PSI Condensed Matter Retreat 2019 @ FHNW Brugg

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Book of Abstracts

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Poster session / 141

Dynamics of model systems with correlated disorder

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In condensed matter, frustration emerges from the impossibility to satisfy all constraints simultaneously. Oft-times, this leads to exotic phases of matter with quasi-particle excitations. One such example is the Coulomb phase of spin ice which has emergent monopole excitations. The Coulomb phase has a highly degenerate ground state but with long-range correlation whose signature are the pinch points appearing in the (static) structure factor. In this project, we are interested in one such material, $CsNiCrF_6$[1], which is described by not one but three Coulomb phases: charge ice, displacement ice and a pyrochlore Heisenberg-like spin liquid. One characteristic property of this material is the structural correlated disorder. This provides an environment for the study of the interplay between frustrated magnetism and correlated disorder. We investigate both the magnetic and vibrational dynamics of model systems with correlated disorder of the type found in $CsNiCrF_6$.

[1] Fennell *et al.*, Nature Physics **15**, 60 (2019)
[2] Robert *et al.*, PRL **101**, 117207 (2008)

Position:

Postdoc

Poster session / 146

Spontaneous reduction of polydispersity and self-healing colloidal crystals

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[1] *Paul Scherrer Institut*

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[3] *Georgia Institute of Technology*

Crystallization is often suppressed by point defects due to larger impurity particles. Surprisingly, microgels can overcome this limitation: Large microgels can spontaneously deswell to fit into the crystal lattice of smaller but otherwise identical microgels. We find this unique reduction of polydispersity and particle deswelling to be triggered by a difference in osmotic pressure, Π, between the inside and the outside of the microgel particles. Π is set by the counterions of charged groups on the microgels. Although pNIPAM is uncharged, pNIPAM microgels carry charged groups originating from the starter for their synthesis. A Π-difference between inside and outside of a microgel builds up when the counterion clouds of neighboring particles overlap at high concentration. This causes an increase of Π in the space between particles, which is not compensated inside the particles. With increasing concentration, this Π-difference exceeds the bulk modulus of the softest and largest microgels and makes them deswell, enabling crystallization. We find the freezing point of polydisperse and bidisperse pNIPAM suspensions to be linked to particle deswelling: A reduction of polydispersity due to particle deswelling is required for crystallization. Compared to monodisperse suspensions, this causes the freezing point to shift to higher concentrations. In comparison to hard, incompressible colloidal particles, this particle deswelling mechanism fundamentally changes the role of polydispersity in microgel suspensions.

Position:

Scientist

Poster session / 128

Multiple Coulomb Phase in the Fluoride Pyrochlore CsNiCrF6

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Frustrated magnets are a particularly promising class of materials for studying emergent phenomena in condensed matter. The construction of field theories describing the correlations and excitations of spins on a pyrochlore lattice is a prominent example. Such theories are typically based on a Coulomb phase, in which a non-divergent field with power-law correlations encodes the correlation function. Well known possibilities include emergent magnetostatics with monopoles in classical spin ice, or emergent electrodynamics with magnetic photons and charges in quantum spin ice. However, other types of Coulomb phase based on different degrees of freedom are possible, and this work describes an investigation of a material in which Coulomb phase correlations are simultaneously present in both the structural and magnetic degrees of freedom. We present the results of neutron and x-ray scattering experiments on the structural and magnetic correlations, and magnetic dynamics in CsNiCrF6, and basic models of the correlations, which show that this is a crystalline solid with highly correlated disorder that can be described by three Coulomb phases: a charge ice, displacement ice, and pyrochlore Heisenberg antiferromagnet-like spin system [1]. CsNiCrF6 is a member of a large class of compounds (AMM'F6), and these may be of broader general interest - correlated structural disorder should be a feature of many materials with mixed cations, and may well help to develop novel functionalities, such as new thermoelectrics [2].
[1] Fennell *et al.*, Nature Physics **15**, 60 (2019)
[2] Overy *et al.*, Nature Communications **7**,10445 (2016)

Position:

Scientist

Poster session / 125

Structural phases of elemental Gallium: universal relations in conventional superconductors

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The pressure induced superconductivity in Ga-II phase of elemental Gallium (the transition temperature $T_c \simeq 6.45$ K) was studied experimentally by means of muon-spin rotation. Experiments reveal that Ga-II is the type-I superconductor with the zero temperature ther-modynamic critical field $B_c(0) = 64.07(1)$ mT. The analysis of $B_c(T)$ data within the phenomenological α-model, ref [1], allows to estimate $T_c = 6.448(2)$ K, the zero-tempeature value of the superconducting energy gap $\Delta = 1.121(1)$ meV, and the coupling strengths $2\Delta/k_B T_c = 4.024(2)$.

Correlations between the thermodynamical critical field B_c and the transition temperature T_c (see Fig.1) as well as between the coupling strength $\Delta/k_B T_c$, the ratio $B_c(0)/T_c\sqrt{\gamma_e}$ (γ_e is the normal state specific heat coefficient), and the specific heat jump $\Delta C(T_c)/\gamma_e T_c$ were found to hold for varios phonon-mediated superconductors. The corresponding quantities for the pressure stabilized Ga-II phase, obtained from the temperature dependence of the thermodynamic critical field $B_c(T)$ and of the specific heat $C(T)$ follow quite precisely the above mentioned scaling laws. These relations can be well understood taking into account strong coupling adjustments of BCS universal parameters and can naturally explain the empirical scaling of thermodynamic critical field and critical temperature of phonon-mediated type-I superconductors.

References

[1] H. Padamsee, J. Low Temp. Phys., **12**, 387 (1973).
[2] J.W. Rohlf, Modern physics from α to Z, Williey (1994).

Figure 1. Correlation between the thermodynamical critical field B_c and the transition temperature T_c in single-element superconductors (after [2]). The various Ga phases are denoted by red starts.

Position:

Scientist

Poster session / 117

Quantum interference between multi-triplon continua and bound states in quasi-one-dimensional cuprate Sr14Cu24O41

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In atomic physics, interactions between single-particle state and multi-particle continuum leads to distinct ionization processes interfering with each other, leads to the so-called Fano resonance. Similar concepts have also been materialized in nanostructured systems, such as semiconducting quantum dots or frustrated magnets. The later shows renormalized energy levels of the single-particle bound state to repel from the continuum boundary. Here we demonstrate an experimental realization from two-triplon (2T) excitations in quasi-one-dimensional ladder Sr14Cu24O41 probed by resonant inelastic X-ray scattering (RIXS). The energy-dependent RIXS spectra reveals the the collective triplon excitations distinct from the incoherent particle-hole-like continua, which well describes the renormalized energies of ΔS=1 (ΔS=0) 2T bound state away from the lower boundary of 2T continuum at Cu L3-edge (O K-edge). Furthermore, we clearly observe a suppressed spectral weight of ΔS=0 bound state for qLadder < 0.15 (2π/cLadder), which matches the crossing region with continuum boundary where the bound state ceases to exist. These findings are in good agreement with theoretical works using continuous unitary transformation (CUT) method. Moreover, our RIXS study on 2T excitations in Sr14Cu24O41 spin ladder demonstrates a novel approach for investigating interacting quantum systems in micro-scale.

Position:

Phd

Poster session / **134**

Towards the understanding of the dynamics and the Raman effect of strained germanium lasing

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Thanks to its CMOS compatibility and “near” direct bandgap, Germanium (Ge) has been for long in the race for the development of a fully Si-compatible light source, as an alternative to the traditional III-V-on-Si laser integration. The offset ΔE = E(Γ)-E(L) = 140 meV of Ge can be reduced by tensile strain and/or by alloying with Sn, increasing the radiative recombination efficiency. GeSn was shown to be a successful platform for lasing back in 2015 [1] and a rapid development of the field pushed the operational limit almost to room temperature [2]. However, the first demonstration of lasing in elemental strained Germanium was only recently achieved by our group in PSI [3]. We showed highly efficient lasing between 3.20 and 3.66 μm in Ge microbridges highly strained along the <100> direction, up to 100 K and upon pulsed excitation of 100 ps. Interestingly, lasing could not be achieved in alike conditions under continuous wave (CW) excitation, indicating that, on the contrary of many previous theoretical models, the band gap is only marginally closed even at almost 6 % of strain. We thus propose that lasing is obtained thanks to a non-equilibrium distribution of the carriers, which evidentially takes place on a time scale longer than the excitation pulse length, and also only at sufficiently low temperatures. We are currently investigating the scattering time of the carriers between the Γ and L valleys by studying the lasing response of the microbridge under a pump-probe like excitation scheme. We will also show the appearance of Raman lasing, which seems to compete with the traditional population inversion lasing.

Position:

Phd

Poster session / **90**

Topochemical synthesis of the 2M-WS_2

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Transition metal chalcogenides (*TMCh*), which exhibit a wide spectrum of novel physical phenomena, are of vital importance in fundamental research and in many fields for future technological applications including spintronics, topological electronics, Motttronics, etc. Metastable, monoclinic tungsten diselenide (*2M*-WS_2) is the *TMCh* family member. It has been identify as a Dirac semimetal, exhibiting superconductivity and topological surface states [1]. Design, synthesis, and single crystal growth of the materials with a certain chemical stoichiometry and crystal structure play a key role in desire electronic phase realization. Preparation of a compound, with intriguing physical properties can be achieved by applying a unique set of optimized growth process conditions. We succeed to form *2M*-WS_2 phase by the topochemical synthesis method. Structural evolution trough a synthetic route and studies of superconducting state properties under ambient and elevated pressures will be presented.

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[1] Zurab Guguchia, Dariusz J. Gawryluk, Marta Brzezinska, Stepan S. Tsirkin, Rustem Khasanov, Ekaterina Pomjakushina, Fabian O. von Rohr, Joel A. T. Verezhak, M. Zahid Hasan, Titus Neupert, Hubertus Luetkens, Alex Amato, "Nodeless superconductivity and its evolution with pressure in the layered dirac semimetal *2M*-WS_2", npj Quantum Materials 4 50 (2019)
https://doi.org/10.1038/s41535-019-0189-5

Position:

Scientist

Poster session / **101**

GdFeCo nanoparticles for all-optical magnetization switching

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All optical switching (AOS) of the magnetization, discovered over a decade ago in GdFeCo ferrimagnetic alloy, is a hot topic in ultrafast condensed matter science due to high potential for implementation in data storage technology, substituting the writing head by ultrashort laser pulses in magnetic hard drives. However, most of study was on thin films, where the switched area is compatible with laser beam size. The alternative is to use magnetic nanoparticles (NP) as a working media for AOS. Magnetic NP with size in order of several tenth of nm are good candidates to move the optically switched state to nanoscale levels. While synthesis of homogeneous NP is well established, creation of GdFeCo magnetic NP remains unexplored. Here, we present our findings on synthesis and testing of GdFeCo magnetic nanoparticles, in scope of using them for AOS, with PEEM and high field soft X-ray spectroscopy techniques. We demonstrate that most of NP are in an oxidized state when deposited, however we could avoid it if NP deposited on Si3N4 substrate.

Position:

Postdoc

Poster session / **108**

Disentangling charge and spin excitations in RIXS spectra and their evolution in the phase diagram of Bi2Sr2CaCu2O8+x superconducting cuprate

Authors: Wenliang Zhang[1] ; Yi Tseng[2] ; Eugenio Paris[2] ; Enrico Giannini[3] ; Thorsten Schmitt[4]

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The knowledge of the elementary excitations is vital for understanding the physics of superconducting cuprates. Nowadays, Resonant Inelastic X-ray Scattering (RIXS) plays an increasingly important role in studying various excitations especially the spin excitations in cuprates. However, the interpretation of the measured excitations is still controversial. One obstacle is that the measured low-energy excitations in doped cuprates are usually of mixed charge and spin character, making the correct assignment of the spectral profile to individual excitations difficult. Using the recent proposed azimuthal dependent RIXS measurement, we resolved the accurate spectral profiles of the charge and spin excitations in Bi2Sr2CaCu2O8+x, and studied their doping and temperature responses separately in the phase diagram. These results help to elucidate the nature of the spin and charge excitations in doped cuprates and their possible correlations to the superconductivity.

Position:

Postdoc

Poster session / **148**

Synchrotron studies for optimization of Selective Laser Melting manufacturing of alumina parts

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[3] *EMPA*

Applying the Selective Laser Melting (SLM) technology to ceramics is challenging due to not understood mechanisms of interaction of the powder with laser light, high melting temperature and low thermal shock resistance. FUORCLAM (Fundamental Understanding of Oxide Refractory Ceramics and Laser Additive Manufacturing) is a project in collaboration between PSI, ETH and EMPA, which aims to establish SLM manufacturing technology of alumina. The approach used in this project is to utilize small amounts of metal oxide additives in in alumina granules to enable the efficient absorption of laser light.
In order to optimize the process, studies of micro- and macrostructure of the ingredient powder and the printed parts are essential. This is achieved by employing advanced synchrotron techniques. The powder used for SLM is composed of spray-dried alumina granules. The composition and crystallographic structure of the granules and printed parts is studied by means of combined micro-XRD/micro-XRF 2D and 3D imaging (microXAS) and high-resolution powder diffraction (MS beamlineI). These studies demonstrated a uniform dopant distribution in as-produced alumina granules and capability to modify it prior to laser treatment. Quantitative analysis of porosity and cracks is performed by synchrotron tomography (TOMCAT).

Position:

Postdoc

Poster session / 121

Disordered skyrmion phase stabilized by magnetic frustration in a chiral magnet Co7Zn7Mn6

Authors: Jonathan White[1] ; Kosuke Karube[2] ; Daisuke Morikawa[3] ; Charles Dewhurst[4] ; Robert Cubitt[5] ; Akiko Kikkawa[3] ; Xiuzhen Yu[3] ; Yusuke Tokunaga[6] ; Taka-hisa Arima[7] ; Henrik Ronnow[8] ; Yoshinori Tokura[7] ; Yasujiro Taguchi[3]

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Magnetic skyrmions are vortex-like topological spin textures often observed to form a triangular-lattice skyrmion crystal in structurally chiral magnets with the Dzyaloshinskii-Moriya interaction. Recently, beta-Mn structure–type Co-Zn-Mn alloys were identified as a new class of chiral magnet to host such skyrmion crystal phases, while beta-Mn itself is known as hosting an elemental geometrically frustrated spin liquid. Here we report detailed small-angle neutron scattering, ac susceptibility and Lorentz microscopy measurements that show the intermediate composition system Co7Zn7Mn6 to be a unique host of two disconnected, thermal-equilibrium topological skyrmion phases; one is a conventional skyrmion crystal phase stabilized by thermal fluctuations and restricted to exist just below the magnetic transition temperature Tc, and the other is a novel three-dimensionally disordered skyrmion phase that is stable well below T . The stability of this new disordered skyrmion phase is argued to be due to a cooperative interplay between the chiral magnetism with Dzyaloshinskii-Moriya interaction, and the frustrated magnetism inherent to beta-Mn [1].

[1] K. Karube, *J.S. White*, D. Morikawa, C. D. Dewhurst, R. Cubitt, A. Kikkawa, X.Z. Yu, Y. Tokunaga, T. Arima, H. M. Rønnow, Y. Tokura, and Y. Taguchi, Science Advances 4, eaar7043 (2018).

