TT 56: Focus Session: Electronic Properties of Spin-Orbit Driven Oxides

Relativistic correlated materials such as iridates present a substantial challenge to theory and experiments since several relevant energy scales converge to the level of 0.5–1 eV: one-electron hopping t, spin-orbit coupling λ, onsite Coulomb repulsion U, and Hund's rule magnetic coupling J. This is often accompanied by nontrivial geometries, such as honeycomb, pyrochlore or triangular lattice structures. Many phenomena, intuitively understood in the non-relativistic $3d$ transition metal oxides or weakly relativistic $4d$ systems, become highly nontrivial and challenging in $5d$ materials. This Focus Session will review recent progress made in this internationally active field of research.

Organizers: Roser Valenti (Uni Frankfurt), Jeroen van den Brink (IfW Dresden)

Time: Wednesday 9:30–12:15 Location: HSZ 03

Invited Talk TT 56.1 Wed 9:30 HSZ 03
Exotic Magnetism of J_{eff}=1/2 Iso-Spins in Complex Ir Oxides — •Hidenori Takagi — Department of Physics, University of Tokyo, Tokyo, Japan — Max Planck Institute for Solid State Research, Stuttgart, Germany

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_2IrO_4, spin-orbital Mott state with J_{eff}=1/2 is realized due to the novel interplay of those energy scales [1, 2]. Despite the strong entanglement of spin and orbital degrees of freedom, surprisingly isotropic, two-dimensional Heisenberg character of J_{eff}=1/2 iso-spins was observed in Sr_2IrO_4 with 180 deg Ir-O-Ir bonds, by the recent resonant magnetic x-ray diffuse scattering and the magnetic susceptibility measurements [3]. Complex Na-Ir oxides with honeycomb and more recently identified hyper-honeycomb lattices, where 90 deg Ir-O-Ir bonds are realized, are candidates for Kitaev spin liquid. Such exotic magnetism was recently shown to be tailored using super-lattice structure [4]. In this talk, we review these phases of interest.

[1] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008)
[2] B. J. Kim et al., Science 323, 1329 (2009)
[3] S. Fujiyama et al. , Phys. Rev. Lett. 108, 247212 (2012)
[4] J. Matsuno et al., submitted.

Invited Talk TT 56.2 Wed 10:00 HSZ 03
Isospin Dynamics in Sr_2IrO_4 Revealed by Resonant Inelastic X-Ray Scattering — •Jungho Kim — Argonne National Lab, Argonne, IL, 60565 USA

Iridium oxides with strong relativistic spin-orbit coupling have received much attention due to intriguing sets of novel electronic and magnetic phases and phenomena, which were imagined for a long time but not realized in real world. Among many materials, Sr_2IrO_4 provides a model case for investigating essential aspects of the magnetic exchange interactions of the so-called J_{eff}=1/2 isospin states, which were established by various spectroscopic studies such as angle-resolved photoemission and magnetic x-ray scattering. In this talk, I will review on resonant inelastic x-ray scattering (RIXS) technique at the Ir absorption edges and novel aspects of iridium oxides with strong relativistic spin-orbit coupling. Low energy excitation spectra of Sr_2IrO_4 by RIXS will be discussed. The J_{eff}=1/2 isospin dynamics of Sr_2IrO_4 can be well described by the isotropic Heisenberg model, which renders the low-energy effective physics of Sr_2IrO_4 much akin to that in superconducting cuprates. Higher dd excitations between J_{eff}=1/2 and 3/2 are found to be dispersive in the same way as the single hole propagates in an antiferromagnetic background.

Topical Talk TT 56.3 Wed 10:30 HSZ 03
Honeycomb Lattice Iridates — •Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Iridates, in particular those crystallizing in a honeycomb structure have recently created much interest due to the proposal of new topological states such as Kitaev-Heisenberg magnet with dynamic spin liquid phase or correlated topological (quantum spin Hall) states. Experimentally, both Na_2IrO_3 and Li_2IrO_3 are Mott insulators with antiferromagnetic ground states. We report single crystal structural, microscopic and magnetic experiments in combination with band-structure calculations for variously doped honeycomb iridates to explore the possibility of tuning these systems into topological states.

Work in collaboration with Soham Manni, Friedrich Freund, Yogesh Singh, Sungkyun Choi, R. Coldea, F. Luepke, M. Wenderoth, M. Altmeyer, H.O. Jeschke, I. Mazin and R. Valenti. Financial support through DFG SPP 1666 and the Helmholtz virtual institute 521 is acknowledged.

15 min. break.

Topical Talk TT 56.4 Wed 11:15 HSZ 03
Novel Magnetic States in Spin-Orbit Coupled Mott Insulators — •Giniyat Khaliullin — Max-Planck-Institut FKF, Stuttgart

In late transition metal compounds such as Ir, Rh, Os oxides, large spin-orbit coupling entangles the spin and orbital subspaces and may lead to unusual interactions and ground states. In this talk, after some basic introduction to spin-orbital physics, the following topics will be addressed: (i) Magnetic ordering and excitations in single layer Sr_2IrO_4 and bilayer $Sr_3Ir_2O_7$ iridium perovskites; (ii) Exchange interactions in a hexagonal lattice iridates, Kitaev-Heisenberg model, its phase diagram including spin-liquid states; (iii) Excitonic magnetism and spin-orbit driven magnetic QCP in Van Vleck-type d4 Mott insulators.

Topical Talk TT 56.5 Wed 11:45 HSZ 03
Electronic Structure of Honeycomb Iridates and Rhodates from a Density Functional Theory Perspective — •Harald O. Jeschke[1], I. I. Mazin[2], K. Foyevtsova[1], D. Khomskii[3], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany — [2]Naval Research Laboratory, Washington, USA — [3]II. Physikalisches Institut, Universität zu Köln, Germany

Taking a complementary point of view to previous studies that classify the hexagonal iridate Na_2IrO_3 as a realization of the Heisenberg-Kitaev model with dominant spin-orbit coupling, we show that this system represents a highly unusual case in which the electronic structure is dominated by the formation of quasi-molecular orbitals (QMOs), with substantial quenching of the orbital moments [1]. The QMOs consist of six atomic orbitals on an Ir hexagon, but each Ir atom belongs to three different QMOs. We discuss both limiting descriptions for Na_2IrO_3, the itinerant QMO limit valid at small SO coupling and the localized relativistic orbitals limit at large SO coupling and show that the description of Na_2IrO_3 lies in an intermediate regime [2]. We demonstrate that the electronic structure of Na_2IrO_3 is exceptionally sensitive to structural details and analyze role of the various structural distortions. We discuss the application of the QMO picture to Li_2RhO_3 [3].

[1] I. I. Mazin, H. O. Jeschke, K. Foyevtsova, R. Valenti, D. I. Khomskii, Phys. Rev. Lett. **109**, 197201 (2012)
[2] K. Foyevtsova, H. O. Jeschke, I. I. Mazin, D. I. Khomskii, R. Valenti, Phys. Rev. B **88**, 035107 (2013)
[3] I. I. Mazin *et al.*, Phys. Rev. B **88**, 035115 (2013)