# MA 31: Frustrated Magnets - Strong Spin-Orbit Coupling 1 (joint session TT/MA)

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

**Invited Talk** MA 31.1 Wed 9:30 HSZ 304

**Field-induced magnetic order in the Kitaev material $\alpha$-$RuCl_3$** — •Lukas Janssen — Technische Universität Dresden, Dresden, Germany

$\alpha$-$RuCl_3$ has recently been intensely debated in the context of a potential field-induced spin-liquid phase. However, interesting physics can be observed in this material also at field strengths below and above the putative spin-liquid regime. In this combined experimental and theoretical work, we demonstrate the existence of a novel ordered phase at intermediate field strengths, characterize its nature, and discuss implications for the dominant exchange interactions present in this material.

*Talk includes results obtained with Christian Balz, Stephen E. Nagler, and Matthias Vojta.*

MA 31.2 Wed 10:00 HSZ 304

**Field-induced quantum phase transitions in $\alpha$-$RuCl_3$** — •Sebastian Bachus[1], Yoshifumi Tokiwa[1], Vladimir Tsurkan[2], Alois Loidl[2], Anton Jesche[1], Alexander A. Tsirlin[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Recently the observation of a half-integer quantized thermal Hall effect in the Kitaev material $\alpha$-$RuCl_3$, possibly indicating chiral Majorana edge modes, attracted considerable attention [1]. It arises in a finite field range exceeding the critical field for long-range antiferromagnetic order. We utilize a high-resolution alternating field method for the precise determination of the truly adiabatic magnetocaloric effect or magnetic Grüneisen parameter down to $\sim 1$ K and in magnetic fields up to 15 T. Together with accompanying heat capacity measurements, it allows us to determine the entropy evolution when tuning the system into and out of the presumed topological Kitaev quantum spin liquid regime as a function of the applied field. We present a comprehensive analysis of the thermodynamic data and comparison to [2].

Work supported by the German Science Foundation via Project No. 107745057 (TRR80).

[1] Y. Kashara *et al.*, Nature 559, 227-231 (2018).
[2] C. Balz *et al.*, Phys. Rev. B 100, 060405(R) (2019).

MA 31.3 Wed 10:15 HSZ 304

**High-Field Quantum Disordered State in $\alpha$-$RuCl_3$** — •Anuja Sahasrabudhe[1], David Kaib[2], Stephan Reschke[3], Raphael German[1], Thomas Koethe[1], Jonathan Buhot[4], Dmytro Kamenskyi[4], Ciarán Hickey[5], Petra Becker[6], Vladimir Tsurkan[3,7], Alois Loidl[7], Seung-Hwan Do[8], Kwang-Yong Choi[8], Markus Grüninger[1], Stephen Winter[2], Zhe Wang[1,9], Roser Valentí[2], and Paul van Loosdrecht[1] — [1]Institute of Physics II, University of Cologne — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [4]High Field Magnet Laboratory (HFML - EMFL), Radbound University, Nijmegen — [5]Institute for Theoretical Physics, University of Cologne — [6]Institute for Geology and Mineralogy, University of Cologne — [7]Institute of Applied Physics, MD2028 Chisinau — [8]Department of Physics, Chung-Ang University, Seoul — [9]Institute of Radiation Physics, Helmholtz Zentrum Dresden-Rossendorf

Layered $\alpha$-$RuCl_3$ does not show a true Kitaev quantum spin liquid state due to the presence of additional interactions leading to magnetic ordering at low temperature. This ordering can be suppressed by applying a moderate in-plane magnetic field, leading to a novel high field phase. Using Raman and THz spectroscopy, combined with an exact diagonalization study, we show that the induced high field state can be identified as a partially-polarized quantum disordered magnetic state characterised by a gapped multi-particle continuum out of which a bound-state emerges as well as a sharp single-particle response.

