MA 21: Correlated Electrons: Frustrated Magnets - Strong Spin-Orbit Coupling 1

Time: Tuesday 9:30–13:00 Location: HSZ 304

MA 21.1 Tue 9:30 HSZ 304

Quantum spin liquid ground state in $Ba_3InIr_2O_9$: A combined NMR and μSR study — •Mayukh Majumder[1], Tusharkanti Dey[1], Jean-Christophe Orain[2], Norbert Buettgen[3], Alexander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP-VI, EKM, University of Augsburg, Germany — [2]Paul Scherrer Institute, Switzerland — [3]EP-V, EKM, University of Augsburg, Germany

5d Iridium based systems have drawn a lot of attention because of the presence of similar energy scales of crystal field splitting, spin-orbit coupling and on-site Coulomb interaction which give rise to unconventional ground states. In the present compound $Ba_3InIr_2O_9$ (Ir has an average of +4.5 oxidation state), Ir-dimers aligned along crystallographic c-axis form a triangular lattice which promotes frustration. The magnetization and specific heat show no evidence of long-range magnetic ordering down to 400 mK. We have employed ^{115}In (I=9/2) NMR and μSR to study the microscopic nature of the ground state. ^{115}In Knight shift and line width exhibit a temperature independent behavior below 1.4 K down to 25 mK which indicates no static correlations are developing down to such a low temperature whereas the nuclear spin-lattice relaxation rate ($1/T_1$) shows a dynamical behavior in the same temperature range and follows a $T^{2.2}$ power law. Furthermore, we have carried out μSR experiments which also discarded the presence of any static long-range ordering and provide the evidence of dynamical fluctuations down to 25 mK. Altogether, local probes provide strong evidence for gapless quantum spin liquid ground state in $Ba_3InIr_2O_9$.

MA 21.2 Tue 9:45 HSZ 304

Spin liquid behavior in the triangular lattice iridate $Ba_3InIr_2O_9$ — •Tusharkanti Dey[1], Mayukh Majumder[1], Anatoliy Senyshyn[2], Panchanan Khuntia[3], Alexander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP-VI, EKM, University of Augsburg, Germany — [2]Munich University of Technology, Germany — [3]Universite Paris-Sud, Orsay, France

Materials with the general formula $Ba_3MIr_2O_9$ (M is a trivalent ion) crystallize in a hexagonal structure containing face-sharing Ir_2O_9 bi-octahedra forming Ir-Ir dimers along the crystallographic c-axis. These dimers build a triangular lattice in the crystallographic ab-plane. In these materials, Ir has a single crystallographic site with an average charge state +4.5. Therefore the two Ir sites within the dimer share one electron among them. This fractional charge state combined with the frustrated geometry give rise to many interesting properties like magnetoelastic effect, spin gap behavior and magnetic ordering. We have recently synthesized polycrystalline sample of $Ba_3In^{3+}Ir^{4.5+}{}_2O_9$ and studied its structural, magnetic and thermodynamic properties in detail. Our magnetic susceptibility data show the absence of magnetic ordering down to 0.4 K which is very small compared to the Weiss temperature. The magnetic heat capacity shows a hump at 1.6 K and follows power law with temperature below 1 K. In this presentation, we will discuss these results suggesting a quantum spin liquid ground state for this material.

MA 21.3 Tue 10:00 HSZ 304

Magnetism of honeycomb ruthenate $Ag_3LiRu_2O_6$ without singlet dimers — •Tomohiro Takayama[1,2] and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]FMQ3, University of Stuttgart, Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Tokyo, Japan

Honeycomb-based transition-metal oxides currently attract interests as novel quantum magnets. 5d honeycomb iridates were theoretically proposed to host quantum spin liquid state owing to bond-dependent magnetic coupling (Kitaev coupling)[1], and experimental verifications of such spin liquid state are intensively under way. On the other hand, honeycomb ruthenate Li_2RuO_3 is known to form spin-singlet dimers and the ground state is non-magnetic insulator [2].

By using ion-exchange reaction, we have synthesized silver-intercalated honeycomb ruthenate $Ag_3LiRu_2O_6$ [3]. Possibly due to the formation of strong O^{2-}-Ag^+-O^2- between the honeycomb layers, the singlet-dimer formation is suppressed in $Ag_3LiRu_2O_6$, and Ru^{4+} magnetism survives down to low temperatures. Despite Curie-Weiss like behavior observed at high temperatures ($\theta_{CW} \sim$ -40 K), we did not see any magnetic order down to 2 K in magnetization and heat capacity measurements. We discuss the possible magnetic ground state of this honeycomb ruthenate.

