PAUL SCHERRER INSTITUT

PSI

2nd PSI Condensed Matter Retreat

15th & 16th November, 2017

Fachhochschule Nordwestschweiz FHNW
Campus Brugg-Windisch

Program Overview

Wednesday, 15 November 2017

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08:45	*Overview: LMN*	J. Gobrecht	
08:55	*Overview: SwissFEL*	L. Patthey	
09:10	*Overview: NUM*	C. Rüegg	
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15:00-15:40	Poster Session (odd #'s) and Coffee Break / 5.OH06

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Thursday, 16 November 2017

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Poster Session Overview

Wednesday, 15 November 2017

15:00-15:40 Poster Session and Coffee Break / 5.OH06

and

17:00-18:15 Poster Session and Prize / 5.OH06

Oral Contributions

On the importance of electric quadrupole interactions in rare-earth based frustrated magnets

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In the modelling of magnetic insulators, one often assumes only the interactions between dipolar moments. However, in f-electron systems, multipolar interactions can be of importance [1]. The multipoles correspond to magnetic dipoles, electric quadrupoles, magnetic octupoles, etc. Recent examples of multipolar interactions in frustrated magnets are found in the rare-earth pyrochlores. The effects of electric quadrupole interactions have been enlighten in Pr-based pyrochlores [2, 3]. The presence of a quadrupolar order has also been reported in off-stoichiometric $Tb_2Ti_2O_7$ [4].

We here report the effects of electric quadrupole interactions in another family of frustrated magnets, the SrR_2O_4 compounds. Their magnetic properties are dominated by rare-earth magnetic ions R that form frustrated zigzag chains [5, 6]. Neutron scattering measurements on $SrDy_2O_4$ and $SrHo_2O_4$ reveal diffuse scattering patterns that can be related to the correlations between the dipolar magnetic moments. For these two compounds, the effects of electric quadrupolar interactions appear in the excitation spectrum measured by inelastic neutron scattering.

Specifically, in $SrDy_2O_4$, a crystal-electric field level exhibits a dispersion with an energy scale that is an order of magnitude larger than the energy scale of the dipolar magnetic correlations. This observation can be explained by a large quadrupole-quadrupole coupling. This 'hidden' energy scale can exist because the Kramers ground state doublet is insensitive to quadrupolar interactions. In $SrHo_2O_4$, a complete description of the excitation spectrum also requires to consider quadrupole-quadrupole coupling. Furthermore, a direct coupling between the quadrupolar degrees of freedom and the lattice appears in the Ho analogue. This is observed by hybrid magnetoelastic modes formed from crystal-electric field levels and acoustic phonons. These results indicate the importance to consider multipolar interactions in f-electron systems, where competing multipolar interactions could lead to novel phenomena.

[1] P. Santini, *et al.*, Rev. Mod. Phys. **81**, 807 (2009).
[2] S. Onoda & Y. Tanaka, Phys. Rev. Lett. **105**, 047201 (2010).
[3] S. Petit, *et al.*, Phys. Rev. B **94**, 165153 (2016).
[4] H. Takatsu, *et al.*, Phys. Rev. Lett. **116**, 217201 (2016).
[5] A. Fennell, *et al.*, Phys. Rev. B **89**, 224511 (2014).
[6] N. Gauthier, *et al.*, Phys. Rev. B **95**, 134430 (2017).

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$LiY_{1-x}Ho_xF_4$ - a candidate material for the implementation of solid state qubits

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The model magnet $LiY_{1-x}Ho_xF_4$ has been shown to exhibit a variety of quantum many-body phenomena, such as quantum phase transitions [1], quantum annealing [2], long lived coherent oscillations [3] and long-range entanglement [4], making it a promising candidate for the implementation of solid state qubits. The derivation of the lowest lying energy states of the magnetic Ho^{3+} ion is shown in Fig. 1a. The degeneracy of the free-atom electron states is lifted by the tetragonal crystal symmetry of the lattice (point group S4) and subsequently further split by the hyperfine interaction with the nuclear spin $I = 7/2$. Earlier Ref. [5] optically probed the transition from the eightfold hyperfine-split ground state to the second excited state in a Fourier transform infrared (FTIR) spectrometer with a lab infrared source and 1.2 m optical path difference (OPD), hence with limited signal to noise ratio and resolution. Here, we present data using high brilliance SLS light in the far infrared regime and the world record high resolution FTIR spectrometer featuring 11 m OPD allowing us to probe the hyperfine state lines with unprecedented precision as shown in Fig. 1b. The average line width for $x = 0.1\%$ doping was found to be 0.006 cm^{-1}, which corresponds to 180 MHz and a lower bound lifetime of 0.46 ns. As a next step, we push towards the examination of the absorption line shapes and intensities as well as measurements of other compounds with sharp absorption lines in the infrared regime.

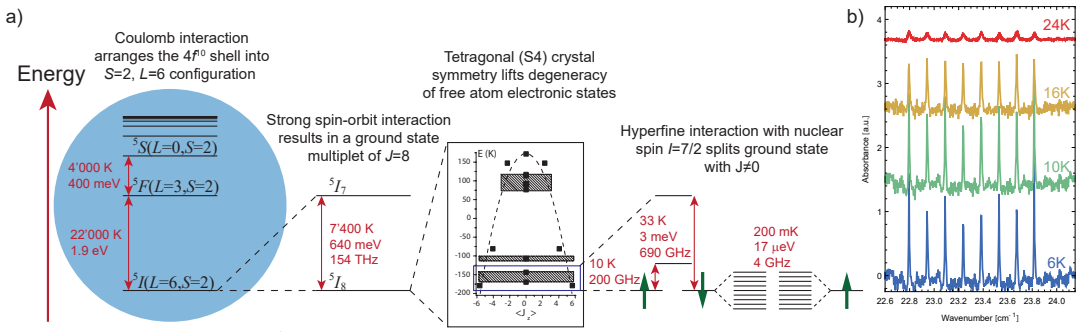

FIG. 1: a) Derivation of Ho^{3+} energy levels. b) FTIR detection of the eightfold-split ground state to second excited state transition of $LiY_{0.999}Ho_{0.001}F_4$ at four temperatures

[1] H. M. Rønnow *et al.*, Science **308**, 389 (2005).
[2] J. Brooke *et al.*, Science **284**, 779 (1999).
[3] S. Ghosh *et al.*, Science **296**, 2195 (2002).
[4] S. Ghosh *et al.*, Nature **425**, 48 (2003).
[5] G. Matmon *et al.*, Phys. Rev. B **94**, 205132 (2016).

*Electronic address: adrian.beckert@psi.ch

Pressure-control of magnetic exchange and its dimensionality in metal-organic coordination polymers

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Applying external pressure provides an efficient route to control structural and in turn magnetic properties of metal-organic coordination compounds. In this presentation, I will show how key properties can be accessed experimentally by x-ray and neutron scattering and susceptibility measurements in high magnetic fields. In a model-square lattice Heisenberg antiferromagnet we observe a giant pressure dependence and dimensionality switch of the magnetic properties from quasi-two dimensions to quasi-one dimension [1], see Figure 1. The microscopic picture can be understood by combining first principles calculations and Quantum Monte Carlo simulations.

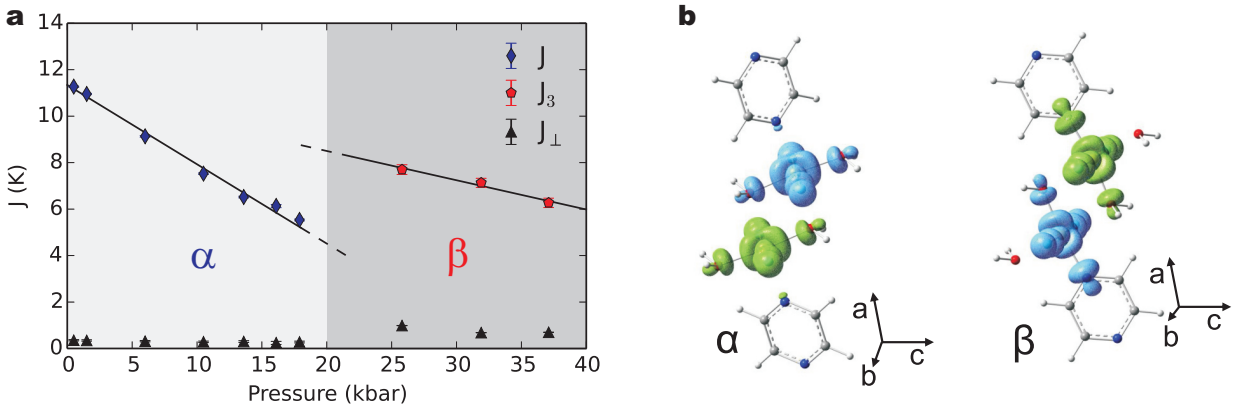

FIG. 1: Magnetic exchange parameters (**a**) and spin density distribution (**b**) in the α- and β-phase of $(CuF_2(H_2O)_2)_2$pyz.

[1] B. Wehinger, C. Fiolka, D. Graf, W. A. Coniglio, A. Grockowiak, J.-H. Chen, J. Gukelberger, M. Skoulatos, K. Kr¨amer, S. Tozer, C. Mudry, and C. R¨uegg, Giant pressure dependence and dimensional crossover in a metal-organic Heisenberg antiferromagnet, arXiv:1606.08344 (2016).

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Reversible Magnetoelectric switching by Lithium intercalation

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During my Flash Talk I will introduce my PhD-project since I just started my PhD at PSI recently.

Manganites (Manganese based perovskites) of the composition $A^{III+}_{1-x}B^{II+}_{x}MnO_3$ 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 A^{III+} and B^{II+} and the ratio of Mn^{III+}/Mn^{IV+} results in local variation of the mechanisms mentioned earlier.

During this PhD-project we want to cross magnetic phase boundaries reversibly by chemical doping and monitor the process in operando. To achieve this, we want to use electrochemical Lithium intercalation and deintercalation (using a Li-Ion half-cell). The material of choice during the first steps is $La_{1-x}Sr_xMnO_3$ (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 deintercalation.

Furthermore, the in-operando measurements are carried out using Polarized Neutron Reflectometry. With this method we investigate the distribution of the Lithium and the magnetic profile. Another goal is to relate these phenomena to the Mn^{III+}/Mn^{IV+} 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.

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Tunable Spin Correlations in 2D Kagomé Ice

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The geometrically frustrated pyrochlore spin ices $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$, provide an experimentally accessible environment for a variety of phenomena including residual entropy [1, 2] and magnetic monopole excitations [3]. Applying a medium strength magnetic field in the (111) direction splits the rare earth tetrahedra into triangular and kagome planes, precipitating a field-induced phase change [4, 5]. Competition between the ice rule and the applied field in the kagome phase limits the 3D spin ice degeneracy to the kagome plane, creating a 2D spin ice analog complete with a distinct Coulomb phase and associated pinch point scattering [6–8].

The possible spin configurations of kagomé ice map to a hexagonal dimer model, in which an unconventional phase transition was predicted as a consequence of modifying dimer activity on different families of links [9]. Tilting the field slightly away from the (111) axis alters the relative energies of kagomé plane spins, leading to a Kasteleyn transition whose signature is visible in the drifting of peaks across the scattering plane [4, 5, 10]. Polarized neutron experiments on $Ho_2Ti_2O_7$ allow us to observe both the spin ice correlations and those of an Ising antiferromagnet on the kagome lattice, opening a window onto one of the only experimental procedures to study the Kasteleyn transition and frustration on a true 2D spin ice. An investigation of the tunable algebraic Ising correlations via non-trivial diffuse scattering and their equivalency to a Kasteleyn transition will be presented.

[1] Pauling, J. Am. Chem. Soc. **57**, 26802684 (1935).
[2] Ramirez et al., Nature **399**, 333335 (1999).
[3] Castelenovo et al., Nature **451**, 7174 (2008).
[4] Moessner & Sondhi, Phys. Rev. B. **68**, (2003).
[5] Harman-Clarke, UCL (University College London), 2012).
[6] Henley, Annual Review of Condensed Matter Physics **1**, 179210 (2010).
[7] Fennell et al., Science **326**, 5951 (2009).
[8] Bramwell & Harris, J. Phys.: Condens. Matter **10**, L215 (1998).
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[10] Fennell et al., Nat. Phys. **3**, 8 (2007).

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Signatures of emergent quantum electrodynamics in a quantum spin ice

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In a quantum spin liquid (QSL), the magnetic moments of the constituent electron spins evade classical long-range order to form an exotic state that is quantum entangled and coherent over macroscopic length scales [1]. Quantum spin ice (QSI) is an appealing proposal of one such state, in which a quantum field theory describes the ground state properties and excitations [2]. An emergent $U(1)$ gauge structure endows this quantum-coherent regime with quasiparticles that are predicted to behave like magnetic and electric monopoles, along with a gauge boson playing the role of an artificial photon. We present neutron scattering measurements of the pyrochlore $Pr_2Hf_2O_7$ [3] that provide evidence for a QSI ground state [4]. We find a quasielastic structure factor with pinch points - a signature of a classical spin ice - that are partially suppressed, as expected in the quantum-coherent regime of the lattice field theory at finite temperature [5]. Our result allows an estimate for the speed of light associated with magnetic photon excitations. We also reveal a continuum of inelastic excitations, a property of the fractionalized excitations defining QSLs, which relate to the monopole excitations of the QSI. Our results constitute an experimental discovery of a condensed matter system whose low-energy physics can be described by emergent quantum electrodynamics. The observation of a QSI provides a concrete example of a three-dimensional QSL, a topical state of matter, which so far has only been reported in lower dimensionalities.

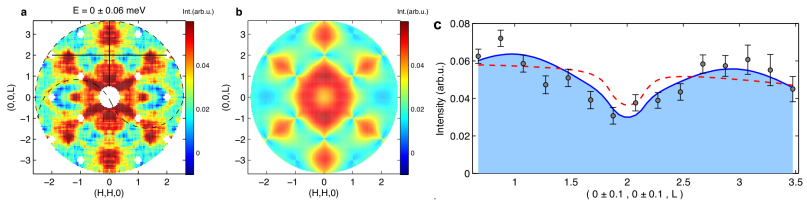

FIG. 1: Quasi-elastic scattering observed in $Pr_2Hf_2O_7$ (**a**) [4] and calculated using a Quantum Spin Ice (QSI) model (**b**) [5]. Panel **c** shows a cut in panel **a** (grey points with error bars) compared to calculations for the QSI model (solid blue line) and classical near-neighbor spin ice model (dashed red line) [4].

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[1] L. Savary & L. Balents, Rep. Prog. Phys. **80**, 016502 (2016).
[2] M. J. P. Gingras & P. McClarty, Rep. Prog. Phys. **77**, 056501 (2014).
[3] R. Sibille *et al.*, Phys. Rev. B **94**, 024436 (2016).
[4] R. Sibille *et al.*, arXiv:1706.03604.
[5] O. Benton, O. Sikora & N. Shannon, Phys. Rev. B **86**, 075154 (2012).

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Incommensurate magnetic order and magnetic diffuse scattering in the frustrated magnet TmB_4

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TmB_4 is a physical realization of a frustrated magnet on the two dimensional Shastry Sutherland lattice (SSL), leading to complex ground states and exotic phases of matter. TmB_4 belongs to a rare-earth tetraborides family of metallic frustrated magnets which crystallize in a tetragonal structure with space group P4/mbm. The rare earth moments are placed on an orthogonal dimer network corresponding to the 2D SSL. Additional interest in TmB_4 is driven by the emergence of fractionalized magnetization plateaus such as in the case of the famous spin realization of the Shastry Sutherland lattice $SrCu_2(BO_3)_2$.