MA 31.4 Wed 10:30 HSZ 304

**Pressure-dependent investigation of the elastic constants in $\alpha$-$RuCl_3$** — •A. Hauspurg[1,2], S. Zherlitsyn[1], T. Yanagisawa[3], V. Felea[1], V. Tsurkan[4], K.-Y. Choi[5], S.-H. Do[5], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Hokkaido University, Sapporo, Japan — [4]Institute of Physics, University of Augsburg, Germany — [5]Department of Physics, Chung-Ang University, Seoul, South Korea

As a paradigmatic example of the realization of Kitaev physics on a honeycomb lattice, $\alpha$-$RuCl_3$ serves for numerous experimental investigations of fundamental physics of this model. Yet it shows a striped AF groundstate with evidence for a field-induced quantum spin liquid state. We performed investigations of the elastic constants by means of propagating ultrasound waves in this intriguing compound. Under variable magnetic fields, temperatures, and pressures we obtain further insight into its phase diagram. We will show evidence of pressure-dependent contributions of competing Kitaev and Heisenberg terms, which results in a suppression of the antiferromagnetically ordered phase at low temperatures.

MA 31.5 Wed 10:45 HSZ 304

**Pressure-induced dimerization and Kitaev spin liquid regime of $\alpha$-$RuCl_3$** — •Quirin Stahl[1], Gaston Garbarino[2], Tobias Ritschel[1], Francisco J. Martinez-Casado[3], Gilberto Fabbris[4], Joerg Strempfer[4], Maximilian Kusch[1], Anna Isaeva[1,5], Thomas Doert[5], Randirley Beltrán Rodríguez[6], Rajyavardhan Ray[6], Silvina P. Limandri[7], Maria Roslova[5], Liviu Hozoi[6], Ravi Yadav[6], Jeroen van den Brink[6,8], Gaël Bastien[6], Anja U.B. Wolter[6], Bernd Büchner[1,6], and Jochen Geck[1] — [1]IFMP, TU Dresden, Germany — [2]ESRF, Grenoble, France — [3]ILL, Grenoble, France — [4]APS, Argonne National Laboratory, USA — [5]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [6]IFW Dresden, Germany — [7]IFEG, National University of Córdoba, Argentina — [8]Institute of Theoretical Physics, TU Dresden, Germany

Recently, the honeycomb material $\alpha$-$RuCl_3$ has been identified as a possible realization of the Kitaev model, rendering this material an ideal platform for exploring Kitaev magnetism experimentally. However, the onset of long-range magnetic order at $T_N = 7$ K and ambient pressure, i.e. the absence of a spin liquid ground state, implies that $\alpha$-$RuCl_3$ deviates from the ideal Kitaev model under these conditions. We therefore set out to elucidate whether $\alpha$-$RuCl_3$ can be driven into the true Kitaev regime by means of hydrostatic pressure. Our x-ray diffraction and extended x-ray absorption fine structure studies reveal a rich structural phase diagram, including pressure induced Ru-Ru dimerization as well as a high-symmetry rhombohedral phase. The latter is indeed found to be very close to the ideal Kitaev model.

MA 31.6 Wed 11:00 HSZ 304

**Giant coupling between phonons and Majorana fermions in a Kitaev spin liquid** — •Dirk Wulferding[1,2], Youngsu Choi[3], Yann Gallais[4], Clément Faugeras[5], Peter Lemmens[1,2], Seung-Hwan Do[6], and Kwang-Yong Choi[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]Chung-Ang Univ., Seoul, Korea — [4]Univ. Paris-Diderot, Paris, France — [5]LNCMI Grenoble, France — [6]Oak Ridge National Lab, USA

In the Kitaev honeycomb candidate material $\alpha$-$RuCl_3$ a continuum of fractionalized Majorana fermions exists which can be directly probed by Raman spectroscopy [1-5]. In-plane magnetic fields gap the continuum, thereby confining it energetically to the regime of optical phonons. Using high-field Raman spectroscopy [6], we shine a light onto the interplay of Majorana fermions and phonons, which results in a drastic reduction of the phonon lifetimes together with a renormalization of phonon energies.

