5th Swiss-Sino Workshop

4th – 5th May, 2015
FHNW Brugg-Windisch
Switzerland

Sponsored by Swiss National Science Foundation

Organisers:
Paul Scherrer Institut: Shi Ming, Nolting Frithjof, Fueglister Martina (secretary)
Institute of Physics: Ding Hong, Yang Shulei (secretary)

Table of Contents

Daily Programme Monday 4th May 2015

FHNW Brugg-Windisch, Room 6.1H13

08:15 – 08:45	Matt Ch. & Shi M.	***Registration***
08:50 – 10:20	***Session 1***	***Chair Nolting Frithjof***
08:50 – 09:05	Mesot J. *PSI & EPFL & ETHZ*	Opening
09:05 – 09:30	Aeppli G. *PSI & EPFL & ETHZ*	Large research facilities at PSI and Photon Science
09:30 – 09:55	Xue Q-K. *Tsinghua U*	Molecular beam epitaxy-scanning tunneling microscopy of high Tc superconductivity
09:55 – 10:20	Patthey L. *PSI*	The New Femto Second X-ray Laser Source at PSI
10:20 – 10:50		***Coffee break***
10:50 – 12:30	***Session 2***	***Chair Fang Zhong***
10:50 – 11:15	Rice M. *ETHZ*	The Exotic Pseudogap Phase in the Cuprate Super-conductors
11:15 – 11:40	Wang Y. *Tsinghua U*	Electronic structure in parent and lightly doped cuprates studied by STM
11:40 – 12:05	Guguchia Z. *PSI & Zurich U*	Hydrostatic pressure and oxygen isotope effects on the static spin-stripe order and superconductivity in $La_{2-x}Ba_xCuO_4$ ($_X$ = 1/8)
12:05 – 12:30	Miao H. *IOP*	Observation of strong electron pairing on band without Fermi surface
12:30 – 14:00		***Lunch***
14:00 – 15:40	***Session 3***	***Chair Abela Rafael***
14:00 – 14:25	Normand B. *Renmin U*	Finite-temperature dynamics of highly frustrated quantum spin ladders
14:25 – 14:50	Rueegg Ch. *PSI & Geneva U*	Quantum Critical Points in Systems with Effective Singlet Ground-States
14:50 – 15:15	Fennell T. *PSI*	Emergent monopoles and photons in pyrochlore magnets
15:15 – 15:40	Sun L. & Zhao Z. *IOP*	Superconductivity emerging from suppressed large magnetoresistant state in WTe_2
15:40 – 16:10		***Coffee break***
16:10 – 17:50	***Session 4***	***Chair Xue Qi-Kun***
16:10 – 16:35	Zhou X. *IOP*	ARPES on $FeSe/SrTiO_3$ Films, Topological Insulators and Silicene
16:35 – 17:00	Biswas P. *PSI*	Superconducting and magnetic properties of single layer FeSe grown on STO revealed by Muon spin rotation spectroscopy
17:00 – 17:25	Dreiser J. *PSI & EPFL*	Lanthanide Single-Ion Molecular Magnets: Getting Control of the Molecule-Metal Interface
17:25 – 17:50	Vaz C. *PSI*	Inducing interfacial couplings in multiferroic heterostructures
19:15 – ~ 22:00	Hotel Blume Baden, l	***Pre-dinner drinks followed by workshop dinner***

Daily Programme Tuesday 5th May 2015

FHNW Brugg-Windisch, Room 6.1H13

08:40 – 10:20	***Session 5***	***Chair Aeppli Gabriel***
08:40 – 09:05	Zhoung F. *IOP*	Topological Semimetals
09:05 – 09:30	Ding H. *IOP*	Discovery of Weyl semimetal TaAs
09:30 – 9:55	Xu N. *PSI*	(S-)ARPES investigation on the electronic and spin structures of the first topological Kondo insulator: strongly correlated system SmB_6
09:55 – 10:20	White J. *PSI*	Electric Field-Induced Skyrmion Distortion and Giant Lattice Rotation in the Magnetoelectric Insulator Cu_2OSeO_3
10:20 – 10:50		***Coffee break***

10:50 – 12:30	***Session 6***	***Chair Dai Pencheng***
10:50 – 11:15	Jin Ch. *IOP*	Effects of Pressures on the Superconductivity of Strong Spin Orbital Coupling System
11:15 – 11:40	Pomjakushina E. *PSI*	High oxygen pressure synthesis of transition metal complex oxides at LDM – new instrumentation, first results, future plans.
11:40 – 12:05	Pedrini B. *PSI*	Achievements in 2D protein crystallography at the LCLS
12:05 – 12:30	Milne Ch. *PSI*	Exploring ultrafast chemical and biological reaction dynamics using X-ray techniques
12:30 – 14:00		***Lunch***

14:00 – 15:40	***Session 7***	***Chair Kenzelmann Michael***
14:00 – 14:25	Wang N.-L. *Peking U*	Density waves and superconductivity in $Na_2Ti_2Pn_2O$ (Pn=Sb, As) and $Ba_2Ti_2Fe_2As_4O$: an optical spectroscopy study
14:25 – 14:50	Morin M. *PSI*	Spiral order and ferroelectricity up to 200K in multiferroic $YBaCuFeO_5$: a neutron powder diffraction study
14:50 – 15:15	Gauthier N. *PSI*	Frustrated magnetism in the J_1-J_2 zig-zag chains of $SrDy_2O_4$ compound probed by neutron scattering
15:15 – 15:40	Beaud P. *PSI*	Resonant X-ray diffraction to study ultrafast phase changes in solid matter
15:40 – 16:10		***Coffee break***

16:10 – 17:50	***Session 8***	***Chair Wang Nan-Lin***
16:10 – 16:35	Schmitt Th. *PSI*	Probing the ground state oxygen holes and the metal-insulator transition in strained rare earth nickelate films with Resonant Inelastic X-ray Scattering
16:35 – 17:00	Sibille R. *PSI*	Spin Liquids in Novel Pyrochlore Materials Investigated using Large Facilities
17:00 – 17:25	Embs J.P. *PSI*	Cation Dynamics in Ionic Liquids as Seen by Quasielastic Neutron Scattering
17:25 – 17:50	Dai P. *IOP*	Electronic phase diagrams of Co, Ni, and P-doped $BaFe_2As_2$, and Cu-doped NaFeAs

17:50 – 18:00	Ding H. *IOP*	***Closing remarks***

Abstracts of talks:
Session 1

Large research facilities at PSI and Photon Science

Aeppli G.[1,2,3]
[1]*Paul Scherrer Institut, Villigen*
[2]*EPF Lausanne, Lausanne*
[3]*ETH Zurich, Zurich*

Abstract:
PSI photon science activities range from development of new accelerators to biology. Accelerator-based photon sources are placed in the context of other sources, some of which were also being developed at PSI, and the challenges and opportunities presented by free electron lasers are presented.

Notes:

Molecular beam epitaxy-scanning tunneling microscopy of high T_c superconductivity

Xue Qi-Kun[1]
[1]*Tsinghua University, Beijing*

Abstract:
Searching for superconducting materials with high transition temperature (T_C) is one of the most exciting and challenging fields in physics and materials science. By using molecular beam epitaxy (MBE) technique, we are able to prepare stoichiometric and superconducting FeSe single crystalline films on various substrates, which enables us investigate superconductivity mechanism of FeSe thin films in well-controlled way. Most importantly, by using scanning tunneling spectroscopy (STS), a superconductive gap as large as 20 meV and the vortex state under magnetic field are revealed in the single unit-cell thick FeSe films on $SrTiO_3$(001) substrate. Such an interface enhanced high T_c superconductor is further confirmed by recent transport measurements. The work not only demonstrates a way for finding new superconductors with high T_C, but also provides a well-defined platform for systematic study of the pairing mechanism of unconventional superconductivity by using different superconducting materials and substrates.