In this context, magnetization studies and a neutron powder diffraction experiment were carried out [1, 3], from which a rich field-temperature phase diagram of TmB_4 was elaborated, which includes AFM order, possible incommensurate phases and a fractionalised plateau phase. Previous single crystal neutron scattering experiment showed some rich diffractions patterns both in and out of field [2].

We have carried neutron scattering experiments with a single crystal of TmB_4 on the cold diffractometer DMC and the diffractometer Zebra. The obtained results allows us to establish the magnetic order and temperature dependence of two incommensurate and one commensurate phase in zero field, as well as that of the fractional plateau and a second commensurate phase in applied field. In addition, our result show clear ring-like magnetic diffuse scattering around the magnetic Bragg peaks, which points towards a co-existence of the magnetic order with short range order correlations induced by the frustrated interactions in TmB_4.

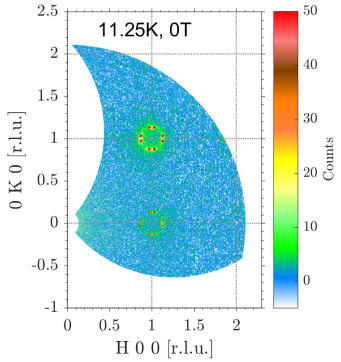

FIG. 1: Magnetic diffuse scattering of TmB_4 from DMC in one of the incommensurate phase at 11.25K.

[1] S. Michimura et al. J. Phys. Soc. Jpn., Vol. 78 2009
[2] K. Siemensmeyer et al. PRL 101, 177201 2008
[3] S. S. Sunku et al. PRB 93, 174408 2016

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Nature of $Ba_3MIr_2O_9$ (M=Sc,Y,In) ground state probed by μSR.

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The $Ba_3MIr_2O_9$ family offers a tremendous playground to study the influence of spin orbit coupling (SOC) in the stabilization of a spin liquid ground state. We present here the μSR study of the $J = 1/2$ compounds (M=Y,Sc,In) synthesized in the 6H lattice. The magnetism is held by iridium dimers based on a triangular lattice [1, 2].

We did zero field μSR measurements in order to probe the nature of the ground state in the different compounds. For the Y and Sc ones we found an homogeneous ordered ground state, with transitions at 4.5 K and 10 K respectively, as expected from the susceptibility, heat capacity and NMR measurements [1]. On the contrary, for the In one, we found no sign of frozen magnetism down to 20 mK despite interactions of about 130 K, which could be the sign of a spin liquid ground state. Moreover, our transverse field measurements point out a local susceptibility for the muon similar to our squid and NMR experiments, enlightening the absence of defects. In addition, our NMR and heat capacity measurements are in favor of a gapless spin liquid ground state [3].

On the theoretical side, a first principle calculation study on the Y compound pointed out the stabilization of an ordered ground state due to a small SOC value in regard to the Heisenberg interaction [4]. As each studied samples present the same lattice and effective spin one could expect a similar ratio between the SOC and the Heisenberg interaction. Nevertheless, a more careful study of the interactions between the Ir dimers enlighten two interactions, J_T in the (ab) plane and J_H along the (c) direction. We propose that the ratio among J_H and J_T drives the transition from an ordered ground state to a spin liquid one. Indeed, the Y and Sc compounds magnetism could be modeled by a triangular lattice ($J_T \ll J_H$) whereas a more complex model with a mix between honeycomb and triangular lattice ($J_T \propto J_H$) has to be taken into account for the In material.

[1] T. Dey *et al*, Phys. Rev. B **89**, 205101 (2014)
[2] T. Sakamoto *et al.*, Journal of Solid State Chemistry **179**, 2595-2601 (2006)
[3] T. Dey *et al*, ArXiv:1702.08305v2 (2017), to be published in Phys. Rev. B
[4] S. K. Panda *et al.*, Phys. Rev. B **92**, 180403(R) (2015)

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Strain manipulation of the $J_{eff} = \frac{1}{2}$ state of Sr_2IrO_4

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The Sr_2IrO_4 material has been in the lime light during last years due to the discovery of a novel $J_{eff} = 1/2$ Mott insulating state in the large spin-orbit regime. The sensitivity of this quantum state to local coordination and structural distortions suggests strain and confinement as ideal routes for studying and manipulating its properties. Our group has recently demonstrated that, due to the metal-ligand hybridization, oxygen K-edge resonant inelastic X-ray scattering (RIXS) can capture the elementary excitations in 5*d*-oxides. The low penetration depth makes this technique very suitable for the investigation of thin films. From O K-edge RIXS on thin films of Sr_2IrO_4 grown on several substrates by pulsed laser deposition, we detected the low-energy elementary excitations encompassing single magnons, bimagnons and spin-orbital excitations and their dispersion relations as a function of strain. In particular, we observe a change in the dispersion of the spin wave excitations, indicating renormalization of the exchange interaction upon strain. By measuring the particle-hole excitation across the Mott gap we observe that the strength of electron-electron correlations is also tuned. We find clear evolution in the crystal field excitations upon strain, reflecting the tuning of local crystal structure and spin-orbit coupling strength. Our study provides direct evidence that epitaxial strain effectively tunes all the energy scales which are relevant for the stability of the $J_{eff} = 1/2$ state.

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Nodeless-to-nodal superconductivity in $LaOFeAs_{1-x}P_x$ synthesized under high pressure

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Similar to chemical doping, pressure produces and stabilizes new phases of known materials, whose properties may differ greatly from those of their standard counterparts [1]. Here, by considering a series of $LaOFeAs_{1-x}P_x$ iron-pnictides synthesized under high-pressure high-temperature conditions, we investigate the simultaneous effects of pressure and isoelectronic doping in the 1111 family. Results of numerous macro- and microscopic technique measurements, unambiguously show a radically different phase diagram (see Fig. 1) [2] for the pressure-grown materials, characterized by the lack of magnetic order and the persistence of superconductivity across the whole $0.3 \leq x \leq 0.7$ doping range. This unexpected scenario is accompanied by a branching in the electronic properties across $x = 0.5$, involving both the normal and superconducting phases. Most notably, the superconducting order parameter evolves from nodeless (for $x < 0.5$) to nodal (for $x \geq 0.5$), in clear contrast to known 1111 and 122 iron-based materials grown under ambient pressure conditions [3, 4].

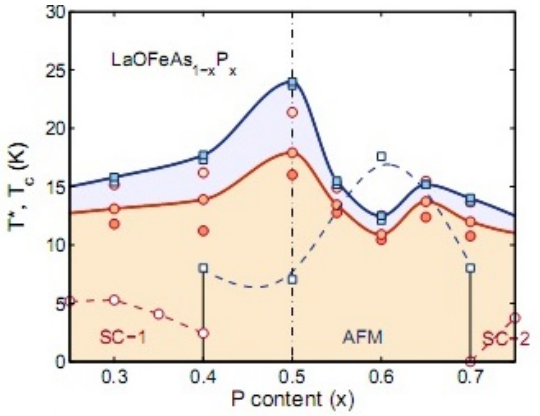

FIG. 1. Phase diagram of $LaOFeAs_{1-x}P_x$ showing the critical temperature T_c and that of the spin-fluctuation maxima T* at different applied magnetic fields (top to bottom: 0, 3.5, and 7 T).While the onset of superconductivity is suppressed by the applied field, the T* values remain unaffected. Empty symbols and dashed lines refer to the phase diagram of the material grown at ambient pressure, exhibiting two SC phases separated by an antiferromagentic phase. For clarity, the latter temperature values were reduced by half.

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Pressure effects on the magnetic order $Ba(Fe_{0.946}Co_{0.054})_2As_2$

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Cobalt substitution for iron in antiferromagnetic $BaFe_2As_2$ produces a superconducting ground state – first in coexistence with, then in the absence of, long range magnetic order – with indications that antiferromagnetism (AFM) and superconductivity (SC) compete for the same itinerant electrons [1, 2]. The AFM in $BaFe_2As_2$ is thought to be driven by nesting between hole-like and electron-like fermi surface pockets at the Brillouin zone center and edge, respectively [3].

Partial substitution of cobalt for iron changes the relative sizes of the two pockets [4] with two effects: 1) the magnitude of the ordered moment decreases with increasing cobalt concentration [5]; 2) beyond a critical concentration commensurate nesting is lost and a small transverse incommensurability appears which maintains long range magnetic order [6].

Magnetic susceptibility and resistivity measurements in applied pressure show suppression of AFM and appearance of SC above 3.5 GPa in $BaFe_2As_2$ [7] and, similarly, suppression of AFM and enhancement of SC below 2 GPa in $Ba(Fe_{1-x}Co_x)_2As_2$ [8]. Such measurements could not determine if the suppression of AFM via pressure is due to reduced fermi surface nesting, leaving whether the mechanisms which produce SC in $BaFe_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ are the same undetermined.

Neutron diffraction evinces loss of commensurate (C) fermi surface nesting by observation of the appearance of incommensurate (IC) magnetic peaks [6], and can be carried out on samples encased within massive pressure cells. The nature of the magnetic order in $BaFe_2As_2$ could therefore be directly tracked in applied pressure via neutron diffraction but for the high AFM suppression pressure. By selecting a $Ba(Fe_{1-x}Co_x)_2As_2$ composition with substitution-suppressed AFM which remains C, it is possible to use available pressure cells to further suppress AFM via applied pressure.

Presented here are single crystal neutron diffraction measurements under applied pressure which track the suppression of AFM order and reveal the presence of IC spin density wave order in $Ba(Fe_{0.946}Co_{0.054})_2As_2$. Coexistence of IC and C order is observed at all applied pressures with a continuous IC increase with pressure; suggesting that the mechanisms of suppression of AFM and appearance of SC in $Ba(Fe_{1-x}Co_x)_2As_2$ and $BaFe_2As_2$ are similar.

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Phase mixture and pseudogap behavior in the bismuthate high Tc superconductors

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Unconventional superconductivity often emerges from an adjacent parent compound phase, such as anti-ferromagnetic, charge density wave or spin density wave. However the inter-relation between these phases is poorly understood, and in some cases, it is still uncertain the existence of the parent compound correlation in the superconducting state. Here we report a comprehensive study of the bismuthate high-temperature superconductor using angle-resolved photoemission and transport measurements. We find that at temperature T* higher than Tc, superconducting $Ba_{1-x}K_xBiO_3$ exhibits a very bad to better metal transition in transport measurements and associated with a pseudogap seen by Angle-resolved photoemission. We argue that this behavior marks phase separation related to the changes in the crystal structure between being orthorhombic and tetragonal.

Distinct domain switching in $Nd_{0.05}Ce_{0.95}CoIn_5$ at low and high fields

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Heavy-fermion systems are prime candidates for complex superconducting order parameters that feature a strong interplay with magnetism. The series $Nd_{1-x}Ce_xCoIn_5$ reveals a competition between static magnetic order and superconductivity at zero field [1]. 5% Nd doped $CeCoIn_5$, however, features an auxiliary field-induced magnetic phase (Q-phase) that is only stable within the superconducting condensate, and that collapses in a first-order transition at the upper critical field [2]. This behavior provides evidence for a cooperative magneto-superconducting ground state in the Q-phase that is separated from the low-field SDW-phase via a quantum phase transition (QPT) [2]. Since both magnetic phases feature the same magnetic symmetry, it is an open question by which fluctuations the QPT is driven.

Using neutron diffraction we demonstrate that the population of the two magnetic domains in the two phases is affected differently by the rotation of the magnetic field in the tetragonal basal plane [3]. In the low-field SDW-phase the domain population is only weakly affected while in the high-field Q-phase they undergo a sharp switch for fields around the a-axis. Our results provide evidence that the anisotropic spin susceptibility in both phases arises ultimately from spin-orbit interactions but are qualitatively different in the two phases. This provides evidence that the electronic structure is changed at the quantum phase transition, which yields a modified coupling between magnetism and superconductivity in the Q-phase.

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Interplay of superconductivity and magnetism in $Nd_{1-x}Ce_xCoIn_5$

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The occurrence of a spin density wave (SDW) ordered phase within the superconducting phase of $CeCoIn_5$ is one fascinating example of cooperative interplay of superconductivity (SC) and magnetism [1]. A rich phase diagram is observed with heavy fermion ground state ($x \geq 0.5$), superconductivity($x \geq 0.83$), and magnetism ($x \geq 0.95$) upon substituting with Nd [2]. For 5% Nd substituted $Nd_{1-x}Ce_xCoIn_5$ an incommensurate (ICM) SDW phase is observed at zero field below $T_N = 0.9$ K within the superconducting region. This phase vanishes at 8 T, and another SDW phase with same wave-vector is observed for higher fields indicating towards a magnetically driven quantum phase transition (QPT) at $\mu_0 H = 8$ T [3]. We extend studies on the magnetic structure for 10% and 17 % Nd substituted $CeCoIn_5$ to understand the evolution of the 2 SDW phases with Nd concentration. Our recent neutron diffraction measurements reveal that for $Nd_{0.1}Ce_{0.9}CoIn_5$ a SDW phase is present at $T_N \leq T_c$ which almost completely encloses the SC phase as shown in Fig 1. The AF phase has a propagation vector $Q' = (q, \pm q, 1/2)$, with $q = 0.45$, similar to the Q-phase in $CeCoIn_5$. However, no other typical features of Q-phase is observed. For ($x = 0.17$), the SDW phase is observed at $T_N > T_c$, this seems to indicate that in the doping range $0.1 \leq x \leq 0.17$ SC and magnetic order merely coexist, which is in contrast with $CeCoIn_5$ and $Nd_{0.05}Ce_{0.95}CoIn_5$ where experimental findings suggest a multicomponent order parameter that couples SC and magnetism. The ICM propagation vector is compatible with the SC gap symmetry. It is surprising that the ICM phase persists beyond the SC regime and is present for $Nd_{0.25}Ce_{0.75}CoIn_5$, and crosses over to commensurate (CM) (1/2, 0, 1/2) magnetic phase for higher Nd concentration. The cross-over from CM ($x < 0.6$) to ICM ($x > 0.75$) is not understood fully yet.

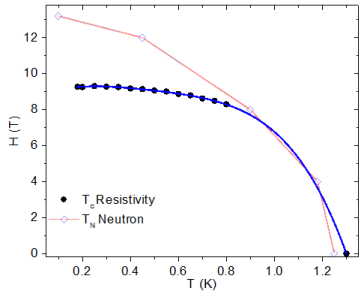

FIG. 1: $H - T$ Phase diagram for $Nd_{0.1}Ce_{0.9}CoIn_5$.

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Evidence for proximity induced p-wave superconductivity in a topological insulator

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At an interface between a topological insulator (TI) and a conventional superconductor, the surface modes have been predicted to rearrange in an interesting fashion. For example, in the region of the TI underneath the core of a vortex excitation in the superconductor, the gapless surface modes may combine to create a Majorana fermion, a collective excitation that is its own antiparticle and is the basic element in a proposal for fault-tolerant quantum computing. Moreover, it was predicted that the induced superconductivity between an s-wave superconductor and a TI develops an order parameter with a p-wave component. Here we present experimental evidence for proximity induced superconductivity in a thin layer of the TI Bi_2Se_3 grown on top of Nb. From depth-resolved measurements below the superconducting transition of Nb, we observe a local enhancement of the magnetic field in Bi_2Se_3 that exceeds the externally applied field, thus supporting the existence of an intrinsic paramagnetic Meissner effect arising from an odd-frequency superconducting state.

