MA 40: Frustrated Magnets - Strong Spin-Orbit Coupling (joint session TT/MA)

Time: Thursday 9:30–13:00 Location: Theater

MA 40.1 Thu 9:30 Theater

Dimerization of the honeycomb iridate α-Li_2IrO_3 under pressure — •Jihaan Ebad-Allah[1,2], V. Hermann[1], M. Altmeyer[3], F. Freund[1], A. Jesche[1], A. A. Tsirlin[1], M. Hanfland[4], P. Gegenwart[1], I. I. Mazin[5], D. I. Khomskii[6], R. Valenti[3], and C. A. Kuntscher[1] — [1]Universität Augsburg, 86159 Augsburg, Germany — [2]University of Tanta, 31527 Tanta, Egypt — [3]Goethe- Universität Frankfurt, 60438 Frankfurt am Main, Germany — [4]European Synchrotron Radiation Facility, BP 220, 38043 Grenoble, France — [5]Code 6393, Naval Research Laboratory, Washington DC 20375, USA — [6]Universität zu Köln, 50937 Köln, Germany

The honeycomb iridates A_2IrO_3 (A= Na, Li) show novel behavior and phases arising from the competition between spin-orbit coupling, magnetization, and dimerization. Here, we show the results of x-ray diffraction and optical spectroscopy measurements under pressure on α-Li_2IrO_3 and Na_2IrO_3 single crystals. In α-Li_2IrO_3, a pressure-induced dimerization of Ir-Ir bonds is observed at P_c=3.8 GPa, concomitant with anomalies in the optical response, while in Na_2IrO_3 this transition is expected at a much higher pressure [1]. The results are discussed in terms of the effect of Ir-Ir bonds on the magnetic and electronic properties and compared to other honeycomb materials.

[1] V. Hermann et al., Phys. Rev. B **97**, 020104(R) (2018)

MA 40.2 Thu 9:45 Theater

Fingerprints of Kitaev physics in RIXS on Na_2IrO_3 and α-Li_2IrO_3 — •Alessandro Revelli[1], Marco Moretti Sala[2], Giulio Monaco[3], Maria Hermanns[4], Petra Becker[5], Ladislav Bohatý[5], Friedrich Freund[6], Anton Jesche[6], Philipp Gegenwart[6], Paul van Loosdrecht[1], Jeroen van den Brink[7], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]ESRF, Grenoble, France — [3]Universitá di Trento, Italy — [4]Stockholm University, Sweden — [5]Abt. Kristallographie, Institut fur Geologie und Mineralogie, Universität zu Köln, Germany — [6]Experimentalphysik VI, Universität Augsburg, Germany — [7]IFW Dresden, Germany

The honeycomb iridates Na_2IrO_3 and α-Li_2IrO_3 are discussed as candidate materials for hosting Kitaev physics. We study the magnetic excitations in these compounds by resonant inelastic x-ray scattering (RIXS) at the Ir L_3 edge, searching for experimental fingerprints of Kitaev physics. In both compounds, we find a broad continuum of excitations centered at q=0. This continuum survives up to 300 K, roughly 20 times the magnetic ordering temperature. The dynamical structure factor shows that spin-spin correlations are restricted to nearest neighbors, a characteristic property of the Kitaev model. Also the polarisation dependence agrees with an interpretation in terms of bond-directional Kitaev exchange interactions.

MA 40.3 Thu 10:00 Theater

Thermodynamic evidence for proximity to the Kitaev QSL in A_2IrO_3 (A = Na, Li) — •Kavita Mehlawat[1,2], A Thamizhavel[3], and Yogesh Singh[1] — [1]Department of Physical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, Mohali 140306, India. — [2]Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany — [3]Department of Condensed Matter Physics and Material Sciences, Tata Institute of Fundamental Research, Mumbai 400005, India

The honeycomb lattice iridates A_2IrO_3 (A = Na, Li) are candidates for the realization of the Kitaev-Heisenberg model although their proximity to Kitaev's quantum Spin-Liquid (QSL) is still debated. We report on heat capacity C and entropy S_{mag} for A_2IrO_3 (A = Na, Li) in the temperature range 0.075 K $\leq T \leq$ 155 K [1]. We find a two-peak structure for the magnetic heat capacity C_{mag} for both materials and S_{mag} shows a plateau between the peaks with a value close to $\frac{1}{2}$Rln2. These features signal the fractionalization of spins into Majorana Fermions close to Kitaev's QSL as predicted recently [2, 3]. These results provide the first thermodynamic evidence for the proximity of A_2IrO_3 to the Kitaev QSL [1].

Financial support: Hallwachs-Röntgen Postdoc Program, UGC-CSIR India.