Notes:

The New Femto Second X-ray Laser Source at PSI

Patthey L.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
Paul Scherrer Institute is building an X-Ray Free Electron Laser (SwissFEL) facility, which will be in operation in 2017 and produce 20 fsec pulses of coherent x-rays in the wavelength range 0.1 to 7 nm, with extremely high peak brightness. These characteristics will provide opportunities for new experiments in chemistry, solid state physics, biochemistry and materials science. After a brief status report, the presentation will focus on novel applications, the description of the fundamental aspects of the planned facility with an emphasis on the photonics part of the project.

Notes:

Abstracts of talks: Session 2

The Exotic Pseudogap Phase in the Cuprate Superconductors

Rice T. M.[1, 2] *
[1]*ETH Zurich, Zurich*
[2]*Brookhaven National Laboratory, Brookhaven*

Abstract:
The transition from a full Fermi surface metallic state at overdoping to the Mott insulator at zero doping, proceeds through an intermediate pseudogap phase with many exotic properties. The opening of the pseudogap breaks up the continuous Fermi surface into 4 separate Fermi arcs (or anisotropic pockets). In addition, the pseudogap phase is characterized by a drop in superconducting Tc, which is preceded by an unusually wide temperature region of superconducting fluctuations reaching up to 3Tc. In recent years a Giant Phonon Anomaly was observed in this fluctuating region, which however disappears below Tc. Many theories have been proposed to explain these anomalies. In this talk I will discuss the role of increasing umklapp scattering as the Mott state is approached as the source of the Fermi surface breakup. This in turn can lead to enhanced fluctuations of the d-wave superconductivity which are responsible for the Giant Phonon Anomaly at T > Tc.

*Work done in collaboration with Y.H.Liu (Zhejiang U & ETH), F.C.Zhang (Zhejiang U), W.S. Wang & Q.H. Wang(Nanjing U).

Notes:

Electronic structure in parent and lightly doped cuprates studied by STM

Wang Y.[1]
[1] *Tsinghua University, Beijing*

Abstract:
Although the mechanism of superconductivity in the cuprates remains elusive, it is generally agreed that at the heart of the problem is the physics of doped Mott insulators. A crucial step for solving the high temperature superconductivity puzzle is to elucidate the electronic structure of the parent compound and the behaviour of doped charge carriers. In this talk we report recent scanning tunneling microscopy studies of the atomic-scale electronic structure of the parent and lightly doped cuprates in the antiferromagnetic insulating regime. In the parent $Ca_2CuO_2Cl_2$ Mott insulator, the full electronic spectrum across the Mott–Hubbard gap is uncovered for the first time. Defect-induced charge carriers are found to create broad in-gap electronic states that are strongly localized in space. In lightly doped Bi-2201 compounds, we show that the main effect of charge doping is to induce a spectral weight transfer from the high energy Hubbard band to the low energy in-gap states. At sufficiently high doping, a sharp energy gap starts to form near the Fermi level, and is accompanied by the emergence of a checkerboard-like charge order. Our results demonstrate that the first ordered phase in the doped Mott insulator is a charge ordered insulator, which will gradually evolve into the superconducting state upon further doping.

Notes:

Hydrostatic pressure and oxygen isotope effects on the static spin-stripe order and superconductivity in $La_{2-x}Ba_xCuO_4$ (x = 1/8)

Guguchia Z.[1,2], Khasanov R.[2], Pomjakushina E.[2], Conder K.[2], Bussmann-Holder A.[3], Shengelaya A.[4], and Keller H.[1]
[1]*University of Zurich, Zurich*
[2]*Paul Scherrer Institut, Villigen*
[3]*Max Planck Institute for Solid State Research, Stuttgart*
[4]*Tbilisi State University, Tbilisi*

Abstract:
Cuprate high temperature superconductors (HTS's) are characterized by a complex interplay between lattice, charge, and spin degrees of freedom, yielding several phases depending on doping level. One of the remarkable phases is a self-organized charge/spin structure, which is known as "stripes" and is observed in some cuprates near 1/8 doping [1]. In the simplest picture stripes are a periodic pattern of 1D charge and spin rivers formed in the 2D CuO_2 planes [2, 3]. Stripe formation involves modulations of charge and spin density. Note that there is no consensus on the microscopic mechanism of stripe formation and the relevance of stripe correlations for high-temperature superconductivity in cuprates at present. The stripes could be caused by purely electronic interactions and/or by a strong electron-lattice coupling.

Studies of the pressure and isotope effects are important to clarify the interplay between superconductivity and static stripe order as well as whether the lattice effects are involved in the formation of the stripe phase [4]. Hence, we studied the oxygen-isotope effects (OIE's) and hydro-static pressure effects on superconducting (SC) and magnetic states in the static stripe phase of 1/8doped $La_{2-x}Ba_xCuO_4$ (LBCO-1/8) by magnetization and muon-spin rotation (μSR) experiments [5]. A substantial OIE's on the SC and the magnetic quantities were observed. Upon replacing ^{16}O with ^{18}O, the SC ordering temperature T_c and the SC fraction V_{sc} decrease, while the static spin-stripe ordering temperature T_{so} and the magnetic volume fraction V_m increase. These results are the first demonstrations of the OIE on the magnetic state in the static stripe phase, suggesting that an electron-lattice interaction plays an important role for the stripes formation in cuprateHTS's. Different signs of observed OIE's for the magnetic and the SC states in LBCO-1/8 provide compelling evidence for a competition between super-conductivity and static magnetic order in the stripe phase of LBCO-1/8. Furthermore, our high-pressure μSR experiments on LBCO-1/8 demonstrated that static stripe order and bulk superconductivity occur in mutually exclusive spatial regions [6].

References:

[1] S.A. Kivelson et: al:, Rev. Mod. Phys. 75, 1201 (2003).
[2] O. Anegawa, et: al:, Phys. Rev. B 63, 140506 (R) (2001).
[3] J.M. Tranquada et: al:, Nature 375, 561 (1995).
[4] H. Keller and A. Bussmann-Holder, Advances in Condensed Matter Physics (2010).
[5] Z. Guguchia et: al:, Phys. Rev. Lett. 113, 057002 (2014).
[6] Z. Guguchia et: al:, New J. Phys. 15, 093005 (2013).

Notes:

Observation of strong electron pairing on band without Fermi surface

Hu M.[1]
[1] *Institute of Physics, Chinese Academy of Sciences, Beijing*

Abstract:
In conventional BCS superconductors, the quantum condensation of superconducting electron pairs is understood as a Fermi surface instability, in which the low-energy electrons are paired by attractive interactions. Whether this explanation is still valid in high-T_c superconductors such as cuprates and iron-based superconductors remains an open question. In particular, a fundamentally different picture of the electron pairs, which are believed to be formed locally by repulsive interactions, may prevail. Here we report a high-resolution angle-resolved photoemission spectroscopy study on $LiFe_{1-x}Co_xAs$. We reveal a large and robust superconducting gap on a band sinking below the Fermi energy upon Co substitution. The observed Fermi surface free superconducting order is also the largest over the momentum space, which rules out a proximity effect origin and indicates that the superconducting order parameter is not tied to the Fermi surface as a result of a Fermi surface instability.

Notes:

Abstracts of talks:
Session 3

Finite-temperature dynamics of highly frustrated quantum spin ladders

Normand B.[1]
[1]*Renmin University, Beijing*

Abstract:
Low-dimensional quantum magnets at finite temperatures present a complex interplay of quantum and thermal fluctuation effects in a restricted phase space. While some limited information about dynamical response functions is available from theoretical studies of the one-triplet dispersion in unfrustrated chains and ladders, little is known about the finite-temperature dynamics of frustrated systems. Experimentally, inelastic neutron scattering studies of the highly frustrated two-dimensional material $SrCu_2(BO_3)_2$ show an almost complete destruction of the one-triplet band at a temperature only 1/3 of the gap energy, accompanied by strong scattering intensities for apparent multi-triplet excitations.

