I: Theory

Chair: Frédéric Mila, EPF Lausanne

16:30 601 Spin-orbit dimers in double perovskites

George Jackeli, FMQ, University of Stuttgart, Pfaffenwaldring 57, DE-70569 Stuttgart

In Mott insulators, unquenched orbital degrees of freedom often frustrate the magnetic interactions and lead to a plethora of interesting phases with unusual spin patterns or non-magnetic states without long-range order. Here, we present a theoretical study of interplay of spin and orbital degrees in double-perovskite compounds with d1 ions occupying the fcc sub-sublattice. We show that the ground state of such a system is non-magnetic dimer pseudo-spin singlet with extensive orientational degeneracy of dimers. We discuss how the pseudo-spin state forming the singlet is altered upon increasing the strength of the relativistic spin-orbit coupling and show that the dimer 'gas' phase remains the ground state throughout. Our theoretical findings support and explain the experimentally observed non-magnetic amorphous valence bond state in Ba2YMoO6 and in related compounds.

17:15 602 First-principles simulations of the electronic and magnetic structure of iridates

Vladimir Mazurenko, Ural Federal University, Mira 19, RU-620002 Ekaterinburg
Igor Solovyev, National Institute for Materials Science, 1-1 Namiki, JP-305-0044 Tsukuba, Ibaraki

The theoretical description of 5d transition metal oxides is a complex computational and methodological problem requiring a whole arsenal of modern numerical techniques. We present the results of density functional theory calculations on the ground state properties of Ba2IrO4, Sr2IrO4 and Sr3Ir2O7. A strong sensitivity of the calculated band structures to the particular magnetic ordering is revealed. We show that the magnetic polarization of the oxygen states plays an important role in formation of the weak ferromagnetism in Sr2IrO4. The pressure-driven insulator-metal transition in Sr3Ir2O7 is analyzed. We discuss recently developed methods for calculating magnetic couplings in the iridates.

18:00 603 Triangular lattice Ising antiferromagnets with long-range interactions: application to Ba3CuSb2O9 and nano-magnet arrays

Andrew Smerald, Frederic Mila, Institute of Physics, EPFL, Rte de la Sorge, 1015 Lausanne

We explore long-range coupled, triangular-lattice, Ising antiferromagnets, concentrating on two examples: the crystal structure of Ba3CuSb2O9, which is thought to support a spin-orbital liquid state, and 2D arrays of nano-magnets. In Ba3CuSb2O9 we suggest that Cu atoms realise stripe-like correlations at short length scales, resulting in a "branch" lattice, and potentially favouring delocalised orphan spins. In nano-magnet arrays we show that an equilibrated system displays a first-order phase transition to a stripe state. However, in reality this is likely avoided in favour of the formation of a glassy state, in part due to a set of topological constraints.

Postersession and Apéro

Public Lecture
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<td>611</td>
<td>Exotic magnetism produced by strong spin-orbit coupling in complex Ir oxides</td>
<td>Hidenori Takagi, Max Planck Institute for Solid State Research, Heisenberg Str. 1, 70659 Stuttgart</td>
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In 5d Iridium oxides, a large spin-orbit coupling of ~0.5 eV, inherent to heavy 5d elements, is not small as compared with other relevant electronic parameters, including Coulomb U, transfer t and crystal field splitting D, which gives rise to a variety of exotic magnetic ground states. In the layered perovskite Sr$_2$IrO$_4$, spin-orbital Mott state with J$_{eff}$ = 1/2 is realized due to the novel interplay of those energy scales [1-3]. Despite the strong entanglement of spin and orbital degrees of freedom, J$_{eff}$ = 1/2 iso-spins in Sr$_2$IrO$_4$ was found to be surprisingly isotropic, very likely due to a super-exchange coupling through almost 180° Ir-O-Ir bonds [4]. The temperature dependence of in-plane magnetic correlation length of J$_{eff}$ = 1/2 iso-spins, obtained from inelastic x-ray resonant magnetic scattering, was indeed well described by that expected for two-dimensional S = 1/2 Heisenberg antiferromagnet [5].


