TT 77: Frustrated Magnets: Strong Spin-Orbit Coupling II

Time: Thursday 15:00–16:30 Location: H 3025

TT 77.1 Thu 15:00 H 3025

Spin-orbit coupling in a half-filled t_{2g} shell: the case of 5d^3 K_2ReCl_6 — •Philipp Warzanowski[1], Marco Magnaterra[1], Gereon Schlicht[1], Quentin Faure[2,3], Christoph J. Sahle[2], Petra Becker[4], Ladislav Bohatý[4], Marco Moretti Sala[5], Giulio Monaco[6], Maria Hermanns[7], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]Institute of Physics II, University of Cologne — [2]ERSF, Grenoble, France — [3]LLB, Paris-Saclay, France — [4]Sect. Crystallography, University of Cologne — [5]Politecnico di Milano, Italy — [6]Università di Padova, Italy — [7]Stockholm University, Sweden

Strong spin-orbit coupling ζ is typically a game changer in 5d transition-metal compounds. The half-filled t_{2g}^3 shell, however, stands out due to its quenched orbital moment. This viewpoint has been tackled by Streltsov and Khomskii for large ζ/J_H, i.e., in the jj-coupling limit [1]. Here, we present our results of resonant inelastic x-ray scattering (RIXS) and optical spectroscopy of the $5d^3$ Mott insulator K_2ReCl_6, studying on-site d-d excitations and overtones thereof, the Mott gap, and charge-transfer excitations [2]. From comparison with single-site multiplet calculations, we determine ζ/J_H and the cubic crystal field-splitting $10Dq$ for this compound and discuss the effect of ζ on the ground state.

[1] S. Streltsov and D. I. Khomskii, PRX 10, 031043 (2020)
[2] P. Warzanowski et al., arXiv:2311.11419

TT 77.2 Thu 15:15 H 3025

Magnetism in Kitaev Quantum Spin Liquid Candidate $RuBr_3$ — Tillmann Weinhold[1], Chennan Wang[2], Felix Seewald[1], Vadim Grinenko[3], Yoshinori Imai[4], Fuki Sato[4], Kenya Ohgushi[4], Hans Henning Klauss[1], and •Rajib Sarkar[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, PSI, Villigen, Switzerland — [3]Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, China — [4]Department of Physics, Graduate School of Science, Tohoku University, Sendai, Japan

We present muon spin rotation (μSR) studies showing that long-range magnetic order takes place in $RuBr_3$ at ≈ 34 K. The observations of clear oscillations in the muon time spectra demonstrate the presence of well-defined internal fields at the muon sites. The magnetic ordering appears to be very robust and static suggesting a more conventional nature of magnetic ordering in the $RuBr_3$ system at zero field. Present investigations prove that in $RuBr_3$ the Kitaev interactions are likely to be weakened at zero field in comparison to the α-$RuCl_3$ system. This proves that it is possible to tune the Kitaev interactions by replacing Cl with heavier halogen elements such as Br.

TT 77.3 Thu 15:30 H 3025

Pressure- and temperature-induced structural evolution of $RuBr_3$ with honeycomb layers — •Victoria A. Ginga[1], Bin Shen[2], Prashanta K. Mukharjee[2], Angel M. Arevalo-Lopez[3], Ece Uykur[4], Philipp Gegenwart[2], and Alexander A. Tsirlin[1,2] — [1]Felix Bloch Institute, University of Leipzig, Germany — [2]EP VI, EKM, University of Augsburg, Germany — [3]University of Lille, France — [4]Helmholtz-Zentrum Dresden-Rossendorf, Germany

$RuBr_3$ received recent attention as a close chemical analog of the Kitaev magnet α-$RuCl_3$. Here, we report on the structural transformations of $RuBr_3$ and the stability ranges of its different polymorphs as a function of pressure and temperature. At ambient pressure, β-$RuBr_3$ forms a chain-like structure where short Ru-Ru bonds prevent the Ru^{3+} ions from being magnetic. In turn, β-$RuBr_3$ can be transformed into layered BiI_3-type magnetic α-$RuBr_3$ (space group R-3) by a high-pressure high-temperature treatment and quenched to ambient conditions. We show that α-$RuBr_3$ is metastable and irreversibly transforms into β-$RuBr_3$ on heating. Additionally, there is a reversible R-3 to C2/m transformation before β-$RuBr_3$ is reached. Upon compression, α-RuBr3 shows a strong tendency toward Ru-Ru dimerization in the triclinic and nonmagnetic α*-$RuBr_3$ (space group P-1).