Position:

Scientist

Poster session / **129**

Magnetic and lattice dynamics in CsNiCrF6

Author: Amirreza Hemmatzade[1]

Co-authors: Alexandra Turrini [2] ; Marek Bartkowiak [1] ; Karim Essafi [3] ; Peter Derlet [1] ; Tom Fennell [4]

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Materials with correlated structural disorder may be viewed as a different material class to conventional crystalline materials with either vanishingly small levels of disorder or, on the other hand, strong random disorder. Both spin and lattice dynamics of a frustrated magnets with an underlying correlated but disordered structure such as a charge ice can be unconventional. In this project, we describe initial efforts to investigate both aspects in CsNiCrF6: the project is at its outset, but we will describe our approach to measuring the spin dynamics and obtaining a realistic spin Hamiltonian for a magnetic charge ice; and thermal conductivity measurements that show the phonons are anomalously strongly scattered for a crystalline material, along with initial measurements of the phonon dispersion relations in which we seek an explanation for this observation.

Position:

Phd

Poster session / **143**

In situ mechanochemistry of hybrid materials

Authors: Manuel Wilke[None] ; Nicola Pietro Maria Casati[None]

Mechanochemistry is increasingly used for solid state reactions because of its advantages like high yields, high conversion rates, the small produce of waste and the good energy consumption, for which it belongs to green chemistry.[1] Nevertheless, the mechanisms behind mechanochemical reactions are still under investigation which is why in situ setups are needed.[2]
Here we present the in situ investigation of the formation of a series of organic-inorganic hybrid materials from mechanochemical synthesis. The compounds are constructed by guanidinium-, lead(II)- and iodide-ions, with the formula (C(NH2)3)nPbI2+n (n = 1, 2, 3, 4).[3] For the in situ investigations a new setup, developed at the MS beamline (PSI, Switzerland) is used.[4] Due to the gained high quality data an automatic quantitative analyses of the time-resolved powder X-ray diffraction patterns was possible and revealed intermediate formations, solid-solid phase transitions and reactions between the guanidinium lead(II) iodides during the syntheses. We consider these discovered pathways to be linked to the respective structural features of the different compounds. Recent results suggest that 3 is a necessary intermediate for the formation of 4 and that both steps have very different energy dependencies.[5]

[1] James et al., Chem. Soc. Rev. 2012, 41, 413-447.
[2] Užarević et al., J. Phys. Chem. Lett. 2015, 4129-4140.
[3] Wilke et al., Chem. - Eur. J. 2018, 24, 17701-17711.
[4] Ban et al., Anal. Chem. 2017, 89, 13176-13181.
[5] Wilke et al., in preparation.

Position:

Postdoc

Poster session / 104

High-resolution neutron imaging of hydrogen concentrations in nuclear fuel claddings

Author: Pavel Trtik[1]

Co-authors: Liliana I. Duarte [1] ; Weijia Gong [1] ; Robert Zubler [1] ; Aaron Colldeweih [1] ; Johannes Bertsch [1]

[1] *PSI*

Hydrogen (hydrides) distribution in the nuclear fuel claddings can often be highly non-uniform because of the high mobility of hydrogen interstitial atoms, raising the risk to the nuclear fuel rod integrity. High-resolution neutron imaging provides an excellent non-destructive tool for the quantification of the hydrogen in nuclear fuel claddings consisting of zirconium based alloys. The spatial resolution of neutron imaging was recently extended down to the sub-5 micrometres domain in 2D and below 10 micrometres in 3D within the 'PSI Neutron Microscope' (NM) project. The high spatial resolution of neutron imaging (equivalent to the scale of the common width of zirconium hydride packets) together with the sub-10 wppm sensitivity to hydrogen is worldwide unique and enabled to reveal clearly the influence of cooling rate on the hydrogen distribution in inactive duplex nuclear fuel cladding rods. Above that, the prototype of a sample container allowing for neutron high-resolution radiography of highly radioactive samples was recently pilot tested using NM and allowed for the acquisition of the first-ever high-resolution neutron radiography of highly radioactive cladding rod that was operated in a (Swiss) nuclear power plant.

Position:

Scientist

Poster session / 110

Stroboscopic neutron diffraction applied to fast time-resolved operando studies on Li-ion battery

Author: Denis Sheptyakov[1]

[1] *Paul Scherrer Institut*

High penetration ability of neutrons and dramatic character of crystal structure modifications occurring in the battery materials during electrochemical cycling make neutron powder diffraction an obvious method to study the reaction mechanisms in rechargeable cells. While basic chemical reactions occurring in batteries upon charge/discharge are mainly understood, the specific processes leading to faster battery degradation upon increasing the charge/discharge rates are under question. We are presenting a practical implementation of the stroboscopic operando neutron diffraction to allow studying the structural and chemical changes occurring in batteries with industrially relevant dimensions and compositions, also at incredibly fast cycling rates. We demonstrate that the graphite lithiation mechanisms at fast and reasonable cycling rates are different, and discuss the possible reasoning for sooner performance fading upon faster charge/discharge. Our stroboscopic method allows to investigate the crystallography of rather short-living states in materials, provided these are possible to be periodically reproduced. The temporal resolution achieved is hereby well below a minute. This stroboscopic mode of collecting the neutron diffraction data is essentially binning the partial low-intensity data from various repetitions of a process into enhanced intensity patterns representing the statistics over many cycles. It offers new possibilities for research into the reproducible changes occurring in solid diffracting materials during the rather short times, otherwise hardly accessible by regular neutron diffraction.

Position:

Scientist

Poster session / 95

Operando observation of structural relaxation in ferroelectric GeTe(111)

Authors: Matthias Kurt Muntwiler[1] ; Juraj Krempasky[2] ; Gunther Springholz[3] ; Jan Hugo Dil[1]

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[2] *SLS*

[3] *Johannes Kepler Universität, Linz*

(Mn,Ge)Te is a remarkable multiferroic material that combines ferroelasticity, ferroelectricity, ferromagnetism and a topological band structure [1,2]. The interplay of these effects via ferroelectric polarization and Rashba spin splitting makes it attractive for device applications in electronics, spintronics and quantum computing. Using photoelectron diffraction (XPD) in an operando setup with applied bias voltage we study the detailed atomic structure of the topmost surface layers of the host material -GeTe and their response to the static electric field. We find that the surface of thin films is particularly susceptible to the electric field and that it is isolated from the bulk by a stable domain wall. A challenge for applications is that the polarization amplitude fades after few switching cycles. The origin of this fatigue is under investigation. Knowing the exact position of the atoms in the active layer is crucial information towards the understanding of the switching and mechanism and the microscopic cause of fatigue.

1. Przybilinska, et al.; Phys. Rev. Lett. 112, 047202 (2014)
2. Krempasky, J, et al.; Phys. Rev. X 8, 021067 (2018)

Position:

Scientist

Poster session / 144

Synthesis of Al-Sc, Al-Zr, and Al-Sc-Zr alloys via SLM from elemental powder blends

Authors: Jennifer Glerum[1] ; Christoph Kenel[1] ; Tao Sun[2] ; David Dunand[1]

[1] *Northwestern University*

[2] *Argonne National Laboratory*

Multiple blends of aluminum and transition metal powders are solidified via selective laser melting (SLM) to create precipitation-strengthened alloys. Previous work has demonstrated the ability to manufacture Ni-base and Ti-Al-Nb oxide-dispersion strengthened (ODS) parts via AM for energy applications (i.e. gas and steam turbines). Al-(Sc,Zr) powders are blended from elemental powders, and then line scans are performed on the powder blends during in-situ x-ray diffraction and imaging at the Advanced Photon Source (APS) at Argonne National Laboratory to create consolidated samples. High-speed x-ray imaging is used to study the behavior and interaction of the particles in the melt pool, the size and shape of the melt pool and keyhole (vapor plume), and any pore formation events across a wide range of powder compositions and process parameters, from conduction to keyhole mode. Results correlating process parameters and keyhole dimensions are compared to existing models for SLM line scans. Complementary in-situ, pre-melting, and post-melting x-ray diffraction are used to study phase evolution in elemental Al-(Sc,Zr) powder blends during SLM to quantify homogenization, second-phase formation, and phase evolution upon multi-pass melting. Additionally, metallography is performed to study microstructural changes induced by varying powder compositions and process parameters. Current work at PSI, in collaboration with Prof. Helena

van Swygenhoven's group, focuses on manufacturing dense, bulk samples from the elemental Al-(Sc,Zr) powder blends and studying the phase evolution via in-situ diffraction. These bulk samples will be compared to their counterparts manufactured from prealloyed powders.

Position:

Phd

Poster session / **145**

Probing the magnetic state of Ni in NdNiO3/La0.7 Sr0.3MnO3 bilayer

Author: Anna Zakharova[1]

Co-authors: Marco Caputo [2] ; Milan Radovic [3] ; Frithjof Nolting [3] ; Cinthia Piamonteze [3]

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Rich phase diagram [1] of oxide heterostructures such as rare earth nickelates (RNiO3) allows to play with their properties. In antiferromagnetic $NdNiO_3$ it has been shown that thickness can influence the type of magnetic ordering [2]. It has been proposed that interface has a strong impact on NNO magnetism. By ARPES and XMCD measurements, it has been shown that 5 u.c. NNO on top of 15 u.c. $La_{0.7}Sr_{0.3}MnO_3$ has different behavior than a single NNO layer. In this bilayer Ni moments are ferromagnetically oriented. The ARPES results suggest that magnetic layer extends far from interface. The aim of this project is to study magnetic state of Ni in NNO in contact with ferromagnetic LSMO as a function of NNO thickness. In order to do that we used X-ray Absorption Spectroscopy, X-ray Linear Dichroism and X-ray Magnetic Circular Dichroism at the Ni $L_{2,3}$ and Mn $L_{2,3}$-edges to estimate magnetic layer thickness. We have probed magnetic properties at NNO(5/8/10/20 u.c.)/LSMO(15 u.c.)//NGO bilayers. Ni moment shows ferromagnetic order even for the thickest NNO layer, Ni magnetic signal from all thicknesses looks surprisingly similar. On the other hand, magnetic signal from LSMO layer has remarkable changes depending on NNO thickness. Our results suggest that the magnetic coupling at NNO/LSMO interface is complex and affects both NNO and LSMO magnetic structure. In this poster we will present our XMCD results and present the next steps planned in order to have further insight in the interface magnetic coupling of this fascinating system.

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Position:

Phd

Poster session / 126

∂-doped silicon devices for quantum electronics and optics

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For solid-state quantum computing the ability to deterministically confine donors in a semiconductor is crucial, not only to create quantum bits defined by the electron or nuclear spin of a dopant, but also to fabricate control systems such as gates mediated by one-dimensional wires or two-dimensional "delta" (∂) layers.
The aim of this work is to achieve two-dimensional confinement of arsenic and phosphorus in silicon, i.e., to create a smooth and conductive ∂ layer. Low-temperature magnetoresistance measurements in up to 9 T magnetic field and 360 degrees sample rotation (rotation axis perpendicular to the magnetic field) is used as a tool to probe the dimensionality and confinement of the electrons in the doped layers [1] and to study other characteristics of these electrons [2]. For example, these characteristics include interactions between dopant atoms, the spin-orbit and spin-spin coupling, the metal-insulator transition, and their dependence on dopant species. The goal is to reduce the dimensionality of the confinement to one and zero dimensions and to create ordered single-atom arrays, as well as to measure their quantum electro-optic properties [3].

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Position:

Phd

Poster session / 106

Enhanced transformation-induced-plasticity in austenitic steel produced by selective laser melting

Author: Efthymios Polatidis[1]

Co-authors: Jan Capek ; Ariyan Arabi-Hashemi [2] ; Christian Leinenbach [2] ; Markus Strobl [3]

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Austenitic stainless steels, such as 304L, exhibit a combination of high strength and ductility and good corrosion resistance and due to their good selective laser melting (SLM) processability, they are ideal candidates for medical applications profiting e.g. from the possibility to manufacture complex geometries. In situ tensile and neutron diffraction tests on the POLDI instrument at the Swiss spallation source, SINQ were undertaken on 304L specimens produced by SLM at Empa, Switzerland. The loading direction was parallel to the build-direction of the specimens. The experimental results indicate high ductility and pronounced strain-induced martensitic transformation, starting at strains higher than 30% engineering strain. The enhanced martensitic transformation is discussed with respect to the crystallographic texture, as revealed by EBSD, and its affinity to martensite formation under uniaxial loading.

Position:

Scientist

Poster session / 135

Nodeless superconductivity and effect of hydrostatic pressure in the charge density wave superconductor SrPt2As2

Author: Ritu Gupta[1]

Co-authors: Catrin Lohnert [2] ; Dirk Johrendt [3] ; Sudip Malick [4] ; Zakir Hossain [5] ; Hubertus Luetkens [6] ; Toni Shiroka [7] ; Chennan Wang [1] ; Rustem Khasanov [6]

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The search of new classes of materials where superconductivity (SC) coexists with other exotic non-magnetic phases is crucial to understand the influence of the latter on SC. Here, we present a detailed investigation of the superconducting gap symmetry on a charge-density-wave (CDW) superconductor SrPt2As2 by means of muon-spin rotation/relaxation technique (μSR) at ambient- and under hydrostatic pressure. Even in presence of a CDW phase around 470 K [1], we detect a superconducting transition at 5 K. The magnetic penetration depth, obtained from transverse-field μSR could be fitted with an isotropic s-wave model, instead of the two-gap s+s wave model reported previously [2]. The observable difference between the muon spectra collected in zero field above and below Tc, suggests the presence of a spontaneous magnetic field in the superconducting state and most likely reflects time-reversal symmetry breaking below Tc. To elucidate the correlation between CDW and SC, we performed μSR experiments under hydrostatic pressure, which provide information on the nature of the superconducting-gap symmetry. Finally, by using AC-susceptibility- and μSR measurements under pressure we could reconstruct the complete pressure-temperature phase diagram of SrPt2As2.

Position:

Postdoc

Poster session / 142

Pd nanoparticles solid-liquid interface study during liquid phase selective hydrogenation by combined XAS and ATR-IR

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Co-authors: Maarten Nachtegaal [1] ; Oliver Kröcher [1] ; Davide Ferri [2]

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[2] *PSI*

Hydrogenation reactions occupy an important place in the realm of catalysis with various functional groups such as double and triple bonds and aldehydes among others which can undergo hydrogenation to produce diverse intermediates and fine chemicals [1]. In the fine chemical industry, these reactions are often performed in liquid phase due to the thermal stability and sensitivity of the compounds. Hydrogenation of furfural in liquid phase was chosen as a model hydrogenation reaction because the conversion and product selectivity are sensitive to both temperature of reaction and solvent [2]. Our aim is to understand the composition of the solid-liquid interface and how solvents and reaction conditions influence on the conversion and the product selectivity of a specific metal.

For this purpose, we used X-ray absorption spectroscopy (XAS) to monitor the oxidation state and local environment of Pd during reduction and reaction in the liquid phase (5 bar). Infrared spectroscopy in the attenuated total reflectance mode (ATR-IR) was exploited to follow the nature of the adsorbed species under similar reaction conditions. A commercial reduced 5 wt.% Pd/Al2O3 was used to perform hydrogenation of furfural in three solvents (isopropanol, cyclohexane and toluene). The Pd nanoparticles were partially oxidized by storage in air but were fully reduced at 125℃ before changing to the hydrogenation reaction conditions. During reduction, the XANES features of Pd metal shifted to lower energy, which together with the increase of the Pd-Pd bond distance from 2.74 Å to 2.81 Å are signatures of the formation of hydrides on the Pd surface. Admittance of the hydrogenation mixture containing furfural consumed these species. The intensity of the XANES features and the Pd-Pd bond distance after reduction of Pd were different depending on the solvent suggesting that the hydrogen coverage is governed by the selected solvent. ATR-IR spectroscopy allowed monitoring the adsorption and reaction of furfural at the surface of the catalyst when admitting the furfural solution to the catalyst after reduction. The observation of adsorbed CO on Pd metal was related to the formation of furan, which is the major product of furfural decarbonylation in cyclohexane and isopropanol. Lower CO signals together with the absence of a-top CO were observed in toluene, in which solvent, furfuryl alcohol is the major product, indicating that hydrogenation of furfural is taking place on specific sites.