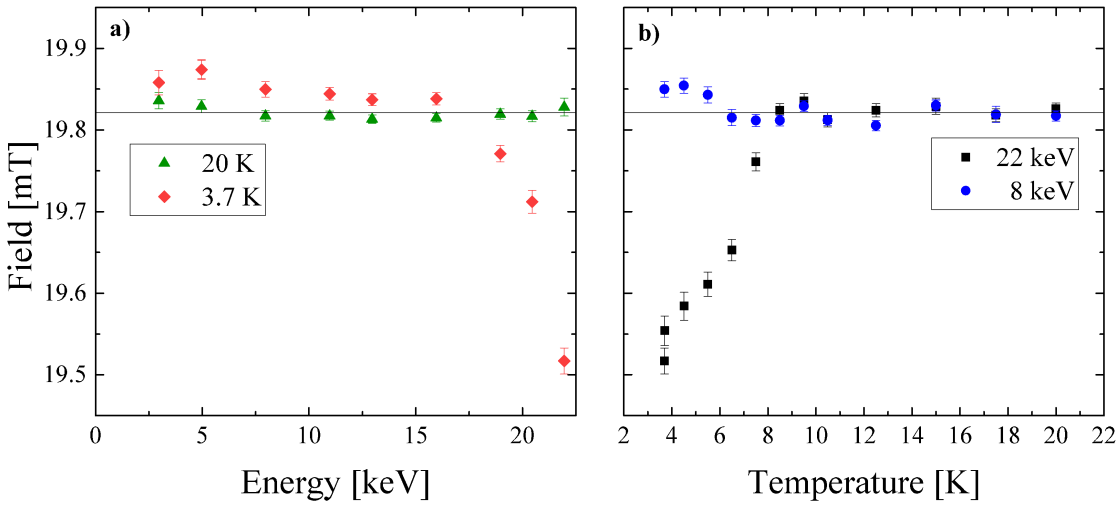

FIG. 1: Energy (a) and temperature (b) dependence of the mean field. The muons implanted at a high energy stop in Nb and see a conventional Meissner screening below 8 K. However, the lower energy muons stopping in Bi_2Se_3 see an increase of the local magnetic field. The solid line shows the energy average of the mean field at 20 K.

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Three-component fermion with Fermi arcs beyond Dirac and Weyl fermion

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Topological Dirac and Weyl semimetals not only host quasiparticles analogous to the elementary fermionic particles in high-energy physics, but also have nontrivial band topology manifested by gapless surface states (SSs), which induce exotic surface Fermi arcs. Recent advances suggest new types of topological semimetals, in which spatial symmetries protect gapless electronic excitations without high-energy analogues. Here using angle-resolved photoemission spectroscopy (ARPES), we observe triply degenerate nodal points (TPs) near the Fermi level (EF) of tungsten carbide (WC) with space group (No. 187), in which the low-energy quasiparticles are described as three-component fermions distinct from Dirac and Weyl fermions. We further observe topological SSs, whose constant-energy contours constitute pairs of Fermi arcs connecting to the surface projections of the TPs, proving the nontrivial topology of the newly identified semimetal state.

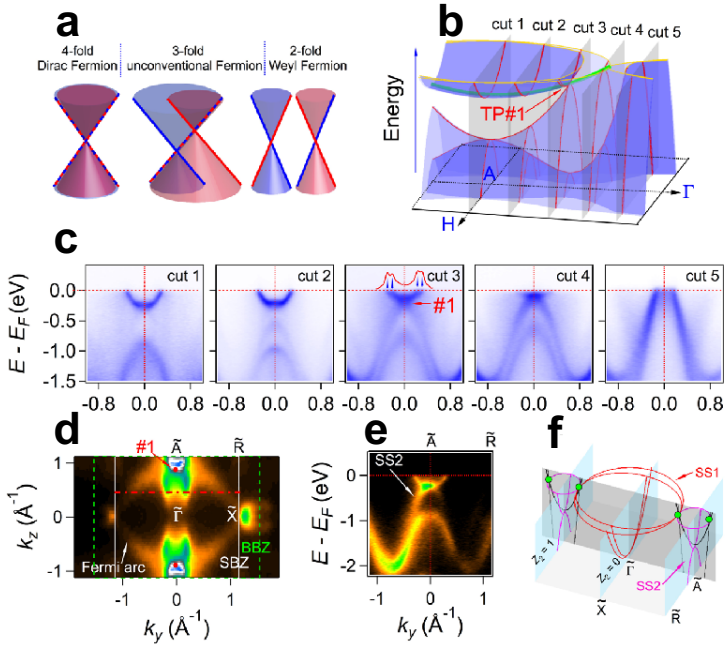

FIG. 1: a, Schematic plots of band structures of 4-fold Dirac fermion, 3-fold unconventional fermion, and 2-fold Weyl fermion. b,Schematic 3D plot of the electronic structure near TP1 in the kx = 0 plane. c. Photoemission intensity plots of band dispersions along cuts 1 to 5, respectively.d, Photoemission intensity plot at -200 meV showing Fermi arcs. e,Photoemission intensity plot showing band dispersions along R-X-R. f,Schematic 3D plot of surface Fermi arcs connecting the surface projections of TP1 (green dots) and SS bands.

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Magnetism in α-$RuCl_3$ under pressure

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Kitaev materials have been an active playground for the physics of bond-frustration and the search for quantum spin liquid states. At the heart of such materials is the bond-directional interaction which was found to be present in transition metal oxides with spin-orbit coupling. In this field of research, the iridates have attracted the most attention so far [1].

Recently, α-$RuCl_3$ was identified as another material where Kitaev interactions play an important role [2]. It does order magnetically at low temperatures with the details of the ordering dependent on further neighbour interactions [3, 4]. Since the nature of the ground state is very sensitive to the relative strength of the different further neighbor interactions, it is tempting to try and tune this system to induce switching between the phases by applying hydrostatic pressure.

In this contribution, I will report on the ongoing investigation of magnetism in α-$RuCl_3$ under pressure. The main tool in this inquiry is the muon spin rotation technique, which offers a microscopic probe of magnetism. In addition to being sensitive to very small moments, it allows to independently estimate the ordered moment and magnetic volume fraction. I will review the already obtained results and comment on the future plans for this project.

Time permitting I will also discuss the high-pressure studies of other Kitaev materials being undertaken in our laboratory.

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Optically induced transient enhancement of a structural order parameter

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We study the ultrafast photoinduced dynamics of an order parameter in a a class of systems where phonon-phonon interactions are believed to be the primary mechanism of the thermodynamic transition. $EuTiO_3$ is a perovskite that undergoes a soft-mode-driven [1] structural phase transition at 280-300K from cubic symmetry (Pm-3m) to tetragonal symmetry (I4/mcm) given by an antiferrodistortive rotation of the oxygen octahedra around the Ti ions (Fig. 1a). We employ above-bandgap femtosecond pulses to excite an $EuTiO_3$ thin film out of its low-temperature equilibrium phase and monitor the subsequent dynamics of the order parameter via the intensity of distortion-induced superlattice reflections using 80-fs hard x-ray pulses (at LCLS). We observe a transient intensity increase in a sub-ps time window (Fig. 1b). This represents an optically induced ultrafast increase of the structural order parameter, which stands in contrast to the reduction of the distortion for an increased internal energy in equilibrium. Preliminary DFT calculations suggest Eu 4f-hole-doping as possible driving force. We compare this behavior to the results obtained in a similar experiment (at FEMTO/SLS) on $SrTiO_3$ which is in its relevant aspects similar to $EuTiO_3$ and exhibits the same type of structurally driven distortion [2]. In contrast, we find an initial rapid decrease of the superlattice reflection on a timescale of 0.2 ps. This is much faster than expected for lattice heating from electronic excess energy.

These results indicate that in systems with phonon-mediated equilibrium phase transitions electronic interactions with the soft mode play an important role in the nonequilibrium case.

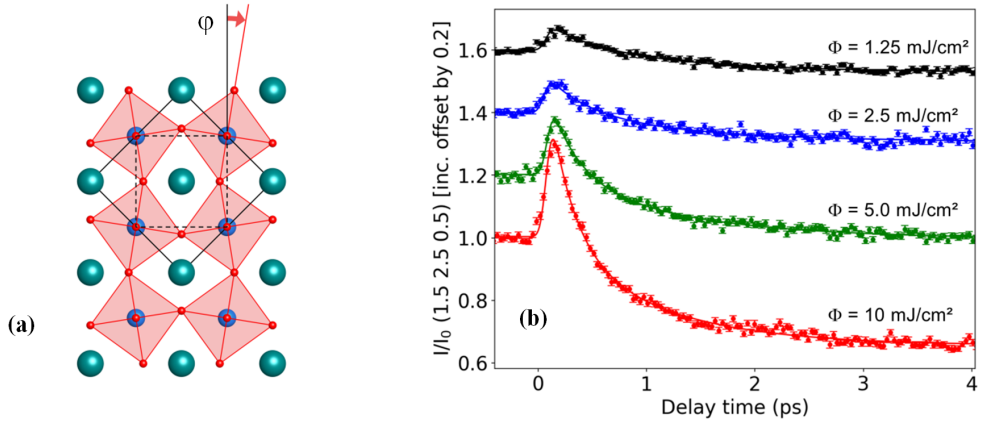

Abbildung 1: Figure 1: (a) Antiferrodistortive phase of $EuTiO_3$ and $SrTiO_3$ as seen along the crystal c-axis. Green: Eu/Sr; Blue: Ti; Red: O. (b) Transient x-ray superlattice reflection of an 40 nm $EuTiO_3$ thin film following photoexcitation with 40 fs pulses centered around 266 nm measured at T = 110 K.

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Orbital character of the mobile and localized electron states at the LAO/STO interface

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The discovery of high mobility two-dimensional electron system (2DES) emergent at the interface between two wide band-gap insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) has put forward new perspectives of oxide electronics where interfacing different materials tunes the interplay of electron, spin, orbital and lattice degrees of freedom characteristic of the transition-metal oxides. Oxygen vacancies (V_Os) at the LAO/STO interface leave two vacant electrons, one of which stays localized at the Ti^{3+}ion and another joins the mobile 2DES. This forms a dichotomic electron system where the localized strongly correlated in-gap electrons coexist with the less correlated mobile ones. The localized electrons in double and higher-order configurations of the V_Os may account for the interface ferromagnetism [1]. The mobile ones, coupled to phonon modes by strong electron-phonon interaction, form large multiphonon polarons fundamentally reducing the 2DES mobility [2]. The latter can however be tuned by the mobile electrons injected by the V_Os which screen the electron-phonon interaction. The V_Os are therefore an important piece of the reach LAO/STO physics in view of potential applications of oxide interfaces in electronics and spintronics.

We use resonant soft-X-ray ARPES experiments at the ADRESS beamline of Swiss Light Source to establish orbital character of the mobile and localized electron states at the LAO/STO interface created by the V_Os. We identify the predominantly Ti e_g- vs t_{2g}-derived orbital character of these two electron systems. Furthermore, we distinguish different chemical states of the in-gap electrons, and demonstrate interface induced orbital selectivity of resonant photoemission allowing separation of the d_{xy}- vs $d_{xz/yz}$-derived bands of the mobile ones. DFT+DMFT calculations agree with the experiment on both energy position and orbital character of the localized and mobile electrons. In contrast to bare STO surface, where these electrons fall into purely e_g and t_{2g} character, at the LAO/STO interface these orbitals significantly hybridize. This finding of a crosstalk between the localized and mobile electron systems sheds new light of the mechanism of magnetism and superconductivity at the LAO/STO interface.

[1] F. Lechermann et al., Physical Review B **90 (8)**, 85125 (2014).
[2] C. Cancellieri et al., Nature Communications **7**, 10386 (2016).

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Manipulation of the 2DEG at Titanates Surfaces

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The two-dimensional electron gas (2DEG) present at the interface and surface of titanates provides a platform to manipulate the 2D transport properties of these systems and explore the interaction of the 2DEG with the versatile physical properties of titanates and related compounds. In this talk, different ways to manipulate the 2DEG of the titanates (001) surface are presented. Crystalline surfaces and films grown by pulsed laser deposition (PLD) are studied by the help of angle-resolved photoelectron spectroscopy (ARPES) to explore the changes in the orbital ordering and band filling of the studied compounds.

In vicinal $SrTiO_3$ and films of $CaTiO_3$, the tetragonal distortion of the TiO_6 octahedra is altered due to the changed surface free energy and chemical strain respectively. With the strong dependence of the formation of the titanates 2DEG on the surface crystal structure, the change in distortion directly affects the energy scale of the orbital ordering of the Ti $3d$ states, that form the 2DEG of these two systems. For thin films of $SrTiO_3$ grown by PLD, the different type of growth defects, compared to crystalline $SrTiO_3$ substrates, are responsible for an observed change in band filling of the 2DEG. The presented results show different ways to manipulate the 2DEG of titanates surfaces and open new paths to engineer the 2DEG and consequently the transport properties of the studied and closely related systems.

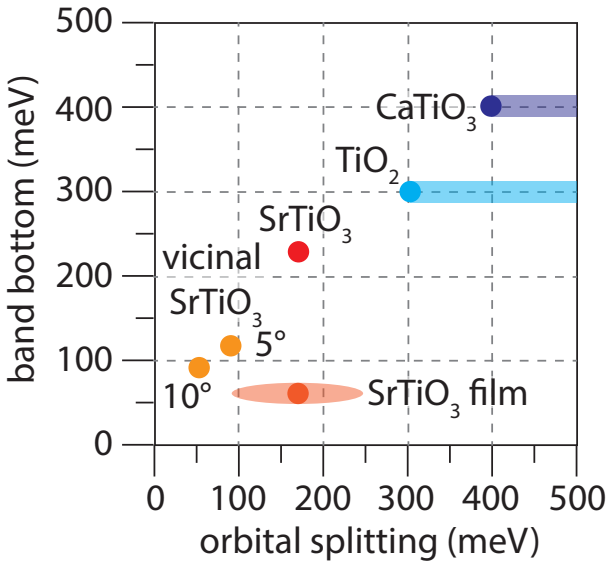

FIG. 1: Graphical summary of different ways to manipulate the properties of the 2DEG at titanates (001) surface showing the resulting changes of the band-filling of the d_{xy} bands and the splitting between the d_{xy} and the d_{xz}, d_{yz} bands.

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Mott Localization in $CaVO_3$

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Resonant Inelastic X-ray Scattering (RIXS) is an element specific probe sensitive to charge excitations in both metallic and insulating thin films. In this talk we will present RIXS measurements at the V L_3-edge across the metal-insulator transition (MIT) that occurs when $CaVO_3$ is synthesized in ultra-thin film form (see Figure 1). We will show that there is a large reduction in the bandwidth of all charge excitations across the thickness-driven MIT. We will also show that the same reconstruction occurs with temperature in a 10 unit cell $CaVO_3$ film, that undergoes a MIT around 200 K.