[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009)
[2] Y. Miura et al., J. Phys. Soc. Jpn., 76, 033705 (2007)
[3] S. Kimber et al., J. Mater. Chem. 20, 8021 (2010)

MA 21.4 Tue 10:15 HSZ 304

Long-range interactions in the effective low energy Hamiltonian of Sr_2IrO_4: a core level resonant inelastic x-ray scattering — •Stefano Agrestini[1], Chang-Yang Kuo[1], Marco Moretti Sala[2], Zhiwei Hu[1], Deepa Kasinathan[1], Pieter Glatzel[2], Tomohiro Takayama[3,4], Hidenori Takagi[3,4,5], Liu Hao Tjeng[1], and Maurits W. Haverkort[1,6] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]ESRF, Grenoble, France — [3]Department of Physics and Department of Advanced Materials, University of Tokyo, Japan — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany — [5]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [6]Institute for theoretical physics, Heidelberg University, Germany

The iridates have received tremendous attention due to the high expectations of finding new exotic phenomena and the long-sought materialization of the Kitaev model. Experimentally, however, most compounds order magnetically. Here we address the puzzle of the ground state in iridates by measuring core-to-core resonant inelastic x-ray spectroscopy on Sr_2IrO_4. From the spectra analysis we found that Sr_2IrO_4 is highly covalent with the effective t_{2g} orbitals very extended spatially. They are not the standard orbitals with nearest-neighbor-only magnetic interactions that most people have in mind. We thus explain why compass models are not realized in most studied iridates and we show a pathway how one can achieve the Kitaev model using other crystal structures or transition metal ions.

MA 21.5 Tue 10:30 HSZ 304

Differences in motion of a single hole and a single electron in the quasi-2D iridates — •Ekaterina Paerschke[1], Krzysztof Wohlfeld[2], Kateryna Foyevtsova[3], and Jeroen van den Brink[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [3]University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1 Canada

We study the motion of a single charge (hole or electron) added to the (Mott) insulating and antiferromagnetically ordered ground state of the quasi-2D iridates, such as Ba_2IrO_4 or Sr_2IrO_4. Using the self-consistent Born approximation applied to the appropriate strong coupling model we show the intrinsic and qualitative differences between the hole and electron cases. On one hand, the added electron forms a spin polaron, which qualitatively resembles the well-known case of the quasi-2D cuprates doped with a single hole or electron. On the other hand, the case with the added hole is far more complex, due to the formation of the $5d^4$ configuration which may carry finite angular momentum J: here the well-known spin polaronic physics is modified due to the additional degrees of freedom and the possibility of the free hole motion between the different AF sublattices. These results have important consequences not only for the photoemission experiments of the undoped quasi-2D iridates but also suggest that the physics of the electron- and hole-doped iridates is fundamentally different.

MA 21.6 Tue 10:45 HSZ 304

Electronic structure of Sr_2IrO_4 probed with low temperature scanning tunneling microscopy — Zhixiang Sun, •Jose M. Guevara, Danny Baumann, Kaustuv Manna, Sabine Wurmehl, Bernd Büchner, and Christian Hess — IFW-Dresden, Helmholtzstrasse 20, 01069

Sr_2IrO_4 is the main example of a spin-orbit assisted Mott insulator. In the family of iridates, Sr_2IrO_4 has also been postulated as a candidate to emulate the physics of the parent compound of the high-temperature superconductors cuprates, where the doping effect in the insulator to metal transition is still not well understood.

In this work, we classify different predominant defects in Sr_2IrO_4, with low temperature STM/S. We probe the spatial structure symmetry of these defects. From the tunneling spectra, we identify the energy of the upper and lower $J_{eff} = 1/2$ Hubbard bands, the Mott gap, and the variation of the electronic structure due to defects. A charge transfer-like behavior for the defect caused ingap states is observed.

Our measurements provide detailed results about the defect effects to the electronic properties of Sr_2IrO_4, which can be important for further understanding of the doping effect in iridates and the insulator to metal transition in Mott insulators.