[1] K. Mehlawat, A. Thamizhavel, and Y. Singh, Phy. Rev. B 95, 144406 (2017)
[2] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. B 92 115122 (2015)
[3] Y. Yamaji, T. Suzuki, T. Yamada, S. I. Suga, N. Kawashima, and M. Imada, Phys. Rev. B 93, 174425 (2016)

MA 40.4 Thu 10:15 Theater

Copper and zinc iridates - new derivatives of the β-Li_2IrO_3 structure — •Alexander O. Zubtsovskii and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Lithium and sodium iridates (A_2IrO_3 where A = Li, Na) form a narrow group of real-world material prototypes of the Kitaev model on the honeycomb and 3D honeycomb-like lattices. Tuning their properties by suitable chemical substituions remains a challenging problem, because only a few A_2IrO_3 iridates can be obtained by high-temperature solid synthesis. Here, we report two new compounds based on the β-Li_2IrO_3 structure and obtained by low-temperature ionic exchange of the Li^+-ions for the nonmagnetic (Zn^{2+}) and magnetic (Cu^{2+}) ions. Crystal structures refined using synchrotron X-ray diffraction data suggest the same motif of IrO_6 octaedra as in the parent compound, but with different positions of Cu^{2+} and Zn^{2+} compared to Li^+. We further report magnetic susceptibility data and discuss the nature of magnetism in these new compounds.

MA 40.5 Thu 10:30 Theater

Microscopic study of the Kitaev material β-Li_2IrO_3 under pressure and magnetic field — •Mayukh Majumder[1], Markus Pritz-Zwick[2], Tushar Kanti Dey[1], Rudra Sekhar Manna[1], Gediminas Simutis[3], Jean-Christophe Orain[3], Friedrich Freund[1], Rustem Khasanov[3], Pabitra Kumar Biswas[4], Norbert Büttgen[2], Aleaxander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP VI, University of Augsburg — [2]EP V, University of Augsburg — [3]PSI, Switzerland — [4]ISIS Pulsed Neutron and Muon Source, UK

β-Li_2IrO_3 with Ir^{4+} moments on a three-dimensional hyperhoneycomb lattice belongs to the class of much-discussed Kitaev materials [1]. At zero-field and ambient pressure, it displays a phase transition at 38 K to an incommensurate non-coplanar and counter-rotating spiral magnetic state [2]. Application of magnetic fields exceeding 2.8 T along the easy b-axis transforms the ground state into a partially polarized quantum paramagnet, which we characterize by thermodynamic as well as ^{7}Li NMR experiments. Furthermore, long-range order (at zero-field) can also be suppressed by the application of hydrostatic pressure. We also discuss our comparative study of bulk and μSR experiments under pressure, which reveal a first-order transition at 1.4 GPa giving way to a new ground state with the coexistence of dynamically correlated and frozen spins [3]. No accompanying structural transition was found and further characterization by ^{7}Li NMR experiments under pressure is intended.

Work supported by DFG through TRR 80.

[1] Phys. Rev. Lett. 114, 077202 (2015)
[2] Phys. Rev. B 90, 205116 (2014)
[3] Phys. Rev. Lett. 120 237202 (2018)

MA 40.6 Thu 10:45 Theater

Structural and magnetic properties of antifluorite $(NH_4)_2IrCl_6$: Candidate J_{eff}=1/2 Mott insulator — •Nazir Khan, Anton Jesche, and Alexander A. Tsirlin — EP VI, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Ammonium hexachloroiridate, $(NH_4)_2IrCl_6$, possesses a face centered cubic (fcc) lattice of the antifluorite K_2PtCl_6-type with isolated and regular $IrCl_6$ octahedra at high temperatures. The lattice symmetry and the 5d magnetic ion (Ir^{4+}) render realization of ideal J_{eff}=1/2 moment on the frustrated fcc lattice that has been predicted to host rich magnetic phases driven by Heisenberg and Kitaev exchanges. Using synchrotron X-ray powder diffraction and dilatometry, we investigate structural effects in $(NH_4)_2IrCl_6$ at low temperatures and in applied magnetic fields. Magnetization measurements indicate long-range antiferromagnetic ordering sets in below T_N=2.2 K. The field dependence of magnetization suggests a field induced magnetic phase transition at a critical field which depends on the crystallographic directions. The estimated effective magnetic moment seems consistent with the J_{eff}=1/2 picture. However, dilatometry shows a sharp drop in the length change along the <111> direction just below T_N. This indicates a possible lattice distortion at low temperature which may result in a deviation from the ideal J_{eff}=1/2 ground state. Magnetostriction measurements show that the field induced magnetization in the compound is strongly coupled to its lattice.