We investigate these questions in the frustrated spin ladder and present numerical results from exact diagonalization for thermodynamic properties and for the dynamical structure factor as a function of temperature. We find significant broadening of the thermodynamic response and suppression of gap and mean energy scales due to the development of multi-triplet excitations, which are particularly low-lying near the quantum phase transition. In the dynamical response we find anomalously rapid transfer of spectral weight out of the one-triplet band and into both broad and sharp spectral features at a wide range of energies. These features are multi-triplet bound states, which are non-dispersive for strongly frustrated ladders and persist at all temperatures. Our results offer new insight into the finite-temperature spectral functions of $SrCu_2(BO_3)_2$ and of many other highly frustrated systems.

Notes:

Quantum Critical Points in Systems with Effective Singlet Ground-States

Rueegg Ch.[1, 2]
[1]*Paul Scherrer Institut, Villigen*
[2]*University of Geneva, Geneva*

Abstract:
Quantum systems with effective singlet ground-states of spin and orbital degrees of freedom have attracted considerable attention in recent years. The singlet may be formed by pairs of quantum spins that are antiferromagnetically coupled (S=0), by more sophisticated mechanisms involving spin-orbit coupling (J=0), or by dynamic processes involving e.g. the Jahn-Teller effect. Phases with various types of long-range spin or orbital order occur in these systems at a quantum critical point, which can be controlled by magnetic field [1-4] or pressure [5]. I will present recent results of experiments testing order, elementary excitations and quantum criticality by neutron scattering on materials with spin and orbital moments.

References:
[1] T. Giamarchi et al., Nature Physics 4, 198 (2008).
[2] B. Thielemann et al., Phys. Rev. Lett. 102, 107204 (2009).
[3] Y. Kohama et al., Phys. Rev. Lett. 109, 167204 (2012).
[4] F. Casola et al., Phys. Rev. Lett. 110, 187201 (2013).
[5] P. Merchant et al., Nature Physics 10, 373 (2014).

Notes:

Emergent monopoles and photons in pyrochlore magnets

Fennell T.[1,]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
The rare earth pyrochlores $R_2Ti_2O_7$ (R = Gd, Tb, Dy, Ho, Er, Tm, Yb) form one of the most interesting and best-studied series of frustrated magnets. The magnetism is due to the rare earth ions, which form a pyrochlore lattice, while the non-magnetic Ti^{4+} ions form a second interpenetrating pyrochlore lattice. The crystal structures are extremely well ordered and large single crystals can be grown, making these ideal model materials for studying various phenomena in frustrated magnetism. I will discuss the examples of R = Ho, Dy, which are the well known spin ices, and illustrate how their dynamics are controlled by an emergent quasiparticle with the properties of a magnetic monopole. I will also illustrate the natural extension of the classical spin ice model to the case including quantum fluctuations, when both monopoles and a collective spin excitation playing the role of the photon are possible. Candidate materials include $Yb_2Ti_2O_7$, and I will review the prospects for the realization of this state.

Notes:

Superconductivity emerging from suppressed large magnetoresistant state in WTe_2

Sun L., Zhao Z.[1,]
[1]*Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, Beijing*

Abstract:
The recent discovery of large magnetoresistance (LMR) in WTe_2 provides a unique playground to find new phenomena and significant perspective for potential applications. The LMR effect originates from a perfect balance of hole and electron carriers, which is sensitive to external pressure. Here we report the suppression of the LMR and emergence of superconductivity in pressurized WTe_2 via high-pressure synchrotron X-ray diffraction, electrical resistance, magnetoresistance, and *ac* magnetic susceptibility measurements. Upon increasing pressure, the positive LMR effect can be gradually suppressed without crystal structure change and turned off at a critical pressure of 10.5 GPa, where superconductivity emerges unexpectedly. The superconducting transition temperature reaches to 6.5 K at ~ 13 GPa and then decreases to 2.6 K at ~ 24 GPa. *In-situ* high pressure Hall coefficient measurements at low temperature demonstrate that elevating pressure decreases hole carriers but increases electron ones. Significantly, at the critical pressure, a sign change in the Hall coefficient is observed, indicating a quantum phase transition of the Fermi surface reconstruction.

In collaboration with Guangming Zhang and Youguo Shi.

Notes:

Abstracts of talks:
Session 4

ARPES on FeSe/$SrTiO_3$ Films, Topological Insulators and Silicene

Zhou X.[1]
[1]*Institute of Physics, Chinese Academy of Sciences, Beijing*

Abstract:
In this talk, I will report our angle-resolved photoemission work on the electronic structure and superconductivity of FeSe/$SrTiO_3$ films [1-4], as well as the electronic structure and spin texture of Bi_2Se_3 topological insulator [5]. I will also present our latest result on direct observation of Dirac cones in single-layer silicene/Ag(111) [6].

References:
[1] Defa Liu, Wenhao Zhang, Daixiang Mou, Junfeng He, Xucun Ma, Qikun Xue and X. J. Zhou et al., Nature Communications 3, 931 (2012);
[2] Shaolong He, Junfeng He, Wenhao Zhang, Lin Zhao, Xucun Ma, Qikun Xue and X. J. Zhou et al., Nature Materials 12, 605 (2013);
[3] Xu Liu, Defa Liu, Wenhao Zhang, Junfeng He, Xucun Ma, Qikun Xue and X. J. Zhou et al., Nature Communications 5, 5047 (2014);
[4] Junfeng He, Xu Liu, Wenhao Zhang, Lin Zhao, Xucun Ma, Qikun Xue and X. J. Zhou et al., PNAS. 111,18501 (2014).
[5] Zhuojin Xie, Shaolong He and X. J. Zhou et al., Nature Communications 5, 3382 (2014).
[6] Ya Feng, Defa Liu, Baojie Feng, Xu Liu and X. J. Zhou et al., arXiv:1503.06278.

Notes:

Superconducting and magnetic properties of single layer FeSe grown on STO revealed by Muon spin rotation spectroscopy

Biswas P.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
Single-layer FeSe thin films grown on $SrTiO_3$ substrates by molecular beam epitaxy, have shown remarkable superconducting properties with very large superconducting gap and higher T_c (65-70 K). Here, I will talk about or recent studies of single-layer FeSe film using low-energy (LE) muon spin rotation/relaxation (μSR) technique. Our results clearly demonstrate that a superconducting gap appears in single-layer FeSe below 65 K. Zero-field μSR data shows that the ground state is non-magnetic and rule out the possible existence of a magnetic gap in this system. Transverse-field (TF)-μSR results reveal that the observed superfluid density can be well described by a simple BCS s-wave model, indicates for nodeless superconducting state in the single-layer FeSe and is consistence with its bulk counterpart. At the end, I will also talk about our future projects in studying proximity effect at the interfaces of topological insulator/superconductor heterostructure using LE-μSR.

Notes:

Lanthanide Single-Ion Molecular Magnets: Getting Control of the Molecule-Metal Interface

Dreiser J.[1, 2]
[1]*EPF Lausanne, Lausanne*
[2]*Paul Scherrer Institut, Villigen*

Abstract:
Single-molecule magnets (SMMs) [1] are quantum objects exhibiting magnetic bistability, perfect monodispersity, and the possibility of tuning their properties by chemical functionalization. This makes them ideal candidates for classical or quantum information processing and data storage applications. Hence it is attractive to study SMMs and in particular mononuclear SMMs, so-called single-ion magnets (SIMs) [2,3], deposited as submonolayers on surfaces on which they can be addressed one-by-one, e.g., by a scanning tunneling microscope (STM) tip. Important questions that need to be answered are how SIMs can be efficiently organized on the surface and how magnetic properties of SIMs are modified by the interaction with the surface.

To this end we are investigating the Er(trensal) SIM (H_3trensal = 2,2′,2″-tris(salicylideneimino) triethylamine) [4–6] which exhibits an electron paramagnetic resonance-accessible ground-state Kramers doublet and attractive optical properties. In this contribution I will report on our results obtained by various X-ray spectroscopies revealing the magnetic and chemical properties of submonolayers of this SIM on metal surfaces [7].