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Position:

Phd

Poster session / 132

Triangular lattice antiferromagnet FeGa2S4

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Co-author: Guratinder Kaur [2]

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Frustrated triangular lattice antiferromagnets show a variety of exotic properties. Experimental observations in NiGa2S4 S=1 system [1] suggest i) presence of quadrupolar correlations [2] in addition to the moderate nearest-neighbor (J1) and strong third-neartest-neighbor (J3) Heisenberg interactions and ii) a topological transition driven by the Z2-vortex binding-unbinding [3].
We study the sister compound FeGa2S4 S=2 [4] by means of neutron scattering. Our aim is to establish the dominant terms in the spin Hamiltonian and to exploit the possibility of multi-k formation.

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Position:

Scientist

Poster session / **140**

Thermoelectric transport properties in magnetically ordered materials

Author: Hans Grimmer[1]

[1] *Multiscale Materials Experiments*

Transport properties of a material like electric or heat conductivity are generally not the same in all directions. The direction dependence can be described by a tensor, the form of which depends on the point group of the material. The Peltier and Seebeck effects describe the interaction between thermal and electric transport properties. If a magnetic field is applied to the material, further effects appear, named after Hall, Righi-Leduc, Nernst and Ettingshausen. These effects exist in all materials, also in dia- and paramagnetic ones, where the spins are not ordered.
In case of magnetically ordered materials, one has to deal also with the spontaneous Hall, Righi-Leduc, Nernst and Ettingshausen effects (which occur without applying a magnetic field) and with the change of these effects in a magnetic field. The effects are determined by tensors invariant under space inversion but changing sign under time inversion, called “magnetic tensors”, which do not vanish only for materials belonging to at most 69 of the 122 space-time point groups.

Making use of the Onsager relations the form of the corresponding tensors has been determined in [1] for all 122 space-time point groups and in [2] for the 21 limit point groups (Curie groups). The results are presented in Nye notation, which immediately shows how many tensor components are independent, which ones are zero and how the non-zero components are related.
The results triggered a recent extension of the information offered on the Bilbao crystallographic server [3].

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Position:

Scientist

Poster session / **119**

Stability of the Q -phase of CeCoIn5 in the presents of localized magnetic impurities

Author: Junying Shen[1]

Co-authors: Damaris Tartarotti Maimone ; Marek Bartkowiak [2] ; Stephane Raymond [3] ; Daniel Gabriel Mazzone [4] ; Gavilano Jorge [2] ; Michel Kenzelmann [2]

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[4] *PSI*

In heavy fermion superconductors, the strong interlocking of charge and spin degrees of freedom creates unconventional superconductivity in the vicinity of complex magnetic ground states - an ideal test bed to study quantum phase transitions. A special case for the coexistence of superconducting and magnetic order is the well-known Q-phase in CeCoIn5 [1] where the antiferromagnetism coexists at low-temperature and high field with the superconducting phase [2] and is a rare example of cooperative coexistence [3]. The magnetic order was evidenced to be an incommensurate spin

density wave (SDW). For a 5% substitution of Ce with Nd, an antiferromagnetic phase is stabilized within the superconducting phase already at zero magnetic field. Previous experimental evidence suggests that both antiferromagnetic phases are separated by a quantum critical point (QCP) that separates two antiferromagnetic states with identical symmetry [3]. We present our recent studies on 2% and 3.5% Nd-doped CeCoIn5 which both feature the Q-phase magnetic order at high-field region along (0.554, 0.554, 0.5) as well as a low-field SDW phase with the same order. Interestingly, the low-field SDW phase vanishes with increasing magnetic fields before the Q-phase is stabilized. This suggests that these two phases are separated by a disordered magnetic phase for low Nd-doped CeCoIn5. The separation of SDW phases represents for two magnetic instabilities in the NdxCe1-xCoIn5 series, suggesting different origins of the two phases. Our study presents a unique case where two magnetic phases of identical symmetry are separated by a disordered phase.

Position:

Postdoc

Poster session / **139**

Multiscale Materials Modelling

Authors: Georg Schusteritsch[None] ; Matthias Krack[None] ; Monica Kosa[None] ; Sergii Nichenko[None] ; Sriram Venkatesan[None]

The Multiscale Materials Modelling (MMM) group is part of the recently established cross-departmental Laboratory for Scientific Computing and Modelling, specializing in inter-disciplinary modelling inside and outside PSI.
The MMM group's expertise is in computational chemistry and materials science simulations for a broad range of materials from energy, pharma, and nuclear fields using state-of-the-art tools in the framework of fundamental and applied research. Specific computational tasks include and are not limited to:
• Chemical reactivity: Reaction mechanisms, Homogeneous and heterogeneous catalysis
• Solid state chemistry: Band gap and band structure calculation, Mechanical response of materials, Polymorph stability, Ionic diffusion in structured solids, electronically challenging materials such as nuclear fuels and perovskite architectures
• Energy Viable Materials: Reduction and oxidation potentials, electrode voltages, electro-catalysis
• Characterization: IR, Raman, Optical absorption spectroscopy, X-ray absorption spectroscopy
• Thermodynamical modelling and database generation

Position:

Postdoc

Poster session / 147

Finite-element mesh generation and simulation of magnetization dynamics in a three-dimensional artificial spin structure

Authors: Sebastian Gliga[1] ; Sven Friedel[2]

[1] *ETH Zürich*

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Magnetic three-dimensional structures on the nanoscale possess static and dynamic properties not found in their 'flat' counterparts. The recent development of three-dimensional lithography and probing techniques (such as X-ray tomography) has enabled the experimental investigation of such structures. Concurrently, simulations need to be developed to gain detailed understanding of the magnetization dynamics. We have developed a finite-element meshing technique involving Eikonal equations, which has allowed us to produce high-quality efficient meshes for to describe a mesoscopic 'Buckyball' made of hollow beams, exemplifying a complex network with tree-fold junctions. Our micromagnetic simulations based on tetrahedral meshes reveal reversal avalanches mediated by the nucleation and propagation of domain walls during the field-driven magnetization reversal in the cylindrical tubes making up the Buckyball.

Position:

Scientist

Poster session / 130

Ultrafast dynamics of antiferromagnetic fluctuations in the spin-chain CuGeO3

Authors: Eugenio Paris[1] ; Christopher Nicholson[2] ; Yi Tseng[1] ; Giacomo Coslovich[3] ; William F. Schlotter[3] ; Sioan Zohar[3] ; Ming-Fu Lin[3] ; Georgi L. Dakovski[3] ; Claude Monney[2] ; Thorsten Schmitt[4]

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[2] *Department of Physics, University of Fribourg*

[3] *SLAC National Accelerator Laboratory*

[4] *Paul Scherrer Institut*

In the edge-shared spin-chain CuGeO3, the relation between charge, spin and lattice degrees of freedom, giving rise to the Spin-Peierls transition, is still unclear. In this regard, Resonant Inelastic X-ray Scattering (RIXS) represent a very powerful tool, capable of probing elementary excitations involving different degrees of freedom in a single experiment. Recently, the advent of Free-Electron Laser sources enabled extending these capabilities to the time domain, allowing pump-probe experiments. In the O K-edge RIXS spectrum of CuGeO3, one of the charge transfer excitations is characterized by a sharp structure associated to the formation of the Zhang-Rice singlet. The probability for such non-local excitation channel depends on the short-range antiferromagnetic (AF) spin correlations between two neighboring CuO4 plaquettes. We use a 266 nm ultrashort laser pump to excite carriers across the charge-transfer gap, removing spin-1/2 holes from the Cu sites and thus perturbing the local spin-correlations. We use O K-edge RIXS to probe the suppression and recovery of the Zhang-Rice singlet excitations, giving insight in the dynamics of the short-range AF magnetic interactions.

Position:

Postdoc

Poster session / 127

Floating zone growth and characterization of topological materials

Author: Pascal Puphal[1]

Co-authors: Jonathan White [2] ; Ekaterina Pomjakushina [3] ; Victor Ukleev [1] ; Vladimir Pomjakushin [4]

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Materials hosting Weyl nodes (a pair of linear crossings in the band-structure, similar to Dirac points) yield an enormous potential for applications since they enable massless electrons leading to fast transport properties. A ferromagnetic Weyl semimetal enables a tuning of the berry curvature by an external field. Bandstructure calculations promise the *R* AlGe family (*R* = La, Ce, Pr) [1] to be a promising candidate.

The tetragonal I41md (#109) structure of *R* AlGe is non-centrosymmetric and its magnetism offers rich possibilities for Weyl fermions since both spatial and time-reversal symmetries are broken. While already discovered in 1992 [2] the interest in the context of topology has only been realized in the last years. Until 2018 only specific heat and magnetization data were published on CeAlGe powder samples while PrAlGe still remained unstudied. Since the theoretical proposal the material class is heavily researched [2-5]. In my talk I will shortly introduce the single crystal growth by floating zone of both CeAlGe (Tc = 5 K) and PrAlGe (Tc = 16 K) [2] and elaborate their physics probed by SANS and elastic neutron diffraction. Reports of large magnetoresistance gives a first hint at the weyl properties of these systems [4,5], in addition to this topology we find a topological magnetic groundstate for CeAlGe with a novel kind of striped meron groundstate quite in contrast to the original ferromagnetic claim. PrAlGe on the other hand has the Γ point groundstate, but still is no simple ferromagnet as we find some diffuse scattering at low q and frequency dependence indicating some sort of spin freezing.

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Position:

Postdoc

Poster session / 133

Emerging molecular magnetic materials

Author: Jan Gui-Hyon Dreiser[1]

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Molecular magnetic materials are coordination compounds, in which metal ions are linked with each other via suitable ligands. These materials exhibit a tremendous variety in their dimensionality, electrical, optical and magnetic properties, giving rise, e.g., to the coexistence of ferromagnetic order and electrical conductivity in layered molecular materials [1], photoswitchable compounds [2], single molecules possessing long magnetization lifetimes [3] and long spin coherence times [4]. In addition, because of their processability they can be incorporated into molecule-inorganic heterostructures [5–7], which constitutes a means of investigating and exploiting their interesting properties attractive for a wide range of possible applications [8]. In this contribution I will show recent developments in this field, with the hope of further stimulating exciting discussions followed by experiments.

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Position:

Scientist

Poster session / 137

Time-resolved X-ray tomography of multiphase systems

Authors: Vladimir Novak[1] ; Christian Matthias Schlepütz[None] ; Marco Stampanoni[2]

[1] *PSI - Paul Scherrer Institut*
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This work is focused on in-situ and time-resolved tomography of multiphase systems. Specifically, transport of liquids and gases in porous structure are investigated. The applications include catalyst coating for air pollution control and pharmaceutical drugs impregnation. The evolution of the studied systems are followed by X-ray tomography in 3D with temporal resolution one second. Necessary environment as sample holders, heating system and experimental cell allowing transport of liquid and gases to the sample during continuous rotation are developed within the project. The aim is to understand interactions between different phases (solid, liquid and gas) in dynamically evolving systems.

Position:

Postdoc

Poster session / 123

The sound of the Q-phase in CeCoIn5 - an ultrasound investigation

Authors: D. T. Maimone[1] ; M. Bartkowiak[1] ; S. Zherlitsyn[2] ; M. Kenzelmann[3]

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Strong correlations in intermetallic compounds containing f-electron elements give rise to a wide variety of ground states. Superconducting states found in heavy fermion materials are candidates for unconventional pairing with intertwined orders [1]. CeCoIn5 is an intriguing example among this class of materials, with a dx2-y2 order parameter. Superconductivity is Pauli limited and coexists with a spin density wave (SDW) at low temperatures and high magnetic fields, in the so called Q-phase [2]. Superconductivity and magnetism are suppressed simultaneously at a first order phase transition, suggesting an unusual cooperative interplay. Inelastic neutron scattering measurements indicate that the Q phase can be interpreted as a field tuned Bose condensation of spin excitons. Intriguingly, this incommensurate SDW order always emerges in a single domain state and the domain selection is hyper sensitive to the direction of the applied magnetic field [3]. The nature of the Q-phase and the mechanism for domain switching remain under debate. In all proposed scenarios, the appearance of the Q-phase will affect the electronic quasi-particle DOS. Since phonons couple to the electronic structure at high frequencies- MHz [4], ultrasound is a suitable technique to investigate the Q-phase and its translational symmetry breaking. Here we investigate the response of elastic constants and attenuation of different modes under rotating magnetic fields.

The ultrasound technique is currently under development at the Paul Scherrer Institute. Traditionally, ultrasound setups rely on analog circuit components. We present our route to establish the technique taking advantage of a commercially available data acquisition card and subsequent digital processing.
[1] M. Kenzelmann et al, Science 321, 186-197 (2008).
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Position:

Phd

Poster session / 138

Investigation of metal-insulator transition in Slater insulator, NaOsO3 using static and time-resolved resonant x-ray diffraction

Authors: Namrata Gurung[1] ; Martin Kubli[2] ; Vincent Esposito[None] ; Susmita Saha[3] ; Federico Pressacco[4] ; Dmitry Ozerov[None] ; Henrik Till Lemke[None] ; Naëmi Leo[None] ; Kazunari Yamaura[5] ; Yves Joly[6] ; Steve Collins[7] ; Makina Yabashi[8] ; Takashi Tanaka[9] ; Tetsuo Katayama[10] ; Tadashi Togashi[11] ; S. Owada[12] ; Urs Staub[13] ; Steven Johnson[13] ; Paul Beaud[13] ; valerio scagnoli[13]

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The metal-insulator transition in 5d transition metal oxide NaOsO3 which occurs concomitantly with antiferromagnetic order (TMIT=TN) has been proposed to be driven by Slater mechanism [1, 2] i.e. it is the onset of the antiferromagnetic order that drives the system into an insulating state [3]. However, there is no consensus and other mechanisms such as a Lifshitz transition have been proposed [4]. We employed static non-resonant and resonant x-ray single-crystal diffraction at the Os L2,3 edges in order to obtain details of the Os electron density deformation across TMIT and to investigate the microscopic mechanism of the phase transition. In the case of a Slater metal-insulator transition, there should be no change in the crystallographic symmetry and, indeed, our off-resonance single crystal x-ray diffraction experiments find no evidence of crystallographic symmetry breaking across the metal-insulator transition. In addition, using an incident x-ray energy corresponding to the Os L3 resonant edge, we observe the emergence of a diffracted intensity of the forbidden re-flection (300), also called ATS (anisotropic tensor of the x-ray susceptibility) reflection at TMIT=TN for a specific energy EA = 10.878 keV. The intensity of this ATS reflection increases continuously with decreasing temperature and is not of magnetic origin. We show that it is due to a change in the Os electron density associated to the onset of long range antiferromagnetic ordering. Thus, the main conclusions of our experimental results namely: the absence of crystallographic symmetry breaking and the presence of antiferromagnetic driven Osmium electron density reconstruction, support the first realization of a Slater insulator, NaOsO3.

We further observed that upon photo-excitation, ultrafast changes in the reflectivity takes place. In order to study the time-evolution of long-range ordering arising from structural, magnetic and electronic ordering, we employed time-resolved resonant x-ray diffraction at the Os L3 edge. From our preliminary data analysis, we observe a significant drop of the antiferromagnetic peak intensity after photo-excitation within the time resolution of the experiment, while the timescale associated with the drop of intensity of a structural reflection is in the order of several picoseconds. As a next step, we aim at comparing the ultrafast dynamics of long range ordering in this system with other transition metal oxides, in order to determine the existence of unified description of a universal time-dependent order parameter in transition metal oxides.