| 17:15 | 612 | Disentangling orbital and magnetic contributions to the exotic Spin Peierls transition in TiPO$_4$ | Marcus Dantz 1, Clemens Wagner 2, Jonathan Pelliciari 1, Jan Trinckaut 2, Xingye Lu 1, Yaobo Huang 1, Xu Lei 2, Liviu Hozoi 1, Jeroen van den Brink 2, Thorsten Schmitt 1
1 Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI
2 Leibniz Institute for Solid State and Materials Research, IFW, DE-01069 Dresden |

We investigate the quasi-one dimensional spin chain compound TiPO$_4$, which has been reported to undergo an exotic spin-Peierls transition that is coupled to a orbital reconstruction [1,2]. We investigate this behavior by using high resolution resonant inelastic x-ray scattering (RIXS) which can probe the involved spin, orbital and lattice excitation simultaneously. By combining RIXS with state of the art quantum chemical calculations, we can identify the orbitals involved and measure the magnetic exchange constant and spin gap directly, settling a conflict in recent literature.


| 17:45 | 613 | Magnetic excitations in the partially stuffed CuO planes of Ba$_2$Cu$_3$O$_4$Cl$_2$ | Sara Fatale 1, Claudia Fatuzzo 1, Peter Babkevich 1, Thorsten Schmitt 2, Henrik Ronnow 1, Marco Grioni 1
1 Institute of Physics, EPFL, Station 3, 1015 Lausanne
2 PSI, 5232 Villigen PSI |

Recent RIXS measurements on edge-sharing tetragonal CuO [1] (fully stuffed planes) show spin waves with the same overall symmetry of corner-sharing cuprates [2] (normal stuffed planes) but with strongly renormalized energies. Boosted by these results, we investigated the spin waves of Ba$_2$Cu$_3$O$_4$Cl$_2$ by Cu L$_3$ edge RIXS. Ba$_2$Cu$_3$O$_4$Cl$_2$ has partially stuffed Cu$_3$O$_4$ layers obtained via the addition of Cu ions to the usual CuO$_2$ planes in a checkerboard pattern. We measured a recovery in the energy of the spin waves and discuss the implication on the description of cuprates.

Asymmetry of collective excitations in ambipolar Y_{0.38}La_{0.62}(Ba_{0.82}La_{0.18})_2Cu_3O_y

Xingye Lu 1, Yaobo Huang 1, Marcus Dantz 1, Jonathan Pelliciari 1, Daniel McNally 1, Shengwei Zeng 2, Vladimir Strocov 1, Ariando Ariando 2, Thorsten Schmitt 1

1 Paul Scherrer Insitut, 5232 Villigen-PSI
2 Department of Physics, National University of Singapore, NUSNNI-Nanocore, Level 11, T-lab building, 5A, Engineering Drive 1, SG-117411 Singapore

We use Cu-L3 RIXS to study the electron-hole asymmetry in cuprates by measuring the doping dependent collective excitations of both electron- and hole- doped Y_{0.38}La_{0.62}(Ba_{0.82}La_{0.18})_2Cu_3O_y, where metal-to-insulator transition (MIT) are realized in both sides. RIXS show clear electron-hole asymmetry in charge ordering and collective excitations. In the hole-doped regime, charge ordering has been observed in superconducting samples with magnetic excitations being heavily damped. The electron-doped samples do not show charge ordering and spin excitations are less damped. Moreover, an extra mode centered at q = 0 appears in the electron doped regime close to the MIT.

Thursday, 25.08.2016, Room A 21

Time | ID |  III: EXPERIMENTS 2  
Chair: Johan Chang, Uni Zürich

11:15 621 Magnetic correlations and implications for topological order in Sm_2Ir_2O_7

Des McMorrow, UCL, LCN, London WC1E6BT, UK

The rare-earth pyrochlore iridates (R_Ir_2O_7, R=rare earth) have been proposed to host a number of exotic electronic states as a consequence of the existence of strong spin-orbit coupling of the Ir^{4+} ion in the presence of significant electron correlations. Of crucial importance to understanding whether any of these states can be realized in practice is to determine the effective low-energy Hamiltonian describing the system. Here we report a comprehensive series of resonant X-ray experiments, both elastic (REXS) and inelastic (RIXS), which reveal the nature of the magnetic order and excitations in single crystals of Sm_2Ir_2O_7.