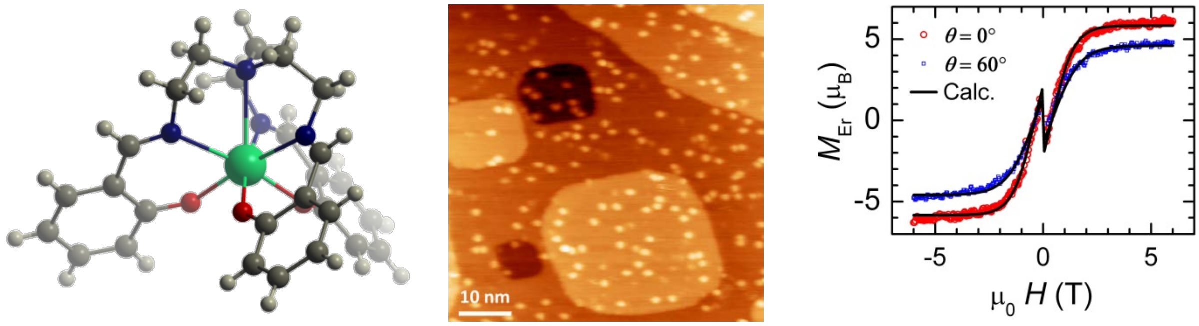

Figure 1. *(left) Molecular structure of the Er(trensal) molecule. Color code: Er: turquoise, N: blue, O: red, C: grey; H: white. (center) STM image of Er(trensal) molecules on a thin film of Ni on Cu(100). The surface coverage is 0.2 monolayers. Imaging conditions: 1.05 V, 60 pA. (right) Er spin and orbital magnetic moment M(H) from XMCD in normal and grazing incidence of the X-rays. The jump around zero field indicates an antiferromagnetic coupling between the Ni film and the molecules.*

References:
[1] D. Gatteschi, R. Sessoli, and J. Villain, Molecular Nanomagnets (Oxford University Press, 2006).
[2] N. Ishikawa, M. Sugita, T. Ishikawa, S. Koshihara, and Y. Kaizu, J. Am. Chem. Soc. 125, 8694 (2003).
[3] J. Dreiser, J. Phys.: Condens. Matter (2015), in press.
[4] B. M. Flanagan, P. V. Bernhardt, E. R. Krausz, S. R. Lüthi, and M. J. Riley, Inorg. Chem. 40, 5401 (2001).
[5] K. S. Pedersen, L. Ungur, M. Sigrist, A. Sundt, M. Schau-Magnussen, V. Vieru, H. Mutka, S. Rols, H. Weihe, O. Waldmann, L. F. Chibotaru, J. Bendix, and J. Dreiser, Chem. Sci. 5, 1650 (2014).
[6] E. Lucaccini, L. Sorace, M. Perfetti, J.-P. Costes, and R. Sessoli, Chem. Commun. 50, 1648 (2014).
[7] J. Dreiser, C. Wäckerlin, M. E. Ali, C. Piamonteze, F. Donati, A. Singha, K. S. Pedersen, S. Rusponi, J. Bendix, P. M. Oppeneer, T. A. Jung, and H. Brune, ACS Nano 8, 4662 (2014).

Notes:

Inducing interfacial couplings in multiferroic heterostructures

Vaz C. A. F.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
There is presently much interest in phenomena which are induced at the interface of artificial heterostructures, where changes in the local coordination, the break in symmetry, and the consequent modications in the electronic structure, result in strong deviations from the bulk properties or to the onset of new characteristics that are intrinsic to the interface [1]. One example is the onset of a magnetoelectric coupling effect across the interface between ferromagnetic and ferroelectric layers, mediated either by charge, spin-exchange, or strain [2,3]. In this talk, I will present results on the multiferroic behaviour of artificial heterostructures based on complex oxide films, whose sensitivity to external parameters, such as charge carrier density and strain, leads to large modulations of the magnetic and electronic state as a function of the applied electric field. In addition, our recent results of the role of strain and doping on the magnetic and transport properties of $La_{1-x}Sr_xMnO_3$ thin films at near half doping show the existence of a very strong sensitivity of the electronic state to strain in this doping range [4], showing that strong modulations in the magnetic state can be achieved with modest applied strains. Such a direct control over the electronic structure is expected to result in time responses that are much faster than typical magnetic precession times.

References:
[1] C. A. F. Vaz, F. J .Walker, C. H. Ahn, and S. Ismail-Beigi. Intrinsic interfacial phenomena in manganite heterostructures. J. Phys.: Condens. Matter, 27:123001, 2015.
[2] C. A. F. Vaz. Electric field control of magnetism in multiferroic heterostructures. J. Phys.: Condens. Matter, 24:333201, 2012.
[3] C. A. F. Vaz, J. Hoffman, C. H. Ahn, R. Ramesh. Magnetoelectric coupling effects in multiferroic complex oxide composite structures. Advanced Materials, 22:2900, 2010.
[4] C. A. F. Vaz, J. A. Moyer, D. A. Arena, C. H. Ahn, and V. E. Henrich. Magnetic and electronic structure of ultrathin $La_{1-x}Sr_xMnO_3$ films at half doping. Phys. Rev. B, 90:024414, 2014.

Notes:

Abstracts of talks:
Session 5

Topological Semimetals

Fang Z.[1]
[1] *Institute of Physics, Chinese Academy of Sciences, Beijing*

Abstract:
Topological semimetals, characterized by Weyl/Dirac nodes in the bulk and Fermi arcs on the surfaces, are new states of three-dimensional (3D) quantum matters, different from topological insulators. Weyl nodes are stable topological objects, and can be viewed as effective magnetic monopoles in the 3D momentum space. Its time-reversal invariant version ---- 3D Dirac node, however, consists of two copies of distinct Weyl nodes with opposite chirality, and requires additional symmetry protection, such as the crystal symmetry. Novel properties, such as negative magneto-resistance and non-local transport, can be expected for such semimetals, due to the presence of chiral anomaly. Recently, several Dirac semimetal (Na_3Bi and Cd_3As_2) and Weyl semimetal ($HgCr_2Se_4$ and TaAs) compounds have been predicted and experimentally verified. In this talk, I will review the theoretical progress with focus on the predictive roles of first-principles calculations in this field. Some recent experimental progress will be also addressed.

Notes:

Discovery of Weyl semimetal TaAs

Ding H.[1]
[1] *Institute of Physics, Chinese Academy of Sciences, Beijing*

Abstract:
Weyl semimetals are recently predicted a class of materials that can be regarded as 3D analogs of graphene breaking time reversal or inversion symmetry. While the bulk band structure of a Weyl semimetal contains pairs of Weyl nodes formed by single-spin-degeneracy 3D Weyl cones, the surface state displays pairs of entangled Fermi arcs at two opposite surfaces. However, the existence of Weyl semimetals has not yet been proved experimentally. In this talk I will report the experimental realization of a Weyl semimetal in TaAs by observing pairs of 3D Weyl cones in the bulk states and Fermi arcs formed by the surface states using ARPES. Our first-principles calculations, matching remarkably well with the experimental results, further confirm that TaAs is a Weyl semimetal.

Notes:

(S-)ARPES investigation on the electronic and spin structures of the first topological Kondo insulator: strongly correlated system SmB_6

Xu N.[1], Biswas P. K.[1], Dil J. H.[3], Dhaka R. S.[1,3], Landolt G.[4], Muff S.[4], Matt C. E.[1], Shi X.[1,2], Plumb N. C.[1], Radović M.[1], Pomjakushina E.[1], Conder K.[1], Amato A.[1], Borisenko S.V.[5], Yu R.[2], Weng H.-M.[2], Fang Z.[2], Dai X.[2], Mesot J[1,3]., Ding H.[2] and Shi M.[1]

[1]Paul Scherrer Institut, Villigen

[2]Institute of Physics, Chinese Academy of Sciences, Beijing

[3]EPF Lausanne, Lausanne

[4]University of Zurich, Zurich

[5]IFW Dresden, Dresden

Abstract:

Recent theoretical investigations have suggested SmB_6, in which electrons are strongly correlated, can possibly host topological nontrivial surface states with a true insulating bulk, forming a special group of TIs known as topological Kondo insulators. The truly bulk insulating behavior of SmB_6 make it possible for applications as spintronic materials, and for creation of exotic novel phenomena like Majorana fermions. Furthermore, the strong correlation in SmB_6 enable it serve as an ideal platform for the systematic study of the interplay between novel topological quantum states with emergent effects and competing order induced by strongly correlated electrons.

