EPFL - EPF Lausanne); MILA, Frédéric (EPFL); GIRIAT, Gaétan (EPFL); SIMUTIS, Gediminas (PSI - Paul Scherrer Institut); RØNNOW, Henrik (EPFL); LASS, Jakob (PSI - Paul Scherrer Institut); KAKURAI, Kazuhisa (CROSS); MUNAKATA, Koji (CROSS); BARTKOWIAK, Maciej (HZB); BOEHM, Martin (ILL); ZAYED, Mohamed (Carnegie Mellon University Qatar); PROKHENKO, Oleksandr (HZH); GAAL, Richard (EPFL SB ICMP EPSL); HANSEN, Thomas (ILL)

**Presenter:** FOGH, Ellen (EPFL - EPF Lausanne)

**Session Classification:** Morning Session

Contribution ID: 5

Type: **Talk**

## Giant pressure-enhancement of multiferroicity in $\text{CuBr}_2$

*Wednesday 22 November 2023 13:45 (15 minutes)*

Type-II multiferroic materials, in which ferroelectric polarization is induced by inversion-nonsymmetric magnetic order, promise new and highly efficient multifunctional applications based on the mutual control of magnetic and electric properties. Although this phenomenon has to date been limited to low temperatures, we have found a giant pressure-dependence of the multiferroic critical temperature in  $\text{CuBr}_2$ , specifically from 73.5 K at ambient pressure to 162 K at 4.5 GPa. Not only is this to our knowledge the highest value yet reported for a nonoxide type-II multiferroic but its growth also shows no sign of saturating, and the dielectric loss remains small, at these pressures. We establish the structure under pressure and demonstrate a 60% increase in the two-magnon Raman energy scale up to 3.6 GPa. First-principles structural and magnetic energy calculations provide a quantitative explanation in terms of dramatically pressure-enhanced interactions between  $\text{CuBr}_2$  chains. These large, pressure-tuned magnetic interactions motivate structural control in cuprous halides as a route to applied high-temperature multiferroicity.

**Author:** Dr NORMAND, Bruce (LTC, SCD, Paul Scherrer Institute)

**Presenter:** Dr NORMAND, Bruce (LTC, SCD, Paul Scherrer Institute)

**Session Classification:** Afternoon Session 1

Contribution ID: 6

Type: **Talk**

## Complex Order Parameter Tuning in Superconducting $\text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4$

*Wednesday 22 November 2023 16:15 (15 minutes)*

High-temperature superconducting cuprates are a model system to examine the relationship between intertwined quantum phases. The competition has, however, been difficult to tune with external stimuli without inducing superconducting vortices by a magnetic field at the same time. In our study, we show that  $c$ -axis strain couples directly to the phase competition between charge stripe order and superconductivity in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO). To track the evolution of charge order upon application of strain at different temperatures, dopings, and magnetic fields, x-ray diffraction measurements were performed at DESY. We show, that compressive  $c$ -axis pressure enhances stripe order only within the superconducting state. The strain furthermore diminishes the magnetic field enhancement of stripe order. It thus provides a fruitful approach to study the interplay between superconductivity and charge order in the cuprates.

**Authors:** KÜSPERT, Julia (University of Zurich); Dr BIAŁO, Izabela (University of Zurich); Dr FRISON, Ruggero (University of Zurich); MORAWIETZ, Alexander (University of Zurich); Dr CHOI, Jaewon (University of Zurich); BUCHER, Damian (University of Zurich); Dr IVASHKO, Oleh (Deutsches Elektronen-Synchrotron DESY Hamburg); Dr ZIMMERMANN, VON, Martin (Deutsches Elektronen-Synchrotron); Dr CHRISTENSEN, Niels B. (Technical University of Denmark); MAZZONE, Daniel Gabriel (PSI - Paul Scherrer Institut); SIMUTIS, Gediminas (PSI - Paul Scherrer Institut); TURRINI, Alexandra Angeline (PSI - Paul Scherrer Institut); THOMARAT, Laure (PSI - Paul Scherrer Institut); TAM, David William (PSI - Paul Scherrer Institut); JANOSCHEK, Marc (PSI - Paul Scherrer Institut); Prof. KUROSAWA, Tohru (Hokkaido University); Dr MOMONO, Naoki (Hokkaido University); Prof. ODA, Migaku (Hokkaido University); Dr WANG, Qisi (University of Zurich); CHANG, Johan

**Presenter:** KÜSPERT, Julia (University of Zurich)

**Session Classification:** Afternoon Session 2

Contribution ID: 7

Type: **Talk**

## Magnetic properties of strained (010)-DyFeO<sub>3</sub> thin films and single crystals

Wednesday 22 November 2023 16:00 (15 minutes)

