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Report of Contributions

Contribution ID : **2** Type : **not specified**

Exploring the phase diagram of the Shastry-Sutherland compound, SrCu2(BO3)2

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 magnets where competing interactions may lead to exotic magnetic states and an external parameter such as magnetic field or pressure can be used to tune the system from one quantum state to another. The Shastry-Sutherland (SS) lattice is such a frustrated system. It consists of spin pairs (dimers) embedded in a square lattice and with inter-dimer coupling, J, and intra-dimer coupling J'. It has an exact dimer product ground state for J'/J ≤ 0.675 [1]. Upon increasing the ratio of J'/J, the system goes through a quantum phase transition to a plaquette singlet state followed by a Néel phase [2]. SrCu2(BO3)2 (SCBO) is a unique material since it is topologically equivalent to the SS lattice [3]. With J'/J ~ 0.6 close to the critical point, SCBO presents remarkable experimental testing grounds for the SS model. The ratio J'/J may be altered by applying pressure and the resulting phase diagram resembles that theoretically predicted for the SS model [4,5]. As a frustrated magnetic system, SCBO exhibits a series of phase transitions upon applying a magnetic field [6,7]. However, with the first transition to the 1/8 magnetization plateau occurring at 27T, these phases are beyond reach for standard neutron scattering experiments and hence direct evidence as to the static and dynamic magnetic behavior is lacking. One way of tuning these magnetic-field-induced transitions to a reachable regime is by applying pressure [8,9]. We demonstrate how to carry out such high-pressure, high-magnetic-field and low-temperature neutron scattering experiment and also discuss the associated challenges with regards to the data analysis.

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Contribution ID : **3** Type : **not specified**

Path-finding for triple-axis spectrometers

Monday, 18 October 2021 16:40 (15)

As part of our efforts in the field of autonomous instrument control, we present a path-finding algorithm and implementation for triple-axis spectrometers. Due to angular constraints in the instrument space, as well as from obstacles such as walls, not every (Q, E) coordinate point is accessible for the instrument. A careful mapping of the available positions is usually required before each experiment to avoid any collisions. The present algorithm is able to automatically find the optimal path for the instrument, keeping it at the furthest possible distance from obstacles. It does so by calculating the Voronoi bisectors of the instrument's angular configuration space. Of these it creates a mesh of possible paths and finds the shortest path along the bisectors.

This work is part of a thesis supervised by Dr. L. Ma and Prof. Dr. Ch. Icking.

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Session Classification : Experimental life – how to perform experiments in future (Chair: Astrid Schneidewind)

Contribution ID : **4** Type : **not specified**

Phonons in hydrid perosvkites

Wednesday, 20 October 2021 10:30 (30)

A.C. Ferreira, S. Paofai, A. Létoublon, J. Ollivier, S. Raymond, B. Hehlen, B. Rufflé, C. Katan, J. Even, and Ph. Bourges

Hybrid organolead perovskites (HOP) have started to establish themselves in the field of photovoltaics, mainly due to their great optoelectronic properties and steadily improving solar cell efficiency. Although much recent attention has been devoted towards unraveling their microscopic optoelectronic properties, the structural dynamics (phonons) are currently still lacking a comprehensive understanding as compared to that already reached for classic semiconductors. Study of the lattice dynamics is then a key in understanding the electron-phonon interactions at play, responsible for the electronic properties. Using inelastic neutron scattering and light (Brillouin and Raman) scattering, we have investigated the phonon spectrum in four different hybrid perovskite single crystals: MAPbBr3, FAPbBr3, MAPbI3 and α-FAPbI3, where MA and FA correspond to methylammonium (CH3NH3) and formamidinium ((CH2)2NH) molecules, respectively.
Previously, we have studied the low energy acoustic phonons and determine the complete set of elastic constants [1,2]. They are characterized by soft elastic constants compared to classic semiconductors, with a particular very soft shear modulus C44. Between room temperature and 240 K, a tendency towards an incipient ferroelastic transition is also observed in FAPbBr3. A systematic lower sound group velocity is found in the technologically important iodide-based compounds compared to the bromide-based ones. The findings suggest that low thermal conductivity and hot phonon bottleneck phenomena are expected to be enhanced by low elastic stiffness, particularly in the case of the ultrasoft α-FAPbI3
Recently, we investigated the optical phonon spectrum below 40 meV in single crystals of the same four different hybrid lead halide perovskites [3]. Low temperature spectra reveal weakly dispersive optical phonons, grouped in three main bundles of phonons (see figure). These results will be discussed showing that the lowest energies phonons at 2-5 meV seem to be the origin of the limit of the charge carrier mobilities in these materials. The temperature dependence of the neutron spectra reveals a significant anharmonic behaviour, resulting in optical phonon overdamping at temperatures as low as 80 K, questionning the validity of the quasi-particle picture for the low energy optical modes at room temperature where the solar cells actually operate.