We compare our results with electronic structure calculations and suggest that the thickness-driven MIT in $CaVO_3$ is due to a combination of both strain and thickness. In contrast, structural or magnetic effects alone are suggested as the cause of the MIT as a function of temperature in the 10 u.c. $CaVO_3$ film. We interpret the measured crystal field excitations in the thinner $CaVO_3$ in terms of formation of local moments with an increase in V^{3+} character. These local moments may order in the thinner films. The presented results emphasize the importance of strain and dimensionality in the modern field of rational design of heterostructures of correlated materials.

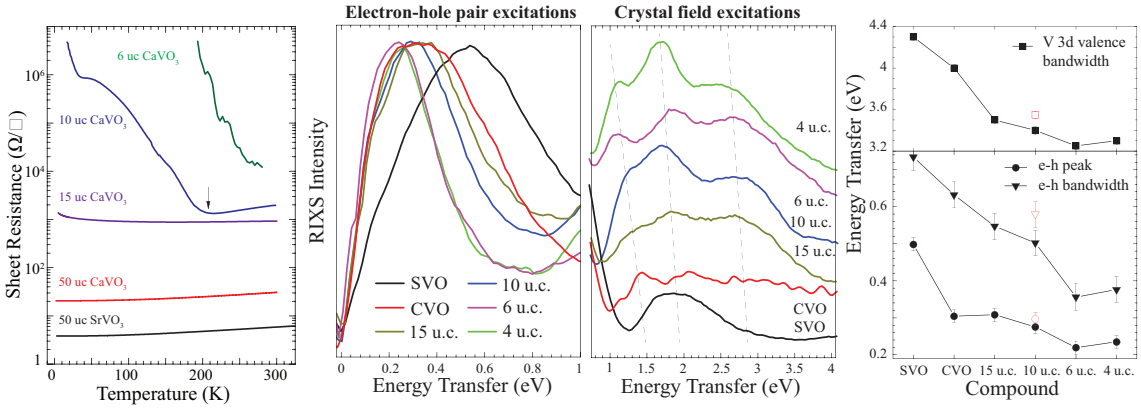

FIG. 1: (a) Resistance as a function of temperature for the films indicated. (b,c) Resonant inelastic x-ray scattering (RIXS) at the Vanadium L_3 edge results on the same films. The excitations shown are Raman-like modes (energy transfer independent of incident energy) (d) Extracted bandwidth and peak of the electron-hole pair excitations shown in (b) as well as the V 3d bandwidth extracted from higher energy fluorescence peaks (not shown here)

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CAMEA - A novel multiplexing analyzer for neutron spectroscopy

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The neutron spectrometer CAMEA (Continuous Angle Multiple Energy Analysis) will be installed as a new analyzer system on the cold-neutron TAS RITA-2 at SINQ, PSI [1]. CAMEA is optimized for efficiency in the horizontal scattering plane enabling detailed and rapid mapping of excitations [2]. As a novelty the design employs a series of several sequential upward scattering analyzer arcs. Each arc is set to a different, fixed final energy scattering towards position sensitive detectors (PSDs). Thus, neutrons with different final energies are collected simultaneously over a large angular range. For CAMEA in a single data-acquisition several entire constant-energy lines in the horizontal scattering plane are recorded for a quasi-continuous angular coverage of about 60, whereby tremendous gains in data collection rates can be achieved. With a large combined coverage in energy and momentum, this will result in a very powerful and efficient spectrometer, which will be particularly suited for parametric studies under extreme conditions with restrictive sample environments (high magnetic field magnets or pressure cells) and for small samples of novel materials. We will present the analyzer concept, performance simulations, technical solutions and prototype verifications.

[1] F. Groitl *et. al.*, Rev. Sci. Instrum. **87**, 035109 (2016).
[2] P.G. Freeman *et. al.*, EPJ Web of Conferences **83**, 03005 (2015).

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New applications of contrast variation in neutron reflectometry

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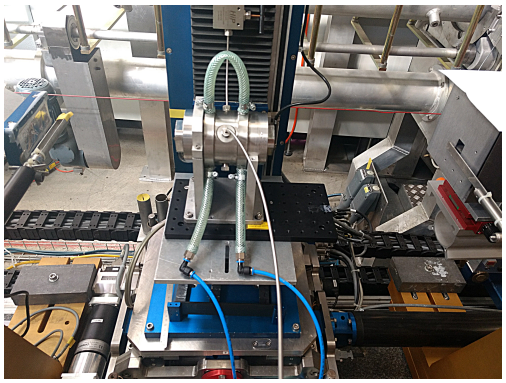
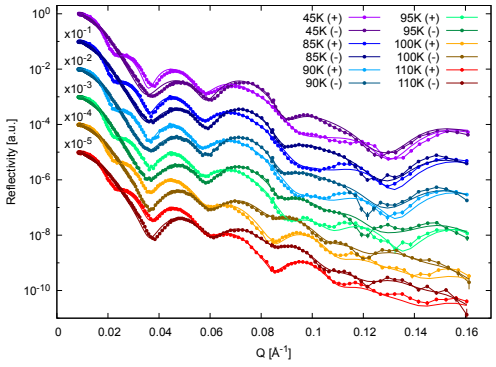
Neutron reflectometry allows to employ the unique sensitivity of the radiation to magnetism and elemental as well as isotopic composition to investigate surfaces and thin film interfaces on the nanometer scale. The unique contrast of different isotopes is often used to highlight certain aspects of a system or even making otherwise indistinguishable materials visible. Such contrast variation is also employed to circumvent a fundamental limitation of such a scattering technique; the phase problem. As only the intensity of the neutron wave-field is measured by the detector, the actual structure can't be directly determined from the measurement but has to be assumed and then refined by modeling the measured intensity. For systems with several unknown parameters like density, roughness and thickness of a set of layers it is often impossible to find a unique solution with only one reflectivity profile. Changing the contrast for structurally identical samples can be used to lift that ambiguity. Isotope exchange is the most often applied technique, but it is also common to use a magnetic reference layer between substrate and investigated system together with spin-resolved measurements, allowing two contrasts to be measured on the same sample.

We have performed two experiments that highlight the possibilities for such contrast variation experiments in new systems. For the investigation of structural phase transition in spontelectric films, materials that form spontaneous electric dipole moments upon condensation out of the gas phase, we have employed magnetic as well as isotope contrast variation. Using hydogenated and deuterated methyl formate on a Co/Pt coated substrate we were able to measure film density and thickness. When heating these deposited films above a phase transition the density change as well as intra-layer diffusion could be observed, challenging the previous model of a glass to crystal transition. In a proof of concept experiment we have employed a high pressure gas chamber to vary the contrast between the ambiance and the film surface. This technique will allow the investigation of hard matter materials using various contrasts, in-situ and without altering the sample structure.



(a) Setup used for pressure contrast variation



(b) Measurement series of magnetic and isotope contrasted system

FIG. 1

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Soft X-ray ptychography for condensed matter research

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With the miniaturization of modern electronic devices comes an increasing demand for understanding and for achieving an accurate control over materials properties down to the atomic scale. Synchrotron-based microscopy such as X-ray photo-emission electron microscopy (X-PEEM) or scanning transmission X-ray microscopy (STXM) have been proven as important tools for spectromicroscopic investigation of materials and condensed matter systems at the nanoscale. However, currently available X-ray based microscopy techniques do not provide the spatial resolution being required to address important phenomena occuring for instance at the scale of the magnetic exchange interaction or in the vicinity structural defects such as dislocations.

In this contribution we present our plan to develop a soft X-ray ptychographic microscopy set-up for the SLS. Ptychography is an innovative microscopy technique which circumvents the difficulties with imperfections in optical elements by means of numerical reconstruction of diffraction patterns recorded over overlapping regions of a specimen [1, 2] . The soft x-ray ptychography endstation will particularly benefit from recent developments on pixelated X-ray detectors, instrumentation, and powerful ptychographic reconstruction techniques carried out at PSI and promises spectromicroscopy with spatial resolution below 5 nm. In magnetism, such a development will allow one to directly investigate phenomena such magnetic skyrmions, Dzyaloshinskii-Moriya interactions, or the internal spin structure of nanomagnets. We will motivate the need for such investigations based on recent insights obtained by X-PEEM and STXM at the SIM and Pollux beamlines of the SLS. We will further outline the potential of soft x-ray ptychography for the wider condensed matter and materials research community, in particular in the context of SLS-2.

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Electronic structure of buried heterostructure and impurity systems explored by soft-X-ray ARPES

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Pushing ARPES into the soft-X-ray energy range (SX-ARPES) extends its **k**-resolving abilities from surface physics to buried heterostructure and impurity systems [1]. This results from enhancement of the photoelectron escape depth and a possibility of resonant photoexcitation. This overview illustrates SX-ARPES research at the ADRESS beamline of SLS.

Oxide interfaces. $LaAlO_3/SrTiO_3$ is a paradigm oxide interface embedding mobile 2D electrons. Resonant SX-ARPES resolves band structure of the interface charge carriers and identifies their polaronic nature [2] where electron coupling to different phonon modes limits low-temperature mobility and causes a dramatic mobility drop with temperature. Doping with oxygen vacancies opens ways to tune the interfacial mobility.

Semiconductor interfaces. AlGaN/GaN high electron mobility transistors (HEMTs) are an example of buried semiconductor interfaces. SX-ARPES experiment finds there significant anisotropy of the Fermi surface, band dispersions and effective mass of the interfacial quantum well states that results from piezoelectrically active atomic relaxation. SX-ARPES intensity as a function of emission angle and photon energy informs Fourier composition of the interfacial wavefunctions.

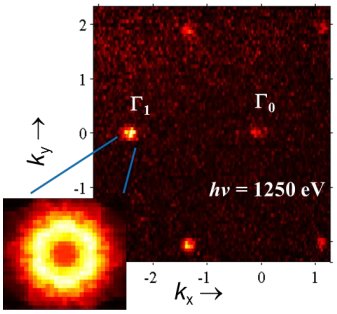

FIG. 1: Experimental Fermi surface of GaN-HEMT heterostructures.

Magnetic impurity systems. Doping of various materials with magnetic impurities is in the heart of spintronics. Resonant SX-ARPES reveals electronic structure of Mn doped magnetic semiconductors GaMnAs and InFeAs [3] and ferroelectric Rashba semiconductor GeMnTe, V doped topological insulator Bi_2Se_3, etc shading light on the elusive mechanism of ferromagnetism.

Unfolding the spectroscopic potential of SX-ARPES, further examples include multiferroic $BaTiO_3/La_{1-x}Sr_xMnO_3$ interfaces, EuO/Si spin injectors, Al/InAs interfaces as prototypes of Majorana fermions and other systems for future electronic and spintronic devices.

[1] V.N. Strocov *et al*, Synchr. Rad. News **27** No.2, 31 (2014)
[2] C. Cancellieri *et al*, Nature Comm. **7**, 10386 (2016)
[3] M. Kobayashi *et al*, Phys. Rev. B **89**, 205204 (2014)

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Time-Streaking for Investigation of Ultrafast Dynamic Processes at X-ray Free Electron Lasers

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X-ray free electron lasers (FELs) exhibit unique capabilities to conduct resonant X-ray spectroscopy techniques on ultrafast time scales. Up to now, pump-probe experiments are generally done in multiple-shot mode, restricting the technique from observing phenomena where the initial state cannot be reset. Utilizing diffractive optical elements, the pathlength difference inherent to diffraction in combination with focusing can be exploited to streak the arrival time of an x-ray probe along a geometric dimension in an individual shot. This concept has been applied in a pioneering experiment in reflection geometry at FLASH with a time resolution of 120 fs [1].
Adapting the experiment to a transmission geometry, we investigated demagnetization dynamics of a CoDy film (see FIG. 1). This geometry is espically appealing for observation of changes in magetization probed by X-ray magnetic circular dichroism. The time window reachable with this setup is 1.5 ps, with a time resolution that is in the femtosecond range. In our experiment, the time resolution is limited by the duration of the pump pulse of approx. 100 fs.
Extending this scheme to take advantage of the other spatial dimension, more advanced experiments become possible, such as single-shot, time-resolved spectroscopy. The new large-bandwidth operation mode of the Athos branch at SwissFEL thus opens a whole new perspective for ultrafast spectroscopy of dynamic effects in condensed matter.

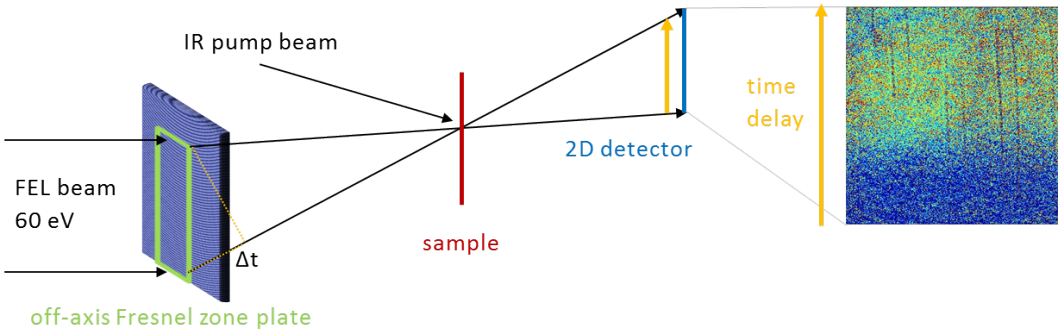

FIG. 1: Time-streaking setup in transmission. An incoming X-ray beam is diffracted at an off-axis Fresnel zone plate and focused onto the sample, inducing a time delay according to a pathlength difference of lambda times the number of zone pairs, which is dispersed in one direction on a 2D detector.

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Solar fuels: new materials and device configurations

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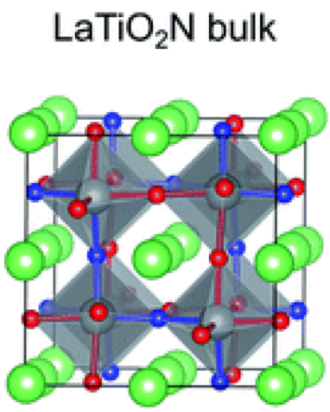
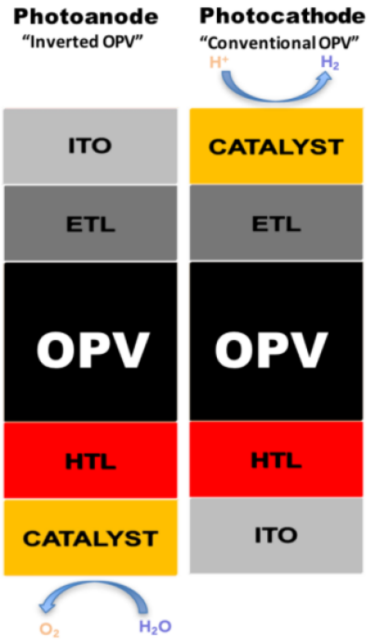
In this presentation I will outline the rationale behind solar fuels as an alternative energy source and cover some of my present and past work on the same subject. I will particularly focus on my recent development of proof-of-concept organic photovoltaic photoelectrodes for water splitting during my Masters. Moreover, I will also outline some my recent work and plans for upcoming research at PSI on visible-bandgap (∼1.8eV) Oxynitride materials for water splitting.