Strain in antiferromagnetic orthoferrite thin films is predicted to significantly change magnetic properties and result in a polar response up to room temperature. Orthorhombic DyFeO<sub>3</sub> is of particular interest since the Fe-spins undergo a spin-reorientation with transition temperatures depending strongly on the Dy-Fe interaction and a magnetic field induced ferroelectric phase below the Dy ordering temperature of 4K. To gain an understand of the magnetic properties of highly strained, coherently grown (010)-oriented DyFeO<sub>3</sub> thin films we studied the pressure dependence of a DyFeO<sub>3</sub> single crystal at the thermal triple-axis spectrometer EIGER, SINQ. The scattering experiments were conducted in the  $(0kl)$  scattering plane in the temperature range between 1.5 and 100K. For the pressure dependent measurements, a helium gas pressure cell has been used with a max reachable pressure of 5 kbar to study the spin reorientation transition ( $T_{SR}$ ) at 40K under uniaxial pressure conditions. In the temperature regime of interest, the He-pressure cell has the advantage that the pressure medium is still liquid and the applied pressure therefore truly isostatic. For the single crystal we measure an increase in  $T_{SR}$  with a rate of 1K/500bar. As a rule of thumb, a lattice mismatch between film and substrate of 1% corresponds roughly to a chemical pressure of 10kbar. Hence a  $T_{SR}=70K$  equals a measured film lattice change of approximately 3%. Overall, pressure dependent magnetic data for a DyFeO<sub>3</sub> single crystal are in broad agreement with values obtained for highly strained thin films.

**Author:** SCHNEIDER, Christof (PSI - Paul Scherrer Institut)

**Co-authors:** BISWAS, Banani (PSI - Paul Scherrer Institut); Dr NAUMOV, Pavel (PSI); Mr STUHR, Uwe Hans-Arnim (PSI - Paul Scherrer Institut); HAUTLE, Patrick (Paul Scherrer Institut); BARTKOWIAK, Marek (Paul Scherrer Institut); LIPPERT, Thomas (Paul Scherrer Institut)

**Presenter:** SCHNEIDER, Christof (PSI - Paul Scherrer Institut)

**Session Classification:** Afternoon Session 2

Contribution ID: 9

Type: **Talk**

## THz control of quantum materials under pressure

*Wednesday 22 November 2023 13:15 (15 minutes)*

Quantum materials exhibit rich phase diagrams, strongly sensitive to external parameters, which include intriguing properties such as magnetic and ferroelectric order, electronic correlations, superconductivity, and spin and charge order. These macroscopic properties arise from the complex interactions between electronic, structural, spin and orbital degrees of freedom. While key in defining the unique response of quantum materials, the complexity of these couplings and interactions poses a tremendous challenge for the physical understanding, theoretical modeling and technological device applications of these systems.

One approach that has proven successful in decoupling the effect of different degrees of freedom is to perform time-resolved measurements, which yield the out-of-equilibrium response of different components of the system following an ultrafast perturbation. Of particular interest is photoexcitation by a terahertz pulse, where the low photon energy ensures that the out-of-equilibrium sample remains closer to its electronic ground state than when e.g. an optical pump is used. Another approach to address the complexity of quantum materials is to reduce the available parameter space by choosing one external parameter, such as pressure, which can be continuously controlled (contrary to doping) while preserving thermal equilibrium (contrary to temperature). Pressure has been used extensively to draw phase diagrams in equilibrium but only to some extent with ultrafast measurements.

Combining terahertz spectroscopy or terahertz photoexcitation with pressure poses significant technological challenges, which has led to slow progress in this field despite its great potential. I will discuss our preliminary results in mapping out the pressure and temperature dependence of the THz response of Cr-doped  $V_2O_3$ , a canonical Mott insulator.

**Authors:** SUTER, Tim (ETH Zürich); DÖSSEGGGER, Janine (ETH Zürich); JOHNSON, Steven (ETH Zurich); ABREU, Elsa (ETH Zürich)

**Presenter:** ABREU, Elsa (ETH Zürich)

**Session Classification:** Afternoon Session 1

Contribution ID: 10

Type: **Talk**

## Pressure tuning of quantum matter: A local-probe perspective

*Wednesday 22 November 2023 16:30 (15 minutes)*

The demanding experimental conditions required to access the quantum critical behavior of many materials (including high magnetic fields, high pressures, and ultra-low temperatures), make their microscopic investigation often problematic. Over the years, techniques such as the nuclear magnetic resonance and muon-spin rotation/relaxation have emerged as complementary, well suited (and often unrivalled) methods up to the challenge.

Here, we focus on the effects of high pressure on strongly-correlated quantum matter, as observed from the local-probe perspective of nuclei (NMR) and muons ( $\mu$ SR). Pressure tuning is used to establish phase diagrams, induce phase transitions, and identify critical points. By means of selected examples, comprising low-dimensional magnets [1,2], unconventional superconductors [3], and heavy-electron systems [4], we show how the delicate balance between competing ground states, reflecting close-lying energy scales, is modified by pressure. We conclude with recent developments in uniaxial strain experiments, where the breaking of rotational lattice symmetry can provide access to the underlying symmetries.