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Session Classification : Science cases (Chair: Andrew Wildes)

Contribution ID : **5** Type : **not specified**

Pyrochlores magnets, spin ice and quantum spin ice physics: the neutron scattering perspective

Tuesday, 19 October 2021 14:35 (30)

Pyrochlores magnets, spin ice and quantum spin ice physics: the neutron scattering perspective

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Magnetic frustration, the inability of a system to simultaneously satisfy all of its interactions, is the subject of much research in condensed matter physics. This phenomenon, which can be related to the topology of the crystalline network or to the competition between interactions, constitutes the source of new exotic states of matter, the description of which goes beyond the classical models. Spin ice and its quantum analogues are an emblematic example of this physics. The crystallographic structure of these materials is based on a pyrochlore-type network, formed by a set of tetrahedra connected by their vertices, each node being occupied by a magnetic rare earth ion (Tb, Dy, Ho, Pr, etc.). In these compounds, the relevant electronic orbitals have the shape of a very thin needle, elongated towards the centres of each tetrahedra. The magnetic moment of each ion can then only point inward or outward, much like the ±1 states of an Ising variable. The classical ground state of such a system is very peculiar in that it is infinitely degenerate. Indeed, the only prescription for constructing it is to follow a local organizing principle, which states that each tetrahedron must have two spins "in" and two "out". In recent years, theoretical physicists have proposed a new vision of the problem, noting that the "two in-two out" rule is actually analogous to the conservation law of a fictitious magnetic flux (div B=0) in electromagnetism [1]. The analogy is complete when quantum fluctuations are incorporated. Indeed, the fluctuations of the fictitious magnetic field B, create by virtue of the Lenz law curl E=- dB/dt an "emergent" electric field E. According to theoretical predictions, a quantum spin ice should have a particular excitation spectrum characterized by a photon-like mode. Using examples from the literature and from our own recent research, we will show in this presentation how inelastic neutron scattering has contributed to a better understanding of this physics. We will especially discuss the case of $Tb_2Ti_2O_7$, $Pr_2Zr_2O_7$, $Er_2Ti_2O_7$, as well as $Nd_2Zr_2O_7$.

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Session Classification : Science cases (Chair: Philippe Bourges)

Contribution ID : **6** Type : **not specified**

The need for realistic simulations of phonon intensities in inelastic neutron and x-ray scattering – an experimentalist's perspective

Monday, 18 October 2021 17:50 (20)

The advent of inelastic neutron scattering in the middle of the last century enabled detailed studies of lattice vibrations, i.e. phonons, in condensed matter. Initially focused on simple structures [1,2], inelastic neutron scattering has been instrumental for our understanding of superconductivity in A15 compounds [3] and more recent conventional superconductors [4,5]. However, many materials of current interest have a large number of atoms in the crystallographic unit cell, which results in an even larger number of phonon dispersion lines. Having obtained a data set from inelastic neutron or x-ray scattering, the experimenter relies heavily on model calculations for an understanding of the observed intensities. Naturally, such calculations become more demanding or even impossible with large unit cells.

Here, I will discuss various investigations of lattice dynamical properties by inelastic neutron and x-ray scattering in which ab-initio and other model calculations have been indispensable for a detailed understanding. I will highlight the way in which model calculations have been employed but also point out limitations. Finally, I will discuss based on these examples the need for more realistic simulations of phonon intensities requiring an improved link between lattice dynamical modelling and the experimental setup, i.e., evaluating resolution effects on the calculated phonon dispersion and intensities.

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Session Classification : Experimental life – how to perform experiments in future (Chair: Astrid Schneidewind)

Contribution ID : **7** Type : **not specified**

Exploiting symmetry with brille

Tuesday, 19 October 2021 18:40 (10)

Modern time-of-flight neutron spectrometers routinely collect datasets covering volumetric reciprocal space. By taking advantage of multiplexing techniques or parametric studies datasets can exceed one billion independent observations. Software exists to facilitate collecting observations from volumetric datasets in arbitrary, user-defined, regions of reciprocal space; which can often be compared directly to theoretical models for the double differential cross section. Such comparisons benefit from existent software to account for instrumental resolution effects; however, the large number of observations makes the evaluation costs prohibitively high for typical physical models.

The open-source software package brille has been developed to facilitate faster evaluation of arbitrary physical models by exploiting the irreducible Brillouin zone symmetry of crystal samples. Typically, brille stores a cache of model eigenvalues and eigenvectors at the vertices of a conformal grid and later linearly interpolates between the cached values. Due to the possibility of atom-labelling permutations under application of a lattice symmetry operation, brille must typically be tailored to a model. Thus far brille can reliably interpolate the eigenvalues and eigenvectors of the grand dynamical matrix and has been used successfully to speed-up phonon calculation with Euphonic. Future developments will enable brille to handle second-quantized systems as well, with an eye towards speeding-up linear-spinwave calculations with SpinW.