12:00 622 Orbital Selective Mott Physics in Ca_2RuO_4:
An Angle Resolved Photoemission Spectroscopy Study

Denys Sutter 1, Johan Chang 1, Titus Neupert 1, Fabio Cossalter 1, Claudia Fatuzzo 2, Rosalba Fittipaldi 3, Alfredo Vecchione 4, Marco Grioni 2, Tay-Rong Chang 4, Gianmarco Gatti 2, Nicholas Plumb 5, Ming Shi 5, Christian Matt 5, Moritz Hoesch 6, Timur Kim 6, Henrik Rønnow 2

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2 EPFL, Institute for Condensed Matter, 1015 Lausanne
3 Università di Salerno, Dipartimento di Fisica, IT-84084 Salerno
4 National Tsing Hua University, Departement of physics, 300 Hsinchu City, Taiwan
5 Paul Scherrer Institut, Swiss Light Source, 5232 Villigen
6 Diamond Light Source, Harwell Science & Innovation Campus, Oxfordshire, UK

An orbital selective Mott transition has been proposed, but lack of experimental knowledge of the band structure has precluded direct test of that scenario. Here we present a detailed angle resolved photoemission spectroscopy study of the Ca_2RuO_4 band structure. With a mix of matrix element effects, band structure calculations, and direct observation we resolve the orbital character of the bands. We show that a significantly stronger Mott gap acts on the oxy states than on the dxz and dyz states. This result sheds light on the orbital physics reinforcing the scenario of orbital selective Mott physics in Ca_2RuO_4.
Synchrotron Spectroscopic Experiments on Ruthenates

Claudia Fatuzzo 1, Marcus Dantz 2, Sara Fatale 1, Oleh Ivashko 1, Paul Olalde-Velasco 1, Noore E. Shaik 1, Bastien Dalla Piazza 1, Sandor Toth 4, Jonathan Pelliciari 2, Rosalba Fittipaldi 5, Antonio Vecchione 3, Naoki Kikugawa 6, James S. Brooks 7, Henrik M. Rønnow 1, Marco Grioni 1, Christian Rüegg 4, Thorsten Schmitt 2, Johan Chang 3

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2 Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI
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5 Dipartimento di Fisica “E.R. Caianiello”, Università di Salerno, Via Giovanni Paolo II, 132, IT-84084 Fisciano SA
6 National Institute for Materials Science, 1-2-1 Sengen, 121 Tsukuba, Japan
7 National High Magnetic Field Laboratory, 1800 E Paul Dirac Dr, 32310 Tallahassee, USA

Ruthenate-oxide materials attract much attention due to the interesting ground states they exhibit, such as unconventional superconductivity in Sr2RuO4 or Mott physics in Ca2RuO4 [1]. The role of electron correlations, Hund's coupling and spin-orbit interactions is still being debated and explored [2,3]. In this talk, we present a combined XAS and RIXS study on the Ru 4d-orbital occupation and excitations in (Ca/Sr)2RuO4, to elucidate the electronic and orbital structure. In particular, the implication of spin-orbit interaction on the t2g states will be discussed.


ARPES study of the exotic insulating phase in the high-\(T_c\) superconductor parent compound BaBiO3

Nicholas Plumb 1, Dariusz Gawryluk 2, Yan Wang 1, Zoran Ristic 1, Jihwey Park 1, Baiqing Lv 1, Zhiming Wang 1, Christian Matt 1, Nan Xu 1, Tian Shang 2, Kazimierz Conder 2, Joël Mesot 1, Ming Shi 1, Milan Radovic 1

1 Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI
2 Laboratory for Scientific Developments & Novel Materials, Paul Scherrer Institut, 5232 Villigen PSI
3 Department of Physics and Astronomy, University of Tennessee, 1408 Circle Drive, Knoxville, TN, 37996, USA
4 Paul Scherrer Institut, 5232 Villigen PSI