Despite the many challenges involved with high-pressure experiments, once the associated technical difficulties are overcome, even conventional materials are shown to exhibit extraordinary properties, as demonstrated by the record-breaking  $T_c$  superconducting hydrides [5,6].

### References

1. N. Barbero et al., *Phys. Rev. B* **93**, 054425 (2016).
2. G. Simutis et al., *Phys. Rev. B* **98**, 104421 (2018).
3. T. Shiroka et al., *Nature Commun.* **8**, 156 (2017).
4. G. Lamura et al., *Phys. Rev. B* **101**, 054410 (2020).
5. A. P. Drozdov et al. *Nature* **525**, 73 (2015).
6. D. V. Semenov et al., *J. Phys. Chem. Lett.* **9**, 1920 (2018).

**Author:** SHIROKA, Toni (PSI - Paul Scherrer Institut)

**Presenter:** SHIROKA, Toni (PSI - Paul Scherrer Institut)

**Session Classification:** Afternoon Session 2

Contribution ID: 11

Type: **Talk**

## Study of Background Noise in High-Pressure Neutron Scattering Experiments

*Wednesday 22 November 2023 15:45 (15 minutes)*

Advanced high-pressure neutron scattering experiments demand a high neutron flux and precise phase space at small sample volumes, while maintaining a high signal-to-noise ratio. This work is dedicated to a comprehensive evaluation of background noise in high-pressure neutron scattering experiments, employing simulations and benchmark experiments. McStas 3.2 with the Union component is used to simulate the sources of background noise and its effects on high-pressure experiments. Validation experiments are conducted at the CAMEA (Cold Neutron Triple-Axis Spectrometer) at SINQ (Swiss Spallation Neutron Source), utilizing Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> powder samples placed in a 5 mm diameter × 19 mm height container. The container is then housed within a CuBe clamp cell, which is subsequently placed in orange cryostats. Simulations and tests are compared to understand the sources of background noise and assess its impact on high-pressure experiments. Furthermore, the potential solutions to reduce background noise from pressure cells are discussed.

**Author:** MA, Zhanwen (PSI - Paul Scherrer Institut)

**Co-authors:** MAZZONE, Daniel Gabriel (PSI - Paul Scherrer Institut); LASS, Jakob (PSI - Paul Scherrer Institut); SIMUTIS, Gediminas (PSI - Paul Scherrer Institut); BARTKOWIAK, Marek (Paul Scherrer Institut); Dr BERTELSEN, Mads (3. European Spallation Source ERIC); WILLENDRUP, Peter (Technical University of Denmark, Physics Department); FILGES, Uwe (PSI - Paul Scherrer Institut); KLAUSER, Christine (PSI - Paul Scherrer Institut)

**Presenter:** MA, Zhanwen (PSI - Paul Scherrer Institut)

**Session Classification:** Afternoon Session 2

Contribution ID: 12

Type: **Poster**

## Probing pressure-driven phase transitions using THz time domain spectroscopy

We describe recent progress in developing a setup in which we use a diamond anvil cell (DAC) to explore phase transitions under high pressure and ultrafast photoexcitation in combination with terahertz time-domain spectroscopy (THz TDS). We aim to access pressures of up to 10 GPa at temperatures as low as 10 K.

We will present our investigation of the Mott insulator  $(V_{1-x}Cr_x)_2O_3$ . This compound exhibits a pressure-driven insulator-to-metal transition and a temperature-dependent transition to an antiferromagnetic insulator phase. We present recent measurements on samples with 5% and 10% Cr doping, crossing the insulator-to-metal transitions at room temperature and pressures of 1.7 GPa and 2.7 GPa respectively and crossing the transition to the antiferromagnetic insulator phase at 140 K and 3.5 GPa (10% doping). These transitions have previously not been studied using THz TDS and demonstrate our capability to control both pressure and temperature separately.

As the sample chamber in a DAC is only a few hundred microns wide and thick, pressure dependent studies are limited to small samples, which poses a challenge to THz spectroscopy measurements: (i) Given that the size of the focused THz spot is also on the order of a few hundred microns, the external part of the THz beam is necessarily cut off. Careful referencing between measurements is therefore required, and a larger THz bandwidth is preferred as the size of the THz focal spot is thereby reduced. (ii) Reflections of the THz beam inside the sample lead to features that overlap with the main pulse in the time domain, hindering a simple Fourier transform analysis. We will present the technical and analytical approaches we are exploring to address these two issues.