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Session Classification : Poster session

Contribution ID : **8** Type : **not specified**

From one- to two-magnon excitations in the S = 3/2 magnet β-$CaCr_2O_4$

Tuesday, 19 October 2021 17:40 (10)

Decades of theoretical, numerical and experimental studies have sought quantum systems, beyond the classical picture of conventional magnetism, focusing on low-dimensional S = 1/2 materials. The characteristic features of such systems are the lack of long-range magnetic order and the presence of deconfined fractional spin-1/2 excitations called spinons. Owing of the exact solution of the spin- chain model, theoretical and experimental works have led to a fairly comprehensive understanding of spin dynamics in the simplest quantum system, the Heisenberg antiferromagnetic chain of S = 1/2 spins. As spinons are created in pairs, the excitation spectrum for such spin chain is characterised by a continuum of excitations. Introducing a magnetic coupling between individual S = 1/2 chains forces spinon excitations to confine into bound states, called magnons, thus leading to a dimensional crossover between a quantum one-dimensional to a semi-classical three-dimensional regime. Yet, what happens when increasing the spin fractional quantum number is not known. Here we present neutron scattering experiments for a weakly coupled S = 3/2 chain compound, β-$CaCr_2O_4$. In the ordered state, the low-energy spin fluctuations resemble large-S linear spin-waves from the incommensurate groundstate. However, at higher energy, these semi-classical and harmonic dynamics are replaced by an energy and momentum broadened continuum of excitations. Applying kinematic constraints, required for energy and momentum conservation, sum rules of neutron scattering and comparison against exact diagonalization calculations, we show that the dynamics at high energy resemble low-S one-dimensional quantum fluctuations. β-$CaCr_2O_4$ therefore represents a unique example of a magnet at the border between classical Néel and quantum phases, hosting dual behaviors. As studies on low-dimensional magnets with intermediate spin values are scarce, we show that this system provides a rich playground to explore the physics beyond the usual quantum/classical dichotomy.

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Session Classification : Poster session

Contribution ID : **9** Type : **not specified**

Domain-Aware Gaussian Processes and High-Performance Mathematical Optimization for Optimal and Autonomous Data Acquisition

Monday, 18 October 2021 15:40 (20)

Gaussian Processes and Gaussian-Process-Related stochastic processes have shown to be a powerful tool for autonomous control of data acquisition due to their robustness, analytical tractability, and natural inclusion of uncertainty quantification. In this talk, I want to present our work on a general, flexible, and powerful GP-driven framework for autonomous data acquisition. The focus will lie on making Gaussian processes domain aware, how this awareness can be used for decision-making, and the computational and mathematical challenges that come with domain awareness.

Primary author(s) : NOACK, Marcus

Presenter(s) : NOACK, Marcus

Session Classification : New algorithms and Machine learning: relevance to inelastic neutron scattering (Chair: Toby Perring)

Contribution ID : **10** Type : **not specified**

MIEZE - Neutron spin-echo optimized for magnetic materials

Tuesday, 19 October 2021 18:10 (10)

Highest resolution in classic TAS and TOF techniques always comes at the price of decreased flux. This challenge has been tackled by the development of neutron spin-echo, where the resolution is completely decoupled from the wavelength spread of the instrument. Conventional neutron spin echo reaches an energy resolution down to < 1 neV. However, classical NSE is limited in the range of high energy transfers and depolarizing samples/sample environments.

MIEZE on the other hand is in essence a high-resolution, spin-echo, time-of-flight technique. In contrast to classical neutron spin-echo, all beam preparation and therefore all spin manipulation is done BEFORE the sample, opening up the possibility of introducing depolarizing conditions at the sample position.Therefore, magnetic, or strongly incoherently scattering samples can easily be measured without loss of signal. Additionally, large magnetic fields can be applied to the sample, making MIEZE an excellent tool for studying quasi-elastic and inelastic processes in quantum matter, such as fluctuations at quantum phase transitions, magnon dynamics in ferromagnets, or the melting of superconducting vortex lattices.
With the introduction of the field-subtraction coils, it has been possible to push the technique to shorter spin-echo times and higher energy transfers making it even more attractive for spectroscopic studies of quasi-elastic and inelastic processes.
As a very young technique MIEZE is still not well known in the TAS/TOF community and the I2NS meeting is the ideal place to discuss future developments and collaboration in this area.

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Presenter(s) : JOCHUM, Johanna

Session Classification : Poster session

Contribution ID : **11** Type : **not specified**

ALSA – Automatic Laue Sample Aligner

Tuesday, 19 October 2021 18:00 (10)

Each of you will be familiar with the well-known chart of the dependence of the flux of large synchrotron and neutron infrastructures on time. While synchrotron power continues to increase by orders of magnitude, neutrons reached their highest power 50 years ago at ILL and it will be slightly surpassed with the help of ESS. Therefore, scientists have been trying for decades to optimize optics, measurement strategy or build multi-detector systems to take advantage of every possible neutron to measure weaker fluctuations on smaller samples.