Like parent compounds of some other unconventional and/or high-\(T_c\) superconductor families, BaBiO3 (BBO) is an unexpected insulator that becomes superconducting (> 30 K) when doped. To explain BBO’s insulating phase, theories have invoked, e.g., charge ordering, attractive Hubbard interactions, reverse charge transfer, and bipolarons. Our ARPES studies of BBO thin films show the existence of known BiO6 breathing distortions, but not the Bi3+/Bi5+ ordering often thought to accompany them. Combining with DFT, states near EF are shown to be primarily oxygen-derived, while the occupied Bi states mostly lie at deeper energy. We find BBO is a “bond-disproportionated” insulator, with hole pairs condensed on combinations of the O 2p orbitals.
scattering for dominant bond-directional interactions in antiferromagnetic Na$_2$IrO$_3$. In particular, we observe the three spin components exhibiting short-range correlations along distinct crystallographic directions. This spin- and real-space entanglement directly provides a direct connection between honeycomb iridates and Kitaev physics.

14:45 632 High pressure crystal growth, structure and properties of Sr$_3$Pt$_{23}$As$_{11}$ and Sr$_2$Pt$_8$As.

Sergiy Katrych, Edoardo Martino, Andrea Pisoni, Ivica Zivkovic, Janusz Karpinski, László Forró, Institute of Physics, EPFL, Station 3, 1015 Lausanne

We present the first results on investigation of ternary Sr-X-As (X = Pt, Ir) systems in the range of compositions close to SrX$_3$As. The existence of the phase SrX$_3$As was not confirmed. However, two new compounds were found in the Sr-Pt-As system: Sr$_3$Pt$_{23}$As$_{11}$ ($a = b = c = 17.0995$ Å, space group: $Fm$-3$m$, structure type: Ce$_3$Pt$_{23}$Si$_{11}$) and Sr$_2$Pt$_8$As ($a = 8.0299$ $b =17.9971$ $c = 5.6588$ Å, space group: amm2, superstructure of Sr$_2$Pt$_8$P structure). The structures of both compound was determined employing single crystal x-ray diffraction data and will be shown in detail. Magnetic and electrical transport properties and influence of different possible dopant's will be presented as well.

15:15 633 The interplay of ferromagnetic and antiferromagnetic exchanges in the the 3d-5d transition metal oxides Sr$_2$MIrO$_6$ (M = Ni, Cu, Zn)

Katharina Rolfs $^1$, Ekaterina Pomjakushina $^1$, Sandor Toth $^2$, Kazimierz Conder $^1$

$^1$ Laboratory for Scientific Developments and Novel Materials, PSI, 5232 Villigen PSI

$^2$ Laboratory for Neutron Scattering and Imaging, PSI, 5232 Villigen PSI

To understand the influence of spin orbit coupling (SOC) on the electronic ground state the focus also turned to mixed 3d-5d systems, which gives the possibility to disentangle SOC effects from common charge-spin-orbital physics, and may also introduce new properties. One interesting group within these candidates are Ir-based double perovskites A$_2$MIrO$_6$ (M=3d TM). Here the SOC of 5d elements could change the exchange topology. We successfully synthesized Sr$_2$MIrO$_6$ (M = Ni, Cu, Zn), which are high oxygen pressure compounds. We will discuss the magnetic properties based on bulk magnetization, transport measurements and neutron diffraction.

15:45 634 Ab initio quantum chemical approach to spin-orbit excitations and magnetic interactions in 4d and 5d transition metal compounds

Vamshi Mohan Katukuri, École polytechnique fédérale de Lausanne

Density functional theory in conjunction with dynamic mean field theory are often used to describe certain material properties such as spectral properties and the metal-insulator transition in materials with strongly correlated electrons. However, such methods still depend on parameters such as the onsite Coulomb interactions and the Hund’s exchange, etc. which are often difficult to estimate for materials with 4d and 5d transition elements. I will talk about an alternative ab initio approach based on the calculation of many-body wave function using configuration-interaction methods and what it offers in understanding the spin-orbit coupled ground state, excitations and magnetic exchange in spin-orbit coupled Mott insulating materials.

16:30 END