Our high-resolution ARPES study [1] revealed that the two dimensional surface states reside within the Kondo band gap (20 meV relative to E_F), and form three Fermi surfaces in the first surface Brillouin zone (SBZ), one is centered at the SBZ ($\bar{\Gamma}$ point) and two (viewed as four half-Fermi surfaces) encircle the midpoints of the SBZ boundaries ($\bar{X}$ points). The odd number of surface bands crossing the Fermi level fulfills the necessary condition of topologically nontrivial surface states, and the observed surface state dispersions are in good agreement with theoretical calculations of the topologically non-trivial states, indicating that SmB_6 could be a topological Kondo insulator. Using spin-resolved ARPES (SARPES), we investigated the spin texture of the surface states around the X points in the SBZ of SmB_6 [2]. The surface states are spin polarized with strong *k* dependence, and the spin-helical structure fulfills the requirement of time-reversal symmetry. Our results prove that SmB_6 is the first realization of strongly correlated topological Kondo insulator. Exotic Kondo crossover in a wide temperature region (30 ~ 110 K) is also carefully investigated by high resolution ARPES [3]. We also studied another rare earth hexaboride YbB_6 [4], which is predicted to be a correlated TI too. Our (S-)ARPES results indicate that spin polarized topological surface states do exist in YbB_6. The bulk states of YbB_6 are also probed by the bulk sensitive soft X-ray ARPES, which suggest a distinct topological mechanism (*d-p* band inversion) in YbB_6.

References:

[1] N. Xu et al. Phys. Rev. B 88, 121102(R) (2013).
[2] N. Xu et al. Nat. Commun. 5, 4566 (2014).
[3] N. Xu et al. Phys. Rev. B 90, 085148 (2014).
[4] N. Xu et al. arXiv:1405.0165 (2014).

Notes:

Electric Field-Induced Skyrmion Distortion and Giant Lattice Rotation in the Magnetoelectric Insulator Cu_2OSeO_3

White J.S.[1,3]. Prša K.[1], Huang P.[1], Omrani A. A.[1], Živković I.[2], Bartkowiak M.[1], Berger H.[3], Magrez A.[3], Gavilano J. L.[1], Nagy G.[1], Zang J.[4] and Rønnow H. M.[1]
[1]*Paul Scherrer Institut, Villigen*
[2]*Institute of Physics, Bijenička, Zagreb*
[3]*EPF Lausanne, Lausanne*
[4]*Johns Hopkins University, Baltimore*

Abstract:
Skyrmions are magnetic spin vortex-like objects that can be stabilized in chiral magnets with Dzyaloshinskii-Moriya (DM) interactions. Due to their topological property and nanometric size (~10–100 nm), Skyrmions presently attract attention as candidate components of new spin-based applications. Key to their implementation in real devices is the ability to control their motion. Indeed, spin-transfer torques generated by either magnon currents, or ultra-low electric currents, are well-established to cause Skyrmion motion. Despite these breakthroughs, it remains of paramount importance to discover new control mechanisms which may also be considered for use in efficient Skyrmion-based functionalities.

Among the known Skyrmion lattice host materials, Cu_2OSeO_3 is the only insulator. This makes Cu_2OSeO_3 a model system in which to explore the control of Skyrmions in the absence of conduction electrons. Importantly Cu_2OSeO_3 also displays a magnetoelectric coupling, which allows the mutual control of the electric and magnetic degrees of freedom via the application of a single controlling electric or magnetic field. Taken together, these properties naturally raise the unique prospect of addressing questions concerning the ability to manipulate Skyrmions using electric fields, this being more efficient than using electric currents that are subject to resistive losses.

Here, we explore the electric field coupling to the magnetoelectric Skyrmion lattice phase and study the response using small-angle neutron scattering. Taking advantage of a novel experimental protocol, giant electric field-induced rotations of the Skyrmion lattice are achieved that span a range of ~25°. Our data can be well-described by the expectations of an analytic model which shows that an electric field-induced Skyrmion distortion lies behind the lattice rotation. Overall, we present a new approach to Skyrmion control that makes no use of spin-transfer torques due to currents of either electrons or magnons.

Reference:
[1] J.S. White et al., Phys. Rev. Lett. 113, 107203 (2014)

Notes:

Abstracts of talks: Session 6

Effects of Pressures on the Superconductivity of Strong Spin Orbital Coupling System

Jin C.[1]
[1]*Institute of Physics, Chinese Academy of Sciences, Beijing*

Abstract:
Systems of strong spin orbital coupling (SOC) attract growing attention because of many novel physical properties including topological quantum states as well as Rashiba phase. Pressure can be very effective to tune the quantum states related to SOC. We will introduce our recent works on SOC compounds especially addressing pressure induced superconductivity in this presentation.

We thank our collaborators for their significant contributions.

References:

[1] X.C. Wang, CQJet al, Solid State Communications 148, 538 (2008)
[2] P. P. Kong, CQJ et al, J. Phys.Condens. Matter 25, 362204 (2013) (Fast Track Communications)
[3] J. J. Wu, J. F. Lin, CQJ et al. Scientific Reports | 4 : 3685 | (2014)
[4] Q.Q. Liu, CQJ et al., J. Am. Chem. Soc. 133, 7892 (2011)
[5] J. L. Zhang, CQJ et al., Proc. Natl Acad. Sci. 108, 24 (2011)
[6] J. Zhu, J. L. Zhang, CQJ et al., Scientific Reports |3 : 2016(2013) | DOI: 10.1038/srep02016
[7] J.J. Wu, J.F. Lin, CQJ et al., Proc Natl Acad Sci 110, 17263 (2013)
[8] P.P. Kong, CQJ et al., Scientific Reports | 4: 6679 (2014)

Notes:

High oxygen pressure synthesis of transition metal complex oxides at LDM – new instrumentation, first results, future plans

Pomjakushina E.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
In my talk I will present a short overview of scientific activity of the Solid State Chemistry Group at LDM, PSI. In particular I will speak about a high oxygen pressure synthesis apparatus recently installed in our group. This setup allows reaching up to 2000 bars of oxygen and temperature of 1200C, which makes possible synthesizing 3, 4 and 5d transition metal complex oxides, where transition metals are stabilized in high or even exotic oxidation states. One of the first successful examples is $Tm_2Mn_2O_7$ pyrochlore, which was synthesized and studied by neutron powder diffraction.

The rare earth manganese (IV) pyrochlores cannot be synthesized at ambient pressure requiring high pressures for the stabilization of the pyrochlore lattice, which is mainly due to the small size of Mn IV compared to trivalent rare earth cations. The reported successful synthesis of $A_2Mn_2O_7$ (A= Y,Tl) by Fujinaka [1] were done in the range 1000-1100 C and pressures 3-6GPa, at pressures 5-8GPa and temperatures 1000-1500 C (A=Sc, Y, In, Tl, Tb-Lu) [2] and A=Y, Dy-Lu by hydrothermal method in sealed gold ampules at 0.3 GPa and 500 C [3]. Later Shimakawa et al. [4] used a hot isostatic press apparatus at 1000–1300 C and only 0.4 kbar for the series A=In, Y, and Lu. All of these materials appear to be ferromagnets and in spite of the variety of preparative conditions, the agreement among the various groups for the structural parameters is excellent, suggesting that sample to sample compositional variation is small [5]. Neutron studies of some selected $A_2Mn_2O_7$ (Y,Ho, Yb) were done, but still more work is needed to understand fully their magnetic ground state.