Our approach tackles the problem from the other end. The goal of **ALSA** is to increase the sample size for inelastic neuron experiments. It will fully automatize the co-alignment process by using a state-of-the-art X-Ray Laue diffractometer, robotized manipulators, real-time camera recognition and special software analysis for crystal placing. The device **ALSA** will be a true game changer in the field of inelastic neutron scattering, because it will drastically speed-up sample preparation.

In my presentation, I will focus on the design of the device, the possible use of artificial intelligence, and discuss a newly developed online 2D irregular bin packing problem with limited rotations used for crystal placement.

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Presenter(s) : Dr. ČERMÁK, Petr (MGML, Charles University)

Session Classification : Poster session

Contribution ID : **12** Type : **not specified**

Panther - a new single-crystal thermal-neutron time-of-flight spectrometer

Tuesday, 19 October 2021 18:20 (10)

Panther is a new thermal-neutron direct-geometry hybrid time-of-flight spectrometer at the Institut Laue-Langevin. Phase-1 of the project is completed, and the design and performance of the instrument will be discussed. Panther is equipped with two double focusing monochromators: a pyrolytic graphite for which the (002), (004), and (006) reflections are routinely used, and a copper monochromator where both the (220) and (331) reflections can be used. The beam is pulsed by a Fermi chopper with a maximum speed of 500 Hz and which can be operated in time-focusing mode. A huge array of 288 position-sensitive 3He detectors of diameter 22 mm and length of 2 m covers angles in the horizontal plane between -16 and +136 degrees and in the vertical plane between -13 and +28 degrees. This corresponds to a solid angle of 2 steradians, making the instrument ideally suited for studies of single crystalline samples. A radial oscillating collimator reduces the parasitic scattering from the sample environment and the evacuated detector tank is shielded by 30 cm of borated high-density polyethylene to reduce background. Incoming energies between 7.5 and 150 meV are currently available. The flux at the sample position for an incoming energy of 19 meV is 5E5 n/cm2/s. The energy resolution at elastic energy transfer varies between 4 and 6% of the incoming energy. In phase-2 of the project, five new disc choppers will be installed upstream from the Fermi chopper and monochromator to reduce background and order contamination, and a device for polarization analysis, PASTIS-3, is being developed.

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Session Classification : Poster session

Contribution ID : **13** Type : **not specified**

Geometry and resolution calculations of the new INS spectrometer at FLNP JINR

Tuesday, 19 October 2021 18:30 (10)

The inverse-geometry inelastic neutron spectrometer NERA has already been operating for more than three decades and during that time has proven to be a very successful machine for broadband chemical spectroscopy with neutrons. To continue the research using the best modern technologies, the project of a new inverse-geometry inelastic neutron spectrometer has been started. New instrument will be located in the Frank Laboratory of Neutron Physics (JINR, Russia) at IBR-2 pulse reactor. Its parameters will significantly outdo the parameters of NERA spectrometer. With solid angle of 6 sr and resolution of the elastic line at the level of 0.55 meV the new instrument will allow to perform chemical spectroscopy with neutrons on a world-class level. Calculations of the secondary spectrometer's geometry and performance were carried out during the design phase of the project and they are presented in this work. The main concept is to place a set of HOPG analysers resembling a bell shape, on both sides of the sample position. Design and optimization of the secondary spectrometer were accomplished using Monte-Carlo ray tracing simulation software McStas and analytical methods.
Project of new INS spectrometer is supported by the Grant from the Polish Plenipotentiary in JINR, Dubna, Russia (Regulation no. 166 of 11.03.2021, article 5).

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Presenter(s) : Mrs. KLEPACKA, M.K. (AMU Poznan / FLNP JINR)

Session Classification : Poster session

Contribution ID : **14** Type : **not specified**

Inelastic Neutron Scattering Measurements of ClathrateHydrates for the HighNESS Project

Tuesday, 19 October 2021 17:30 (10)

Clathrate hydrates are are crystalline water-based solids (similar to ice), which form cages that are able to host guest molecules. The guests are trapped in cavities of the hosts, that are composed of hydrogen-bonded water molecules. Tetrahydrofuran (THF) clathrate hydrates (fully or partially deuterated) seem particularly well suited as a moderation medium for neutron, as they possess low-energy modes with sufficiently large inelastic neutron scattering cross sections [1].

Since THF only occupies the large cages in the clathrate structure, the twice more abundant smaller cages can still be filled with other molecules. This allows a binary clathrate, consisting of two guest molecules within the water structure to be constituted [2]. Of particular interest is oxygen as a second guest molecule. It offers an additional path for moderation via a cooling cascade mechanism that exploits the zero-field splitting of the magnetic triplet ground state of molecular oxygen [3].

In the context of the European project HighNESS [4, 5], whose main mission is the "Development of an High Intensity Neutron Sources at the European Spallation Source (ESS)", we present the first results of measurements of the neutron scattering function $S(q,\omega)$ for clathrate hydrates in absolute units. Both the simple and the binary structure are investigated on the time-of-flight (TOF) spectrometer Panther and IN5 at the ILL. The results include measurements with neutron-wavelengths from 0,1 nm to 0,3 nm, for fully and partially deuterated clathrate samples. With this variation contrast we show the contribution of the different constituents.