**Authors:** DÖSSEGER, Janine (ETH Zürich); JOHNSON, Steven (ETH Zurich); SUTER, Tim (ETH Zürich)

**Co-author:** ABREU, Elsa (ETH Zürich)

**Presenter:** SUTER, Tim (ETH Zürich)

**Session Classification:** Posters + Beers + Wine + Aperó

Contribution ID: 13

Type: Talk

## Mobile interfaces in tubes revealed for three-phase systems containing pressurized methane, p-xylene, and water using neutron imaging

Wednesday 22 November 2023 14:00 (15 minutes)

Interfacial tensions for systems containing model compounds for the freeze out from natural gas can be measured at high pressures by observing the interface shapes in tubes. Mobile interfaces in opaque tubes positioned parallel to gravity are easy to prepare and neutron imaging can provide related system properties (composition, density, etc.). We have observed the phase interfaces in the titanium tubes for the pressurized systems consisting of perdeuterated *p*-xylene (*p*-C8D10) layered over water (10.88 mol.% of H2O in D2O), and exposed to pressurized methane (CH4, 1.0 to 101 bar) at 7.0 to 30.0 °C. The shape of the meniscus through the central plane of the axially symmetric interface follows the Young-Laplace equation

$$z = \frac{\gamma}{\Delta\rho \cdot g} \cdot \left( \frac{z''}{(1+z'^2)^{3/2}} + \frac{z'}{r(1+z'^2)^{1/2}} \right)$$

Figure 1: Young-Laplace equation

The tomographic reconstruction of the meniscus shape were based on the assumption of axial symmetry and derived from the single radiographies (pixel size 20.3 micrometer) using the onion-peeling algorithm [2]. While the shape of the reconstructed meniscus is crucial for the calculation of the interfacial and surface tensions, the swelling and composition of the phases provides information on the density change. Constraints determining the sensitivity and uncertainty of the method will be discussed.

### References

- 1 Dasch, C. J. Applied optics 31, 1146-1152, doi:10.1364/AO.31.001146 (1992).
- 2 Vopička, O., Durďáková, T.-M., Číhal, P., Boillat, P. & Trtik, P. Scientific Reports 13, 136, doi:10.1038/s41598-022-27142-6 (2023).

### Acknowledgement

Authors acknowledge the financial support obtained from GACR and SNSF, project 23-04741K. This work is based on experiments performed at the NEUTRA thermal neutron imaging beamline (proposal 20200129), Swiss spallation neutron source SINQ, Paul Scherrer Institute, Villigen, Switzerland.

**Authors:** VOPICKA, Ondrej (Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czechia); TRTIK, Pavel (PSI - Paul Scherrer Institut)

**Co-authors:** Ms DURDAKOVA, Tereza-Marketa (Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czechia); BOILLAT, Pierre (PSI - Paul

Scherrer Institut); Mr CIHAL, Petr (Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czechia)

**Presenter:** VOPICKA, Ondrej (Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czechia)

**Session Classification:** Afternoon Session 1

Contribution ID: 14

Type: **Poster**

## Uniaxial tuning and NMR

In quantum magnets, simple degrees of freedom with short-range interactions lead to a plethora of emergent many-body phases with different exotic properties. Uniaxial pressure allows tuning these interactions selectively and engineer the underlying Hamiltonians. Hence, the properties of the emergent phases can be controlled on-demand.

One system where such selective tuning is very pertinent is a quantum spin ladder, where only two exchange constants are relevant. In this contribution, we will present our developments of integrating a uniaxial strain device into a Nuclear Magnetic Resonance (NMR).

**Authors:** SIMUTIS, Gediminas (PSI - Paul Scherrer Institut); PHILIPPE, Jonas (PSI - Paul Scherrer Institut); JANOSCHEK, Marc (PSI - Paul Scherrer Institut)

**Presenter:** PHILIPPE, Jonas (PSI - Paul Scherrer Institut)

**Session Classification:** Posters + Beers + Wine + Aperero

Contribution ID: 15

Type: **Talk**

## Pressure tuning and Evolution of Structural, Magnetic and Electronic Properties in TMPX<sub>3</sub> van-der-Waals Compounds

*Wednesday 22 November 2023 13:30 (15 minutes)*

Control of dimensionality in condensed matter continues to reveal novel quantum phenomena and effects. Transition metal phosphorous trichalcogenides  $TM P X_3$  ( $TM = Mn, Fe, Ni, V$ , etc.,  $X = S, Se$ ) have proven to be ideal examples where structural, magnetic and electronic properties evolve into novel states when their dimensionality is tuned with pressure. At ambient pressure, they are two-dimensional van-der-Waals antiferromagnets with strongly correlated physics. Our recent experimental studies [1-4] have shown dimensionality crossover related pressure-induced insulator-to-metal transitions and novel magnetic phases in FePS<sub>3</sub>. To elucidate the relationship between structural transitions, magnetism and electronic properties, we also performed a random structure search using first-principles calculations at high pressures and DFT+U studies [5]. We experimentally explored the coexistence of the low- and intermediate-pressure phases, and we predict a novel high-pressure phase with distinctive dimensionality and possible options for interpreting the origins of metallicity.

We will also present our most recent single-crystal high-pressure synchrotron X-ray study on crystalline structures and the high-pressure neutron scattering study on magnetic structures of FePSe<sub>3</sub>, a similar compound to FePS<sub>3</sub> with reported high-pressure induced superconductivity occurring at 2.5 K and 9.0 GPa [6]. The new work performed at the DIAMOND light source and Institut Laue Langevin finally provides clear crystallographic assignments related to phases which emerge with the application of pressure.