In our recent work [6] we present yet another chemical way of synthesis of $Tm_2Mn_2O_7$ pyrochlore and the studies of its magnetic properties and crystal structure. Neutron powder diffraction study performed at the high-resolution HRPT diffractometer at SINQ neutron spallation source (PSI, Switzerland) has shown, that the resulting compound has a pure pyrochlore cubic phase $Tm_2Mn_2O_7$ (space group Fd-3m) at room temperature. On cooling below 30K there is a transition to a ferromagnetically ordered phase with additional antiferromagnetic canting suggesting the lowering of crystal symmetry to tetragonal one. The magnetic transition is accompanied by well visible magnetostrsiction effect.

At the end our future projects will be also briefly mentioned.

References:
[1] H. Fujinaka, N. Kinomura, M. Koizumi, Y. Miyamoto, and S. Kume, Mater. Res. Bull. 14, 1133 (1979)
[2] I.O. Troyanchuk, V.N. Derkachenko, and E.F. Shapovalova, Phys. Stat. Sol. (a) 113, K243 (1989)
[3] M.A. Subramanian, C. C. Toradi, D. C. Johnson, J. Pannetier, A. W. Sleiht. J. Solid State Chem. 72, 24 (1988)
[4] Y. Shimakawa, Y. Kubo, N. Hamada, J. D. Jorgensen, Z. Hu, S. Short, M. Nohara, and H. Takagi, Phys. Rev. B 59, 1249 (1999).
[5] Jason S. Gardner, Michel J. P. Gingras, John E. Greedan REVIEWS OF MODERN PHYSICS 82, JANUARY–MARCH (2010)
[6] E. Pomjakushina, K. Rolfs, V. Pomjakushin, J. Karpinski and K. Conder, to be published

Notes:

Achievements in 2D protein crystallography at the LCLS

Pedrini B.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
Most high-resolution protein structures have been obtained by X-ray diffraction of three-dimensional crystals. Especially for membrane proteins, two-dimensional crystals may however offer a more close-to-physiological environment for the protein molecules. Indeed, the lipids that connect the molecules mimic the natural environment on the cell membrane. Until recently, X-ray diffraction on two-dimensional protein crystals data was out of reach, because, due to the very limited diffraction power, radiation damage occurs much before sufficient diffraction signal can be accumulated. Therefore, meaningful experiments on two dimensional crystals could be conducted only by electron microscopy at cryogenic temperatures (cryo-EM), which is more favorable from the point of view of radiation damage.

X-ray free electron lasers (X-FELs), which have become operational after 2009, nowadays provide a mean to overcome the damage limitation by exploiting the “diffract-before-destroy” concept, which has already been applied extensively to three-dimensional crystals. Because of the ultrashort and ultraintense pulses, the diffraction signal is generated with sufficient signal-to-noise ratios before the sample is damaged. The success achieved in particular with submicrometer sized crystals triggered us to attempt the analog experiment with the even weaker diffracting two-dimensional protein crystals. We report here on the results from beamtimes at the CXI experimental station of the Linac Coherent Light Source X-FEL. The measurements were performed on bacteriorhodopsin two-dimensional crystal samples, kept at almost physiological conditions within a sugar layer. The collected data demonstrate that the samples diffract to at least 4 Å. However, given the weakness of the measured Bragg reflection, it appears that significant progress towards high resolution structure determination depends on substantial increase of the per-pulse X-ray intensity delivered to the sample. The findings will be discussed in the light of the complementarity of cryo-EM and X-FEL techniques, which highlights the role of the latter for time-resolved and room temperature investigations.

Notes:

Exploring ultrafast chemical and biological reaction dynamics using X-ray techniques

Milne Ch.[1], Szlachetko J.[1], Knopp G.[1], Czapla-Masztafiak J G.[1], Penfold T.[1], Patterson B.[1] and Abela R.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
X-ray free electron lasers (XFELs) are 4th-generation X-ray sources, which produce very large numbers of x-ray photons (10^{11}-10^{12}) in very short pulse durations (1-100 femtoseconds).[1] This makes them ideal for certain types of experiments, including time-resolved pump-probe experiments[2,3], single-shot experiments[4], and nonlinear x-ray experiments[5]. The Swiss hard X-ray free electron laser SwissFEL started construction at the Paul Scherrer Institute in late 2012, with a planned startup date of 2017 for the ARAMIS hard x-ray undulator section. In this talk I will present an overview of the design of Experimental Station A (ESA), which will be the first experimental station to come online in early 2017.[6] This instrument is designed to investigate ultrafast photochemical and photobiological processes using a range of X-ray techniques, including both scattering and spectroscopy. I will also present examples of our recent research where we have applied these techniques to investigate the nature of ultrafast charge-trapping in photoexcited metal-oxide semiconductor nanoparticles and to identify the long-lived electronic states responsible for the photochemical activity of these functional materials[7]. I will conclude with an outlook on how we expect ESA to allow researchers to perform investigations into a variety of fields, with a specific focus on ultrafast photobiology using a unique combination of tender X-ray spectroscopy in the 2-5 keV photon energy range and serial femtosecond crystallography[8].

References:
[1] C. Pellegrini and S. Reiche, in Digital Encyclopedia of Applied Physics (Wiley-VCH Verlag GmbH & Co.KGaA, 2003).
[2] C. J. Milne, T. J. Penfold, and M. Chergui, Coordination Chemistry Reviews 277, 44 (2014).
[3] P. Beaud, S. L. Johnson, E. Vorobeva, C. J. Milne, A. Caviezel, S. O. Mariager, R. A. De Souza, U. Staub, and G. Ingold, Chimia 65, 308 (2011).
[4] J. Szlachetko, C. J. Milne, J. Hoszowska, J. C. Dousse, W. Błachucki, J. Sa, Y. Kayser, M. Messerschmidt, R.Abela, S. Boutet, C. David, G. Williams, M. Pajek, B. D. Patterson, G. Smolentsev, J. A. van Bokhoven, and M. Nachtegaal, Struct. Dyn. 1, 021101 (2014).
[5] K. Tamasaku, E. Shigemasa, Y. Inubushi, T. Katayama, K. Sawada, H. Yumoto, H. Ohashi, H. Mimura, M.Yabashi, K. Yamauchi, and T. Ishikawa, Nature Photonics 8, 313 (2014).
[6] B. D. Patterson, P. Beaud, H.-H. Braun, C. Dejoie, G. Ingold, C. J. Milne, L. Patthey, B. Pedrini, J. Szlachetko,and R. Abela, Chimia 68, 73 (2014).
[7] M. H. Rittmann-Frank, C. J. Milne, J. Rittmann, M. Reinhard, T. J. Penfold, and M. Chergui, Angew. Chem.Int. Ed. 53, 5858 (2014).
[8] J. C. H. Spence, U. Weierstall, and H. N. Chapman, Rep Prog Phys 75, 102601 (2012).

Notes:

Abstracts of talks:
Session 7

Density waves and superconductivity in $Na_2Ti_2Pn_2O$ (Pn=Sb, As) and $Ba_2Ti_2Fe_2As_4O$: an optical spectroscopy study

Wang N.-L.[1]
[1]*Peking University,Beijing*

Abstract:
We present an optical spectroscopy study on single crystals of $Na_2Ti_2Pn_2O$ (Pn=Sb, As) and $Ba_2Ti_2Fe_2As_4O$. $Na_2Ti_2Pn_2O$ (Pn=Sb, As) are sister compounds of superconducting titanium oxypnictide $Na_2Ti_2Sb_2O$ and have the density wave (DW) ground state, while $Ba_2Ti_2Fe_2As_4O$ is a newly discovered superconductor showing a coexistence of superconductivity and DW order. The study reveals significant spectral weight changes and formation of energy gaps across the DW phase transitions in those compounds. The ratio of the DW energy gap over the transition temperature, $2\Delta/_{kB}T_{DW}$, is considerably larger than the mean-field value of BCS weak-coupling theory. For the compound of $Ba_2Ti_2Fe_2As_4O$, further spectral change associated with the superconducting condensate was identified. The low frequency optical conductivity could be well modeled within the Mattis-Bardeen approach with two isotropic energy gaps. The study reveals that the superconducting properties of $Ba_2Ti_2Fe_2As_4O$ are similar to those of $BaFe_{1.85}Co_{0.15}As_2$.