TT 77.4 Thu 15:45 H 3025

Pressure effect on several Kitaev materials — •Bin Shen[1], Faranak Bahrami[2], Fazel Tafti[2], Philipp Gegenwart[1], and Alexander A. Tsirlin[3] — [1]EP VI, EKM, University of Augsburg, Germany — [2]Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — [3]Felix Bloch Institute, University of Leipzig, Germany

Kitaev quantum spin liquids host quantum entanglement and non-Abelian anyonic excitations. However, experimentally, the ground state of these Kitaev candidates is all magnetically ordered mainly thanks to other competing interactions beyond pure Kitaev exchange. Boosting the Kitaev term and driving the system towards Kitaev limit is a subject of current interest. Here, we present our pressure-tuning results on several Kitaev materials [β-Li_2IrO_3 (B. Shen et al., PRB 104, 134426), α-Li_2IrO_3 (B. Shen et al., PRB 105, 054412), and α-$RuBr_3$ (unpublished)] and reveal a generic behavior for the majority: a sudden suppression of the magnetic order due to structural dimerization. We also show one exception [$Ag_3LiRh_2O_6$ (unpublished)] in which the magnetic order is gradually suppressed without the interference of structural dimerization.

TT 77.5 Thu 16:00 H 3025

Band structure study of the magnetic ground state of pyrochlore iridates — •Alexander Yaresko, Aleksandra Krajewska, Tomohiro Takayama, and Hidenori Takagi — Max Plank Institute for Solid State Research, Stuttgart, Germany

Most of pyrochlore $R_2Ir_2O_7$ iridates, where R^{3+} is a rare-earth ion, undergo a transition to non-collinear magnetically ordered state with Ir moments pointing either to or from the center of a tetrahedron. This all-in-all-out (AIAO) order is thought to be stabilized by strong Dzyaloshinskii-Moriya interaction (DMI) allowed on the pyrochlore lattice. Recently, a new $In_2Ir_2O_7$ iridate was synthesized in which the trigonal distortion and Ir-O-Ir bond bending is even stronger than in $Lu_2Ir_2O_7$. Thus, one would expect that also in this compound strong DMI stabilizes AIAO order.

In order to verify this we performed LDA+U calculations for $In_2Ir_2O_7$ and $R_2Ir_2O_7$ (R=Y, Lu, Nd) with different non-collinear magnetic structures. For $R_2Ir_2O_7$, in agreement with neutron diffraction data the lowest energy was obtained for AIAO order. For $In_2Ir_2O_7$, however, non-collinear coplanar Palmer-Chalker order is found to be the most favorable one. This prediction is supported by recent neutron diffraction experiments. Comparison of exchange parameters estimated from the calculations suggests that the change of the magnetic ground state in $In_2Ir_2O_7$ may be caused by competition between DMI and local easy plane anisotropy which becomes allowed because of strong trigonal splitting of Ir d t_{2g} states.

TT 77.6 Thu 16:15 H 3025

Metallic conductivity on Na-deficient structural domain walls in the spin-orbit Mott insulator Na_2IrO_3 — •Franziska Breitner, Julian Kaiser, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

Charge carrier doping of spin-orbit Mott insulators and Kitaev magnets is considered as promising route towards the realization of exotic quantum phases. Here we focus on the prototypical system Na_2IrO_3, for which previous ARPES and STM studies revealed indications of a high tunability of its electronic properties. We thus performed a combined structural and electrical resistivity study of Na_2IrO_3 single crystals [1]. Laue back-scattering diffraction indicates twinning with $\pm 120°$ rotation around the c^*-axis while scanning electron microscopy displays nanothin lines parallel to all three b-axis orientations of twin domains. Energy dispersive x-ray analysis line-scans across such domain walls indicate no change of the Ir signal intensity, i.e. intact honeycomb layers, while the Na intensity is reduced down to $\sim 2/3$ of its original value at the domain walls, implying significant hole doping. The temperature dependent electrical resistance of individual domain walls contacted via focused-ion-beam microstructuring demonstrates the tuning through the metal-insulator transition into a correlated-metal ground state by increasing hole doping.

[1] F. A. Breitner, J. Kaiser, A. Jesche, Ph. Gegenwart, https://arxiv.org/abs/2311.07275