### References:

- [1] C. R. S. Haines, *et al.*, Phys. Rev. Lett., 121, 266801 (2018).
- [2] M. J. Coak, *et al.*, J. Phys. Condens. Matter, 32, 124003 (2020).
- [3] M. J. Coak, *et al.*, Phys. Rev. X, 11, 011024 (2021).
- [4] D. M. Jarvis, *et al.*, Phys. Rev. B, 107, 54106 (2023).
- [5] S. Deng, *et al.*, SciPost Phys. 15, 020 (2023).
- [6] Y. Wang, *et al.*, Nat. Commun. 9, 1914 (2018).

**Author:** DENG, Shiyu (University of Cambridge)

**Co-authors:** Dr R. S. HAINES, Charles (University of Cambridge; University of East Anglia); Dr J. COAK, Matthew (University of Cambridge; University of Birmingham); Dr HAMIDOV, Hayrullo (University of Cambridge; Navoi State University of Mining and Technologies); Dr DAISENBERGER, Dominik (Diamond Light Source); Dr WARREN, Mark (Diamond Light Source); Mr LIU, Cheng (University of Cambridge); Mr ZHANG, Xiaotian (University of Cambridge); Dr M. JARVIS, David (University of Cambridge; Institut Laue-Langevin); Dr WILDES, Andrew (Institut Laue-Langevin); Prof. ARTACHO, Emilio (University of Cambridge; CIC Nanogune BRTA and DIPC; Ikerbasque, Basque Foundation for Science); Dr S SAXENA, Siddharth (University of Cambridge; British Management University)

**Presenter:** DENG, Shiyu (University of Cambridge)

**Session Classification:** Afternoon Session 1

Contribution ID: 16

Type: **Talk**

## **On the study of the phase behavior of salts in water by high-pressure differential scanning calorimetry to prevent clogging in the hydrothermal conversion of wet biomass to biogas and biocrude.**

Hydrothermal liquefaction (HTL) and catalytic hydrothermal gasification (cHTG) have drawn considerable attention in recent years as a clean and renewable biocrude and synthetic natural gas (bio-SNG) production technology, respectively. Under the temperature (350-450°C) and pressure (200-300bars) typically used, water acts as the solvent and reactant, hence no drying step is required to convert biomass feeds of high moisture content, leading to high energy efficiency compared to conventional conversion technologies. Operating near or beyond the critical point of water brings several challenges that have been the topic of several research projects recently in the catalyst process engineering group at PSI.

One of them relates to the complex phase behavior of salts in hot and pressurized water, which is severely impacted by the rapid decrease of the dielectric constant of pressurized water with increasing temperature. This can lead to the precipitation of salts present in the biomass stream processed, leading to clogging of pipes. I will cover our recent studies in high-pressure differential scanning calorimetry (HP-DSC) used as an accurate technique to investigate the phase behavior of such solutions under hydrothermal conditions. HP-DSC allowed us to collect phase behavior data for unknown binary, ternary, or more complex mixtures, to discover liquid-liquid immiscibility in several of them, and establish the dependence of the phase behavior to the composition of the cations present in a mixture. I will also describe the technology developed at PSI to continuously extract salts during the process and the different strategies followed to optimize such extraction and prevent clogging based on the data obtained from these analyses.

**Author:** BAUDOUIN, David (PSI - Paul Scherrer Institut)

**Co-author:** Prof. VOGEL, Frédéric (PSI - Paul Scherrer Institute)

**Presenter:** BAUDOUIN, David (PSI - Paul Scherrer Institut)

**Session Classification:** Afternoon Session 1

Contribution ID: 17

Type: **Poster**

## A Tool to Simulate Muon Stopping Fractions in Hydrostatic Pressure Cells.

External parameters have been shown to be a powerful tool for tuning the electronic or magnetic ground state of a material. Hydrostatic pressure is a widely used external parameter but can lead to issues in the experimental procedure, such as a large background or spurious responses. Specifically, within muon spin rotation ( $\mu$ +SR), a significant share of the incoming muons can stop inside the pressure cell instead of the sample, giving a large background signal, and with non-magnetic samples the signal from the sample can be lost inside the background, with it being difficult to extract within the fit. This all makes it incredibly difficult to align the muon momentum to the sample. In response to these issues, we have developed a tool to aid in simulating muon stopping fractions with the use of pySRIM. The setup is specifically designed for the setup at the GPD spectrometer in the  $\mu$ E1 beamline at the Paul Scherrer Institute. This is presented as a GUI, so that users can easily calculate the stopping fractions of their samples for various muon momentums in order to be able to fit their data and align their sample.