Work done with Y. Huang, Y. G. Shi, H. P. Wang, T. Dong, X. B. Wang, R. Y. Chen, Y. L. Sun and G. H. Cao.

Notes:

Spiral order and ferroelectricity up to 200K in multiferroic $YBaCuFeO_5$: a neutron powder diffraction study

Morin M.[1], Scaramucci A.[1,2], Bartkowiak M.[1], Pomjakushina E.[1], Deng G.[1,3], Sheptyakov D.[1], Keller L.[1], Rodriguez-Carvajal J.[4], Spaldin N.A.[1,2], Kenzelmann M.[1] Conder K.[1] and Medarde M.[1]
[1]*Paul Scherrer Institut, Villigen*
[2]*ETH Zurich, Zurich*
[3]*Bragg Institute, ANSTO, Lucas Heights Australia*
[4]*Institut Laue Langevin, Grenoble*

Abstract:
The discovery of materials where magnetic and ferroelectric orders are strongly coupled has raised a great deal of interest in view of its possible use in data storage technologies. Nevertheless, while their potential for applications was rapidly recognized, the possibility of combining ferroelectricity with ferromagnetism has been obscured by two facts: on one side, most of them are antiferromagnetic, on the other, their transition temperatures, typically below 40K, are too low for most practical applications.

The oxygen-deficient double perovskite $YBaFeCuO_5$ constitutes a remarkable exception. Spontaneous electric polarization has been recently reported to exist below an unusually high temperature of $T_C \approx$ 240K [1] coinciding with the occurrence of a commensurate - to - incommensurate reorientation of the Fe^{3+} and Cu^{2+} magnetic moments [2,3]. From a more fundamental point of view the observation of incommensurable magnetic order in a tetragonal material at such high temperatures is rather surprising. In particular, the nature of the relevant competing magnetic interactions and its possible link to low dimensionality or geometrical frustration is not understood at present.

Although the existence of the spin reorientation in this material is known since 1995 [2], the low temperature incommensurate magnetic structure has not been reported. Using neutron powder diffraction we have recently been able for the first time to propose a spiral model - which satisfactorily reproduces the observed magnetic intensities below T_C [3]. Further, investigation of the crystal structure showed the existence of small anomalies in the lattice parameters and some interatomic distances at T_C. The relevance of these findings for the magnetoelectric coupling, the direction of the polarization, the modification of the different exchange paths in the structure and the stabilization of the incommensurate magnetic order below T_C will be discussed.

References:
[1] B. Kundys et al., Appl. Phys. Lett. 94, 072506, (2009).
[2] V. Caignaert et al., J. Solid State Chem. 114, 24, (1995).
[3] M. Morin et al., Phys. Rev. B 91, 064408 (2015)

Notes:

Frustrated magnetism in the J_1-J_2 zig-zag chains of $SrDy_2O_4$ compound probed by neutron scattering

Gauthier N.[1], Fennell A.[1], Désilets-Benoît A.[2], Prévost B.[2], Bianchi A.D.[2], Niedermayer C.[1], Zaharko O.[1], Frontzek M.[1], Baines C.[1], Ollivier J.[3], Regnault L.-P. [3], Nilsen G.[3], and Kenzelmann M.[1]
[1]*Paul Scherrer Institut, Villigen*
[2]*Université de Montréal, Montréal*
[3]*Institut Laue Langevin, Grenoble*

Abstract:
Competing interactions in geometrically frustrated magnets can lead to ground states with large degeneracies and open the way to novel states of matter. Compounds of SrR_2O_4 family (*R*=Gd, Tb, Dy, Ho, Er, Tm and Yb) have first been pointed out to be candidates for frustrated magnetism in 2005[1]. Since then, various interesting properties have been observed in these systems: spinliquid- like groundstates, coexistence of two different magnetic orderings, low-dimensional correlations, magnetization plateaus and magnetic field induced order.

Zig-zag chains in the structure are thought to be an important source of frustration in these compounds. The physics in the zig-zag chains is equivalent to a 1D chain with nearest neighbor J_1 and next-nearest neighbour J_2 interactions, usually called Ising J_1-J_2 chain model[2]. The presence of two inequivalent rare earth sites in the structure probably leads to the coexistence of two different orders in compounds such as $SrHo_2O_4$ and $SrEr_2O_4$[3,4].

The $SrDy_2O_4$ compound is especially interesting because it does not feature long range order down to 50 mK, thus showing a high degree a frustration. Different neutron scattering techniques have been used to characterize the low temperature properties of $SrDy_2O_4$ and to understand the absence of long range order. Diffuse scattering indicates short range correlations mainly along the c-axis originating from only one of the two inequivalent sites. Inelastic neutron scattering reveals the presence of a dispersive crystal field level and a gap opening at 60 mK, whose origin is not understood at present. Under applied field, a 1/3 magnetization plateau has previously been observed. This field-induced phase features a propagation vector consistent with the up-up-down state expected from theory.

References:
[1] H. Karunadasa et al. Physical Review B 71, 144414 (2005).
[2] A. Fennell et al., Physical Review B 89, 224511 (2014).
[3] O. Young et al., Physical Review B 88, 024411 (2013).
[4] T. Hayes, et al. Physical Review B 84, 174435 (2011).

Notes:

Resonant X-ray diffraction to study ultrafast phase changes in solid matter

Beaud P.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
Strongly correlated electron systems exhibit very strong interactions between structural and electronic degrees of freedom leading to complex phase diagrams that show technologically highly relevant properties. These properties are often intrinsically related to symmetry changes of the atomic lattice and to intriguing ordering patterns of the spins, orbitals and charges. Therefore the study of long range order using diffraction techniques has been for many years an essential tool for the characterization of correlated materials. Recent developments in ultrashort x-ray sources now open the opportunity to extend these techniques into the femtosecond time domain to directly study the coupling between the lattice and the electronic subsystems as they develop in time. One goal of these studies is to advance our understanding of the underlying correlations, another to find ways using ultrashort pulses of light to control the technologically highly relevant properties of these materials on an ultrafast time scale [1-3].

An extreme example is the so-called `ultrafast' phase transition, where a persistent symmetry change is induced by a sudden impulsive interaction from a laser pulse lasting only a few femtoseconds. In this case, different coordinates of the phase transformation, that in equilibrium are tightly linked to the conventionally defined order parameter, can undergo quite different dynamics. To address this issue, we investigated the dynamics of the ultrafast phase transition in an epitaxially grown film of $Pr_{0.5}Ca_{0.5}MnO_3$, a perovskite-type manganite. Here the application of an intense optical pulse induces an ultrafast insulator-to-metal transition [3]. Initial diffraction experiments performed at the SLS slicing source demonstrated a concomitant change of structural symmetry occurring on a sub-picosecond time scale [4-5]. In a recent experiments at the LCLS free electron laser we were not only able to study in more detail the lattice dynamics, but also the changes in long-range order of the electronic subsystems by tuning the x-ray energy ‘to’ and ‘off’ an atomic resonance [6]. We find that although the actual change in crystal symmetry associated with this transition occurs over different timescales characteristic of the many electronic and vibrational coordinates of the system, the dynamics of the phase transformation can be well described using a single time-dependent ‘order parameter’ that depends exclusively on the electronic excitation.

References:

[1] D. Fausti et al., Science 331, 6014 (2011).
[2] T. Kubacka et al., Science 343, 1333 (2014).
[3] D. Polli et al., Nature Mater. 6, 643 (2007).
[4] P. Beaud et al, Phys. Rev. Lett. 103, 155702 (2009).
[5] A. Caviezel et al., Phys. Rev. B 86, 174105 (2012); Phys. Rev. B 87, 205104 (2013).
[6] P. Beaud et al., Nature Mater. 13, 923 (2014).