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[5] N. Gurung, et al., Physical Review B 98, 115116 (2018)

Position:

Phd

Poster session / 73

Probing solid-liquid interfaces with tender X-rays

Authors: Zbynek Novotny[1] ; Dino Aegerter[2] ; Emiliana Fabbri[3] ; Luca Artiglia[3] ; Jörg Raabe[3] ; Thomas Huthwelker[3] ; Juerg Osterwalder[4]

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Many important chemical and biological processes occur at the interface between a solid and a liquid, which is difficult to access for chemical analysis. The large inelastic scattering cross section of electrons in the condensed matter makes X-ray photoelectron spectroscopy (XPS) highly surface sensitive but less sensitive to buried interfaces. This limitation can be overcome by stabilizing an ultrathin layer of liquid with a thickness in the order of a few tens of nanometres and by employing tender X-rays (photon energy ranging between 2-8 keV) that can be used to probe the buried solid-liquid interface. We have recently built and commissioned a new instrument at the Swiss Light Source that combines ambient-pressure XPS with in-situ electrochemistry. With this new setup, we can stabilize a thin liquid layer on a solid surface by a dip&pull method [1], and by using tender X-rays (2-8 keV) from the Phoenix beamline, we can probe the properties and chemistry at the solid-liquid and liquid-gas interface while having a potential control over the ultrathin electrolyte film. The capabilities of this new instrument were demonstrated during the first commissioning beamtime, where we stabilized a thin electrolyte layer (0.1 M KOH) over the Ir(001) electrode. The dip&pull technique was used for the first time using well-defined single-crystalline surfaces (see Supplementary document). Core-level binding energy shifts following the applied potential were observed for species located within the electrolyte film. This included the oxygen 1s level from liquid water, potassium, and, interestingly, also an adventitious carbon species, while the interface was carbon-free. We will present the results from the first commissioning beamtime and outline the future directions we are going to pursue using this new instrument.
[1] S. Axnanda, E. J. Crumlin et al., Sci. Rep. 5, 09788 (2014).

Position:

Scientist

Poster session / 69

Evidence of large polarons in photoemission band mapping of the perovskite semiconductor CsPbBr3

Authors: Nicola Colonna[1] ; Michele Puppin[2] ; Serhii Polishchuck[2] ; Andrea Crepaldi[3] ; Dmitry Dirin[4] ; Olga Nazarenko[4] ; Riccardo de Gennaro[5] ; Gianmarco Gatti[3] ; Silvan Roth[3] ; Thomas Roland Barillot[6] ; Luca Poletto[7] ; Rui Patrick Xian[8] ; Laurenz Retting[8] ; Maximilian Walf[8] ; Ralph Ernstorfer[8] ; Maksym Kovalenko[9] ; Marzari Nicola[5] ; Grioni Marco[3] ; Majed Chergui[6]

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Lead-halide perovskite (LHP) semiconductors rival conventional semiconductors in multiple optoelectronic applications. The origin of such outstanding transport propeties are howerer not yet fully understood. We find signatures of large polaron formation in the electronic structure of the inorganic LHP $CsPbBr_3$ by means of angle-resolved photoelectron spectroscopy. The experimental valence band dispersion shows a hole effective mass 0.26 ± 0.02 m_e, 50% heavier than the bare mass m_0=0.17 m_e predicted by density functional theory. Calculations of electron-phonon coupling indicate that phonon dressing of the carriers mainly occurs via distortions of the Pb-Br bond with a Fröhlich coupling parameter α=1.82. A good agreement with our experimental data is obtained within the Feynmann polaron model, validating a viable theorical method to predict the carrier effective mass of LHPs $ab\,initio$.

Position:

Postdoc

Poster session / 98

Addressing Electronic and Spin Transitions of Switchable Molecules in the Monolayer Range

Authors: Niéli Daffé[1] ; Juan-Ramón Jiménez[2] ; Amina Benchohra[2] ; Michal Studniarek[None] ; Jessem Landoulsi[3] ; David Kreher[2] ; Rodrigue Lescouëzec[2] ; Jan Gui-Hyon Dreiser[1]

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Switchable molecules exhibiting tunable physical properties as a function of external stimuli (electric or magnetic fields, temperature, light or pressure) have drawn a considerable interest for their useful functionalities [1,2]. Nevertheless, with the considerable attraction for those systems, some fundamental and practical challenges arise in view of their integration in molecule-based electronic devices such as molecular switches, sensors or qubits. An example of a present day challenge is the preservation of the switchable functionalities of the molecules while being adsorbed on surfaces [3,4]. Promising bistable properties have emerged from the so-called Fe spin-crossover group of compounds and Fe/Co molecular complexes exhibiting concomitant changes in their optical and magnetic properties (see Fig.1) induced by spin transition and charge transfer respectively [5,6]. In order to address the switchable properties of those systems on surfaces, we have explored different solutions to prepare monolayers of these complexes consisting of ultra-high vacuum compatible techniques and deposition in solutions. By means of X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism, we follow the oxidation state changes of the transition metals upon application of laser light and temperature and investigate whether the molecules keep their switchable properties when adsorbed on a suitable surface. The results obtained on the monolayers show results different from the bulk phases of the same complexes depending on *i)*the technique used to prepare the monolayer, *ii)* the nature of the substrate and/or *iii)* the intrinsic properties of the molecules.

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Position:

Postdoc

Poster session / 76

Revisiting the magnetic structure of R1/3Sr2/3FeO3 (R = La, Pr, Nd) by neutron powder and single crystal diffraction combined with spherical polarimetry

Author: Ekaterina Pomjakushina[1]

Co-authors: Fei Li [1] ; Vladimir Pomjakushin [2] ; Romain Sibille [2] ; Bertrand Rössli [2]

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We present our study of a magnetic structure in R1/3Sr2/3FeO3 (R = La, Pr, Nd) system, which is interesting because it has a metal-insulator (MI) transition concomitantly with the magnetic ordering. In our previous paper [1] we have shown that the neutron powder diffraction data can be equally well fitted by two different magnetic space groups, namely a canted helical model P3_221 and a collinear arrangement of the Fe-spins C2/c. The latter model supports the charge ordering, implying that it is responsible for MI-transition. We have performed neutron single-crystal diffraction and neutron spherical polarimetry experiments on La1/3Sr2/3FeO3 single crystals grown by floating zone method, in order to distinguish between the two magnetic models, we proposed. Our single crystal diffraction and spherical polarimetry experiments were able to resolve the above issue, giving the definitive preference to C2/c [2]. This work was supported by SNF project 200021_157009, Fei Li has successfully defended his PhD thesis [3].
[1]. F.Li et al., PHYSICAL REVIEW B 97, 174417 (2018)
[2]. F.Li et al., to be published
[3]. Fei Li: Crystal and magnetic structure of R1/3Sr2/3FeO3 (R = La, Pr and Nd), © 2019, doi: 10.3929/ethz-b-000349023

Position:

Scientist

Poster session / 112

Ultrafast dynamics of structural and orbital order in TiSe2

Authors: Max Burian[1] ; Michael Porer[None] ; José Renato Linares Mardegan[None] ; Vincent Eposito[2] ; Valerio Scagnoli[3] ; Namrata Gurung[4] ; Tadashi Togashi[5] ; Urs Staub[3]

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Charge density waves (CDWs) comprise a class of collective phenomena that find their roots in the interplay of (i) a materials electron density and (ii) its underlying atomic lattice. In the prominent reference system TiSe¬2, numerous experimental and theoretical studies have looked at the emergence of the CDW phase – yet until today the microscopic mechanisms remain elusive.[1,2] Based on our previous research [3], we performed ultrafast resonant X-Ray diffraction experiments at the Se K edge, tracking the structural and orbital order of TiSe2 after optical excitation. We observe similar transient dynamics of structural and orbital response, yet the dependency on pump fluence appears remarkably different. Furthermore, we find a strong oscillatory lattice deformation in the high fluence regime – likely the result of a coherently driven L1 phonon mode. Current efforts are directed towards theoretical considerations and calculations, which will put the experimental findings into context with existing hypotheses. Here, we hope that our findings will help to understand if (i) electron-phonon interactions or (ii) exciton correlations are the main driving mechanism for the formation of the CDW in TiSe2.

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https://doi.org/10.1038/nmat4042
[2] E.Möhr-Vorobeva, S.L.Johnson, et al.; Nonthermal Melting of a Charge Density Wave in TiSe2. Physical Review Letters 107, 036403 (2011).
http://doi.org/10.1103/PhysRevLett.107.036403
[3] P.Beaud, A.Caviezel, et al.; A time-dependent order parameter for ultrafast photoinduced phase transitions. Nature Materials 13, 923-927 (2014).
https://doi.org/10.1038/nmat4046

Position:

Postdoc

Poster session / **94**

Influence of Selective Laser Melting strategies and post treatment on the residual stresses and microstructure of Alloy 718

Author: Jan Capek[None]

Co-authors: Efthymios Polatidis [1] ; Pederson Robert [2] ; Markus Strobl [3]

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Selective Laser Melting (SLM) provides valuable prospects for nickel-based superalloys that are used in many applications in aerospace or automotive, chemical and nuclear industry. SLM involves numerous building parameters and subsequently, numerous post-building treatment options that affect the geometrical integrity, surface quality, microstructure and mechanical behavior. Coin-shaped samples of Alloy 718, were built with different SLM building strategies. Residual stresses in the bulk of the specimen were measured by neutron diffraction experiment at the POLDI instrument at the Paul Scherrer Institute. In addition, X-Ray diffraction was measured to study the precipitates and electron microscopy was used to investigate the effect of building conditions on the microstructure, crystallographic texture and chemical variations.

Position:

Postdoc

Poster session / **91**

Operando high energy XRD of Cu/La0.5Sr0.5CoO3 TWC under oscillating feed

Authors: Ivo Alxneit[1] ; Alberto Garbujo[2] ; Davide Ferri[3] ; Giovanni Carollo[2] ; Antonella Glisenti[2]

[1] *PSI - Paul Scherrer Institut*

[2] *Università degli Studi di Padova, Dipartimento di Scienze Chimiche*

[3] *PSI*

Copper is considered a possible candidate to replace precious metals in future three-way catalysts. Its performance as catalyst was assessed in operando conditions. A 20 wt% $CuO/La_{0.5}Sr_{0.5}CoO_3$ catalyst was studied under oscillating redox conditions while subjected to a temperature cycle $100-400-100^{o}C$. Mass spectrometry was used to monitor gas compositions while time-resolved XRD diffraction data was used to monitor phase transitions and structural changes. Rietveld analysis of the data reveals the irreversible decomposition of CuO to Cu_2O and Cu and reversible conversion of the perovskite support to a brownmillerite phase at high temperatures. The perovskite host itself is also sensitive to the redox environment, thus the oscillations of the gas feed are reflected in the phase composition. The redox oscillations are also responsible for the increased NO reduction activity. The analysis is complcated by the presence of some not yet identified decomposition products and the rather low resolution in 2Θ.

Position:

Scientist

Poster session / 78

Time-of-arrival detection for time-resolved STXM imaging

Authors: Simone Finizio[None] ; Sina Mayr[1] ; Jörg Raabe[1]

[1] *Paul Scherrer Institut*

The quest for faster and more efficient magnetic data storage devices has recently ignited numerous studies of sub-ns magnetodynamical processes such as e.g. antiferromagnetic spintronics [1], high frequency spin waves [2], and ultrafast SOT-induced processes [3]. Time-resolved scanning transmission X-ray microscopy (STXM) is a popular technique for the investigation of such processes, as it combines a high spatial resolution with the possibility to efficiently carry out pump-probe experiments. Up to now, time-resolved STXM imaging relies on the assumption that the X-ray photon flashes generated by the synchrotron light source illuminate the sample at a specific, infinitesimally small, time point. This is, however, not the case, as the X-ray flashes generated by the synchrotron light source exhibit, at the SLS, a FWHM on the order of 70 ps, having the consequence that high frequency excitations (above 6 GHz) are inaccessible. A possible workaround to this problem is to employ shorter X-ray pulses, offered e.g. by operating the synchrotron with low-alpha optics, but this approach is both not practical and not sustainable in the long term: with the upcoming upgrade to the diffraction-limited source SLS 2.0, the operation with low-alpha optics will no longer be possible, and it is expected that the X-ray bunch length will remain unvaried from the current 70 ps value. Therefore, we present here a different solution, based on the measurement of the time-of-arrival of the X-ray photons. This will enable the measurements of high frequency excitations (with "low alpha performance") using the normal optics. Faster measurements at high excitation frequencies will therefore be possible, thanks to the higher photon flux offered by the standard optics and, with the upgrade to SLS 2.0 in sight, such a solution would guarantee the long-term competitiveness of the SLS in time resolved studies down to 1-10 ps resolutions.

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[2] G. Dieterle et al., Physical Review Letters 122, 117202 (2019)
[3] M. Baumgartner et al., Nature Nanotechnology 12, 980 (2017)

Position:

Postdoc

Poster session / 113

Spin reorientation in ferromagnetic type-II Weyl Fe3Sn2.

Authors: Neeraj Kumar[1] ; Yeong-Ah Soh[2]

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[2] *PSI*

Fe3Sn2 is a predicted type-II Weyl semimetal which orders ferromagnetically below TC= 646 K. It undergoes a spin reorientation transition (SRT) between 300K-100 K which together with recently shown coupling between its easy axis and the band structure paves the way of external control of its bulk properties. By probing anisotropic magnetoresistance, and bulk magnetization, we understand its domain structure together with evolution of easy axis during the SRT. We are able to clearly establish the nature of SRT to be of first order and accurately determine the transition temperature.

[1] Kumar et al. arXiv 1908.03927 (2019).

Position:

Postdoc

Poster session / 131

Momentum Signatures of Site Percolation in disordered 2D Ferromagnets in low and high defect density regimes

Author: Zhi Jian Daniel Tay[1]

Co-author: Christian Miniatura [2]

[1] *ETH Zurich*

[2] *Center for Quantum Technologies (CQT)*

As real devices necessarily contain defects, it is of interest to study wave propagation in disordered systems. In this work, we start from a 2D square lattice of magnetic spins with nearest-neighbour interactions and replace a fixed proportion of magnetic sites with nonmagnetic defects ('Site Percolation Model'). We are primarily interested in the disorder-averaged momentum signatures that occur at low and high defect densities when an initial spin wave with fixed momentum propagates through the disordered system.

At low defect densities, the system consists of a single percolating cluster with some small disconnected clusters. In this regime, we expect that the usual predictions of Anderson localization [1] should apply. Indeed, we observe two peaks in the momentum distribution: A Coherent Forward Scattering (CFS) peak in the same direction as the initial plane wave, as well as a Coherent Backward Scattering (CBS). These phenomena are consistent with existing literature on the momentum signatures of Anderson Localization in random disorder [2-3].

At high defect densities, we move into uncharted territory. In this regime, we observe that the system increasingly breaks down into multiple disconnected clusters. The formation of these disconnected clusters gives rise to a unique momentum signature in the form of oscillations in the CFS peak. These oscillations occur at frequencies consistent with the energies of the clusters and provide a unique momentum signature of cluster formation due to defects in magnetic systems.