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Novel study of monolayrs of FeCo photomagnetic cages adsorbed on surfaces with X-ray Magnetic Spectroscopy

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Over the past decade there has been considerable interest in the development of molecular switches that exhibit bistability in their physical properties as a function of external stimuli. Prussian blue analogs (PBA), are found to be very good candidates to exhibit concomitant changes in their magnetic and optical properties based on a metal-to-metal electron transfer when they are submitted to a temperature or light stimulus [1], such as in molecular cubes based on Co and Fe linked by cyanide bridges (see Fig.1). Indeed, these molecules display a reversible conversion between the diamagnetic (Fe^{II}_{LS}-CN-Co^{III}_{LS}) pairs and the paramagnetic (Fe^{III}_{LS}-CN-Co^{II}_{HS})) ones [2]. Interestingly, the electron transfer phenomena can be easily tuned through modification of the compositions [3] or the nature and polarity of a solvent [4]. We propose a novel study based on the exploration of the electronic configuration and the magnetic properties of CoFe photomagnetic cages when adsorbed at surfaces at orders of monolayer coverages. X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) measured at the $L_{2,3}$ edges of 3d transitions metals is a powerful method to answer the question regarding the spin and oxidation states of the metals ions, and also to probe the nature of the Co-Fe magnetic interaction inside the molecule [5, 6]. The question whether the molecules keep their charge-transfer property when adsorbed on a suitable surface is still without answer. To this end, we are currently performing the first XAS and XMCD study to follow the thermal- and photo-induced electron transfer of these unique molecular switches deposited as monolayers.

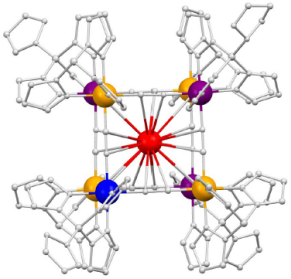

FIG. 1: CoFe photomagnetic cage. Blue : Co(II), Yellow : Co(III), Purple : Fe (II), Red : Cs.

[1] D. Aguila *et al.*,Chem. Soc. Rev., **45**, 203 (2016)
[2] D. Garnier *et al.*, Chem. Sci. **7**, 4825, (2016)
[3] J.-D. Cafun *et al.*, J. Am Chem. Soc. **132**, 11552-11559, (2010)
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[5] S. F. Jafri, *et al.*, Inor. Chem., **55**, 6980-6987, (2016)
[6] M. L. Baker, *et al.*, Inor. Chem., **52**, 13956-13962, (2013)

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All-optical switching of FeGdCo nanoparticles

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Currently employed magnetic recording technologies are relying on magnetic fields to switch the magnetization and are approaching fundamental limitations of recording speed and information density. Therefore alternative ways to read and write information in magnetic nanostructures are intensively investigated. Of particular interest are ultrafast all-optical schemes, which could replace current read-write head technology. FeGdCo is a ferrimagnetic alloy well known to show all-optical switching in the form of thin films or sub-micrometer structures. However, much less is known about the properties of this material at the nanoscale.
Here we report on preliminary SQUID, TEM (compare Fig. 1) and PEEM (compare Fig. 2) investigations of FeGdCo nanoparticles with sizes ranging from 5 nm to 25 nm. The combination of PEEM with complimentary experimental techniques allows for both detemination of single nanoparticle and nanoparticle ensemble properties. Furthermore, we outline steps for the continuation of these experiments, and ultimately for the investigation of deterministic all-optical nanoparticle switching, induced by a fs laser.

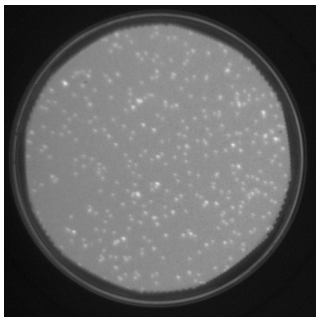

FIG. 1: PEEM image at Fe L_3 edge of FeGdCo nanoparticles, 20 μm aperture

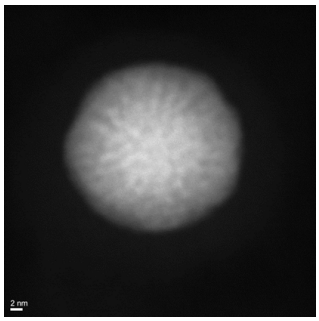

FIG. 2: TEM image of a single FeGdCo nanoparticle

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Tuning magnetization relaxation of single-molecule magnets using functional oxide films

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Single-molecule magnets[1] including a trivalent lanthanide ion[2] are attracting much attention due to their large energy barrier for magnetization reversal, opening a path toward potential applications in spintronic devices and high-density data storage[3]. This further intensified research on the properties of these species on surfaces.

Recently, Wäckerlin *et al.*[4] demonstrated a three-Tesla hysteresis opening on a sub-monolayer of $TbPc_2$ (Pc - phthalocyanine) on a thin MgO film. This was attributed to the preserved high symmetry of the molecules by the weakly interacting oxide surface as well as to the suppressed interaction with the conduction band electrons of the underlying Ag(100) substrate. A similar, but less tremendous effect was observed for $DyPc_2$ and Tb_2Pc_3 molecules on MgO.

In a near perspective we are planning to study single-molecule magnets on functional substrates, *i.e.*, in which properties such as electron density at the surface, can be varied by external means (*e.g.*, applied voltage). By that, we aim to gain control over molecule-substrate interaction, and to tune the magnetic properties of single-molecule magnets towards their incorporation into devices. Our ongoing experiments focus on the utilization of thin films of $LaAlO_3$ on $SrTiO_3$ substrates which provide a 2D electron gas at their interface, and whose properties can be altered by stimuli such as gate voltage, light, or magnetic field.

For a further perspective, within a collaborative effort on functional molecular devices, we are interested in substrates which allow control over the subtle interplay between fragile magnetism of adsorbed molecules and molecule-surface interaction. The desired features are: weakly interacting surface (*e.g.* oxide), low roughness (required flat adsorption of molecules), and capability to externally modify the surface properties (surface charge, electric polarization, etc.)[5, 6].

The aim of the talk is to introduce the progress of the group in the field, present the current focus of the study, and draft the possible ideas which could be realized within a PSI-internal collaboration.

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X-ray free-electron lasers – a new tool for the exploration of condensed matter

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Nearly a decade of user operation at x-ray free-electron lasers (FEL) has proven the potential for new science that is enabled by this generation of accelerator-based photon sources – particularly also in solid state physics. For studies of condensed matter systems the extremely brilliant, coherent and ultrashort x-ray pulses are primarily used to map out the femtosecond dynamics in so-called pump-probe experiments. But the x-ray pulses also permit for single-shot detection of ground states and correlation spectroscopy. To sketch this potential in condensed matter research, I will first review some x-ray FEL-based techniques and approaches that have earlier been used by PSI collaborations and others, for example to reveal photo-excited coherent dynamics of phonons and magnons, but also to detect structural order in extreme environments.

Then, I will focus on plans for condensed matter experiments at SwissFEL. Its hard x-ray beamline ARAMIS will see first pilot experiments by the end of this year and regular user operation from autumn 2018 on. Of particular interest for studies of correlated electron systems will be the availability of intense THz pulses, whose energy scale matches those of many quantum phases (1 THz $\sim$ 4.14 meV) and allow for access of charge-neutral excitations. The investigation of the femtosecond dynamics of electronic and magnetically ordered states will be a focus at the BERNINA endstation, where also dedicated instrumentation is already foreseen as a next step, including pulsed high magnetic fields and resonant inelastic x-ray scattering. The first allows probing the structure of ordered states in distant corners of phase diagrams, whereas the latter will be used to map out the dynamics of coherently driven low-energy excitations.

Finally, from 2020 on soft x-rays will be available at the ATHOS beamline of SwissFEL. There, the flexibility of the operation modes will allow tailoring the properties of the x-ray pulses to the needs of a particular experiment, for example in terms of polarization, bandwidth or pulse duration. To illustrate these capabilities, I will elaborate on several time-domain approaches that are currently being discussed, including single-shot and imaging resonant elastic and inelastic x-ray scattering, Fourier transform spectroscopy, x-ray magnetic circular dichroism or the use of transient gratings to imprint periodic potentials, e.g. on charge/spin ordered correlated electron systems.

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Poster Contributions

Laser induced magnetization dynamics in multiferroic $CoCr_2O_4$

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Recently, multiferroic materials have attracted significant attention, primarily because the coupling between the electric and magnetic order parameters presents the possibility of controlling magnetic properties by applying electric fields (and vice versa). $CoCr_2O_4$(CCO), a type II multiferroic, is rare within the type II classification as it retains a macroscopic magnetic moment M alongside its electric polarization P. Here, we present a dynamic study about the influence of long range magnetic order CCO in ultrafast time scale. A pump probe experiment was performed, inducing demagnetization in CCO by a femtosecond laser pulses, studying the demagnetization effect below and above the transition temperature in the multiferroic phase. It has been observed a possible influence of the magneto-electric coupling on picosecond time scale.

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μSR study on high-T multiferroic $YBaCuFeO_5$

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The discovery of materials where magnetic order and ferroelectricity are strongly coupled - the so-called multiferroics – has raised a great deal of interest during the last decade. Indeed, the possibility of combining these two properties in the same material can be exploited in applications requiring the control of magnetism (preferable ferromagnetism) by an electric field or vice versa. Unfortunately, the promising multifunctionalities of multiferroics have been obscured by two facts: on one side, most of the materials reported to date are antiferromagnetic. On the other, their transition temperatures are too low for most practical applications (typically below 40 K).

Recently, the oxygen-defficient double perovskite YBaFeCuO5 constitutes a remarkable exception. This material displays simultaneous incommensurate magnetic order and ferroelectricity below $T_{N2} \simeq 200$ K, and its magnetic spiral temperature has been increased beyond room temperature by control of the Fe/Cu disorder. Up to now, the local magnetic properties of this material is still missing. As a local probe technique, we did ^{63}Cu and ^{89}Y NMR measurements on this material. Unfortunately, due to the disappearance of the NMR signal caused by fast magnetic fluctuations, these attempts proved unsuccessful. Here we use μSR technique to investigate its local magnetic environment.

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New magnetic phase in the nickelate perovskite $TlNiO_3$

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The nickelate perovskites ($RNiO_3$) are an archetypal class of correlated electron materials [1]. They order antiferromagnetically at a composition-dependent "Néel" temperature T_N. While it is known that the magnetic structure has a period of four Ni spins along each (pseudo)cubic crystal axis, the arrangement of these spins is still under debate, especially in view of the conjecture of ferroelectricity in the antiferromagnetic phase.

Our recently published results of nuclear magnetic resonance and muon spin rotation (SR) experiments on $TlNiO_3$, a nickelate with non-magnetic A-site cation, reveal the presence an unexpected second magnetic phase transition at a temperature above T_N [2]. The temperature-dependence of the zero-field (ZF) μSR frequencies, displayed in Fig. 1, clearly shows both the previously known transition at $T_N = 104\,\mathrm{K}$ and the new transition at $T_N^* = 202\,\mathrm{K}$. The new phase is suppressed by magnetic fields on the order of at most 1 T.

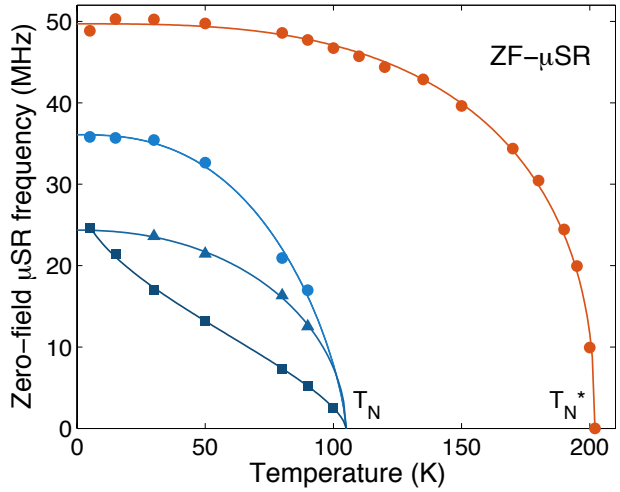

FIG. 1. Zero-field muon spin rotation frequencies, here plotted as a function of temperature, show the presence of two magnetic phase transitions.

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Magnetic Symmetry and Field-Induced Spin-Textures in Chiral Multiferroic $Ba_3TaFe_3Si_2O_{14}$

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Multiferroic langasites, which crystallize in a chiral space group, have attracted attention due to their doubly-chiral magnetic ground state [1]. We present the results of resonant soft X-ray and neutron diffraction studies on the triangular antiferromagnetic langasite $Ba_3TaFe_3Si_2O_{14}$ (BTFS). In the absence of an external magnetic field, we observe the satellite reflections $(0, 0, \tau)$, $(0, 0, 2\tau)$, $(0, 0, 3\tau)$ and $(0, 0, 1 - 3\tau)$ where $\tau \approx 0.140 \pm 0.001$. The dependence of the scattering intensity on X-ray polarization and azimuthal angle indicate that the odd harmonics are dominated by the c-axis spin-canting while the $(0, 0, 2\tau)$ originates from orbital distortions [2]. On application of the magnetic field along the *ab*-plane, above a critical field $\mu_0 H_c = 4\,T$, the system undergoes a phase transition indicated by the appearance of a second incommensurate modulation $(\delta, 0, 0)$ where $\delta \approx 0.0040 \pm 0.0006$ [Fig. 1]. We explore the spin structure and symmetry in the field-induced phase and present the H-T phase diagram of BTFS.

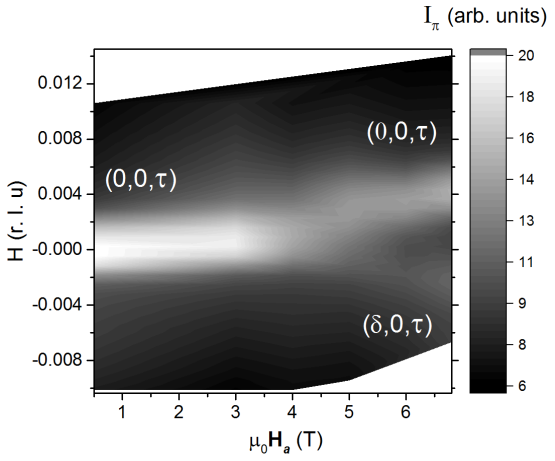

FIG. 1: Reciprocal space map showing the splitting of the $(0, 0, \tau)$ reflection along an orthogonal direction above the critical field at T = 5 K.

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Electric field control of skyrmionic bubbles and interfacial magnetic anisotropyin Pt/Co/Ta heterostructures using Si_3N_4 as gate dielectric

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Metals with large spin orbit coupling (Pt = 0.0368 eV, Ta = 0.0125 eV), give rise to an asymmetric exchange interaction at metal/magnetic interface from the Dzyaloshinskii-Moriya interaction (DMI) which contributes to the net surface/interface anisotropic energy. Pt/Co/Ta has different metal interfaces with a non-zero DMI value which results in the formation of spiral like domains known as skyrmions. The objective of this study is to investigate field effects on the DMI or interfacial anisotropy in Si_3N_4/Pt/Co/Ta heterostructures. The Pt/Co/Ta layers are grown on Si_3N_4 membrane and an electric field is applied out of plane resulting in interfacial charge modulation in Co layer. Here we demonstrate using x-ray photoelectron emission microscopy (XPEEM) the creation and annihilation of skyrmionic bubbles with applied electric field (Fig. 1). Furthermore, a change in the interfacial anisotropy resulted in a controllable domain wall motion (Fig. 2). These results suggest a modulation in the net anisotropy of the system due to a change in interfacial anisotropy. Further spectroscopic data/experiments are required to verify the change in DMI from this effect.