**Authors:** DAS, Debarchan (Paul Scherrer Institute); ELSON, Frank (KTH, Royal Institute of Technology); SIMUTIS, Gediminas; Prof. WEISSENRIEDER, Jonas (KTH, Royal Institute of Technology); MÅN-SON, Martin; FORSLUND, Ola Kenji; Dr PALM, Rasmus (KTH, Royal Institute of Technology); Ms MINIOTAITE, Ugne (KTH, Royal Institute of Technology); SASSA, Yasmine

**Presenter:** ELSON, Frank (KTH, Royal Institute of Technology)

**Session Classification:** Posters + Beers + Wine + Aperol

Contribution ID: 18

Type: **Poster**

## Molecular dynamics simulations of surface tension of mixtures under high pressures

In this contribution we present theoretical framework for quantitative modeling of surface tension of liquids and their mixtures under high pressures. We perform molecular dynamics (MD) simulations (in GROMACS 1) and apply statistical thermodynamics of solutions (namely Kirkwood-Buff theory) [2,3]. This allows us to describe solution structure (distribution functions) not only in coexisting liquid phases, but also at the interface, and importantly build its connection to macroscopic thermodynamics (surface tension, chemical potential, etc.).

We will illustrate this framework on MD simulation data of liquid-gas equilibrium of pure methane at a series of subcritical temperatures, presenting surface tension, vapor pressure, and solution structure of coexisting phases.

This methodology is general with respect to number and complexity of components. Thus, once calibrated to experimental data, it will provide atomic insight in novel, industrially relevant, systems studied within the joint GACR-SNSF project "Properties of liquids exposed to pressurized methane, ethane and hydrogen"

Authors acknowledge the financial support obtained from Czech Science Foundation (GACR) and Swiss National Science Foundation (SNSF) within the research project **23-04741K**.

### References:

[1] Abraham, M. J., Murtola, T., Schulz, R., Páll, S., Smith, J. C., Hess, B., & Lindah, E. (2015). Gromacs: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. *SoftwareX*, 1–2, 19–25.

[2] Smith, P. E., Matteoli, Enrico., & O'Connell, J. P. (2013). *Fluctuation Theory of Solutions: Applications in Chemistry, Chemical Engineering, and Biophysics*. CRC Press.

[3] Chen, F., & Smith, P. E. (2008). Theory and Computer Simulation of Solute Effects on the Surface Tension of Liquids. *The Journal of Physical Chemistry B*, 112(30), 8975–8984.

**Authors:** Mr MELČÁK, Martin (University of Chemistry and Technology, Prague); DURDAKOVA, Tereza-Marketa (Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czechia); HEYDA, Jan (University of Chemistry and Technology, Prague); VOPICKA, Ondrej (Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czechia); TRTIK, Pavel (PSI - Paul Scherrer Institut)

**Presenter:** Mr MELČÁK, Martin (University of Chemistry and Technology, Prague)

**Session Classification:** Posters + Beers + Wine + Aperol

Contribution ID: 19

Type: **Talk**

## Resolving spin reorientation of CrCl<sub>3</sub> induced by high-pressure with MuSR and neutron diffraction

*Wednesday 22 November 2023 14:15 (15 minutes)*

Researches on two-dimensional (2D) materials have attracted tremendous attention both from fundamental and applied sciences since accelerated by the discovery of graphene. Among a large number of 2D materials, chromium trihalides CrX<sub>3</sub> (X = Cl, Br, I) van der Waals (vdW) magnets have also raised a large interest due to the existence of many magnetic subtleties that cannot be explained by their magnetic and/or structural transitions.

Numerous studies were performed on CrI<sub>3</sub>, but only a few have been reported so far on its analogue CrCl<sub>3</sub>. The 2D vdW CrCl<sub>3</sub> compound is stabilized under a rhombohedral symmetry, consisting of 2D Cr layers arranged in a honeycomb web fashion and surrounded by octahedrally coordinated Cl, with weak vdW inter-layer coupling. This makes CrCl<sub>3</sub> an ideal system to study under external stimuli such as pressure or magnetic field, where new intriguing states can be unveiled. Expectantly, studies of CrCl<sub>3</sub> under high pressure and room temperature have been reported. However, its spin dynamics at low-temperature and high-pressure regimes remain unexplored. Motivated by the variability of the spin degree of freedom and spin dynamics under such conditions, we performed muon spin rotation (MuSR) and neutron powder diffractions (NPD) on ambient and hydrostatically pressured CrCl<sub>3</sub> up to 23 kbar down to 2 K. [2,3]

In this study, by incorporating the two techniques and high-pressure, we resolved a suppression of the magnetic ground state and a stronger relaxation rate by MuSR. Within the magnetically ordered states, a spin reorientation was also observed by NPD at high pressure. A linear extrapolation points toward the suppression of magnetism at about  $p_c = 30$  kbar indicating the possible existence of a critical point at  $p_c$ . [3]

[1] Ahmad, A., et al. *Nanoscale* 12.45 (2020): 22935-22944.

[2] Forslund, O., et al. *arXiv:2111.06246* (2021).

[3] Ge, Y., et al., in preparation.