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Position:

Phd

Poster session / 88

Dzyaloshinskii-Moriya Interaction in Nanocrystalline Vitroperm

Author: Yifan Quan[1]

Co-authors: Ben van den Brandt [2] ; Joachim Kohlbrecher [2] ; Andreas Michels [3] ; Patrick Hautle [2]

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The Dzyaloshinskii-Moriya interaction (DMI) is believed to be operative in low-symmetry crystal lattices lacking inversion symmetry. However, already in 1963, Arrott pointed out that even in a high symmetry lattice, where the DMI would normally vanish, this interaction is present in the vicinity of any lattice defect. Based on these considerations and recent theoretical work, first experimental studies of the impact of the DMI on the spin-polarized magnetic small-angle neutron scattering (SANS) on polycrystalline magnets exhibiting a large density of microstructural defects have been performed. They demonstrated that an asymmetry in the difference between the two half polarized SANS cross sections is induced by the DMI in nanocrystalline terbium and holmium as well as in mechanically deformed microcrystalline cobalt. Here we present an additional case, the nanocrystalline soft magnet Vitroperm ($Fe_{73}Si_{16}B_7Nb_3Cu_1$), where the SANS cross section exhibits the polarization dependent asymmetric term originating from the DMI. The effect has a magnetic field dependence and is less pronounced at higher fields until it eventually vanishes reaching full saturation. The result supports the generic relevance of the DMI for the magnetic structure of defect-rich ferromagnets. Furthermore it shows that polarized SANS is a particularly powerful tool for investigating defect-induced DMI, due to it's unique dependence on the chiral interactions.

Position:

Phd

Poster session / 100

Determination of Molybdenum Species Evolution during Non-Oxidative Dehydroaromatization of Methane and its Implications for Catalytic Performance

Authors: Miren Agote Aran[1] ; Ines Lezcano-Gonzalez[2] ; Anna Kroner[3] ; Andrew Beale[2]

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[2] *UCL*

[3] *Diamond Light Source*

Methane dehydroaromatisation reaction (MDA) is of increasing industrial interest to convert methane directly into benzene, valuable precursor for the chemical industry. Mo-containing zeolites are promising catalysts for MDA, Mo species activate methane while the zeolite pores provide shape selectivity to benzene; however, the rapid material deactivation due to carbon deposit accumulation compromises the commercialisation of the reaction.
In order to shed light into the catalyst working mechanism/deactivation, the evolution of Mo species in Mo/zeolites has been investigated by means of operando X-ray absorption/diffraction techniques (XAS/XRD). XAS results revealed that in contact with methane, initial tetrahedral Mo-oxo species attached to the zeolite are carburised to MoxCy, which showed to be selective to aromatics. XAS/XRD studies evidenced the detachment of MoxCy from the zeolite and their migration outside the pores; this would result in the loss of shape selectivity to aromatics explaining the increased carbon deposit formation overtime and catalyst deactivation.
At short reaction times, MoOx and MoOxCy species are believed to coexist and to show selectivity to ethylene, also of interest for the chemical industry. Collaboration with SuperXAS to perform

modulated quick-XAS measurements combined with multivariate curve resolution (MCR) analysis will help to discriminate among the different Mo species evolving under reaction conditions and to evaluate their selectivity/stability.

Position:

Postdoc

Poster session / 70

Neutron-based research on additive manufactured materials at the Paul Scherrer Institute

Author: Efthymios Polatidis[1]

Co-authors: Jan Capek ; Manuel Morgano [2] ; Pavel Trtik [3] ; Markus Strobl [2]

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[3] *PSI Villigen*

Additive manufacturing (AM) processes allow the building of three-dimensional (3D) parts by progressively adding thin layers of materials guided by a digital model. AM processes are known for the complexity of the processing parameters which can greatly influence the materials properties such as porosity, residual stresses, microstructure and mechanical behavior.

Within the Neutron Imaging and Applied Materials (NIAG) group at the Paul Scherrer Institute, a synergy of multiscale characterization techniques is applied for studying components processed by AM. Neutron diffraction studies are undertaken at the instrument POLDI for residual stress characterization while the novel deformation rigs (uniaxial and multiaxial) are used for in-situ investigations of the deformation behavior of AM materials. The imaging beamlines ICON and NEUTRA and the novel "Neutron Microscope" installed on POLDI, ICON or BOA beamlines are employed for the characterization of the internal structures in length-scales ranging from about 10 μm to cm. Finally, diffraction contrast imaging on the BOA beamline is undertaken for mapping the phase, strain and texture distribution with high spatial resolution.

In this contribution reference cases and various characterization methods applied to different materials, produced by AM techniques will be showcased. Specific examples of characterization of the mechanical behaviour, porosity and strain/stress distribution with respect to the material, processing parameters and building methods will be presented.

Position:

Scientist

Poster session / 92

Observing dynamics in photoexcited states of photocatalysis/photoelectrodes studied by transient XAS in XFELs

Authors: Yohei Uemura[1] ; Ahmed Ismail[2] ; Frank de GRoot[2] ; Kiyotaka Asakura[3] ; Toshihiko Yokoyama[4] ; Sang Han Park[5] ; Soonnam Kwon[6] ; Tetsuo Katayama[7] ; Makina Yabashi[8]

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Photocatalysts and photoelectrodes play an important role to promote the decomposition of water to hydrogen (H2) and oxygen(O2). Various kinds of photocatalysts/photoelectrodes have been proposed for the last several decades. However, new materials are still explored to enhance its catalytic efficiency for our daily use. Fundamental studies on the mechanisms of photocatalysts/photoelectrodes have been based on theoretical calculations, electrochemical methods and spectroscopic studies. Although these studies have achieved important discoveries on photocatalytic materials, the detailed mechanisms of the photocatalytic materials are not well understood yet. X-ray absorption spectroscopy (XAS) is relatively a new methodology to understand the excited states of photocatalytic materials. XAS can address local structures and electronic states of a target element, which can provide different information from optical spectroscopies. Recently, x-ray free electron lasers (XFELs) have been established in some countries (USA, Japan, Germany, South Korea, Switzerland) and they have been utilized for time-resolved experiments because they provide ultrashort x-ray pulses (<10 fs).

We have already demonstrated that time-resolved x-ray absorption spectroscopy (tr-XAS) in XFELs are useful to understand dynamic changes in the valence states or local structures of photocatalytic materials. In WO3, there were different two kinetic processes observed after the photoexcitation.1 It was found that an intermediate state was formed after the photoexcitation and it recovered to its ground state with a lifetime of 2 ns. In BiVO42, it was found that a structural change occurred after the photoexcitation, which could be induced by coherent oscillations. Recently, we have measured time-resolved XAS of several different materials: WO3, CuWO4 and Fe2O3. For WO3, we employed the arrival timing monitor to correct the timing jitter between each x-ray pulse and laser pulse and a fast decay process was observed just after the photoexcitation (< 1 ps). For CuWO4, we employed both the hard x-ray (SACLA, Japan) and soft x-ray XAS (PAL-XFEL, South Korea) and successfully observed the changes in the valence state of Cu. Our hard x-ray and soft x-ray results give new insights into the origin of photoexcited electrons in CuWO4. For Fe2O3, we employed soft x-ray XAS and 2p3d resonant inelastic x-ray scattering (RIXS) to understand the changes in Fe2O3. In addition to XAS, RIXS for the photoexcited Fe2O3 was successfully observed. RIXS can give more information about the changes of the photoexcited Fe and the interactions between the Fe and the surrounding atoms. In this presentation, we would like to discuss these new XFELs based time-resolved studies.

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1. Y. Uemura et al. *Angew. Chem. Int. Ed.* 2016, **55**, 1364-1367
2. Y. Uemura et al. *Chem. Comm.* 2018, **53**, 7314-7317

Position:

Postdoc

Poster session / **83**

Analysis of Silicon Carbide ultra-thin (<2um) x-ray sensors for synchrotrons beam position monitors applications

Authors: Maria del Mar Carulla[1] ; Massimo Camarda[None]

Co-authors: Selam Nida [2] ; Alexander Tsibizov [2] ; Thomas Ziemann [2] ; Beat Meyer [1] ; Dario Ferreira Sanchez [3] ; Mario Birri ; Oliver Bunk [3] ; Claude Pradervand [3] ; Daniel Grolimund [3] ; Grossner Ulrike [2]

[1] *PSI*

[2] *APS-ETH*

[3] *Paul Scherrer Institut*

In this work, we present a systematic theoretical and experimental investigation of the use of Silicon Carbide thin (thicknesses between 500nm and 10µm) low-doped large area (>10mm2) membranes as X-ray sensors for beam position monitoring (XBPM) applications at synchrotron light sources (SLS).

Position:

Scientist

Poster session / **80**

Single spin-polarised Fermi surface in $SrTiO_3$ films

Author: Eduardo Bonini Guedes[1]

Co-authors: Stefan Muff [1] ; Mauro Fanciulli [2] ; Andrew Weber [2] ; Marco Caputo [1] ; Zhiming Wang [3] ; Nicholas Plumb [4] ; Milan Radovic [4] ; Jan Hugo Dil [4]

[1] *Paul Scherrer Insitut*

[2] *Ecole Polytechnique Federale de Lausanne*

[3] *Ningbo Institute of Materials Technology and Engineering*

[4] *Paul Scherrer Institut*

The 2D electron gas (2DEG) formed at the surface of $SrTiO_3$(001) has attracted great interest because of its fascinating physical properties and promise as a novel electronic platform, but up to now has eluded a stable way to tune its properties. Using angle-resolved photoemission spectroscopy with and without spin resolution we here show that the band filling can be controlled by growing thin $SrTiO_3$ films on $SrTiO_3$(001) substrates with different Nb doping levels. This results in a single spin-polarised 2D Fermi surface in a superconducting system, which can be used as platform for Majorana physics. Based on our results it can furthermore be concluded that the 2DEG does not extend more than 3 unit cells into the film and that its properties are determined by the dielectric response of the system.

Position:

Postdoc

Poster session / 79

Thin Film Deposition With The Sputtering Lab @ LIN

Authors: Christine Klauser[1] ; Uwe Filges[2] ; Michael Horisberger[2]

[1] *PSI - Paul Scherrer Institut*

[2] *PSI*

Thin film deposition is a technique useful in many scientific domains.

Our sputtering lab provides their coating services for all PSI groups, developing novel thin layers, lending support in sample preparation and manufacturing of instrument components.

The lab is equipped with 2 sputtering plants that have 3 target stations each and cover 50x200 mm^2 and 400 x 580 mm^2 respectively. Both DC magnetron and HF-sputtering are possible, including reactive sputtering.

We specialize in multilayer and supermirror deposition for neutron optical applications. Recent successes include m=6 Ni-Ti supermirrors and 10B coatings.

We would like to push the development of supermirrors further and would benefit from additional expertise in thin layer characterization.

Position:

Scientist

Poster session / 86

CO2 alcoholysis to organic carbonates over Zr-based catalysts: an in situ ATR-IR study

Authors: Matteo Signorile[1] ; Davide Ferri[2] ; Valentina Crocellà[3] ; Francesca Bonino[3]

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Beside the reduction of CO2 emissions by switching from fossil to renewable energy sources, alternative strategies to limit the greenhouse effect are represented by its storage and/or utilization. Among the various proposed utilization reactions, a potentially viable route is the direct CO2 fixation in organic carbonates, whose industrial interest as green chemicals is growing [1].
This work focuses on the synthesis of simple organic carbonates through the direct reaction of CO2 and alcohols: the main challenge is the high energy barrier of this reaction, which requires the development of effective catalysts to make it viable. We focus here on the development of specific heterogeneous catalysts, based on Zr4+ supported over high surface area silica, as inspired from the results on the corresponding pure oxide [2]. Furthermore, post-synthetic functionalization with amines is exploited to enhance the capture capabilities toward CO2. A graphical concept of the catalyst is given in the attached Figure.
Beside the basic characterization outcomes, the first fundamental results on the interaction of the pure reactants (CO2 and alcohols) with the proposed catalyst have been obtained by means of liquid phase in situ ATR-IR spectroscopy. The complex datasets have been treated also taking advantage of reference materials and is further corroborated by applying advanced analysis tools, such as concentration modulation experiments and multivariate curve reconstruction. Preliminary results concerning the reaction will be discussed too.
A valuable contribution to this project would result from the quantitative evaluation of the catalytic

performances of the designed catalysts compared to ones of a reference, since only qualitative data are presently available.

[1] M. Aresta, A. Dibenedetto and A. Angelini, Chem. Rev., 2014, 114, 1709–1742.
[2] K. Tomishige, Y. Ikeda, T. Sakaihori, K. Fujimoto, J. Catal., 2000, 192, 355–362.

Position:

Postdoc

Poster session / **114**

Bragg coherent diffractive imaging of one-dimensional topological strings in multiferroic barium hexaferrite nanocrystals

Authors: Dmitry Karpov[1] ; Edwin Fohtung[2]

[1] *PSI - Paul Scherrer Institut*

[2] *Rensselaer Polytechnic Institute*

Studies of topological strings is important both for condensed matter physics and cosmology, where they share the universality class with cosmic strings. Until recently these studies were bound to the surface phenomena or to destructive studies where layers of material were removed and imaged, thus preventing researchers to look into time-dependent behavior. We combined group-theoretical analysis, first-principle density functional calculations, Landau phase-field theory and Bragg coherent diffractive imaging technique at synchrotron light source to visualize and interpret three-dimensional distribution of topological strings in barium hexaferrite nanoparticle under applied external electric field. We expect that our results will be used in future experiments on topological defects in many condensed matter systems where volumetric information is of critical importance.

Position:

Postdoc

Poster session / **77**

Spin uctuation induced Weyl semimetal state in the paramagnetic phase of EuCd2As2

Author: J.-Z. Ma[1]

Co-authors: J. Jandke [1] ; T. Shang [2] ; M. Medarde [3] ; J. Mesot [1] ; Y. G. Shi [4] ; T. Qian [4] ; H. Ding [4] ; C. Mudry [5] ; M. Müller [5] ; M. Shi [1]

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Weyl fermions as emergent quasiparticles can arise in Weyl semimetals (WSMs) in which the energy bands are nondegenerate, resulting from inversion or time-reversal symmetry breaking. Nevertheless, experimental evidence for magnetically induced WSMs is scarce. Here, using photoemission spectroscopy, we observe that the degeneracy of Bloch bands is already lifted in the paramagnetic phase of EuCd2As2. We attribute this effect to the itinerant electrons experiencing quasi-static and

quasi long-range ferromagnetic fluctuations. Moreover, the spin nondegenerate band structure harbors a pair of ideal Weyl nodes near the Fermi level. Hence, we show that long-range magnetic order and the spontaneous breaking of time-reversal symmetry are not essential requirements for WSM states in centrosymmetric systems and that WSM states can emerge in a wider range of condensed matter systems than previously thought.

Position:

Postdoc

Poster session / 81

Switching a cryo-memory cell in less than half a picosecond

Author: Jan Ravnik[1]

Co-authors: Igor Vaskivskyi [2] ; Yaroslav Gerasimenko [2] ; Michele Diego [2] ; Jaka Vodeb [2] ; Yevhenii Vaskivskyi [2] ; Anze Mraz [2] ; Tomaz Mertelj [2] ; Viktor Kabanov [2] ; Dragan Mihailovic [2]

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Cryo-cooled supercomputers and quantum computation are prospective directions of IT development, which both face the same barrier: No high-performance storage memory is available for low-temperature operation. A promising candidate for a future ultrafast memory device is the layered transition metal dichalcogenide 1T-TaS2, which has undergone a recent resurgence of interest with the discovery of a topologically protected stable hidden state [1]. We performed three pulse write-pump-probe experiments and have directly measured the time evolution of the hidden state after the crystal is hit by a laser pulse [2]. In addition, multiple fluence dependent (optical pump-probe and scanning tunnelling microscopy) switching experiments at different temperatures show us a time-resolved phase diagram of the hidden state. We find that the phonon frequency changes in about one oscillation period (~400 fs), making the material the fastest known switching device. The switching is controllably reproducible and the threshold switching fluence is constant at all temperatures, suggesting that only a sufficient number of induced carriers is important for the transition. The material is of great technological interest especially due to the easy readout of the hidden state, as its resistivity is up to three orders of magnitude lower than that of the virgin state.