MA 21.7 Tue 11:00 HSZ 304

New pyrochlore iridate $In_2Ir_2O_7$ stabilised by high pressure — •Aleksandra Krajewska[1,2], Tomohiro Takayama[1,2], Robert Dinnebier[2], Alexander Yaresko[2], Kenji Ishii[3], and Hidenori Takagi[1,2] — [1]Institut für Funktionelle Materie und Quantentechnologien, University of Stuttgart, 70550 Stuttgart, Germany — [2]Max-Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [3]QST, Hyogo 679-5148, Japan

In 5d transition metal oxides Coulomb repulsion, crystal field splitting and spin-orbit coupling are comparable which leads to a variety of exotic electronic states. Pyrochlore iridates with chemical formula $A_2Ir_2O_7$ (A= Y, rare earth) consist of A and Ir corner-sharing tetrahedral networks and are predicted to exhibit Weyl semimetal or topological insulator states. Their properties depend on the ionic radius of A^{3+}, where the system is driven from metallic to insulating regime with decreasing A^{3+} size. Those effects are likely related to diverging degree of local lattice distortion. In our work in order to explore small A^{3+} limit we synthesised new pyrochlore $In_2Ir_2O_7$ using high pressure. Structural analysis shows its octahedra are the most distorted among $A_2Ir_2O_7$ family which is in agreement with its insulating behaviour. It shows magnetic order at T_N = 55 K with $\theta_{CW} \sim$ -400 K, which suggests strong frustration and is in large contrast with $Y_2Ir_2O_7$ (T_N = 155 K, $\theta_{CW} \sim$ -130 K). Our band calculation shows that despite large distortion $In_2Ir_2O_7$ is in proximity to pure $j_{eff} = 1/2$, unlike $Y_2Ir_2O_7$, which shows strong hybridisation of $j_{eff} = 1/2$ and $j_{eff} = 3/2$. We will discuss the possible origin of almost pure $j_{eff} = 1/2$ state in $In_2Ir_2O_7$.

15 min. break.

MA 21.8 Tue 11:30 HSZ 304

Magnetic ground state of the pyrochlore iridate $Nd_2Ir_2O_7$ — •Hanjie Guo[1], Clemens Ritter[2], Kazuyuki Matsuhira[3], Isao Watanabe[4], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]Kyushu Institute of Technology, KitaKyushu, Japan — [4]RIKEN, Wako, Japan

Pyrochlore iridates are of interest due to the interplay between the relatively large spin-orbit coupling and electron-electron correlations which may induce novel phases such as Weyl semimetals. One important task for understanding the properties of these compounds is the determination of the magnetic structure which is challenging due to the small size of Ir^{4+} moments and maybe also due to the neutron absorption from Ir atoms. Our μSR studies on $Nd_2Ir_2O_7$ clearly show two transitions below about 30 and 9 K related to the Ir and Nd sublattices, respectively. The full magnetic structure including the Ir sublattice has been determined by means of powder neutron diffraction at the high flux D20 diffractometer at the ILL. Our magnetic structure refinement unravels a so-called all-in/all-out magnetic structure for both the Nd and the Ir sublattices. The ordered magnetic moments at 1.8 K amount to 0.34(1) μ_B/Ir^{4+} and 1.27(1) μ_B/Nd^{3+}.

[1] H. Guo, C. Ritter and A. C. Komarek, Phys. Rev. B **94**, 161102(R) (2016).

MA 21.9 Tue 11:45 HSZ 304

Synthesis and magnetic properties of double perovskites with Ir(IV)-states — •Michael Vogl[1], Tusharkanti Dey[1,2], Laura Teresa Corredor Bohorquez[1], Saicharan Aswartham[1], Anja Wolter-Giraud[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research , Dresden, Germany — [2]EP-VI, Electronic Correlations and Magnetism, University of Augsburg, Germany

With strong spin-orbit coupling 5d-based iridates exhibit many interesting phenomena and ground states. Here, we synthesized and investigated two series of 5d-based double perovskites $La_2Co_{1-x}Zn_xIrO_6$ and $La_2Cu_{1-x}Zn_xIrO_6$. Polycrystalline samples of the substitution series were synthesized by conventional solid state reaction and characterized by structural, magnetic and specific heat measurements. In both parent compounds (x=0) complex magnetic interactions between the strongly spin-orbit coupled 5d-ion Ir^{4+} and a magnetic 3d-transition metal ion (Co/Cu) are present. Dilution with non-magnetic Zn^{2+} is used to further study this interaction.

The evolution of the magnetic properties throughout both series is discussed. A strong shift of the transition temperatures to lower temperatures can be observed with increasing Zn-content. The magnetic phase diagram for both the series is mapped out.