Notes:

Abstracts of talks: Session 8

Probing the ground state oxygen holes and the metal-insulator transition in strained rare earth nickelate films with Resonant Inelastic X-ray Scattering

Schmitt Th.[1], Bisogni V.[1], Catalano S.[2], Gibert M.[2], Scherwitzl R.[2], Huang Y.[1], Strocov V.[1], Zubko P.[2], Green R.J.[3], Balandeh S.[3], Sawatzky G.[3] and J Triscone J.-M.[2]
[1]*Paul Scherrer Institut, Villigen*
[2]*University of Geneva, Geneva*
[3]*University of British Columbia, Vancouver*

Abstract:
The metal-insulator transitions (MIT) and the intriguing magnetic properties of rare-earth perovskite nickelates have attracted considerable attention in recent years. Nonetheless, a complete understanding of these materials remains elusive, in particularly due to the difficulties in describing their electronic ground state (GS). Taking compressive and tensile strained $NdNiO_3$ thin film as representative examples, we utilize soft x-ray spectroscopy to investigate the electronic structure across the MIT and the complex electronic GS properties of the nickelates.

High-quality epitaxially strained $NdNiO_3$ films of 30nm thickness were prepared by off-axis radiofrequency magnetron sputtering on a variety of substrates and were fully characterized by x-ray diffraction measurements, atomic force microscopy, transport and soft x-ray scattering measurements.

By combining results from x-ray absorption (XAS) and resonant inelastic x-ray scattering (RIXS) at the Ni L_3-edge, we clearly identify the coexistence of strong spectral contributions from both localized bound and delocalized continuum states in all samples, contrasting with earlier studies which suggested the XAS spectra to be dominated by local multiplet excitations. Furthermore, we disentangled the continuum features into charge transfer and electron-hole excitations, suggesting the latter to arise due to the presence of a ground state containing holes in the oxygen 2p band. The electron-hole excitations were shown to gain spectral weight in the low energy loss regime above the metal-insulator transition temperature and extend down to zero energy.

Using an Anderson impurity model interpretation, we show that these distinct spectral signatures arise due to the presence of a unique Ni $3d^8$ ground state along with holes in the formally full oxygen valence band ($Ni3d^8\underline{L}$), confirming suggestions that these materials exhibit a negative charge transfer energy gap which is closely linked to their unusual properties. In this scenario the MIT is realized by a bond disproportionation leading to two Ni sites, i.e. $Ni3d^8$ and $Ni3d^8\underline{L}^2$, differing in the hybridization with the O 2p hole states yet leaving the charge at the nickel sites almost equal.

Notes:

Spin Liquids in Novel Pyrochlore Materials Investigated using Large Facilities

Sibille R.[1]
[1]Paul Scherrer Institut, Villigen

Abstract:
Insulating pyrochlore oxides, denoted by the general formula $A_2B_2O_7$ where A is a rare-earth magnetic ion and B is a transition metal ion or a group IV ion, have attracted much attention because both A and B sites form a network of corner-sharing tetrahedra, a wonderful landscape for the study of magnetic frustration in three dimensions. The case of rare-earth ions having a strong uniaxial anisotropy constrained to be pointing along the <111> direction of the cubic unit-cell (Pr^{3+}, Tb^{3+}, Dy^{3+}, Ho^{3+}) reverses, in theory, the roles of ferromagnetic and antiferromagnetic couplings with regard to frustration: the ferromagnetic case becomes highly frustrated, and can lead to the spin ice state, while the antiferromagnetic one is not frustrated. However, pyrochlore Ising antiferromagnets have proved able to markedly defy these expectations of long-range ordering. A famous example is the enigmatic terbium titanate, $Tb_2Ti_2O_7$, which forms a so-called spin liquid state with power-law correlations and magnetoelastic excitations. I will firstly present ongoing investigations on the Hafnium analogue of this compound, which displays striking similarities with its historical counterpart despite the existence of a substantial amount of disorder. Secondly, I will show recent results on the largely unexplored case of a Ce^{3+} pyrochlore. In particular, I will demonstrate that $Ce_2Sn_2O_7$ is characterized by an isolated Kramers doublet at low temperature, and that this leads to a system of small Ising magnetic moments on the pyrochlore lattice. In this material, antiferromagnetic exchange interactions one order of magnitude larger than the expected ferromagnetic dipolar couplings strongly suggest that the correlated dynamical ground state which is retained down to 20 mK finds its origin in enhanced quantum fluctuations.

Results from the PSI large scale facilities (SINQ, SμS, SLS) will be used to illustrate a prospective materials approach having the aim of discovering and characterizing novel spin liquid states.

Notes:

Cation Dynamics in Ionic Liquids as Seen by Quasielastic Neutron Scattering

Embs J. P.[1]
[1]*Paul Scherrer Institut, Villigen*

Abstract:
Ionic Liquids (ILs) as a class of compounds have aroused a burgeoning scientific interest in the past decades due to their benign properties for many present and potential industrial applications: high thermal stability and electrochemical stability, negligible vapor pressure, wide liquid range, non-flammability under ambient conditions, good solvents for polar solutes, and tunable catalytic ability. The properties of ionic liquids result from a complex interplay of intermolecular interactions between ions, their geometry and charge distribution. All possible universal (Coulomb, van der Waals, dipole-dipole) and specific (for example H-bonding) intermolecular interactions can define the behaviour of ILs. A structural variation of the cation or anion may lead to a new IL with targeted functionality ("designer solvents"). Quasielastic neutron scattering (QENS) and inelastic neutron scattering (INS), which have been demonstrated to be an informative tool for studying different materials, can be applied to yield comprehensive information about various stochastic processes in ILs. Incoherent neutron spectroscopy is particularly sensitive to hydrogen atoms and can be applied to unravel the dynamics of hydrogen-rich materials. Moreover, the (E,Q)-range covered in QENS and INS corresponds to the range probed in molecular dynamic simulations, so that this experimental method can be used to prove the accuracy of computations.

In my talk I will review our recent results obtained on dedicated ILs. I will demonstrate which dynamical processes can be observed in ILs presenting results from QENS and backscattering experiments.

Notes:

Electronic phase diagrams of Co, Ni, and P-doped $BaFe_2As_2$, and Cu-doped NaFeAs

Dai P.[1]
[1]*Institute of Physics, Chinese Academy of Sciences, Beijing*

Abstract:
In this talk, I will speak about our recent experiments determining the electronic phase diagrams of iron pnictide superconductors. We use X-ray, neutron scattering and NMR experiment to establish universal phase diagrams of electron-doped and isovalent doped iron pnictides, and reveal an avoided quantum critical point. Furthermore, we show that Cu-doped NaFeAs induces an insulating antiferromagnet near 50%, suggesting the presence of a Mott insulator near iron pnictide superconductors.

Notes:

List of Participants

PSI: Paul Scherrer Institut, Switzerland

(last name, first name)

Abela Rafael
Aeppli Gabriel
Beaud Paul
Biswas Pabitra Kumar
Dreiser Jan
Embs Jan Peter
Fennell Tom
Gauthier Nicolas
Guguchia Zurab
Kenzelmann Michel
Matt Christian
Mesot Joël
Mickael Morin
Milne Chris
Nolting Frithjof
Patthey Luc
Pedrini Bill Francesco
Pomjakushina Ekaterina
Rice T. Maurice
Rüegg Christian
Schmitt Thorsten
Shi Ming
Sibille Romain
Vaz Carlos
White Jonathan
Xu Nan

IOP: Institute of Physics, Chinese Academy of Sciences, China

(last name, first name)

Dai Pengcheng
Ding Hong
Fang Zhong
Hu Miao
Jin Changqing
Normand Bruce
Sun Liling
Wang Yayu
Wang Nan-Lin
Xue Qi-Kun
Zhou Xingjiang