[1] L. Stojchevska, et al.; Ultrafast Switching to a Stable Hidden Quantum State in an Electronic Crystal. Science 344, 177 (2014) https://doi.org/10.1126/science.1241591
[2] J. Ravnik, et al.; Real-time observation of the coherent transition to a metastable emergent state in 1T-TaS2. Physical Review B 97, 075304 (2018)
https://doi.org/10.1103/PhysRevB.97.075304

Position:

Postdoc

Flash talks / 93

Direct correlation between magnetic field and cycloidal rotation on CoCr2O4 and Ge doped CoCr2O4

Author: Nazaret Ortiz[1]

Co-authors: Sergii Parchenko ; José Renato Linares Mardegan ; Michael Porer ; E Schierle [2] ; E Weschke [2] ; Milan Radovic [3] ; Urs Staub [3]

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[3] *Paul Scherrer Institut*

The large interest from the scientist community on the magnetoelectric multiferroics comes, mostly, from the technological prospects on those [1,2]. Especially, the type II multiferroics, where the magnetic order drives the electric polarization, being both order parameters strongly correlated. The strong correlation gives the possibility of switching the magnetization by electric field or vice versa. This can be understood as low energy consumption, more energetically efficient and faster-switching devices.

CoCr2O4 (CCO), type II multiferroic, is one of the few magnetoelectric multiferroics which exhibits a transversal conical magnetic structure, giving as a result of a net polarization and magnetization [3]. Here, we present a study using soft x-ray scattering under high and low magnetic fields, to characterize a Ge doped CCO compound, to compare with pure CCO and follow their conical order of the multiferroic phase under high magnetic fields. We report the unexpected control of the spin spiral direction, and as a consequence the polarization direction, via the field cooling process. This effect is observed in Ge-CCO as in CCO. In addition, the (qq0) magnetic modulation vector of Ge-CCO presents a double feature with opposite sign, which may describe a scenario of multiple spiral sublattices.

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[1] N. A. Spaldin et al., “The Renaissance of Magnetoelectric Multiferroics, Science”, vol. 309, 391-392 (2005).
[2] M. Fiebig, et al., ‘’The evolution of multiferroics’’, Nature Reviews Materials, vol.1, p. 16046, 2016.
[3] Y. Yamasaki et al., Magnetic Reversal of the Ferroelectric Polarization in a Multiferroic Spinel Oxide. Phys.Rev. Lett. 96, 207204 (2006).

Position:

Phd

Flash talks / 96

Laser induced magnetization dynamics in antiferromagnetically coupled ferromagnetic thin films

Authors: Jingyuan Zhou[1] ; Susmita Saha[2] ; Zhaochu Luo[3] ; Eugenie Kirk[4] ; valerio scagnoli[5] ; Laura Heyderman[6]

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Combining magnetic thin films such that two ferromagnetic layers couple antiferromagnetically via a nonmagnetic spacer layer lead to the discovery of new physical properties, such as the giant magnetoresistance effect [1], that are not present in bulk materials. In addition, the magnetization dynamics in these multilayer films are modified by the interlayer coupling [2]. Such systems are proposed to support a nonreciprocal spin-wave dispersion and achieve the unidirectional propagation of spin waves [3]. As a first step to ascertain the spin-wave nonreciprocity in such systems, we have measured the uniform precessional dynamics in a series of antiferromagnetically coupled CoFeB/Ru/CoFeB trilayer films using time-resolved magneto-optical Kerr effect (TRMOKE). We have observed both the acoustic and optical modes, together with a transient mode that is caused by laser induced decoupling between the two ferromagnetic layers. In order to quantitatively explain our observation, we calculated the precessional dynamics expected in our trilayer films based on the Landau-Lifshitz equation. We found, in agreement with the experimental observation, three different field regions where the frequency relation between the three modes are qualitatively different. Such distinct responses are the results of the competition between the interlayer coupling and Zeeman energy.

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[1] G Binasch, P Grünberg, et al. Phys. Rev. B 39.7 4828 (1989)
[2] Z Zhang, et al. Phys. Rev. B 50,6094 (1994)
[3] K Di, et al. Sci. Rep. 5 10153 (2015)

Position:

Phd

Flash talks / 116

Reversible magnetoelectric switching by electrochemical lithium intercalation

Authors: Gesara Bimashofer[None] ; Jochen Stahn[1]

[1] *PSI*

Manganese based perovskites (“maganites”) of the composition A1-xBxMnO3 appear in various electronic and magnetic phases, with features like colossal magnetoresistance. Those phases are composition and temperature dependent as shown in complex phase diagrams. The complexity of this system originates from competition between order mechanisms, magnetic interactions and structural aspects. The macroscopic phase diagram is believed to be an overlap of small phases where the disorder that is induced by the distribution of A3+ and B2+ and the ratio of Mn3+/Mn4+ results in local variation of the mechanisms mentioned earlier. During this project, we want to cross magnetic phase boundaries reversibly by chemical doping and monitor the process in-situ. To achieve this, we want to use electrochemical lithium intercalation and de-intercalation. The material of choice is La1-xSrx MnO3 (LSMO) where Lithium would replace part of lanthanum or strontium. At a composition of 50% strontium and at room temperature LSMO shows a phase transition between ferro- and paramagnetism. It is believed that one could switch between those magnetic states by lithium inter- and de-intercalation. Furthermore, the in-situ measurements are carried out using polarized neutron reflectometry (PNR) and resonant X-ray techniques as well as elechtrochemical characterization. With PNR, we investigate the distribution of the Lithium and the magnetic induction profile. Another goal is to relate these phenomena to the Mn3+/Mn4+ ratio. Because the process should be reversible we want to investigate the same sample in various states along the phase transition border using various methods and connect the different appearing phenomena as mentioned above to each other.

Position:

Phd

Flash talks / 85

Anomalous magnetotransport in materials with strongly anisotropic Fermi surfaces

Author: Zhi Jian Daniel Tay[1]

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Recent experiments probing the magnetic-field dependence of the resistivity $\rho(H)$ of selected charge-density-wave (CDW) materials including GdSi, Cr, $SrAl_4$, $NbSe_3$ and $(PO_2)_4(WO_3)_{2m}$ etc, revealed a linear-in-H variation of $\rho(H)$ at low fields and at temperatures below the CDW transition [1]. The classical theory of magnetoresistance (MR), based on Boltzmann’s transport theory [2], however, predicts a quadratic-in-H variation of $\rho(H)$ at low fields. Attempts to adapt existing models involving, e.g., the linear dispersion of Dirac cones [3] failed to predict the observed $\rho(H)$ feature.

In this talk, we outline a simple 2D model which predicts the linear variation of $\rho(H)$ to arise from a strongly anisotropic Fermi surface [4] here assumed to consist of a rectangular cross section with rounded corners. This is an extension of Pippard’s original model [2] where the corners are 90° angles. Our model considers that the corner regions may adopt light or heavy effective masses. While both variants of the model invariably reproduce the linear MR in low fields, the model predicts a saturating longitudinal MR and a nonzero Hall resistance for the “light-corner” variant but the opposite

for the "heavy-corner" variant. New forthcoming experiments are expected to further improve the understanding of this intriguing feature of CDW materials.

[1] Y. Feng et al. "Linear magnetoresistance in the low-field limit in density-wave materials", Proc. Natl. Acad. Sci. 116, 11201 (2019).
[2] A. B. Pippard, Magnetoresistance in metals, Vol. 2 (Cambridge University Press, Cambridge, 1989).
[3] A. A. Abrikosov, "Quantum linear magnetoresistance", Europhys. Lett. 49 789 (2000).
[4] L. Zou, S. Lederer, and T. Senthil, "Theory of anomalous magnetotransport from mass anisotropy", Phys. Rev. B 95 245135 (2017).

Position:

Phd

Flash talks / **102**

A quantum liquid of magnetic octupoles on the pyrochlore lattice

Author: Victor Porée[1]

Co-authors: Nicolas Gauthier [2] ; Elsa Lhotel [3] ; Sylvain Petit [4] ; Vladimir Pomjakushin [1] ; Jacques Ollivier [5] ; Russell A. Ewings [6] ; Toby G. Perring [6] ; Clemens Ritter [5] ; Thomas Hansen [5] ; Andrew Wildes [5] ; David A. Keen [6] ; Gøran J. Nilsen [6] ; Lukas Keller [1] ; Tom Fennell [1] ; Romain Sibille [1]

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The search for spin liquid ground states in frustrated magnets has held a considerable place in condensed matter physics over the last decades as it represents a large playground for both theoreticians and experimentalists [1-3].
Quantum Spin Liquids (QSLs) have been and still are of particular interest as they evade long-range magnetic order down to zero temperature, being instead characterized by emergent gauge fields and fractionalized quasiparticle excitations [4-6].
The Ce2Sn2O7 pyrochlore stands as a serious candidate for the realization of a special type of QSL – the octupolar quantum spin ice [7].
Using macroscopic as well as microscopic probes, the dipolar-octupolar nature of the degrees of freedom was found. This led to substantial efforts aiming at isolating and characterizing the type of correlations developing below 1 Kelvin in Ce2Sn2O7, the results demonstrating that a quantum liquid of magnetic octupoles forms, in agreement with the octupolar quantum spin ice scenario.

[1] - J. Villain, Insulating Spin Glasses, Z. Physik B 33,31-42 (1979).
[2] - P.W. Anderson, The Resonating Valence Bond State in La2CuO4 and Superconductivity, Science, Vol. 235, Issue 4793, pp. 1196-1198 (1987) .
[3] - L. Balents, Spin Liquids in frustrated magnets, Nature volume 464, pages 199–208 (2010).
[4] - O. Benton & al., Seeing the light: Experimental signatures of emergent electromagnetism in a quantum spin ice, Physical Review B 86, 075154 (2012).
[5] - S. Lee & al., Generic quantum spin ice, Physical Review B 86, 104412 (2012).
[6] - M.J.P. Gingras and P.A. McClarty, Quantum spin ice: a search for gapless quantum spin liquids in pyrochlore magnets, Report on Progress in Physics. 77 056501 (2014).
[7] - R. Sibille & al., Candidate Quantum Spin Liquid in the Ce3+ Pyrochlore Stannate Ce2Sn2O7, Physical Review L 115, 097202 (2015).

Position:

Phd

Flash talks / 97

Elucidation of the complex (de-)lithiation reactions of SnO_2 in all-solid-state battery using operando X-ray photoelectron spectroscopy

Authors: Marta Mirolo[1] ; Xiaohan Wu[2] ; Carlos Vaz[3] ; Petr Novák[3] ; Mario El Kazzi[3]

[1] *PSI - Paul Scherrer Institut*

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[3] *Paul Scherrer Institut*

For the successful employment of Li-ion batteries at large scale, e.g. for electrical vehicles or stationary energy storage, a crucial point is to increase of energy density in the battery. In order to increase this parameter, anode conversion-alloy materials, such as SnO_2 with a specific capacity of ~ 1500 mAh/g, are a serious choice, in particular when mixed with graphite. Despite the theoretical predictions of the different SnO_2 conversion and alloy reactions during (de-)lithiation, the experimental identification of those electrochemical reactions and the formation of intermediate species (e.g. Li_aSnO_b, Li_xSn and Li_2O) is not fully understood,[1] mainly due to their possible relaxation and conversion to other byproducts during disassembling of the cycled cell in *post mortem* analysis.[2] In this contribution we explore the capabilities of our recently developed *operando* X-ray photoelectron spectroscopy (o-XPS) to monitor in real time the evolution of the electrolyte-electrode interface and the (de-)lithiation processes of the active materials during solid state Li-ion battery operation.[3] In particular, we present the results of our study on the (de-)lithiation of the SnO_2 particles in a working electrode composed of SnO_2 nanoparticles, $(Li_2S)_3$-P_2S_5 (LPS)[4] solid electrolyte (SE) and Super P as conductive carbon cycled versus $InLi_x$ counter electrode (Figure 1a). The analysis of the Sn 3d (Figure 1b), Sn 4d, O 1s (Figure 1c) and Li 1s spectra reveals the progressive conversion of the SnO_2 particles to form Sn^0 and the simultaneous formation of the Li_xSn alloy. When the potential is below 0.4 V (vs. Li^+/Li), the Li_2O phase is formed and grows until the full lithiation at 0.01 V (vs. Li^+/Li), where the only species observed are Li_2O and Li_xSn. During the de-lithiation process, the partial reversibility of the conversion-alloy reactions takes place, where Li_xSn is converted to SnO_x at 2.5 V (vs. Li+/Li). The S 2p and P 2p core levels reveal the presence of reduced Li_2S byproduct species below 1.6 V (vs. Li+/Li), in accordance with previous studies.[4]

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[1] Y. Cheng, A. Nie, L.-Y. Gan, Q. Zhang, U. Schwingenschlögi, *J. Mater. Chem. A*, **2015**, 3, 19483
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[3] X. Wu, C. Villevieille, P. Novák, M. El Kazzi, *Phys. Chem. Chem. Phys.*, **2018**, 20, 11123
[4] X. Wu, M. El Kazzi, C. Villevieille, *J. Electroceram.*, **2017**, 38, 207-214

Position:

Phd

Flash talks / **71**

Epitaxial growth and electrical control of antiferromagnetic materials

Author: Zhentao Liu[1]

Co-authors: Charles-Henri Lambert [2] ; Zhaochu Luo [1] ; Benjamin Jacot [2] ; Laura Heyderman [1] ; Pietro Gambardella [2] ; Aleš Hrabec [1]

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Having the advantages of immunity to external magnetic fields and fast spin dynamics, antiferromagnetic materials open a new door towards the next generation of high-speed data storage devices. Here, we optimized the growth condition of epitaxial Mn2Au and NiO films, an antiferromagnetic metal and an insulator film, which can be controlled electrically with two different spin-orbit torque mechanisms [Ref.1, ref.2]. The materials are consequently patterned into star shaped devices for electrical switching measurements. Due to current-induced switching of Neel vectors, we observe a change of Anisotropic Magnetoresistance (AMR). This Neel vector switching offers a platform to investigate magnetization dynamics in antiferromagnetic materials.

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[1] J. Železný et al., Phys. Rev. Lett. 113, 157201 (2014)
[2] X. Z. Chen et al., Phys. Rev. Lett. 120, 207204 (2018)

Position:

Phd

Flash talks / **84**

Strain Induced Ferroelectricity in Orthorhombic REFeO3 Thin Films

Author: Banani Biswas[1]

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The search for materials being simultaneously ferroelectric and magnetic, ideally at room temperature, gained interest about a decade ago for its potential applications in energy efficient electronic devices [1]. Materials in which magnetic order induces ferroelectric order, also called multiferroics, are of interest because of their typically strong magnetoelectric coupling [2], such as orthorhombic REMnO3. Orthorhombic bulk REFeO3 has a similar crystal structure like REMnO3 and is expected to show similar physical properties. Theoretical calculations for bulk REFeO3 have shown that this class of materials can gain a large electrical polarization of up to 90 μC/cm2 at RT under large lattice misfit strain [3]. To verify the theoretical predictions, we are growing orthorhombic REFeO3 thin films on different single crystalline substrates using pulse laser deposition. We are using X-ray diffraction (XRD) for crystal structure analysis, for magnetic measurements a superconducting quantum interface device (SQUID), and to measure the electrical polarization a have a home-build Tower-Sawyer set-up. The films we have investigated so far are epitaxially grown (010) oriented DyFeO3 on (010) YAlO3 substrates. All films show ferromagnetic and antiferromagnetic properties and in some films we have been able to induce ferroelectricity at low temperatures.