MA 40.7 Thu 11:00 Theater

Syntheses and magnetic properties of two sodium ruthenates: Na_3RuO_4 and Na_2RuO_3 — •Vera P. Bader, Alexander Tsirlin, Anton Jesche, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Ruthenates show a diversity of magnetic phenomena, e.g. due to strong Ru-O covalency in the case of Ru^{5+} [1] and due to the non-magnetic $J = 0$ state potentially leading to Van Vleck excitons in Ru^{4+} [2]. Additionally, geometrical frustration may affect the magnetic properties. We focus on two ruthenates with the Ru-ions in the oxidation state 5+ and 4+, respectively. In Na_3RuO_4 the $Ru^{5+}O_6$ octahedra condense into tetramers which are composed of two equilateral triangles. In Na_2RuO_3 the Ru^{4+} ions form honeycomb layers. We prepare powder samples of Na_3RuO_4 via solid state reaction in a controlled atmosphere. The measurement of the magnetic susceptibility shows an antiferromagnetic transition at 30 K and suggests suppression of the magnetic order. Specific heat measurements reveal two consecutive phase transitions at 25 K and 28 K. Na_2RuO_3 powder is synthesized by thermal decomposition of a precursor in argon. Due to the layered structure the compound is prone to stacking faults. To improve the quality of the sample different synthesis routes have been compared.

[1] A. Hariki *et al.*, PRB 96, 155135 (2017)
[2] G. Khaliullin, PRL 111, 197201 (2013)

15 min. break.

MA 40.8 Thu 11:30 Theater

Bilayer Kitaev models: Phase diagrams and novel phases — •Urban F. P. Seifert[1], Julian Gritsch[2], Erik Wagner[3], Darshan G. Joshi[4], Wolfram Brenig[3,1], Matthias Vojta[1], and Kai P. Schmidt[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — [3]Institut für Theoretische Physik, Technische Universität Braunschweig, Germany — [4]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We study the fate of $\mathbb{Z}_2$ spin liquid phases in differently stacked bilayer versions of Kitaev's honeycomb model. Increasing the inter-layer Heisenberg coupling $J_\perp$ (at fixed Kitaev couplings $K^{x,y,z}$) eventually destroys the topological spin liquid in favor of a paramagnetic dimer phase. We establish phase diagrams as a function of $J_\perp/K$ and Kitaev coupling anisotropies using Majorana-fermion mean-field theory, and employ different expansion techniques in the limits of small and large $J_\perp/K$. For strong anisotropies, we use effective models for the different layer stackings to discuss the quantum phase transition out of the Kitaev phase. The phase diagrams depend sensitively on the nature of the stacking and anisotropy strength. In some stackings and at strong anisotropies we find a single transition between the Kitaev and dimer phases. Importantly, for other stackings we prove the existence of two novel macro-spin phases which can be understood in terms of Ising chains which can be either coupled ferromagnetically, or remain degenerate, thus realizing a classical spin liquid. We also suggest the existence of a flux phase with spontaneous inter-layer coherence.

MA 40.9 Thu 11:45 Theater

Magnetic Frustration in Cd-substituted $HoInCu_4$ — Maximilian Wolf[1], Christina Baumeister[1], Sebastian Bachus[1], Jens-Uwe Hoffmann[2], Oliver Stockert[3], and •Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$HoInCu_4$ is one of the rare examples of a partially frustrated magnetic metal [1, 2], due to the Ho ions forming an fcc lattice, with alternating antiferromagnetic planes along [100], which are separated by frustrated planes. The substitution of In with Cd in $HoInCu_4$ yields a breakdown of magnetic frustration, resulting for $HoCdCu_4$ in a fully ordered magnetic structure of ferromagnetic planes, stacked antiferromagnetically along the [111] direction [3, 4]. We have investigated the evolution of magnetic order and magnetic frustration in $HoIn_{1-x}Cd_xCu_4$ with thermodynamic and transport measurements at low temperatures. Our data indicate the presence of a bicritical point between the frustrated and the unfrustrated phase. Furthermore we present neutron-diffraction data on single crystals of $HoInCu_4$ showing enhanced diffuse scattering as a consequence of magnetic frustration.

[1] V. Fritsch *et al.* PRB **71**, 132401 (2005)
[2] O. Stockert *et al.* unpublished
[3] V. Fritsch *et al.* PRB **73**, 094413 (2006)
[4] O. Stockert *et al.*, Experimental Report, MLZ Garching (2017)

MA 40.10 Thu 12:00 Theater

Discovery of kagome spin ice with crystallized magnetic monopoles in intermetallic compound HoAgGe — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Spin ices are exotic phases of matter characterized by frustrated spins obeying local ice rules that minimize the number of spatially isolated magnetic monopoles, in analogy with the electric dipoles in water ice. In two dimension (2D), one can similarly define ice rules for in-plane Ising-like spins arranged on a kagome lattice, which require each triangle plaquette to have a single monopole, and can lead to a variety of unique orders and excitations at different temperatures.