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Session Classification : Poster session

Contribution ID : **15** Type : **not specified**

Role of correlated disorder on lattice dynamics in negative thermal expansion material, Cadmium Cyanide.

Cubic cadmium(II) cyanide is amongst the most important isotropic negative thermal expansion (NTE) materials, with behavior more than twice as extreme as that of better known systems such as ZrW_2O_8. We investigate the relationship between the geometrically frustrated orientational order of the molecular CN^- anion the system's lattice dynamics. Inelastic neutron scattering (INS) is reported on the system approaching the cyanide order-disorder transition from above and displays non-trivial mode-softening over a wide range of temperatures associated with the correlated cyanide order. The simulation of lattice dynamics in systems with correlated disorder is involved: supercell lattice dynamics (SCLD) are used for simulations on a simple model system. Simplifying approximations are investigated towards the goal of reproducing the INS measured, and understanding the significance of correlated disorder in the NTE mechanism.

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Presenter(s) : BULLED, Johnathan (Inorganic Chemistry Laboratory, Oxford University)

Session Classification : Poster session

Contribution ID : **17** Type : **not specified**

Stroboscopic polarized experiments to study the domain dynamics in multiferroics

Tuesday, 19 October 2021 12:15 (30)

In so-called type-II multiferroics, a complex magnetic structure of chiral character directly drives finite ferroelectric polarization resulting in a close coupling between magnetic and electric order parameters. Therefore, multiferroics allow one to fully control antiferromagnetic domains by external electric fields opening the path to the study of the corresponding domain dynamics. We use a stroboscopic method to analyze the domain relaxation following inversion of external field. Neutron scattering thereby permits the analysis of multiferroic domain relaxation over about 8 orders of magnitude in time. While a first experiment on MnWO4 revealed a strange temperature dependence of the multiferroic domain relaxation [1], our consecutive experiments on TbMnO3 [2] as well as on other type-II multiferroics revealed an astonishingly simple temperature and field dependence. In TbMnO3 the simple combination of an activation law and the Merz law known in ferroelectrics describes the relaxation times in a wide range of electric field and temperature with just two parameters, an activation-field constant and a characteristic time representing the fastest possible inversion [2]. Over the large part of field and temperature values corresponding to almost 6 orders of magnitude in time, multiferroic domain inversion is thus dominated by a single process, the domain wall motion. However when approaching the multiferroic transition other mechanisms yield an accelerated inversion. The combined Merz-activation law was also found to describe the multiferroic relaxation in Ni3V2O8, CuO, (NH4)FeCl5•H2O, and in NaFeGe2O6 [3]. Further perspectives of this technique for the study of multiferroics and of other materials will be discussed.

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In collaboration with: J. Stein[1], S. Biesenkamp[1], M. Baum[1], T. Cronert[1], A.C. Komarek[1], S. Holbein[1,2], P. Steffens[2], K. Schmalzl[2], W. Schmidt[2], Y. Sidis[3], P. Becker- Bohatý [4], L. Bohatý[4], J. Leist[5], and G. Eckold[5]; [2]Institut Laue Langevin, Grenoble; [3]Laboratoie Léon Brillouin, [4]Institut für Kristallographie, Köln; [5]Institut für Physikalische Chemie, Göttingen.

Primary author(s) : BRADEN, Markus

Presenter(s) : BRADEN, Markus

Session Classification : Providing the right experimental conditions - for real (Chair: Arno Hiess)

Contribution ID : **18** Type : **not specified**

Using Generative Adversarial Networks to match experimental and simulated inelastic neutron scattering data

During the past decades, research in materials science has been accelerated by the rapid development of synchrotron and neutron sources.1 Conventional data analysis approaches using minimization techniques, such as least-squares fitting algorithms, cannot keep up with the amount of increasing size of measured datasets. Consequently, data analysis is becoming a bottleneck for research in materials science.2, 3 Therefore, it is of great importance to improve the current state-of-art for data analysis for materials science, particularly utilizing recent developments in artificial intelligence and machine learning (ML).2-4 One of the unsolved problems in this context is to match the simulated datasets that the ML algorithms are trained on to the experimental datasets. This has particularly been a problem for the analysis of inelastic neutron scattering (INS), where it is computationally expensive to ensure that simulated data correctly mimics the experimental signal and background.5 In our project, we are attempting to improve this state through better ML for helping us effectively analyse neutron datasets. More specifically, we are developing generative adversarial networks (GANs) that can learn to make simulated INS data that matches experimental INS dataset under a second. This GAN-based approach, once trained, will be deployed in a range of scenarios for analysing and understanding INS dataset. It can be used to help classify materials structures from the INS datasets and to work with other ML and non-ML (e.g. Spin-W6) algorithms which can estimate magnetic Hamiltonian parameters from INS data. Furthermore, the aim is to expand the algorithm to also match simulated and experimental datasets for other techniques than INS.