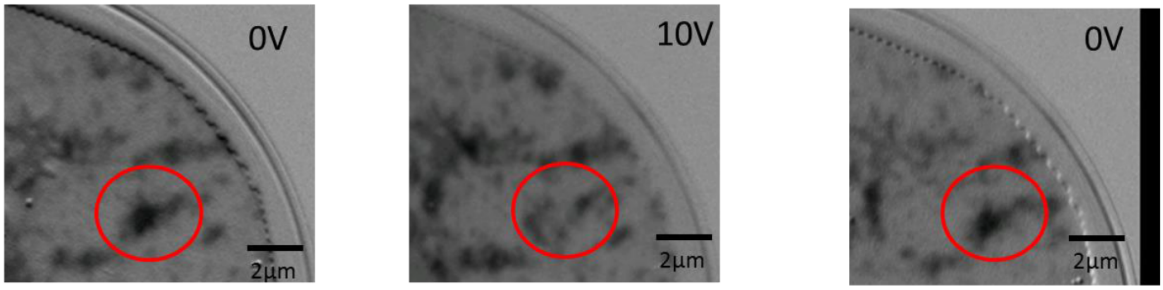

FIG. 1: Creation and annihilation of skyrmionics bubbles (marked in red) with applied electric field.

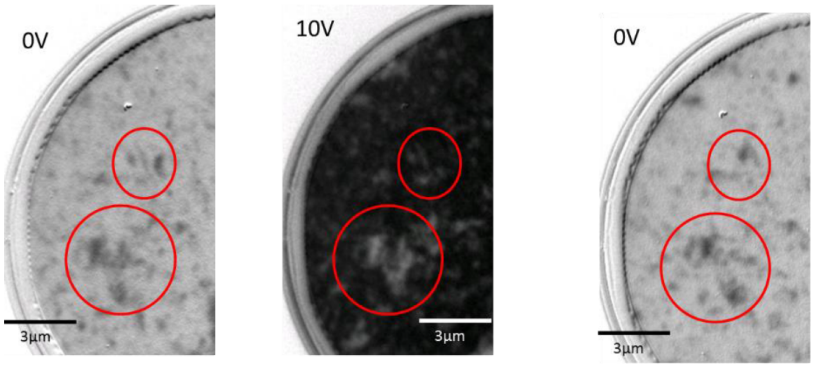

FIG. 2: Nucleation and reverse nucleation of large domain with applied electric field. Red circle indicates pinned skyrmionic bubbles which remain unaffected with applied electric field.

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Correlation between magnetic properties and structural defects in individual cobalt nanoparticles

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Gaining insight in the origin of the frequently observed anomalous magnetic properties of 3d transition metal nanoparticles is important for our fundamental understanding of magnetism at the nanoscale as well as for applications. In fact, despite of considerable experimental and theoretical research efforts, our knowledge about nanoparticle magnetism is still poor. In particular, experimental reports show that the magnetic anisotropy of 3d transition metal nanoparticles can vary over orders of magnitudes [1–3] and, thus, prevent the development of a consistent theoretical description of nanoparticle magnetism. In this contribution, we combine X-ray photo-emission electron microscopy (X-PEEM) with high angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) to correlate magnetic properties with atomic resolution structural characterization of individual cobalt nanoparticles. Our results suggest that structural defects such as twinning or stacking faults are frequent in cobalt nanoparticles and may modify their magnetic energy barriers and spontaneous magnetization axes significantly.

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Toward addressing molecular lanthanide quantum bits on surfaces

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Correlating magnetism and morphology of individual cobalt oxide nanoparticles

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Antiferromagnetic materials are of profound interest for spintronics devices, e.g. spin valves and the development of novel ultra-hard magnetic materials.[1] Recently, instantaneous switching of antiferromagnetic systems has been demonstrated making them a promising candidate for the development of ultra-fast random access memory devices. [2] Although the properties of many antiferromagnetic materials have been well-established in their respective bulk form, the properties of the same materials are poorly understood on the nanoscale.
Here, we study the properties of CoO/Co_3O_4 core-shell nanooctahedra, in order to achieve a deeper understanding of nano-scaled antiferromagnets. Nanoparticles with a core-shell structure are further endorsed with a particular interface between the materials of the core and the shell, which implies novel properties like magnetic moments arising from interfacial strain.[3]
We investigate the CoO/Co_3O_4 core-shell nanooctahedra using X-ray magnetic linear dichroism (XMLD) spectromicroscopy by means of X-ray photoemission electron microscopy combined with scanning electron microscopy in order to correlate the chemical and magnetic properties with the morphology of the nanoparticles. First results indicate a magnetic phase transition around the Néel temperature ($T_N = 285$ K) of CoO in its bulk form. The X-ray linear dichroism (XLD) spectra of the individual cobalt oxide nanoparticles show to interesting features. On one hand we find that the XLD spectra show a distinct anisotropy below T_N. On the other hand we obtain a isotropic XLD above the T_N. This contribution will discuss first results of the investigations on theCoO/CO_3O_4 core-shell nanooctahedra.

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Field and pressure induced quantum phase transitions in $CsFeCl_3$

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$CsFeCl_3$ is a gapped quantum magnet with a singlet ground state that exhibits a putative magnetic field-induced Bose-Einstein condensation of magnons leading to long range antiferromagnetic order. The gap in this system originates from nondimerized $S = 1$ spins where the $S_z = 0$ state is gapped from the doublet $S_z = \pm 1$ state due to the single ion anisotropy D. This compound crystallizes in a hexagonal crystal structure [1], in which the magnetic Fe^{2+} ions are octahedrally coordinated by six Cl^- ions. The Fe ions form ferromagnetically coupled chains along the c-axis and are antiferromagnetically coupled within the hexagonal plane. $CsFeCl_3$ exhibits a magnetic field-induced quantum phase transition into an antiferromagnetic ordered state in fields above H_c = 4 T and at temperatures below $T_N = 2.6$ K [2].

In 2016, the rare case of a pressure-induced quantum phase transition was reported for this system with a critical pressure of 0.9 GPa [3]. Here we report an extensive experimental investigation of the pressure and field induced ordered states with a help of the local probe technique μSR. The pressure dependent measurements have been performed on the GPD spectrometer using a piston-type clamp pressure cell reaching up to 2.0 GPa and temperatures down to 0.25 K in the ^{3}He cryostat. The measurements in field were carried out in the high field instrument HAL-9500 in magnetic fields up to 4 T and temperatures down to 20 mK. These measurements have been performed with the magnetic field parallel to the single ion anisotropy axis (c-axis) for which Bose-Einstein condensation of magnons is predicted.

The obtained results show that $CsFeCl_3$ is in a dynamic magnetic state at low pressures and it possesses static long range magnetic order at pressures above p_c as evidenced by spontaneous zero field μSR oscillations. We have obtained the ordered volume and the Néel temperature as a function of pressure. The high field results confirm the magnetic ordering of the system near the critical field. We will present the extracted parameters of the quantum phase transition as a function of temperature, pressure and field and will discuss them in the framework of a possible Bose-Einstein condensation of magnons.

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Triple Coulomb phase in the fluoride pyrochlore $CsNiCrF_6$

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A Coulomb phase emerges when the configuration of local degrees of freedom in condensed matter can be coarse grained to map onto a magnetic field. These objects may be real magnetic moments as in a spin ice, charges or ions (charge ice), hydrogen bonding networks (in water ice or other ices), or more abstract quantities in classical and quantum spin liquids and dimer models. A Coulomb phase has unconventional dynamics, which include both transverse and longitudinal fluctuations. The transverse fluctuations are cooperative and maintain the non-divergent character of the field, while longitudinal fluctuations correspond to creating and annihilating pairs of particle-like topological defects in the field. In the much discussed cases of quantum and classical spin ice, these excitations correspond to emergent photons and magnetic monopoles respectively, but in other Coulomb phases generalised equivalents should exist.

Fluoride pyrochlores $AMM'F_6$ (with A an alkali metal, M a 2+ and M' a 3+ transition metal cation) are currently not much studied, though $CsNiCrF_6$ was once thought to be a good model material for the pyrochlore Heisenberg antiferromagnet, one of the most highly frustrated classical spin models known. The M and M' cations occupy the sites of the pyrochlore lattice in this structure, and we show that they are correlated according to an ice rule - the first Coulomb phase in $CsNiCrF_6$ is a charge ice. This correlated disorder requires related displacements of the F^- ions, since the average structure does not satisfy the bond valence requirements of any cation in it. This 'displacement ice' is the second Coulomb phase in $CsNiCrF_6$. The spins also obey topological constraints, as in the pyrochlore Heisenberg antiferromagnet, so that the third Coulomb phase is magnetic. Using polarized diffuse magnetic scattering, we separate the structural and magnetic cross sections and show that they are described by models of these three types of Coulomb phase. Using inelastic magnetic scattering, we show that the dynamics are in accord with the expectations of a generalised Coulomb phase.

The $AMM'F_6$ structure type is rather flexible - many combinations of A, M and M' are possible. The A^+ cation resides in a large cage, and we use single crystal neutron and synchrotron powder x-ray diffraction to show that in $CsNiCrF_6$, the Cs^+ cation is highly mobile in this cage. The vibrational dynamics of structures with highly correlated disorder, and the effect on 'rattling' guests in such a host afford an interesting future direction in the study of these materials.

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Kitaev Physics in $RuCl_3$ Under Pressure

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The Kitaev model on a honeycomb lattice is a rare example of an exactly solvable spin Hamiltonian, whose phase diagram includes regions in which the much sought-after spin liquid groundstate is stabilized and excitations are anyonic in nature [1]. Remarkably, it was found [2] that such a Hamiltonian can be realized in real crystal structures satisfying some loose atomic and geometric constraints (namely spin-orbit coupled J_{eff} =1/2 ions in octahedral environments with three-fold connectivity). Initial investigations focused on Iridate compounds Na_2IrO_3 and Li_2IrO_3, where both were found to order magnetically at low temperatures. Though their magnetic structures are highly non-trivial and confirm the presence of anisotropic, Kitaev-like interactions the desired spin liquid groundstate was not forthcoming. Moreover the high absorption of Iridium presents a challenge to neutron scattering – typically the experimental probe of choice for exploring magnetic structures and excitations. Thus, the emergence of a new Kitaev candidate RuCl3, whose honeycomb of Ru^{3+} $4d^5$ ions sit in an octahedral environment of Cl ligands and possess an effective J=1/2 moment, heralded a new surge in experimental and theoretical interest in this field. $RuCl_3$ too orders at low temperatures with a T_N in the range 7-14K depending on stacking faults, however inelastic neutron scattering studies show excitations qualitatively different from the spin waves associated with conventional order [3]. Rather, the spectrum seems to have contributions from fractionalized modes, hinting at the proximity in parameter space to the Kitaev spin liquid. These results prompted experimentalists to see whether perturbing $RuCl_3$ with external stimuli (e.g. magnetic field, hydrostatic pressure) the system could be forced into the spin liquid regime. Here, I will present results of magnetic susceptibility measurements under pressure on a high quality powder sample of $RuCl_3$. Though the work is still on going, preliminary data hints at a reduced magnetic volume fraction with the application of pressure, a result consistent with previous NMR and specific heat results[4, 5]. More than display the results themselves, this work also demonstrates the experimental possibilities of bulk susceptibility measurements up to pressures of 10kbar here at PSI.

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An experimental investigation on the single-band Hubbard model in new fluorides

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A strongly correlated electron system may be described by the single-band Hubbard model [1]. In this project, experimental work on a physical realization of the Hubbard model $NaCuF_3$ has been carried out inspired by recent theoretical calculation [2], aiming to solve the Hubbard model with a more practical approach. Large quantities of $NaCuF_3$ single crystals have been successfully synthesized using solid state chemistry methods. The samples were characterized in-house by means of x-ray powder diffraction and magnetic susceptibility measurements. Those experiments have suggested that rather than a single-band Hubbard model, this fluoride compound actually forms a low-dimensional quantum Heisenberg system with the superexchange pathway going through corner-sharing CuF_6 octahedra with an exchange strength about 17 meV.

Single crystal neutron diffraction experiments were performed and indicated a long range magnetic ordering at 18.85(1) K (FIG 1a). The excitation spectra revealed by recent inelastic neutron scattering experiment, has shown a two-spinon continuum at low temperature, characteristic of a well-isolated antiferromagnetic Heisenberg spin chain (FIG 1b). Details of the synthesis, experiments and interpretation will be presented.

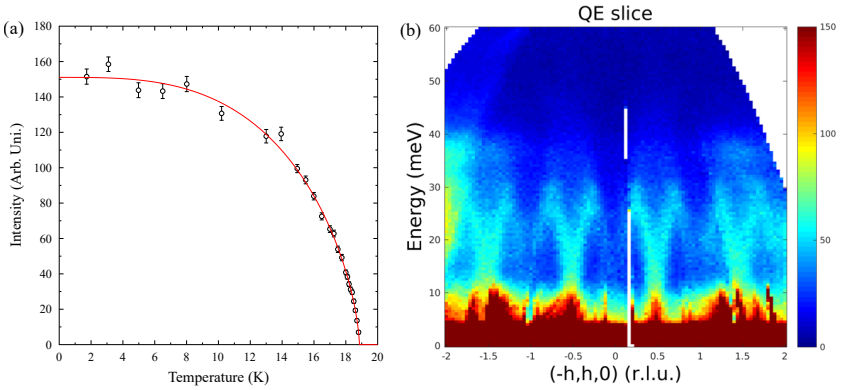

FIG. 1: (a) Extracted magnetic reflection intensity of (-0.5,0.5,0) as a function of temperature from single crystal diffraction experiment (ZEBRA, PSI). The red line represents as a critical fit and $T_N = 18.85(1)$ K. (b) Selected from the inelastic neutron scattering results (MERLIN, ISIS), the neutron intensity is displayed as a function of momentum and energy along the spin chain (-110) direction. Two spinon continuum spectra was observed.

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Studying nano-magnetism with small angle neutron scattering using a novel device for polarization analysis

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Magnetic neutron small angle scattering (SANS) with polarized neutrons and (uniaxial) polarization analysis is presently the only technique which allows one to resolve the spin microstructure on the nanometer length scale (1200 nm) and in the bulk of the magnet. Such experiments became only recently possible with the development of ^3He spin filters that allow the neutron spins from a divergently scattered beam to be analyzed. However, the size and sensitivity for magnetic field inhomogeneities of ^3He spin filters put restrictions on their application. Making use of a recent method of dynamic nuclear polarization (DNP) that employs photo-excited triplet states, we have developed an alternative spin filter based on polarized protons that requires only moderate experimental means, is small in size and insensitive to magnetic field inhomogeneities [1].