Position:

Phd

Flash talks / **111**

Exploring the electron transfer at cuprate/manganite interfaces

Author: Roxana Gaina[None]

Co-authors: Claude Monney [1] ; Christof Niedermayer [2] ; Christian Bernhard [3] ; Edith Perret [4]

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The interface effects in cuprate/manganite multilayers are the subject of many studies, which are focused not only on superconducting properties of antagonistic YBa2Cu3O7(YBCO), but also on its magnetic and electronic properties. In this study we will present our last investigations that proved that in Nd1-x(Ca1-ySry)xMnO3/YBCO/NCSMO (NYN) trilayers, the interfacial electron transfer and the orbital reconstruction of the interfacial Cu ions depend significantly on hole doping x, strontium ratio y, and the subsequent charge/orbital order of the manganite. Driven by the chemical potential difference between NCSMO and YBCO, this interface phenomena can potentially lead to combined superconducting/charge-ordered quantum states in YBCO that can be adjusted via manganite layers and external control parameters like magnetic field or photons.

Position:

Phd

Flash talks / **136**

Evolution of a skyrmion-like state in antiferromagnetic spinel MnSc2S4

Author: Guratinder Kaur[1]

Co-author: Zaharko Zaharko Oksana

[1] *PhD student*

MnSc2S4, a magnetically frustrated thiospinel with Mn forming a diamond lattice, shows multistep long-range ordering as a function of applied field, H and temperature, T [1]. We used neutron scattering to map the H(T), T(K) phase boundaries of the triple-k state for the magnetic field applied along (111) and (110) crystallographic directions and Monte Carlo simulations to examine the additional terms in the spin Hamiltonian, e.g. single ion anisotropy and exchange anisotropy that stabilize this fractional skyrmion topological state.
[1] S. Gao, O. Zaharko, V. Tsurkan, et al. Nature Physics,13,157–161 (2016).

Position:

Phd

Flash talks / **60**

In operando X-ray diffraction during laser 3D printing

Authors: Samy Hocine[1] ; Helena Van Swygenhoven[1] ; Steven Van Petegem[2] ; Cynthia Sin Ting Chang[2] ; Tuerdi Maimaitiyili[2] ; Gemma Tinti[2] ; Dario Ferreira Sanchez[2] ; Daniel Grolimund[2] ; Nicola Pietro Maria Casati[2]

[1] *PSI - EPFL*

[2] *Paul Scherrer Institut*

Selective Laser Melting (SLM) is a well-known process category in Additive Manufacturing in which thermal energy selectively fuses regions of a powder bed. To investigate process parameters for metallic materials in-situ with synchroton X-rays, a miniaturized SLM device has been developped at PSI. The design of the miniaturized SLM device is determined by the requirements for X-ray access and implementability at different beamlines of synchrotron light sources. First in situ X-ray diffraction tests were performed successfully on Ti-6Al-4V samples at the MicroXAS and MS beamlines, located at the Swiss Light Source. By varying the laser power, scanning speed and hatch distance, various energy densities are obtained. The dynamics of the alpha and beta phases during fast heating and solidification are tracked with a time resolution of 50ms. This allows investigating the heating and cooling rates, and the size and shape of the heat affected zone.

Position:

Phd

Flash talks / **118**

Spin Hamiltonian and Dimensionality in (Ba,Sr)CuSi2O6

Authors: Stephan Allenspach[None] ; Pascal Puphal[1] ; Alun Biffin[2] ; Jakob Lass[None] ; Christof Niedermayer[3] ; Gregory Tucker[4] ; Maciej Bartkowiak[5] ; Alsu Gazizulina[5] ; Xinzhi Liu[5] ; Oleksandr Prokhnenko[5] ; Bruce Normand[3] ; Nicolas Laflorencie[6] ; Frédéric Mila[7] ; Ekaterina Pomjakushina[8] ; Christian Rüegg[3]

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The quantum magnet BaCuSi2O6, consisting of stacked spin dimer bilayers, undergoes an anomalous dimensional reduction from 3D to 2D close to the quantum critical point [1]. Mechanisms for this dimensional reduction were proposed based on inter-bilayer frustration resulting from an antiferromagnetic intra-bilayer exchange. Ab initio calculations propose a ferromagnetic intra-bilayer exchange rendering such a frustration impossible [2].
In addition to previous measurements of BaCuSi2O6, we have performed neutron spectroscopy on the child compound Ba0.9Sr0.1CuSi2O6 [3] using the cutting-edge neutron spectrometer CAMEA at PSI. Furthermore, we have measured the phase boundary of the Bose Einstein Condensate phase in BaCuSi2O6, which has a lower critical magnetic field of 23.15T, using neutron diffraction under extreme conditions on HFM/EXED at HZB.
Our results suggest ferromagnetic intra-bilayer exchanges with at least three different dimer types in BaCuSi2O6 and only one dimer type in Ba0.9Sr0.1CuSi2O2. We conclude that the existence of different dimer types in BaCuSi2O6 might lead to the observed quasi 2D behavior.

[1] C. E. Sebastian et al., Nature 441, 617 (2006).
[2] V. V. Mazurenko et al., PRL 112, 107202 (2014).
[3] P. Puphal et al., PRB 93, 174121 (2016).

Position:

Phd

Facilities / **1**

X-radiation from fourth-generation storage rings

Synchrotron light is characterized by its high spectral intensity, small source size, and low divergence, encapsulated in the figure of merit known as 'brilliance'. The next generation of synchrotrons, called 'diffraction-limited storage rings' (DLSRs) promises reductions in the source size and divergence that should combine to improve the brilliance by up to two orders of magnitude. In this talk, I will provide a didactic overview of the machine physics that has allowed this development and how this impacts on synchrotron science, in particular with emphasis on the science envisaged at the SLS after completion of its upgrade in 2025."

Contributed talks / **107**

Universal quantum computing with rare-earth ions

Author: Manuel Grimm[1]

Co-authors: Adrian Beckert [1] ; Gabriel Aeppli [1] ; Markus Müller [1]

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For certain computationally hard problems, quantum computers have a huge speedup advantage compared to their classical counterparts and their successful implementation may lead to drastic advances solid state physics, quantum chemistry and biomedicine, among others.

In this presentation I discuss why rare-earth compounds might be ideal candidates for solid state quantum computation. I address the challenge to realize long-lived, coherent quantum memories, and efficient ways to unprotect those qubits and realize high fidelity gates between them.

Position:

Phd

Contributed talks / 99

Why does a diluted beryllium alloy exhibit a hundred-fold increase in T_c?

Authors: T. Shiroka[1] ; T. Shang[1] ; A. Amon[2] ; D. Kasinathan[2] ; W. Xie[3] ; M. Bobnar[2] ; Y. Chen[3] ; A. Wang[3] ; M. Shi[1] ; M. Medarde[1] ; H.-Q. Yuan[3]

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As one of the lightest elements, beryllium exhibits high-frequency lattice vibrations, a condition for achieving superconductivity (SC) with a sizeable critical temperature. Yet, paradoxically, its $T_c = 0.026$ K is so low, that its SC is often overlooked. Clearly, T_c is affected also by other factors, notably the electron-phonon coupling strength and the density of states (DOS) at the Fermi level $N(\varepsilon_{\rm F})$ (rather low in pure Be). Recently, computational searches have shown that SC is more likely to occur in p^0- and d^1 metals with low-lying empty orbitals. Their electronic properties are predicted to be highly sensitive to structural details, thus resulting in stronger electron-phonon interactions and higher $N(\varepsilon_{\rm F})$ [1]. Based on this intuition, Be-rich alloys may achieve a much higher T_c than elementary Be itself, a prediction which turns out to be true for $ReBe_{22}$, whose $T_c \sim 9.6$ K [2] exceeds by almost 400(!) times that of Be. Here, we report on an extensive study of the physical properties in the normal- and superconducting state of $ReBe_{22}$, by using a series of experimental techniques, in particular muon-spin rotation/relaxation (μSR), as well as numerical density-functional-theory (DFT) band-structure calculations [3]. Our results not only explain the origin of the formidable increase of T_c in $ReBe_{22}$, but also predict exciting developments in case of chemical substitution (of Re with Mo or W) or under high-pressure conditions.

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3. T. Shang et al., *New J. Phys.* **21**, 073034 (2019).

Position:

Scientist

Contributed talks / 87

Oxygen evolution reaction: activity vs. oxygen vacancies in PrBaCo2O5+δ

Authors: Elena Marelli[1] ; Marisa Medarde[2] ; Dino Aegerter[1] ; Dariusz Dawryluk[2] ; Ekaterina Pomjakushina[3] ; Emiliana Fabbri[2] ; Thomas Justus Schmidt[2]

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[2] *Paul Scherrer Institut*

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Cobalt-based layered perovskites have emerged as promising electrocatalysts for the oxygen evolution reaction, but important fundamental questions regarding the reaction mechanisms and the design principles for highly active perovskite electrocatalysts are still open. An important development in this sense has recently emerged in a study by Fabbri et al.[1], who demonstrated that oxygen vacancies can play a critical role in the oxygen evolution reaction mechanism and thus, on the perovskite electrochemical activity.
Double perovskite oxides, such as PrBaCo2O5+δ (PBCO) [2,3], are known to be able to incorporate a large amount of oxygen vacancies, and also to show high oxygen mobility [4-5]. These properties make them ideal candidates for oxygen evolution reaction electrocatalysis. In this work we combine high-resolution neutron and X-ray diffraction, XAS, magnetic and electrochemical analysis to understand the correlation between catalyst activity and oxygen vacancy amount and distribution.

References
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Position:

Postdoc

Contributed talks / 103

Time-Resolved Spectroscopy of Vanadia-Based SCR Catalysts under Transient Conditions

Authors: Rob Jeremiah G. Nuguid[1] ; Davide Ferri[1] ; Oliver Kröcher[1]

[1] *Paul Scherrer Institut*

Understanding the mechanisms behind chemical transformations is key to developing improved catalytic systems. In this context, operando spectroscopy has contributed to advance our molecular view of many reactions at heart of the chemical industry. Here we show the application of complementary spectroscopic techniques to elucidate the mechanism of a reaction that has always occupied a central role in emission control research – the selective catalytic reduction (SCR) of NOx over vanadia-based catalysts. IR spectroscopy revealed that NH3 could adsorb on Lewis and Brønsted-Lowry acid sites as NH3 and NH4+, respectively. Upon NO addition, the SCR reaction started and adsorbed NH3 molecules were consumed preferentially over NH4+ species, thereby suggesting that the Lewis sites are the active sites for SCR. The catalyst also reduced simultaneously as indicated by UV-Vis spectroscopy. Under reaction conditions, vanadyl species (VOx) adopt various states of coordination, as demonstrated by the width of the VOx peak in the time-resolved Raman spectra. However, only the coordinatively unsaturated species (i.e., Lewis sites) were found to be responsible for the SCR activity as their response to repeated NH3 pulses caused their characteristic

signal to appear in the phase-resolved spectra. The synergy between complementary operando techniques, demonstrated here in the particular case of SCR, opens up new possibilities in deciphering the structure-performance relationship of catalysts and other functional materials.

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Figure 1. (a) Complementarity between IR, UV-Vis, and Raman spectroscopies. (b) IR signal of adsorbed NH3 (Lewis) and NH4+ (Brønsted-Lowry) species after NO addition. (c) UV-Vis signal of V4+ species after NO addition. (d) Time-resolved and (e) phase-resolved Raman signal of the V=O stretch.

Position:

Phd

Contributed talks / **82**

RNiO3 perovskites: exploring the TMIT –> 0 limit

Authors: Yannick Maximilian Klein[1] ; Marisa Medarde[2] ; Dariusz Jakub Gawryluk[None] ; Tian Shang[3] ; Denis Cheptiakov[2] ; Lukas Keller[4] ; Nicola Pietro Maria Casati[None]

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Strongly correlated oxides can show a variety of exotic physical behaviour such as metal to insulator transitions, multiferroicity, or high-Tc superconductivity. Here we focus on RNiO3 perovskites (R = trivalent rare earth ions), one of the few transition metal oxide families to display spontaneous metal insulator transitions. Interestingly, superconductivity has been recently reported in the reduced nickelate Nd0.8Sr0.2NiO2, which constitutes the first-ever observation of this property in a Ni-based material1.
The mechanism behind the emergence of superconductivity is just as unclear as the driving force behind the MIT[2][3]. Nickelates with larger rare earth ions (Nd, Pr, LaxPr1-x ; x = 0.1 to 0.5) are candidates to probe the cause of the MIT, as lattice, electric and magnetic degrees of freedom coincide. Here we focus on the role of the lattice that we investigate in the LaxPr1-xNiO3 solid solutions, by exchanging 16O by the 18O isotope.
The presence of huge 16O-18O isotope effects was confirmed in a previous study, where T(MIT) was increased by up to 10K for 18O enriched PrNiO3[4]. The solid solutions of LaxPr1-xNiO3 exhibit an even larger 16O-18O effect in T(MIT) (~20 K), suggesting an increasingly dominant role of the lattice when T(MIT) approaches zero kelvin.
A good understanding of these spectacular and unusual findings require experiment-theory synergies, already established with colleagues from SINQ and SLS at PSI and collaborators from the NCCR MARVEL project.

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Position:

Postdoc

Contributed talks / 105

The role of chains for superconductivity inoptimally doped YBCO thin films: ARPES view

Author: Jasmin Maria Jandke[1]

Co-authors: Muntaser Naamneh [2] ; Marco Caputo [3] ; Eduardo Bonini Guedes [4] ; Yasmine Sassa [5] ; Laura Maurel Velàzquez ; Nicholas Plumb [6] ; Ming Shi [6] ; Milan Radovic [6]

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YBCO is a famous and intensively studied compound belonging to the high-temperature cuprate superconductors. It might sound boring to study such an old system. However, there are many important and unsolved problems to be clarified. For example,the electronic interaction bewteen chains and planes is not yet understood as well as the role of chains for superconductivity. One reason, why the scientific progress for Y123 stagnated in this compound, was the experimental feasibility. In contrast to the Y124 phase [1-3], which has a stable surface after the cleavage of single crystals, the Y123 phase has no natural cleavage plane [4]. As a result, electronic reconstruction occurs and drives the system out of the polar catastrophe scenario [5], leaving behind an overdoped surface. Thus, the optimally doped compound is not accessible in this way.Significant progress was done by Y. Sassa et al., who were able to overcome the polar catastrophe problem and could grew Y123 films for the first time by using a suitable substrate underneath [6,7]. We were now able to optimize the Y123 film growth and could stabilize the nearly optimally doped Ortho-I phase of Y123. In contrast to previous experiments [8-10], the absence of band foldings enables the precise angle-dependent measurement of the chains and planes separately. We find a clear d-wave superconducting gap on the planes, whereas the chains are isotropically gapped. Beeing able to track signals coming from the chains and planes separately, this paths the way for future experiments which could give the additional piece of information to understand superconductivity and/or the role of chains for superconductivity in HTSC cuprates.

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Position:

Postdoc

Contributed talks / 109

Coherent lattice dynamics in LiNbO3 induced by mid infrared laser driven ferroelectric polarization switching

Author: Mathias Sander[1]

Co-authors: Urs Staub [2] ; Roman Mankowsky ; Henrik Till Lemke ; Paul Beaud [2]

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Ferroelectric materials are considered interesting candidates for non-volatile data storage showing below Curie temperature, a macroscopic electric polarization by shifts of oppositely charged ions due to a structural phase transition. Resonant large-amplitude excitation of a polar vibrational mode was recently shown to transiently reverse the ferroelectric polarization of LiNbO3, possibly driven by anharmonic coupling to the ferroelectric mode 1. We have performed fs x-ray diffraction experiments at the swissFEL bernina endstation to investigate accompanied lattice dynamics. The excitation of a LiNbO3 crystal with mid infrared laser pulses triggered coherent lattice dynamics and a long lived shift of the -3-3-6 diffraction peak, depicted in figure 1a,b. Detailed simulations of the induced structure factor change and the triggered lattice dynamics are part of ongoing discussions to pave the way towards the use of LiNbO3 as transducer for the utlrafast control of functional properties in heterostructures.