MA 21.10 Tue 12:00 HSZ 304

Correlating paramagnetic spin centers in the 'nonmagnetic' $5d^4$ compound Ba_2YIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Franziska Hammerath[1], Gizem Aslan Cansever[1], Tushar Dey[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden,D-01171 — [2]Institut für Festkörperphysik, Technische Universität Dresden,D-01062

We will present the electron spin resonance results of the double perovskite Ba_2YIrO_6. This material provides a playground to examine the magnetic interactions in a 5d transition metal oxide with strong spin-orbit coupling. Theory predicts that due to the strong spin-orbit coupling this $5d^4$ iridate should be in a nonmagnetic state. However, static magnetic and NMR measurements evidence the occurrence of paramagnetic spin centers that are correlated at low temperatures. To obtain deeper insight into the magnetic properties of Ba_2YIrO_6 ESR measurements of a polycrystalline sample were carried out for several temperatures and frequencies. This enables to quantify several different paramagnetic spin centers. Two of them correspond to S=1/2 with the g-factor g=1.99 and g=1.90, and the third one to S=3/2 with g=1.49. An overview of the possible origins for the different spin centers and their relevance to the unexpected magnetism of this compound will be given in this talk.

MA 21.11 Tue 12:15 HSZ 304

The iridium double perovskites with Ir^{5+} revised: a combined structural and specific heat study — •Mihai I. Sturza[1], Laura T. Corredor[1], Gizem Aslan Cansever[1], Kaustuv Manna[1], Sebastian Gass[1], Tushar Dey[1], Christian Blum[1], Andrey Maljuk[1], Olga Kataeva[2], Sabine Wurmehl[1], Anja Wolter[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW, Institute for Solid State Research, 01069 Dresden, Germany — [2]A.E. Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Sciences, Kazan, Russia

Recently, the iridate double perovskite Sr_2YIrO_6 has attracted considerable attention due to the report of unexpected magnetism in this Ir^{5+} material, in which according to the Jeff model, a non-magnetic ground state is expected. We present a structural, magnetic and thermodynamic characterization of Sr_2YIrO_6 and Ba_2YIrO_6 single crystals, with emphasis on the temperature and magnetic field dependence of the specific heat. In agreement with the expected non-magnetic ground state of Ir^{5+} ($5d^4$) in these iridates, no magnetic transition is observed down to 430 mK. Moreover, our results suggest that the low temperature anomaly observed in the specific heat is not related to the onset of long-range magnetic order. Instead, it is identified as a Schottky anomaly caused by paramagnetic impurities present in the sample, of the order of 0.5(2) %. These impurities lead to non-negligible spin correlations, which nonetheless, are not associated with long-range magnetic ordering.

MA 21.12 Tue 12:30 HSZ 304

Strain induced changes of electronic properties of B–site ordered Sr_2CoIrO_6 thin films — •Sebastian Esser[1], Chun-Fu Chang[2], Vladimir Roddatis[3], Vasily Moshnyaga[4], Liu Hao Tjeng[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [2]Max Planck Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [3]Institut für Materialphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [4]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Tight-binding calculations for perovskite $SrIrO_3$ indicate a line node near the Fermi energy. Introducing a staggered potential between the iridate layers should gap out the nodal line, leaving a pair of three-dimensional nodal points [1] and providing a strong motivation to synthesize B–site ordered double perovskite iridate materials.

By using a metal-organic aerosol deposition technique we have grown

Sr_2CoIrO_6 thin films on various (pseudo) cubic (001)-oriented substrates to investigate the strain induced changes of the electronic properties. The fully epitaxial strained state of the thin films was verified by x-ray diffraction patterns in combination with reciprocal space mapping and TEM images. HAXPES measurements at SPring-8 indicating a strain induced change of the valence band in the near of the Fermi edge. These changes are also affecting the electrical transport properties, which were investigated down to lowest temperatures.

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[1] J.-M. Carter *et al.*, Phys. Rev. B **85** (2012) 115105.

MA 21.13 Tue 12:45 HSZ 304

Frustrated magnetism and Kitaev exchange on the fcc lattice of K_2IrCl_6 — •Nazir Khan and Alexander A. Tsirlin — EP VI, EKM, Augsburg University, 86159 Augsburg, Germany

Face-centered cubic lattice (fcc) is inherently frustrated, whereas Ir^{4+} ion brings the possibility of Kitaev anisotropy. Synchrotron x-ray study on the powder sample of K_2IrCl_6 shows that the compound retains its room temperature fcc structure (space group Fm-$3m$) and symmetrical Cl_6 octahedral environment down to the low temperature of 20 K followed by 3% volume collapse of the unit cell. Temperature and field dependence of magnetization show that the compound undergoes a paramagnetic to an antiferromagnetic phase transition at T_N=3.14 K. The Curie-Weiss fitting to the high temperature data yields an effective magnetic moment μ_{eff} =1.69 μ_B/Ir ion and Curie-Weiss temperature θ_{CW}=−41.0 K. The frustration parameter, $f = |\theta_{CW}|/T_N$, is found to be 13.0 which suggests presence of significant magnetic frustration. The temperature dependence of electrical resistivity shows that the compound is an insulator with a charge gap close to 0.7 eV.