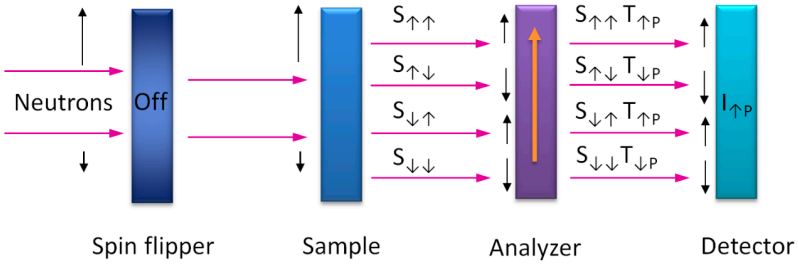

FIG. 1: A schematic drawing of the SANS spin analysis concept. Four channels ↑↑, ↓↓, ↑↓ and ↓↑ are measured to separate the contributions of the non-magnetic and the magnetic scattering of the same nanostructure.

Recently shell-ferromagnetism in Mn-rich antiferromagnetic Heusler-based compounds has been discovered that opens paths to possible functionalities [2]. We have investigated a martensitic Heusler $Ni_{50}Mn_{25}In_5$, which during high temperature annealing under magnetic field segregates and forms paramagnetic $Ni_{50}Mn_{25}In_{25}$ Heusler precipitates that are embedded in a antiferromagnetic $Ni_{50}Mn_{50}$ matrix. A preliminary analysis of the scattering results supports a core shell model that has been proposed to explain the strong shell-ferromagnetism [2]: at the interface with the $Ni_{50}Mn_{50}$ matrix the spins of the precipitate are strongly pinned in the direction of the field applied during annealing, whereas the core spins are paramagnetic.

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Co impurity modification of magnetic correlation in the spin ladder $Sr_{14}Cu_{24}O_{41}$

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Quasi one-dimensional cuprates have attracted a lot of interest due to their rich and unique magnetic and electronic properties. Recently, magnetic susceptibility measurements indicated that Co doping affects the quantum magnetism in the low-dimensional $Sr_{14}Cu_{24}O_{41}$ consisting of chains and ladders [1]. We investigated the effect of Co doping on the two-triplon excitations in the self-doped spin ladder subsystem of $Sr_{14}Cu_{24}O_{41}$ using Cu L_3-edge Resonant Inelastic X-ray Scattering (RIXS). It has previously been demonstrated that RIXS can effectively probe the spin excitations in such ladders [2]. As the intrinsic hole states have been confirmed to be playing a crucial role for the spin ladder [3-5], we followed the impurity-induced evolution of the spin excitations by investigating its correlation with the hole distribution. We observed that the Co-Cu atomic substitution leads to enhanced intensity and energy shift of the two-triplon continuum of the $Sr_{14}(Cu_{1-x}Co_x)_{24}O_{41}$, owing to the combined effect of Co doping and hole redistribution.

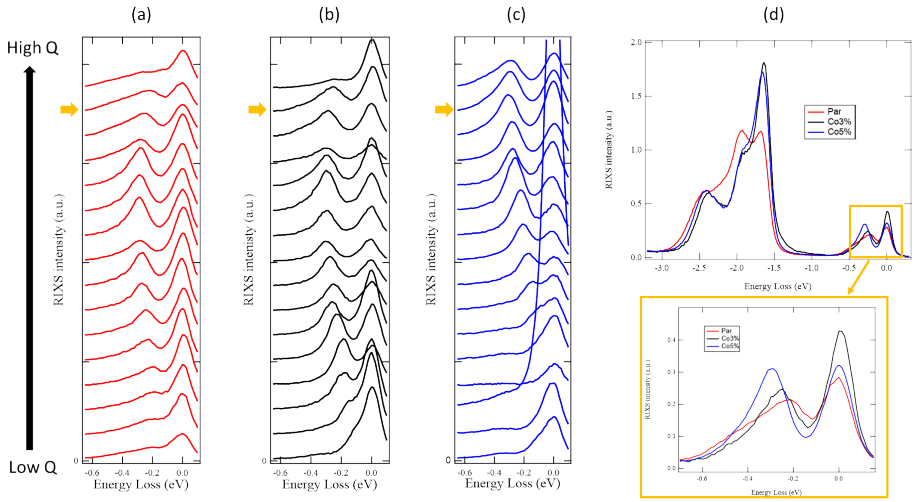

FIG. 1: (a)-(c) RIXS spectra with momentum transfer Q dependence (black arrow) showing two-triplon excitations of $Sr_{14}(Cu_{1-x}Co_x)_{24}O_{41}$ for x = 0, 0.03, and 0.05, respectively. (d) Comparison at Q corresponding to 76 % of the Brillouin zone (orange arrows) and a zoom into the low-energy region below 0 eV.

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Direct probe of magnetism at the γ-$Al_2O_3/SrTiO_3$ interface

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Interfaces between oxides attract tremendous interest as they exhibit a surprisingly colorful palette of physical properties including the emergence of gate-tunable conductivity[1], superconductivity[2], and magnetism[3, 4]. This opens up new opportunities for creating next-generation electronics. The most puzzling property is the magnetic order formed at the interface between non-magnetic insulating oxides such as $LaAlO_3/SrTiO_3$ (LAO/STO)[4] and γ-$Al_2O_3/SrTiO_3$ (GAO/STO). Despite intensive research, it is still poorly understood and challenging to reproduce. Benefiting from the chemical, orbital and orientation selectivity of x-ray dichroism techniques, X-ray Absorption and Magnetic Circular Dichroism (XAS/XMCD) measurements were carried out at the Ti $L_{2,3}$ absorption edges to better understating the magnetic order observed on both transport and scanning SQUID measurements[5]. The XMCD techniques have shown that a small magnetic signal is formed when γ-Al_2O_3 (GAO) is deposited on $SrTiO_3$ substrates (Fig. 1). Using the XAS/XMCD sum rules[6] we could suggest that the Ti 3*d* orbitals are carrying an orbital moment of approximately $m_{orb} = 0.028\ \mu_B$/Ti. This small magnetic moment at the Ti^{3+} ions is due to oxygen vacancies bring a sizable fraction of partially occupied 3*d* states. In addition, the shape of the Ti 3*d* orbitals are strongly influenced by the oxygen vacancy in which for the LAO/STO after the annealing process the linear and circular dichroism drops significantly to zero.

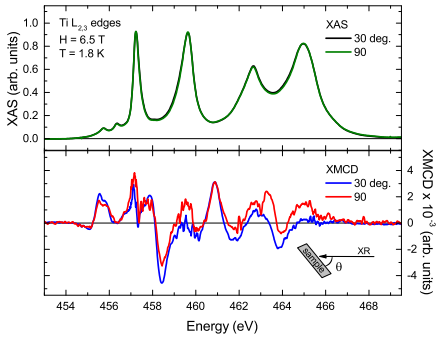

FIG. 1: XAS and XMCD spectra of GAO/STO obtained at 1.8 K and under H = 6.5 T at the Ti $L_{2,3}$ edges.

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Time-resolved imaging of the gyration dynamics of magnetic bubbles and magnetic skyrmioniums in materials with weak perpendicular magnetic anisotropy

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According to micromagnetic simulations, a rich magneto-dynamical behavior is expected when exciting magnetic bubbles and more complex magnetic structures such as the magnetic skyrmionium (or 2π state) e.g. through the application of a magnetic field gradient [1]. However, most of these simulations consider a perfect material without pinning sites, and usually assume a lower damping than those observed on the typical perpendicular magnetic anisotropy (PMA) materials where these magnetic states can be stabilized. The relatively high Gilbert damping (e.g. Pt/Co stacks exhibit damping values of about 0.2 [2]), and the high density of pinning sites (e.g. in Ref [3], one of the magnetic bubbles in the investigated structure is pinned), lead to strong challenges in the experimental observation of the magneto-dynamical behavior of the magnetic states stabilized in these materials. This has the consequence that only a few reported experimental works on the measurement of the magnetization dynamics of magnetic bubbles (e.g. [3, 4]) exist, and none on the dynamics of more complex structures such as the magnetic skyrmionium.

In this contribution, we present micromagnetic simulations and time-resolved measurements of the gyration dynamics in magnetic bubbles and magnetic skyrmioniums stabilized in nanostructured disks fabricated out of a NiFe-based system exhibiting a weak PMA. The gyration dynamics were excited by generating a magnetic field gradient through the injection of a current pulse through an omega-shaped antenna surrounding the nanostructured element.

Thanks to the low damping and low density of pinning sites of this PMA system, we were able to resolve multiple periods of the gyration orbit of the magnetic bubble and of the magnetic skyrmionium, proving that the PMA system employed here is extremely interesting for the investigation of the fundamental properties of complex magnetic and topological structures.

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The photoinduced transition in magnetoresistive manganites: a comprehensive view

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(Dated: October 19, 2017)

We use femtosecond x-ray diffraction to study the structural response of charge and orbitally ordered $Pr_{1-x}Ca_xMnO_3$ (PCMO) thin films across a phase transition induced by 800 nm laser pulses. By investigating the dynamics of both superlattice reflections and regular Bragg peaks, we disentangle the different structural contributions and analyze their relevant time-scales. The dynamics of the structural response are qualitatively different when excited above and below a critical fluence f_c. For excitations below f_c the charge order and the superlattice is only partially suppressed and the ground state recovers within a few tens of nanosecond via diffusive cooling. When exciting above the critical fluence the superlattice vanishes within approximately half a picosecond followed by a change of the unit cell parameters on a 10 picoseconds time-scale. At this point all memory from the symmetry breaking is lost and the recovery time increases by many order of magnitudes due to the first order character of the structural phase transition.

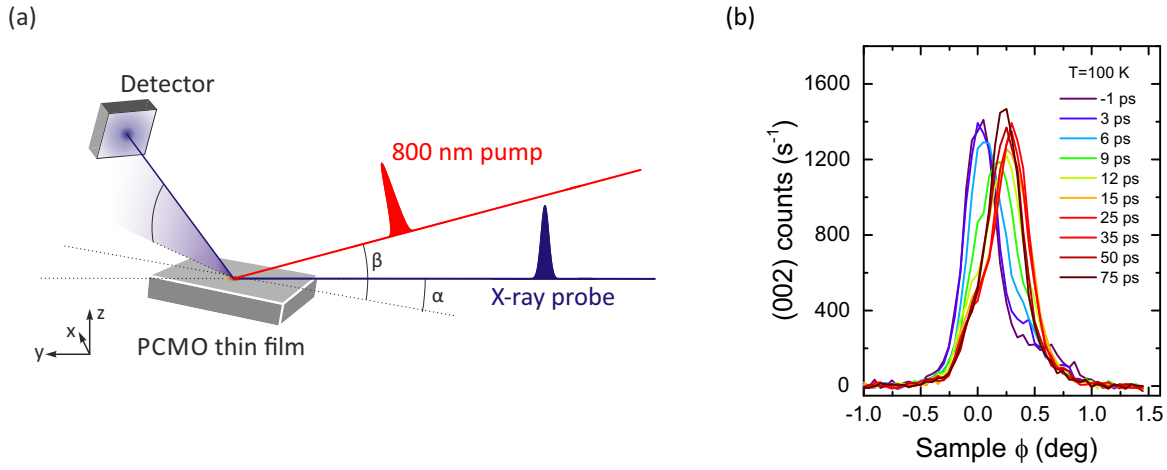

FIG. 1: (a) Experimental setup at the FEMTO slicing source in SLS. (b) Rocking curves of the (002) reflection at various time after excitation above the critical fluence f_c. The peak shift indicates a photo-induced change of the unit cell on a 10 ps time-scale.

Investigation of the metal-insulator transition in $NaOsO_3$ using resonant X-Ray diffraction

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In 5-d transition metal oxides, spin-orbit coupling becomes sizable and its interplay with e.g. the Coulomb interaction has led to the observation of exciting novel ground states. We report here on $NaOsO_3$, which has been proposed to be the first realization of a Slater insulator i.e. a system in which a metal-insulator transition is driven only by antiferromagnetic correlation. We employed Resonant X-ray Diffraction to elucidate the nature of the metal-insulator transition. By a careful study of forbidden reflections, we can exclude the presence of a structural crystallographic change at the phase transition. In addition, we observe an anomaly below the Neel temperature that is indicative of the Slater scenario.

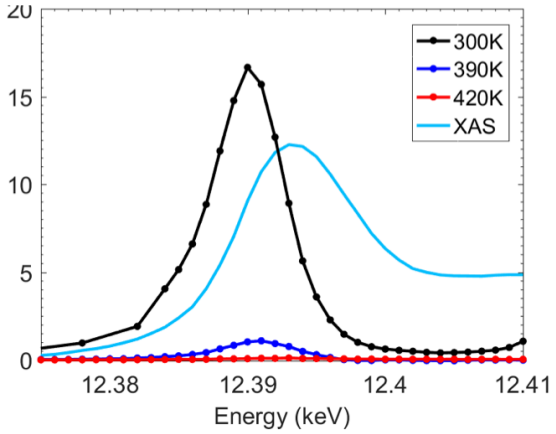

FIG. 1: Temperature dependence of the intensity of the (300) *forbidden* reflection (energy scan at fixed momentum transfer) and X-ray absorption spectrum across the Os L_2 edge, showing the occurrence of a magnetically induced modification in the electronic structure.

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Exploring the boundary between localized and itinerant behavior in rare earth nickelates (III)

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Rare earth nickelates (RNiO$_3$; R = 4f rare earth or Tl^{3+}) which have been of interest for scientists since a long time due to their electronic, magnetic and structural properties. The most significant feature of the RNiO$_3$ family ($R \neq La^{3+}$) is the temperature driven metal to insulator phase transition at critical temperature (T_{MIT}). The T_{MIT} systematically changes with the size of the R ion from 130 K (R = Pr) to 600 K (R = Lu). According to the diffraction studies, the transition is accompanied by subtle structural phase transition (the symmetry of the unit cell decreases from orthorhombic (SG $Pbnm$) to monoclinic (SG $P2_1/n$)) and occurs with charge reordering by the splitting of the unique, nominally Ni^{3+} site into two non-equivalent sites. The mechanism(s) at the origin of the MIT in this system has been the subject of an intense debate since its discovery. However, several experimental results such a gigantic ^{16}O - ^{18}O isotope effect on T_{MIT} point out towards a strong coupling between the lattice and the electronic degrees of freedom. The theoretical predictions of multiferroelectricity and superconductivity additionally triggered the interest by the system.

Up to now, a stabilisation of the formal, high, nickel (III) oxidation state, particularly for the compounds containing R ions smaller than Gd, was achieved by synthesis at high temperatures (up to 1000 °C) and at very high pressures (20 - 60 kbar). Such conditions limit the volume of the synthetized polycrystalline samples. A direct consequence is that many physical properties of the materials have been poorly or never investigated.

Detailed neutron powder diffraction study aimed to re-investigate and to interpret the evolution of the crystal structure of the first member of PrNiO$_3$ in terms of frozen normal distortion modes [1, 2] will be presented. Achievements of moderate oxygen pressure (2 kbar) synthesis, possibility of single crystal growth will be discussed.

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A local-probe perspective on correlated quantum matter

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As a local microscopic probe, magnetic resonance is a well established, complementary technique to those used in large-scale facilities, especially suitable for studying materials under demanding experimental conditions, including high magnetic fields, high pressures, ultra-low temperatures, etc., required to access quantum-critical behaviour.

In our work at the ETH condensed-matter laboratory we regularly make use of this potential to investigate strongly-correlated quantum matter with closely competing energy scales. In this *overview talk* we focus on some of our recent projects, including low-dimensional spin systems, non-centrosymmetric superconductors, two-dimensional antiferromagnets, as well as on ongoing investigations of quantum-spin liquids in honeycomb iridates, field-induced chirality in frustrated spin ladders, etc.