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1 R. Mankowsky et al., Phys. Rev. Lett. 118, 197601 (2017)

Position:

Postdoc

Contributed talks / 120

Manipulating the ground state in nickelates using proximity with magnetic layers

Author: Marco Caputo[1]

Co-authors: Zoran Ristic [2] ; Dhaka Rajej [3] ; Tanmoy Das [4] ; Kim Hongwon [5] ; Jasmin Maria Jandke [1] ; Eduardo Bonini Guedes [6] ; Muntaser Naamneh [7] ; Nicholas Plumb [8] ; Jan Hugo Dil [8] ; Ming Shi [8] ; Joel Mesot [8] ; Marisa medarde [8] ; Cinthia Piamonteze [8] ; Milan Radovic [8]

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[8] *Paul Scherrer Institut*

Transition metal oxides (TMO) are a class of materials where the charge, orbital, magnetic, and spin degrees of freedom are mutually connected. Interfacing different TMOs offers the possibility to act on each of these degrees of freedom, tailoring new materials with desired properties. In this talk, I will show the effect of the presence of a magnetic proximity layer on the ground state of

neodymium nickelate (NNO) interfacing thin NNO films with ferro- and antiferromagnetic manganite layers (strontium doped lanthanum manganite – LSMO) grown via pulsed laser deposition (PLD). Angle resolved photoemission spectroscopy (ARPES) and X-ray magnetic circular dichroism (XMCD), supported by momentum-resolved density fluctuation (MRDF) theory, revealed the suppression of the PM metal – AFM insulator transition in NNO thin films, and the emergence of a new FM metal ground state. This work paves the way for tailoring magnetic properties in different oxides, where already existing magnetic ordering can be tuned using proximity effects.

Position:

Postdoc

Contributed talks / 75

3D Imaging of Advanced Materials using Soft X-ray Laminography at PolLux

Author: Katharina Witte[1]

Co-authors: Andreas Späth [2] ; Simone Finizio [1] ; Claire Donnelly [3] ; Michal Odstrcil [4] ; Manuel Guizar Sicairos [5] ; Mirko Holler [5] ; Benjamin Watts [1] ; Rainer Fink [2] ; Jörg Raabe [1]

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The 3D imaging techniques based on hard X-ray radiation like computed tomography (CT) are commonly used to reveal the inner structure of sophisticated materials and complex objects. Although hard X-ray CT was invented more than 45 years ago1, the use of soft X-rays in 3D imaging is still an exception so far[2], even though soft X-ray radiation involve some advantages in terms of chemical sensitivity and contrast properties[3-6].
We will present the new Soft X-ray Laminography (SoXL) setup implemented at the PolLux beamline going from 2D scanning transmission X-ray microscopy (STXM) to 3D imaging. In addition to a detailed introduction to the new setup, examples of already successful SoXL experiments from various research fields will also be shown. The realization of SoXL at PolLux is based on the fruitful collaboration of different research groups from SLS and their experience concerning 3D imaging. The emphasis of this presentation will be to advertise SoXL to a broader community within PSI and to reach potential users for futures projects.

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Position:

Postdoc

Contributed talks / 89

Visualization of engineered residual strain in additive manufacturing materials by Bragg Edge neutron imaging

Authors: Chiara Carminati[1] ; Efthymios Polatidis[2] ; Manuel Morgano[3] ; Markus Strobl[3] ; Nikola Kalentics[4] ; Robin Woracek[5] ; Roland Loge[4] ; Takenao Shinohara[6] ; Tuerdi Maimaitiyili[3]

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Additive Manufacturing is a quickly developing set of technologies that is revolutionising the manufacturing industry worldwide (by, for example, greatly reducing the number, weight and cost of parts of a finished product and by allowing the manufacture of complex shapes), despite a number of still open problems, such as the introduction of residual tensile stress (in particular on the surface regions of Selective Laser Melting (SLM) produced parts) limiting the fatigue and chemical resistance and causing deformation and cracks.
A post-process technique that has been shown to limit and even counteract this effect is Laser Shock Peening (LSP), which can introduce compressive stress in the surface region of metals through the application of repeated concussive shockwaves using a laser.
Bragg-edge neutron imaging is particularly well suited for investigating the effect of such treatment because it can probe several centimeters of relevant engineering material (such as steel and Nickel) and map with ~100 um spatial resolution the strain state of a finished product. Such technique is here applied to LSP-treated 316L additively manufactured steel samples and the resulting strain field is retrieved and visualized using a specifically design data treatment algorithm.
We therefore demonstrate that the effects of LSP can be successfully mapped with Bragg Edge imaging and we find that its effect reaches down to 200 micrometer, with even the introduction at the surface of a beneficial compressive stress.
After such proof-of-concept measurement demonstrated the usefulness of neutron imaging for additive manufacturing, the natural follow up is to utilize the acquired know-how to optimize the parameters of LSP to achieve the desired strain state depending on the application.

Position:

Scientist

Contributed talks / 115

Neutron imaging of electrochemical energy converters

Author: Pierre Boillat[1]

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To address climate change, air pollution and other environmental issues, as well as our critical dependence on fossil fuels, a profound transformation of the energy landscape is required. This transformation has already begun, at least in given countries, with the rapidly increasing share of renewables in electricity production, as well as the growing popularity of electrification in mobility. However, important challenges remain, such as the long term storage of electrical energy. Electrochemical energy converters can play a significant role in solving this issue, as they build a bridge between the renewable production in form of electricity and the low cost storage in form of hydrogen.
Here, different challenges faced in the understanding of electrochemical systems (fuel cells, electrolysers and batteries) will be presented. The way neutron imaging has been used in the past – at PSI and elsewhere – to address these challenges will be discussed, as well as the applications made possible by advanced measurement modalities such as dark field and energy selective imaging. A particular attention will be given to the opportunities opened by the sensitivity of the cross section to molecular motions of hydrogen compounds, in relation with the inelastic scattering of neutrons: this effect has already been used to distinguish between liquid water and ice, and several further possibilities can be considered. Finally, the possibilities of collaborations within the neutron scattering community in the analysis of imaging measurements with advanced modalities will be discussed.

Position:

Scientist

Contributed talks / 74

Tunable Berry Curvature Effects Through Volume-wise Magnetic Competition in a Topological Kagome Magnet Co3Sn2S2

Author: Zurab Guguchia[1]

Co-authors: Joel Verezhak [1] ; Dariusz Gawryluk [2] ; Stepan Tsirkin [3] ; Jiaxin Yin [4] ; Ilya Belopolski [4] ; Huibin Zhou [5] ; Gediminas Simutis [1] ; Songtian Zhang [4] ; Tyler Cochran [4] ; Guoqing Chang [4] ; Ekaterina Pomjakushina [6] ; Lukas Keller [7] ; Z Skrzeczkowska [6] ; Q Wang [8] ; Hechang Lei [8] ; Rustem Khasanov [1] ; Alex Amato [1] ; Shuang Jia [9] ; Titus Neupert [10] ; Hubertus Luetkens [1] ; Zahid Hasan [4]

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[10] *Department of Physics, University of Z¨urich, Winterthurerstrasse 190, Zurich, Switzerland*

Magnetic topological phases of quantum matter are an emerging frontier in physics and material science. Along these lines, several kagome magnets have appeared as the most promising platforms.

However, the magnetic nature of these materials in the presence of topological state remains an unsolved issue. Here, we explore magnetic correlations in the kagome magnet $Co_3Sn_2S_2$. Using muon spin-rotation, we present evidence for competing magnetic orders in the kagome lattice of this compound. Our results show that while the sample exhibits an out-of-plane ferromagnetic ground state, an in-plane antiferromagnetic state appears at temperatures above 90 K, eventually attaining a volume fraction of 80% around 170 K, before reaching a non-magnetic state (Fig. 1a). Strikingly, the reduction of the anomalous Hall conductivity above 90 K linearly follows the disappearance of the volume fraction of the ferromagnetic state (Fig. 1b-d). We further show that the competition of these magnetic phases is tunable through applying either an external magnetic field or hydrostatic pressure. Our results taken together suggest the thermal and quantum tuning of Berry curvature field via external tuning of magnetic order. Our study shows that $Co_3Sn_2S_2$ is a rare example where the magnetic competition drives the thermodynamic evolution of the Berry curvature field, thus tuning its topological state.

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1 Z. Guguchia et. al., arXiv:1904.09353 (2019).

Position:

Scientist

Contributed talks / 68

Fluctuations in a magnetic metamaterial

Authors: Sandra Helen Skjaervoe[1] ; Valerio Scagnoli[2] ; Oles Sendetskyi[2] ; Naëmi Leo[3] ; Claudio Mazzoli[4] ; Peter Derlet[5] ; Laura Heyderman[2]

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[5] *Paul Scherrer Institut*

In recent years, artificial spin systems, consisting of elongated single-domain ferromagnetic nanomagnets placed on the nodes of two-dimensional lattices and coupled via their dipolar fields, have been used to address open questions in frustrated magnetism. However, the imaging techniques so far used, are severely constrained in terms of temporal and spatial resolution. Using soft resonant x-ray scattering [1,2] we measure magnetic fluctuations in square artificial spin ice (Fig. 1), known to order antiferromagnetically, providing information about the magnetic domain structure evolution beyond what state-of-the-art imaging techniques can. Glassy dynamics were reported in recent experiments with the same technique on similar arrays in which the nanomagnets are only weakly interacting [3], while, anomalous features in the dynamics for long time lags were seen in another similar study on strongly interacting nanomagnets [4]. In particular, the latter results suggest the presence of a crossover from a ballistic to free diffusion regime in the motion of the magnetic domain boundaries. In our data across the transition, we observe re-entrant effects that are not expected for a system with glassy behaviour and two-fold rotational symmetry that has not been observed previously [4]. With further analysis of the data, we aim to identify the nature of fluctuations for our model system, which may, for example, be a result of critical or depinning dynamics.

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[4] Chen, X. M. et al. arXiv:1809.05656 [cond-mat] (2018).

Position:

Postdoc

Contributed talks / 122

Evidence of new mechanism of antiferromagnetic domain selection driven by spin-orbit coupling

Authors: D. T . Maimone[1] ; N. Gauthier[1] ; D. G. Mazzone[2] ; J. Shen[1] ; M. Bartkowiak[1] ; R. Yadav[1] ; R. Sibille[2] ; S. Raymond[3] ; C. Niedermayer[2] ; J. L. Gavilano[2] ; E. Ressouche[3] ; G. Lapertot[4] ; M. Kenzelmann[None]

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The selection and switching of magnetic domains plays a key role in modern data storage and spintronics 1. The selection of antiferromagnetic domains using magnetic fields is less straight-forward than for ferromagnetic domains, and often relies on the Zeeman interaction. Recently, another mechanism was proposed for tetragonal two-band metals featuring antiferromagnetic domains described by an ordering wave-vector k in the basal plane plane, as observed in CeCoIn5 [2]. In CeCoIn5, a spin density wave emerges in the superconducting phase with two domains k = (q,+-q,0.5) and a small rotation of the magnetic field direction around [1 0 0] is sufficient to lift the degeneracy of these two domains and provoke a switching [3]. A Zeeman-induced domain selection can be excluded as its origin, because the ordered moments are perpendicular to the field applied in the tetragonal plane. In this context, two other theories relying on the coupling of the magnetic order with the superconductivity were developed to explain the phenomenon [3,4]. In order to distinguish the different proposed theories, we studied the k-domains in Nd1-xCexCoIn5 for x=0.83 and x =0.25 in the absence of superconductivity using neutron diffraction. We observe a domain selection normal conducting states, ruling out the interpretations based on the coupling with superconductivity. This type of domain selection mechanism should be universal across multiband materials with high symmetry crystal structure displaying itinerant antiferromagnetism modulated in the basal plane. Our results emphasize the important role of spin-orbit interactions for CeCoIn5.
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Position:

Phd

Contributed talks / 72

Spin excitations in the 2D dipolar honeycomb magnet ErBr3

Author: Christian Wessler[1]

Co-authors: Michel Kenzelmann [2] ; Karl Krämer [3] ; Hans-Benjamin Braun [4] ; Bertrand Roessli [2]

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[4] *Dublin Institute for Advanced Studies / ETHZ*

The discovery of Dirac-cones in graphene and related compounds has promoted the search for magnetic Dirac materials. Candidates are the metal tri-halides $CrBr_3$ and CrI_3 which possess topological magnonic band structures [1,2].
Here we report the study of the magnetic ground-state and excitations in isostructural $ErBr_3$.
In this compound magnetic order with propagation vector $\vec{k}$=(1/3,1/3,0) was reported by neutron

diffraction in the temperature range between 50 and 290 mK [3] which has been shown to have two-dimensional (2D) character. Within a mean-field approximation, we show that the spin structure of Er^3+, shown in Fig. 1a, is explained by dipolar interactions consistent with results for a 2D honeycomb lattice [4].
We modeled the spectrum of spin wave excitations in ErBr3 within a random-phase approximation that includes the anisotropy of the crystal-field. The results are shown in Fig. 1b. Our results also show the existence of magnetic Dirac-cones at the K and K'-points in the Brillouin zone. We suggest that this is the consequence of the invariance of the magnetic vortex ground state under combined parity and time reversal symmetry [5].

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Position:

Phd

Facilities / 63

Cristallina-Q: the SwissFEL station for quantum matter in extreme conditions

Position:

45

Plenary

Database-driven discovery and first-principles characterization of novel materials

Nicola Marzari has a « Laurea » degree in Physics from the University of Trieste (1992), and a PhD in physics from the University of Cambridge (1996). He moved to the US as an NSF postdoctoral fellow (Rutgers University, 1996-98), and then as a research scientist first at the Naval Research Laboratory (1998-99) and Princeton University (1999-01). In 2001, he was named assistant professor in computational material science at the Massachusetts Institute of Technology, where he was promoted to associate professor in 2005, and named Toyota Chair of Materials Engineering in 2009. After 10 years at MIT, Nicola Marzari joined the University of Oxford, as its first Statutory (University) Professor of Materials Modelling, and as Director of the Materials Modeling Laboratory. He moved to EPFL in 2011, where he holds the Chair of Theory and Simulation of Materials, and where he directs the Swiss National Centre on Computational Design and Discovery of Novel Materials NCCR MARVEL.

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Perspective Talk

Important topics in condensed matter physics in Switzerland

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Concluding Remarks

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Technology Transfer at PSI: A benefit to scientists ?

Position:

Contributed talks / 18

ENE talk 2

Contributed talks / 19

ENE talk 3

Contributed talks / 17

ENE talk 1

6

Flowers & poster prize

Facilities / **4**

SμS talk

Facilities / **2**

Time resolved Resonant Inelastic X-ray Scattering and X-Ray Diffraction on Quantum Materials at Furka experimental station at Athos

Over the last few years Free Electrons Lasers (FEL) have developed as a powerful tool to perform ultrafast spectroscopy in the XUV, Soft- and Hard- X-ray. In this talk I will introduce the experimental endstation Furka of the soft x-ray beamline (Athos) of the SwissFEL. The Furka experimental endstation will be dedicated to time-resolved X-Ray Diffraction (tr-XRD) and to time-resolved Resonant Inelastic X-ray Scattering (tr-RIXS) experiments in the soft X-ray regime. In particular, tr-RIXS opens new scientific opportunities thanks to its unique capability to probe the energy and momentum time-evolution of elementary excitations in solids.

Facilities / **3**

SINQ talk