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6. https://spinw.org/

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Presenter(s) : Mr. ANKER, Andy Sode (Department of Chemistry, University of Copenhagen, 2100 Copenhagen Ø, Denmark)

Session Classification : Poster session

Contribution ID : **19** Type : **not specified**

Quantum bits and entanglement: a neutron scattering view

Wednesday, 20 October 2021 09:00 (30)

Molecular nanomagnets are model systems to study the spin dynamics and magnetic correlations in low dimensional magnets. The advances in the chemical engineering of magnetic molecules have allowed the synthesis of tailor-made systems which provide promising architectures for the realization of quantum computers.
Molecular nanomagnet can display relatively long coherence time, can host entanglement states and they are scalable, making them very attractive from the quantum computation perspective.
Neutron scattering techniques have been intensively and successfully used to study the microscopic properties of molecular magnets and have enabled to reveal the signatures of their quantum behaviour.
I will show how inelastic neutron scattering (INS) experiments on single crystals of molecular magnets can be used to portray entanglement in weakly coupled molecular qubits [1]. Moreover, INS has been used to study phonons in a molecular qubit to investigate the origin of its decoherence [2].

Primary author(s) : Dr. GUIDI, Tatiana (ISIS Facility, Rutherford Appleton Laboratory (UK))

Presenter(s) : Dr. GUIDI, Tatiana (ISIS Facility, Rutherford Appleton Laboratory (UK))

Session Classification : Science cases (Chair: Andrew Wildes)

Contribution ID : **21** Type : **not specified**

Digital Twins and Virtual Experiments: developments and chances

Monday, 18 October 2021 18:30 (20)

Recent experiences have highlighted that in order to ensure the continued success of neutron scattering as a method, user support must be improved not only at the facilities, but also while users are still in the planning, proposal-writing and preparation stages of an experiment.

Digital twins, which provide a virtual copy of neutron scattering instruments and their user interface(s), are an ideally suited mechanism to familiarize users with the specifics of the instrument as well as the used software, and their features and limitations.

Combined with a realistic simulation of neutron trajectories and scattering behavior at the sample, digital twins can also be made into a powerful tool for the preparation of experiments, e.g. to estimate beamday requirements or feasibility of different configurations.

In this talk, I will show how practical implementation of such digital twins can look like, how to make them accessible to users, and what future developments can be expected in this area.

Primary author(s) : BRANDL, Georg (Forschungszentrum Jülich, JCNS)

Presenter(s) : BRANDL, Georg (Forschungszentrum Jülich, JCNS)

Session Classification : Experimental life – how to perform experiments in future (Chair: Astrid Schneidewind)

Contribution ID : **22** Type : **not specified**

Instrumentation trends for multiplexing continuous-beam spectrometers

Tuesday, 19 October 2021 08:35 (45)

The recent decades have seen a constant and fruitful development of neutron spectrometers of the triple-axis type. Different ways of multiplexing have been implemented and a number of instruments are performing user experiments regularly, while some have recently been replaced by even better instruments. In this overview, I will review the common designs and their typical use cases at a number of facilities. Furthermore, I will point towards the coming interesting developments. Here, I will focus on the development with the CAMEA spectrometer at PSI and the similar (although time-of-flight) instrument BIFROST, under construction at ESS.

Primary author(s) : LEFMANN, Kim (University of Copenhagen)

Presenter(s) : LEFMANN, Kim (University of Copenhagen)

Session Classification : New trends in instrumentation (Chair: Henrik Ronnow)

Contribution ID : **26** Type : **not specified**

From IN8 to THERMES – a thermal three-axis spectrometer commissioned at ILL

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 providing high counting rate even for small and low-scattering samples. The new monochromator unit has been recently commissioned. The device is the fruit of the experience accumulated in the former TAS-group at ILL in using Bragg-focusing beam optics with independently variable and remotely controlled horizontal and vertical focusing (bending) of the crystal reflecting planes. The new monochromator for the thermal neutron beam considerably outperforms the previously used one. It 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, for instance) 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.

Primary author(s) : IVANOV, Alexandre (ILL); PIOVANO, andrea (ILL)

Session Classification : Poster session

Contribution ID : **28** Type : **not specified**

Quantum Critical Phenomena in Metals with Competing Interactions Quantum

Tuesday, 19 October 2021 16:00 (30)

Quantum phase transitions (QPTs) are arguably one of the most intriguing phenomena that can occur when
the electronic ground state of strongly correlated metals are tuned by external parameters such as pressure,
magnetic field or chemical substitution. They define transitions between different states of matter that are
driven by quantum (as opposed to thermal) fluctuations. The strong quantum critical fluctuations that arise at
QPTs often lead to the emergence of macroscopically coherent phases that are at the center of the current
condensed matter research. Thus, microscopic studies of fluctuations across QPTs are central for novel
quantum phenomena, but the microscopic nature of the pertinent fluctuations is unclear in many strongly
correlated materials.
Neutron scattering is expected to continue playing a pivotal role in the research of quantum critical matter,
because the technique allows to directly probe the spatial(Q)- and energy(E)-resolved properties of the
quantum critical fluctuations. The spatial extend of the critical fluctuations, however, has often been
neglected in the past, but has shown to be crucial in materials hosting competing interactions. In this
presentation I will show how modern neutron spectrometers allow clarifying the contribution from different
fluctuating order parameters, and will show potential future paths for the research on quantum critical
phenomena in strongly correlated metals.