After illustrating the new possibilities opened by high-pressure, low-temperature NMR, we highlight our future projects and present possibilities for new collaborations.

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Surface and bulk magnetic gapping in the electronic structure of (V, Fe, Mn) doped BiTeI

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Magnetic doping of topological insulators (TIs) and Rashba systems characterized by enhanced spin-orbit coupling and helical spin structure leads to opening of an energy gap at the Dirac point and formation of new exotic topological quantum effects such as Quantum Anomalous Hall effects, topological surface-state magneto-electric effects and others and can be used in spintronics for manipulation of spin state and induced magnetization without external magnetic field [1]. Here we study magnetically doped polar semiconductor BiTeI with giant Rashba splitting and time-reversal symmetry breaking. BiTeI by itself has a hexagonal crystal structure and is built up of alternating layers of bismuth, tellurium, and iodine atoms stacked along the hexagonal axis. The continuous stacking order of the layers of the three atomic species breaks the inversion symmetry. Therefore, we study the time reversal symmetry breaking in magnetically doped BiTeI. Similar behavior of the surface states takes place in magnetically doped topological insulators [2, 3] the magnetic gap opens at the Dirac point. Combination of the Rashba and magnetic interaction with superconductivity using proximity effect can lead to topologically non-trivial superconductivity and Majorana fermion mode [4].

BiTeI is characterized by bulk and surface Rashba-like states, and thus below the Curie temperature we expect that the magnetic gap can open in both types of states. Measurements of these systems were made by means of UV-ARPES, during which it has been shown the presence of the gap with no zero density of states in the surface Rashba states with the value of 145 meV. In order to investigate the behavior of bulk states we had carried out the Soft X-ray Photoemission Spectroscopy (SX-ARPES). Thus the different photon energies were used to distinguish bulk and surface states. Using high energy that is sensitive to bulk it is possible to conclude with high accuracy that bulk Rashba states of the sample have no magnetic gap. To distinguish the role of the magnetic moment induced by ferromagnetic dopants, we will use V, Fe and Mn L2,3-edge resonant photoemission supported by Circular Dichroism absorption spectroscopy.

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Temperature vs pressure phase diagram of $FeSe_{1-x}S_x$ investigated using μSR

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Application of hydrostatic pressure to the iron based superconductor FeSe suppresses the nematic order and leads to the appearance of static magnetic order for pressures above 0.8 GPa [1]. At the same time, the superconducting T_c increases from 8 K at ambient pressure up to 37 K at approx. 7 GPa [2]. A recent study using high-pressure resistivity measurements suggests that isovalent S substitution for Se up to 17% leads to a faster suppression of the nematic phase while shifting the magnetic dome to higher pressures, which would lead to a complete separation of the two phases as a function of pressure [3]. Here, using muon spin rotation (μSR), we show however that static magnetism is already present at much lower pressures than previously thought in our slightly inhomogeneous sample with x ranging between 7% and 12%, although not with a full volume. In fact, the magnetism seems to develop already at a slightly lower pressure than for pure FeSe. While the relatively large spread of S content in our sample makes quantitative estimation of the ordered moment size difficult, our data clearly indicate an in-creasing moment with increasing pressure, as it has been observed for FeSe, too. This study shows the usefulness of local probe magnetic measurements as a complementary technique.

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The sound of the Q-phase in $CeCoIn_5$ - an ultrasound investigation of the symmetry of the order parameter

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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 complex order parameters [1]. Interesting, magnetic ordered states has been found at the border and unexpectedly completely deep within superconductivity, suggesting that the interplay between magnetism and superconductivity can be rather cooperative then competitive.

$CeCoIn_5$ is an intriguing example among this class of materials, with a $d_{x^2-y^2}$ order parameter. Superconductivity is Pauli limited and coexists with a spin density wave (SDW) at high fields, in the so called **Q**-phase. An additional symmetry breaking observed by the selection of magnetic domains was recently explained in terms of the emergence of a p-wave order parameter in the d-wave condensate [2]. However, the nature of the **Q**-phase is still debated. Since phonons can couple to the electronic structure at high frequencies- MHz [3], ultrasound is a suitable technique to investigate the translational symmetry breaking of the **Q**-phase, as well as phase transitions. So far, we were able to probe the two different domains of the SDW order, $\mathbf{Q}^{\pm}=(q,\pm q,0.5)$. The relative change in sound velocity ($\frac{\partial v}{v}$) reveal opposite signs of the anomaly observed at the transition from the **Q**-phase to the normal conducting phase for $\mathbf{Q}^{\pm}$. Quantum oscillations from 4T to higher fields are observed in $\frac{\partial v}{v}$, as well as in the attenuation (α). The HT-phase diagram was obtained from $\frac{\partial v}{v}$, demonstrating the sensitivity of ultrasound to the intriguing **Q**-phase.

These results encourage us to proceed with an angular dependence investigation and enhance our interest in having the ultrasound technique available at PSI. Intense study on its development is currently in progress.

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Extraordinary Materials: Magneto-Optic and Opto-Electronic Properties of Conjugated Polymers

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Conjugated Polymers (CPs) are organic macromolecules that are characterized by a backbone chain of alternating double- and single-bonds. The overlapping p-orbitals create a system of delocalized -electrons generating a number of remarkable properties. Another advantage of low-cost organic polymer-based materials lies in the modifiability on the molecular level resulting in optimized and customized applications. Therefore, CPs are for example increasingly attractive for future high-technology devices.

An overview of selected applications of CPs will be presented with special attention to magneto-optical properties, superconductivity and multiferriocs. The content is based on some topics of the review by *Timothy M. Swager* [1].

Polymer blends can act as donor and acceptor to create excitons by photoexcitation and exhibit a light-controlled ferroelectricity. Depending on the polymeric composition, the ratio between polarons and bipolarons can be tuned and is among others responsible for susceptibility properties.

Interestingly, magneto-optical Faraday-Rotation effect, which typically occurs in artificial inorganic crystals, can also be observed in CPs. Since classical theories are not applicable for the explanation of this effect in organic materials, novel theory approaches are favoured relating to the inter- and intramolecular structure of polymers.

Furthermore, there is one intrinsic metallic polymer, poly(sulfur nitride) SN_x, that also features superconductivity at low temperatures. The current state of polymer synthesis is promising for future design of intrinsically (super)conducting polymers.

Since the fascinating properties of CPs are closely linked to their intra- and intermolecular structure, current and future research will be focused on this relationship.

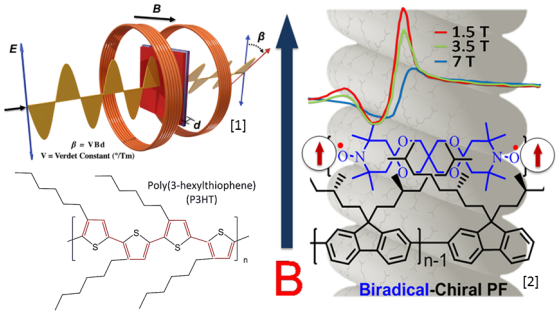

FIG. 1: The Farraday-Effect is one example of the unexpected properties of conjugated polymers.

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Toroidal seeds for investigation of heterogeneous crystal nucleation of colloids

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Toroidal seeds are ideal to investigate the effect of curvature on heterogeneous nucleation of colloids as a torus is positively curved on its outside and negatively curved on its inside. Due to surface tension toroidal droplets will either break [1] [2] into single droplets via the Rayleigh Plateau instabilities and/or shrink [2] to a sphere unless there is an opposing force that stabilizes them. This can be done in a yield stress material [3].

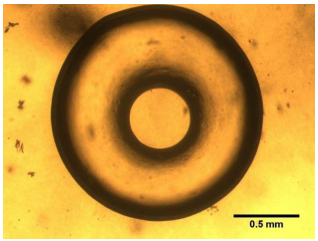

FIG. 1: Toroidal droplet in a yield stress material

Tori are made through the injection of a fluid into another immiscible material, while the two materials are in relative rotational motion. The process of making a torus can be seen as a 3D printing process, where a needles tip is printing into a suitable media. The outer continuous phase is chosen to be a yield stress material in order to stabilize the produced toroidal droplet against the instabilities due to surface tension. Tori can be made in water and oil based yield stress materials. Tori containing NIPAM (N-Isopropylacrylamide) monomers can be polymerized to produce stable toroidal hydrogels. Next the pNIPAM tori are transferred into a solvent in which colloidal particles can be studied.
Stable toroidal hydrogels of various sizes can be made using a 3D printer setup using an automatized stage (XPS Motion Controller and Linear Stages, Newport) and be used for heterogeneous nucleation studies using confocal microscopy.

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Solid state reactions via ball milling

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Ball milling is increasingly used for solid state reactions because of its advantages like high yields, high conversion rates, the easy handling, the small produce of waste and the good energy consumption.[1–3] Metal organic frameworks and cocrystals are the most studied materials. Nevertheless, the mechnisms behind mechanochemical reactions are still under investigation. Recently, setups were developed for monitoring mechanochemical reactions *in situ* using X-ray diffraction[4], Raman spectroscopy[5] or both combined.[6] In all setups the originally steel made milling jar is replaced by a plastic jar.

Here we present the first results of using ball milling for the synthesis of layered hybrid materials. The reactions are conducted as neat grinding in the vibration ball mill Pulverisette 23 (Fritsch GmbH, Germany). For the *in situ* investigations a new setup, developed at the MS beamline is used (Figure 1). Based on the original milling jars of the Pulverisette 23, the setup contains steel jars and a double movement of shaking and rotating. That allows high quality data because of the optimized sampling area.

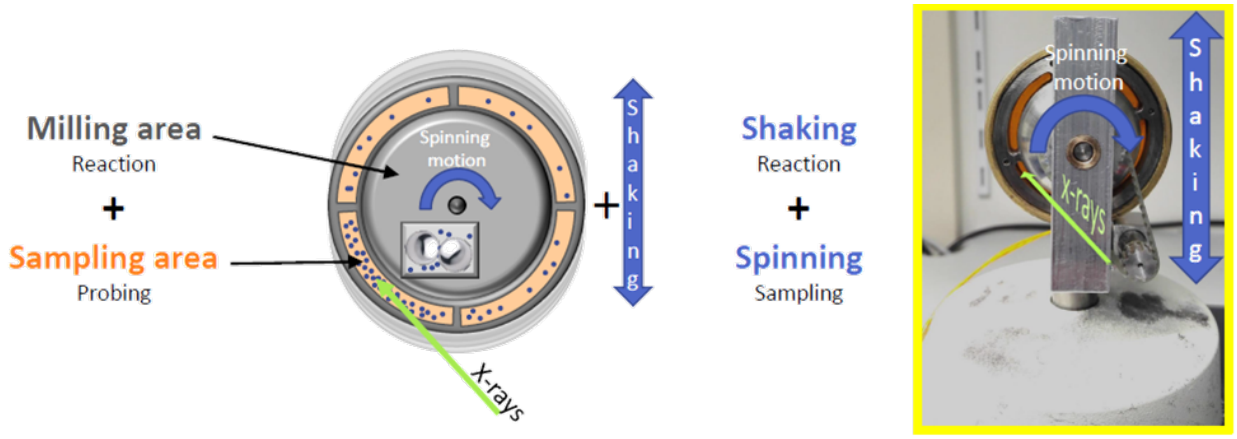

FIG. 1: New *in situ* setup for the investigation of mechanochemical reactions [7]

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High pressure synthesis of iron complex oxides in high oxidation state (Fe^{4+}, Fe^{5+}):mapping between localized and itinerant behavior

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In 1993 colossal magnetoresistance (CMR) was found in $La_{1-x}Ba_xMnO_3$ at the Curie point, where electrical resistance changes by orders of magnitude when a magnetic field is applied. Up to now, most of the known CMR materials are manganese based perovskites mostly $La_{1-x}Sr_xMnO_3$ or $SmBaMn_2O_6$ [1]. Analysis of the potential map that was proposed by Kamata et al. [2] suggests that CMR could also be obtained in $A_xB_{1-x}FeO_3$ (where A=Na, K, Rb and B= Ca, Sr, Ba) perovskites. These proposed iron based compounds should display similar electrical transport properties to the manganese perovskites being in vicinity to metal-insulator border line in the potential map. Additionally, both families should be isoelectronic: Fe^{4+} and Fe^{5+} have the same electron configuration as Mn^{3+} and Mn^{4+} in $La_{1-x}Sr_xMnO_3$. To stabilize these unusually high oxidation states, and to achieve oxygen stoichiometry, $Sr_{1-x}A_xFeO_3$ (A=Na, K) have been synthesized by using a unique oxygen high pressure (HP) system recently relocated and already successfully used in our lab [3]. This HP system allows precise control of temperatures (up to 1200 ^oC), gas pressures (up to 2000 bars) and large production of materials (cm^3). The synthesized materials are phase pure and have structure similar to the parent compound (space group $Pm\bar{3}m$). Measurements of the magnetic susceptibilities, electric properties and magnetic structure for these materials are currently underway.

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A new RIXS analyzer scheme based on transmission zone plates

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Resonant inelastic X-ray scattering (RIXS) is a rapidly developing X-ray spectroscopy technique with the capability to study elementary excitations of electrons, phonons and spins. With rapid progress in brilliance of X-ray sources as well as detection instruments, this technique is a trailblazer in experimental photon science. To date, RIXS instrumentation in the XUV and the soft X-ray range heavily relies on reflecting analyzer VLS gratings that collect the emitted light and disperse it across a detector. Unfortunately, such VLS gratings do not provide imaging capabilities, meaning that no information from the sample is conveyed along the non-dispersive direction of the detector. Therefore, only distributions of scattered photon energies in one direction on the detector can be measured, while the second direction on the detector remains unused.

In this contribution, we present a new analyzer scheme for RIXS, which is based on off-axis transmission Fresnel zone plates. This implementation provides the fundamental advantage of imaging capabilities, which allows for exploiting both directions on the detector. Hence, it opens up a variety of advanced two-dimensional mapping applications. By exciting the sample with a line focus of varying incident energy, we were able to record emission spectra over a range of excitation energies in a parallel manner. Thus, this new analyzer scheme enables efficient hv^2 spectroscopy possibilities. Moreover, by scanning a monochromatic line focus across the sample in one dimension, we efficiently recorded RIXS spectra spatially resolved in 2D. This novel analyzer scheme opens up a variety of new measurement possibilities including ultra-fast time resolved investigations at X-ray Free-Electron Laser Sources.

Study of the influence of doping on CCO

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In this work we studied the temperature dependence of the magnetic moments of doped CoCr2O4 (CCO) thin films, a well known multiferroic system[1]. The epitaxial thin films were grown at SLS using pulsed laser deposition (PLD) technique [2]. We present 2 different types of doping with various concentrations. In a first phase we looked at Fe doped CCO, which replaced atoms in both, Co and Cr sites. In the second phase we investigated the Ge doped CCO which replaced only Co atoms, since Ge prefers the tetrahedral configuration. The absorption measurements were performed at the Resoxs endstation at SIM beamline. In order to probe the magnetic moments, we performed XMCD in which we observed a strong signal at the L2,3 edges at T = 10 K. In addition, temperature dependence revealed a slight increase/decrease of the critical temperature (Tc) for the onset of total magnetic moment. These new findings provide us valuable information regarding how the doping material and its concentration influences the magnetic properties in this system.

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