By integral experimental and theoretical approaches including single crystal synthesis, magnetometry, thermodynamic measurements, neutron scattering and Monte Carlo simulations, we establish the intermetallic compound HoAgGe as the first example of crystalline (i.e. non-artificial) kagome spin ice[1]. It features a variety of partial and fully ordered states and sequence of field-induced phases at low temperatures, all consistent with the kagome ice rule. The multi-stage ordering behavior characteristic of kagome ice are further confirmed by specific heat and magnetic entropy data. Our discovery provides unique possibilities for the study of two-dimensional spin-ice physics.

[1] Zhao, K. et al. submitted (2018)

MA 40.11 Thu 12:15 Theater

Field-induced phases in extended Kitaev models: Insights from hidden symmetries and relevance for real materials — •David Kaib, Stephen Winter, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt

At zero magnetic field, Kitaev's honeycomb model hosts a Z_2 spin liquid with itinerant Majorana fermions. We study a field-induced intermediate phase (IP) in the antiferromagnetic (AFM) Kitaev model, which has been discussed in terms of a gapless $U(1)$ spin liquid [1-3].

In order to characterize the IP, we consider various dynamical correlations, calculated via exact diagonalization (ED). By analyzing hidden symmetries of the model, we discuss which general nonuniform fields retain the IP, and introduce nonuniform fields that relate the field-response of the AFM model to the FM model. Within ED resolution, we find that the IP could represent a line of critical points within the parameter space of such fields.

At last, we turn to models with extended interactions, in order to relate to real materials. Since the candidate materials are thought to realize ferromagnetic (FM) coupling, we identify an extended model with FM Kitaev coupling, that is dual to the pure AFM Kitaev model, and study its vicinity to Hamiltonians of real materials.

[1] C. Hickey et al., arXiv:1805.05953
[2] H.-C. Jiang et al., arXiv:1809.08247
[3] L. Zou et al., arXiv:1809.09091

MA 40.12 Thu 12:30 Theater

Excitations in the high magnetic field phase of the putative Kitaev material $RuCl_3$ — •Anuja Sahasrabudhe[1], Raphael German[1], Thomas C. Keothe[1], Jonathan Buhot[2], Vladimir Tsurkan[3], Alois Loidl[3], Petra Becker[1], Markus Grüninger[1], and Paul H.M. van Loosdrecht[1] — [1]Universität zu Köln, II. Physikalisches Institut. — [2]Radboud University Nijmegen, HMFL. — [3]Universität Augsburg, Institut für Physik.

$RuCl_3$ is discussed as one of the closest realizations of a J=1/2 Kitaev system on a hexagonal lattice. Yet it shows antiferromagnetic (AF) ordering at low temperature signaling the presence of important interactions in addition to the anisotropic Kitaev interactions. AF order can be suppressed by an external magnetic field. The phase diagram and the behavior in high fields are vividly discussed. Here, we probe the magnetic excitation spectrum of $RuCl_3$ with Raman spectroscopy in high magnetic fields. The observed high field excitation spectra yield a detailed insight into the nature of the high field phase.

MA 40.13 Thu 12:45 Theater

Heat transport in the putative Kitaev-Heisenberg spin liq-

uid α-RuCl$_3$ under high magnetic fields — •Matthias Gillig[1], Xiaochen Hong[1], Richard Hentrich[1], Federico Caglieris[1], Maryam Shahrokhvand[2], Uli Zeitler[2], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], Bernd Büchner[1], and Christian Hess[1] — [1]Leibniz Institute for Solid State and Material Research Dresden, Germany — [2]HFML, Radboud University, Nijmegen, Netherlands — [3]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

α-RuCl$_3$ is due to the honeycomb structure of its Ru-sites and the exchange frustration a prime candidate to realize the Kitaev model in a material. The model bears interesting physics with a quantum spin liquid (QSL) ground state and exotic excitations. Although α-RuCl$_3$ orders antiferromagnetically (AFM) below 7 K, indications of a QSL were found experimentally.

We have performed heat transport measurements on α-RuCl$_3$ down to $T = 0.4$ K and up to $B = 33$ T. Below $T = 4$ K thermal conductivity κ is raised in low magnetic fields up to 5 T before it decreases again to a minimum at 8 T. This decline coincides with the suppression of the AFM phase. For $B > 8$ T, κ is strongly enhanced for all temperatures and no sign of saturation is observed. The increase of thermal conductivity can be assigned to a field-induced phase featuring a field-dependent excitation spectrum. More specifically the data suggest the opening of a spin excitation gap which reduces the phononic scattering rate. For the whole T- and B-range investigated the data are consistent with a pure phononic heat transport mechanism.