Presenter(s) : MAZZONE, Daniel

Session Classification : Science cases (Chair: Philippe Bourges)

Contribution ID : **29** Type : **not specified**

Using Generative Adversarial Networks to match experimental and simulated inelastic neutron scattering data

Tuesday, 19 October 2021 17:50 (10)

During the past decades, research in materials science has been accelerated by the rapid development of synchrotron and neutron sources.1 Conventional data analysis approaches using minimization techniques, such as least-squares fitting algorithms, cannot keep up with the amount of increasing size of measured datasets. Consequently, data analysis is becoming a bottleneck for research in materials science.2, 3 Therefore, it is of great importance to improve the current state-of-art for data analysis for materials science, particularly utilizing recent developments in artificial intelligence and machine learning (ML).2-4 One of the unsolved problems in this context is to match the simulated datasets that the ML algorithms are trained on to the experimental datasets. This has particularly been a problem for the analysis of inelastic neutron scattering (INS), where it is computationally expensive to ensure that simulated data correctly mimics the experimental signal and background.5 In our project, we are attempting to improve this state through better ML for helping us effectively analyse neutron datasets. More specifically, we are developing generative adversarial networks (GANs) that can learn to make simulated INS data that matches experimental INS dataset under a second. This GAN-based approach, once trained, will be deployed in a range of scenarios for analysing and understanding INS dataset. It can be used to help classify materials structures from the INS datasets and to work with other ML and non-ML (e.g. Spin-W6) algorithms which can estimate magnetic Hamiltonian parameters from INS data. Furthermore, the aim is to expand the algorithm to also match simulated and experimental datasets for other techniques than INS.

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3. Butler, K. T.; Davies, D. W.; Cartwright, H.; Isayev, O.; Walsh, A., Machine learning for molecular and materials science. Nature 2018, 559 (7715), 547-555.
4. Hey, T.; Butler, K.; Jackson, S.; Thiyagalingam, J., Machine learning and big scientific data. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 2020, 378 (2166), 20190054.
5. Butler, K. T.; Le, M. D.; Thiyagalingam, J.; Perring, T. G., Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data. J. Phys.: Condens. Matter 2021, 33 (19), 194006.
6. https://spinw.org/

Primary author(s) : ANKER, Andy Sode; BUTLER, Keith (RAL); THIYAGALINGAM, Jeyan (STFC); LE, Duc

Presenter(s) : ANKER, Andy Sode

Session Classification : Poster session

Contribution ID : **30** Type : **not specified**

Benchmarking autonomous TAS experiments

Monday, 18 October 2021 17:10 (20)

With the advancement of artificial intelligence and machine learning methods, autonomous approaches are recognized to have great potential for performing more efficient TAS experiments. In our view, it is crucial for such approaches to provide thorough evidence about respective performance improvements in order to increase acceptance within the community. Therefore, we propose a benchmarking procedure designed as a cost-benefit analysis that is applicable not only to TAS, but also to any scattering method sequentially collecting data during an experiment. For a given approach, the performance assessment is based on how much benefit, given a certain cost budget, it is able to acquire in predefined test cases. Different approaches thus get a chance for comparison and can make their advantages explicit and visible. We specify the key components of the benchmarking procedure for a TAS setting and discuss potential limitations.

Primary author(s) : TEIXEIRA PARENTE, Mario

Presenter(s) : TEIXEIRA PARENTE, Mario

Session Classification : Experimental life – how to perform experiments in future (Chair: Astrid Schneidewind)

Contribution ID : **31** Type : **not specified**

Spin-orbital excitations in d-transition metal ion compounds

Tuesday, 19 October 2021 16:30 (30)

We will discuss a framework for modeling and understanding the magnetic excitations in localized, intermediate coupling magnets where the interplay between spin-orbit coupling, magnetic exchange, and crystal-field effects create unconventional ground states. A spin-orbit exciton approach for modelling these excitations is developed based upon a Hamiltonian which explicitly incorporates single-ion crystalline electric field and spin-exchange. We will discuss the application of this to understand neutron spectroscopy data in a series of examples including CaFe2O4 [1], CoO [2], Ca2RuO4 [3], and VI3 [4]. We will further link neutron scattering data with other magnetic probes including x-ray spectroscopic measurements and susceptibility and discuss possible new types of excitations that can be measured and predicted. We will discuss the possible utility of modern neutron spectroscopy instrumentation for the identification and tuning of such excitations.