**Author:** GE, Yuqing (Chalmers University of Technology)

**Co-authors:** MANUEL, Pascal; PAPADOPOULOS, Konstantinos (Chalmers University of Technology); ELSON, Frank (KTH, Royal Institute of Technology); KHALYAVIN, Dmitry; NOCERINO, Elisabetta (Stockholm University); DI BERARDINO, Gaia; KHASANOV, Rustem (PSI - Paul Scherrer Institut); ORLANDI, Fabio; SUGIYAMA, Jun; ABDEL-HAFIEZ, Mahmoud; MÅNSSON, Martin; FORSLUND, Ola Kenji; SASSA, Yasmine

**Presenter:** GE, Yuqing (Chalmers University of Technology)

**Session Classification:** Afternoon Session 1

Contribution ID: 20

Type: **Talk**

## Expanding high-pressure neutron instrumentation capabilities

Wednesday 22 November 2023 15:30 (15 minutes)

The demand for high-pressure equipment has doubled over the last decade at the Institut Laue-Langevin. To cope with this demand and ensure successful experiments, we have enhanced pressure generators and expanded our suite of pressure devices.

First, we have significantly improved the 1 GPa liquid pressure generators with:

- a comprehensive revamp of the automation program improving the reliability,
- a modern user interface easing control and maintenance, additional sensors and controls enhancing safety,
- programmable pressure ramps controlled with greater precision,
- remote control and data archiving capabilities.

These enhancements will also be extended to 1 GPa helium gas pressure generators.

We have also developed a non-magnetic Ø6 mm sample bore double-wall pressure cell accommodating pressures up to 1 GPa with liquid or gas pressure transmitting media. Compared to other cells, it reaches higher pressures and features improved neutron transmission and signal-to-noise ratio. Our processes also now adhere to European Certification standards for answering new safety regulations. Today, we prepare a 2 GPa clamp incorporating in-situ temperature and pressure measurements via Ruby fluorescence [1, 2].

As for cells tailored for NSE and SANS experiments, they have demonstrated exceptional qualities, including ultra-low neutron background and high neutron transmission. While the 50 MPa and 300 MPa versions have proven high reliability, the 500 MPa variant has encountered issues and we actively seek advices and know-how to develop a optimal design.

References:

[1] P. Naumov, R. Gupta, M. Bartkowiak et al., Optical Setup for a Piston-Cylinder Pressure Cell: A Two-Volume Approach. *Phys. Rev. Applied* **17** (2022) 024065

[2] R. Khasanov, M. Elender and S. Klotz. The use of LEDs as a light source for fluorescence pressure measurements, *High Pressure Research* **43** (2023) 192

**Authors:** GONTHIER, Julien (Institut Laue Langevin); CASTILLO, Zeus (Institut Laue-Langevin); LELIÈVRE-BERNA, Eddy (Institut Laue-Langevin); MAURICE, James (Institut Laue Langevin); PAYRE, Claude (Institut Laue Langevin); BARTKOWIAK, Marek (Paul Scherrer Institut); ELENDER, Matthias (Paul Scherrer Institut); KHASANOV, Rustem (Paul Scherrer Institut); NAUMOV, Pavel (Paul Scherrer Institut); GIRIAT, Gaétan (EFPL)

**Presenter:** GONTHIER, Julien (Institut Laue Langevin)

**Session Classification:** Afternoon Session 2

Contribution ID: 22

Type: **Talk**

## Revealing the KDP soft-mode coupling mechanism with infrared spectroscopy under pressure

*Wednesday 22 November 2023 11:00 (30 minutes)*

Potassium dihydrogen phosphate,  $\text{KH}_2\text{PO}_4$  (KDP), is a classic, broadly used ferroelectric material. It is a model system of an order-disorder material, with a Curie temperature  $T_C$  of 123 K. Above this temperature, it is a tetragonal paraelectric. Below, it becomes orthorhombic. In the 1940s, Slater wrote an order-disorder theory to describe rather well the physics of KDP [1]. However, his theory failed to describe why the polarization doesn't change below the ordering temperature, and why  $T_C$  increases when hydrogen is replaced by deuterium. Therefore, it was understood that phonons must also play a role, through coupling to the proton which tunnels in a double well potential [2]. How exactly this happens remained unclear for a long time [3].

In our work, which spanned more than a decade and took place across two continents, we measured the far-infrared reflectivity of KDP up to 2 GPa in its ferroelectric and paraelectric phases. We identified an infrared mode that couples the hydrogen network to the lattice modes, to create the ferroelectric polarization.

[1] J. C. Slater, Theory of the Transition in  $\text{KH}_2\text{PO}_4$ , *The Journal of Chemical Physics* 9, 16 (1941).

[2] J. Pirenne, On the ferroelectricity of  $\text{KH}_2\text{PO}_4$  and  $\text{KD}_2\text{PO}_4$  crystals, *Physica* 15, 1019 (1949).

[3] P. Simon and F. Gervais, Phase-transition mechanism in  $\text{RbH}_2\text{PO}_4$ -type ferroelectrics, *Phys. Rev. B* 32, 468 (1985).