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Primary author(s) : Dr. STOCK, Chris (University of Edinburgh)

Presenter(s) : Dr. STOCK, Chris (University of Edinburgh)

Session Classification : Science cases (Chair: Philippe Bourges)

Contribution ID : **32** Type : **not specified**

Beyond the basics - complex sample environment for neutron spectroscopy

Tuesday, 19 October 2021 10:35 (25)

Neutron spectroscopic methods are indispensable tools to study dynamical processes such as diffusion, magnetic excitations and even electronic excitations.
The small signal size and the flux limitation of neutron sources result in long counting times. Moreover, the requirement of special sample environment to perform spectroscopic studies at extreme conditions affects the signal to noise ratio negatively and efforts that counteract the direct and indirect negative effects
caused by complex sample environment equipment are worth to consider.
I will give an overview over the efforts that have been done in the last years and
present exemplary solutions that have been adapted.

Primary author(s) : BARTKOWIAK, Marek (Paul Scherrer Institut)

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

Session Classification : Providing the right experimental conditions - for real (Chair: Arno Hiess)

Contribution ID : **33** Type : **not specified**

Exploring the Shastry-Sutherland compound, Sr2Cu(BO3)2, by using inelastic neutron scattering with high pressures and high magnetic fields

Tuesday, 19 October 2021 15:05 (30)

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 magnets where competing interactions may lead to exotic magnetic states and an external parameter such as magnetic field or pressure can be used to tune the system from one quantum state to another. The Shastry-Sutherland lattice is such a frustrated system. It consists of spin pairs (dimers) embedded in a square lattice. It has an exact dimer product ground state when the ratio between the inter and intra-dimer couplings is sufficiently low [1]. Upon increasing this ratio, the system goes through a quantum phase transition to a plaquette singlet state followed by an antiferromagnetic phase [2]. Sr2Cu(BO3)2 is a unique material since it is topologically equivalent to the Shastry-Sutherland lattice [3] and it is close to the critical point to the plaquette phase. Sr2Cu(BO3)2 therefore presents remarkable experimental testing grounds for the Shastry-Sutherland model where the couplings may be altered by applying pressure to obtain a phase diagram which resembles the one theoretically predicted [4]. As a frustrated magnetic system, Sr2Cu(BO3)2 also exhibits a series of transitions upon applying a magnetic field with the first one occurring at 27T [5] . The transition field may be tuned to a range achievable in neutron scattering experiments by applying pressure [6]. I will thus present our recent experimental effort to characterize the first magnetization plateau of Sr2Cu(BO3)2 by carrying out neutron scattering experiments with high pressure, high magnetic field and low temperatures, all simultaneously. I will also show you results from inelastic neutron scattering experiments performed with the aim to explore the plaquette and antiferromagnetic phases and where even higher pressures were needed.

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Presenter(s) : FOGH, Ellen

Session Classification : Science cases (Chair: Philippe Bourges)

Contribution ID : **35** Type : **not specified**

High Field Magnets using High Temperature Superconductors

Tuesday, 19 October 2021 11:00 (25)

Soon after their discovery at the end of the 80's, Cuprate High Temperature Superconductors (HTS) were expected to trigger a revolution in high field magnets thanks to their extremely high irreversibility field at low temperature. The difficulty to make these brittle ceramics into practical conductors led to a 20 years delay, with the first significant high field HTS magnet prototypes appearing after 2010. In the last 5 years, a few all-superconducting solenoids with field high than 23.5T were tested, with the latest ones exceeding 30T.

We will present an overview of recent HTS conductor performances and availability. We will then introduced the HTS high field magnet performances expected in the near future in a few major ongoing projects and explain why there is still much to do to fully exploit HTS conductor's specifications.
Finally, we will try to translate the performances of these magnets, which are mostly solenoids for NMR and/or magneto-science, into plausible Neutron Scattering Magnet specifications in order to sketch a possible roadmap for HTS Neutron Scattering Magnets.

Primary author(s) : BADEL, Arnaud (CNRS); CHAUD, Xavier (CNRS); Prof. AWAJI, Satoshi; Prof. TIXADOR, Pascal

Presenter(s) : BADEL, Arnaud (CNRS)

Session Classification : Providing the right experimental conditions - for real (Chair: Arno Hiess)

Contribution ID : **36** Type : **not specified**

AI Tools that Auto-generate Materials Databases for Building Data-science Platforms

Monday, 18 October 2021 14:50 (20)

This presentation will introduce and exemplify the artificial intelligence tools that my group have been developing with ISIS. These use data-mining and machine-learning methods to build data-science platforms that aid materials characterisation and materials application methods. These include the incorporation of neutron scattering data. I will also show some examples of how these data-science platforms can lead to the data-driven prediction and discovery of new materials.

References to our AI tools

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Presenter(s) : COLE, Jacqueline (University of Cambridge and ISIS Neutron and Muon Facility)

Session Classification : New algorithms and Machine learning: relevance to inelastic neutron scattering (Chair: Toby Perring)