**Authors:** AKRAP, Ana (University of Fribourg); HOMES, Christopher (National Synchrotron Light Source II, Brookhaven National Laboratory); SANTOS, David (Department of Physics, University of Fribourg); CAPITANI, Francesco (Synchrotron Soleil); LOBO, Ricardo (ESPCI Paris); NASRALLAH, Serena (Department of Physics, University of Fribourg)

**Presenter:** AKRAP, Ana (University of Fribourg)

**Session Classification:** Morning Session

Contribution ID: 23

Type: **Talk**

# Tuning and understanding correlated quantum phases of layered materials

*Wednesday 22 November 2023 11:30 (30 minutes)*

The classification and deep understanding of phases of quantum matter is a necessary premise for utilizing quantum materials in all areas of modern and future electronics in a controlled and optimal way. In this respect, layered systems with highly anisotropic electronic properties have been found to be potential hosts for rich, unconventional and tunable exotic quantum states. Prominent classes of layered materials are cuprates, transition metal dichalcogenides (TMDs) and kagome-lattice systems.

In this talk, I will provide brief overview of systems, from different material classes, with novel electronic and magnetic properties, where the application of temperature, magnetic field, hydrostatic pressure, and uniaxial strain lead to large and unexpected effects. These include the topological kagome magnet  $\text{TbMn}_6\text{Sn}_6$  [1] (where we show that the topological electronic properties tied to the spin-polarized Dirac dispersion is promoted only by true static out-of-plane ferrimagnetic order and is washed out by the slow commensurate magnetic fluctuations), the topological kagome metals  $\text{AV}_3\text{Sb}_5$  ( $A=\text{K,Rb}$ ) [2-4] (where we found intertwining of a TRSB charge ordered state with tunable unconventional superconductivity), the cuprate system  $\text{La}_2 - x\text{Ba}_x\text{CuO}_4$  [5] (where an extremely low uniaxial stress of 0.1 GPa induces a dramatic rise in the onset of 3D superconductivity), and superconducting TMDs  $2\text{H-NbX}_2$  ( $X=\text{Se,S}$ ) [6] (where a strong strain/hydrostatic pressure effect on the superfluid density and its unconventional scaling with the critical temperature were observed). I will discuss these results using a combination of muon-spin rotation under pressure/strain/field, magnetization, transport, and diffraction techniques.

[1] Mielke et. al., and Guguchia, *Communications Physics* **5**, 107 (2022).

[2] Mielke et. al., and Guguchia, *Nature* **602**, 245-250 (2022).

[3] Guguchia et. al., *Nature Communications* **14**, 153 (2023).

[4] Guguchia et. al., *NPJ Quantum Materials* **8**, 41 (2023).

[5] Guguchia et. al., *Physical Review Letters* **125**, 097005 (2020).

[6] Rohr et. al., and Guguchia, *Science Advances* **5(11)**, eaav8465 (2019).

**Author:** GUGUCHIA, Zurab (PSI - Paul Scherrer Institut)

**Presenter:** GUGUCHIA, Zurab (PSI - Paul Scherrer Institut)

**Session Classification:** Morning Session

Contribution ID: 24

Type: **Poster**

## Uniaxial-pressure devices for scattering experiments

Over the last years, we have developed and implemented a few different designs of uniaxial pressure devices, specifically optimized for scattering experiments.

I will present the relevant considerations for such experiments, discuss selected recent results and introduce new in-situ devices available for the user program at SINQ.

[1] GS et al., to appear in Swiss Neutron News, vol. 62 (2023)

[2] GS et al., Communications Physics 5, 296 (2022)

[3] GS et al., Review of Scientific Instruments 94, 013906 (2023)

[4] Guguchia et al., arXiv:2302.07015 (2023)

[5] Thomarat et al., under review.

[6] Küspert et al., under review.

**Author:** SIMUTIS, Gediminas (PSI - Paul Scherrer Institut)

**Presenter:** SIMUTIS, Gediminas (PSI - Paul Scherrer Institut)

**Session Classification:** Posters + Beers + Wine + Aperero

Contribution ID: 25

Type: **Poster**

## Take it up a notch - Sample Environment at SINQ

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 acquisition 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.

<sup>1</sup> 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

**Author:** BARTKOWIAK, Marek (Paul Scherrer Institut)

**Presenter:** BARTKOWIAK, Marek (Paul Scherrer Institut)

**Session Classification:** Posters + Beers + Wine + Aperero

Contribution ID: 26

Type: **Poster**

## BYO Beamline Experiment with 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. It is designed to build up complex setups for beamline experiments as well as for lab based measurements. It enables users of large scale facilities to integrate their own setups into the facility data acquisition work flow utilizing the sample environment communication standard SECoP.

SECoP is already in use at SINQ/PSI and FRMII/MLZ and will become available at many other user facilities world wide.

**Author:** Dr ZOLLIKER, Markus (PSI)

**Presenter:** Dr ZOLLIKER, Markus (PSI)

**Session Classification:** Posters + Beers + Wine + Aperero