*Work supported by QUANOMET NL-4 and DFG LE967/16-1.*

[1] Sandilands, et al., Phys. Rev. Lett. 114, 147201 (2014)
[2] Knolle, et al., Phys. Rev. Lett. 113, 187201 (2014)
[3] Glamazda, et al., Phys. Rev. B 95, 174429 (2017)
[4] Glamazda, et al., Nat. Commun. 7, 12286 (2016)
[5] Sahasrabudhe, et al., arXiv:1908.11617 (2019)
[6] Wulferding, et al., arXiv:1910.00800 (2019)

**15 min. break.**

MA 31.7 Wed 11:30 HSZ 304

**Thermal Transport of the Kitaev spin-liquid candidate**

**$\alpha$-$RuCl_3$** — Richard Hentrich[1], •Matthias Gillig[1], Xiaochen Hong[1], Federico Caglieris[1], Maria Roslova[2], Anna Isaeva[1,2], Thomas Doert[2], Uli Zeitler[3], Matija Culo[3], Maryam Shahrokhvand[3], Bernd Büchner[1,4], and Christian Hess[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [3]High Field Magnet Laboratory (HFML-EFML), Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands — [4]Center for Transport and Devices, TU Dresden, Germany

$\alpha$-$RuCl_3$ currently is the best known candidate material for realizing Kitaev physics. Previous experiments on the longitudinal thermal conductivity revealed a strong coupling of he magnetic and phononic subsystems which results in a strongly magnetic field dependent thermal conductivity due to the field-induced opening of a gap [1]. Furthermore, a sizeable thermal Hall effect has been observed which triggered the search for signatures of fractionalized thermal transport due to topological edge modes near an in-plane field value of 8 T where long-range magnetic order is suppressed but the spin gap is still small [2]. Here we focus on low-temperature and high-field (up to 30 T) studies of the thermal transport which suggest the persistence of low-energy field-dependent modes up to the highest field studied at 30 T.

[1] R. Hentrich et al., Phys. Rev. Lett. **120**, 117240 (2018)
[2] Y. Kasahara et al., Nature **559**, 227 (2018)

MA 31.8 Wed 11:45 HSZ 304

**Magnetic properties of two sodium ruthenates $Na_2RuO_3$ and $Na_3RuO_4$** — •Vera P. Bader[1], Alexander A. Tsirlin[1], Anton Jesche[1], Clemens Ritter[2], and Philipp Gegenwart[1] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Institut Laue-Langevin, Grenoble, France

Ruthenates show a diversity of magnetic phenomena, e.g. due to transitions between the non-magnetic $J = 0$ state and excited $J = 1$ levels in $Ru^{4+}$ [1] or due to strong Ru-O covalency in the case of $Ru^{5+}$ [2]. Powder samples of $Na_2RuO_3$ and $Na_3RuO_4$ were prepared via solid state reactions in a controlled atmosphere. The $Ru^{4+}$ ions in $Na_2RuO_3$ form honeycomb layers which are stacked along the crystallographic c-axis. The measured diffraction pattern could be simulated under the assumption of stacking faults. The inverse susceptibility deviates from the Curie-Weiss behaviour and shows a downward bending in the high temperature region indicating a paramagnetic Van Vleck contribution which would be expected for a $J = 0$ ground state. In $Na_3RuO_4$ the $Ru^{5+}$ ions form isolated tetramers which are composed of two equilateral triangles. The magnetic susceptibility reveals an antiferromagnetic transition at 30 K while the heat capacity data show two successive phase transitions at 25 K and 28 K. Up to now, the origin of the two phase transitions is not known. Neutron diffraction reveals the absence of symmetry lowering upon both transitions and the development of incommensurate magnetic order.

[1] J. Chaloupka et al., arXiv:1910.00074 (2019)
[2] A. Hariki et al., PRB 96 155135 (2017)

MA 31.9 Wed 12:00 HSZ 304

**On the charge transfer energy in iridates: a HAXPES study** — •Daisuke Takegami[1], Deepa Kasinathan[1], Klaus Wolff[1], Simone Altendorf[1], Chun-Fu Chang[1], Katharina Hoefer[1], Anna Meléndez-Sans[1], Yuki Utsumi[1], Federico Meneghin[1], Thai Duy Ha[1], Chien-Han Yen[1], Kai Chen[2], Chang-Yang Kuo[1,3], Yen-Fa Liao[3], Ku-Ding Tsuei[3], Ryan Morrow[4], Sabine Wurmehl[4], Beluvalli E. Prasad[1], Martin Jansen[5], Alexander Komarek[1], Philipp Hansmann[1], and Liu Hao Tjeng[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Physics II, University of Cologne, Cologne, Germany — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]Leibniz Institute for Solid State and Materials Research IFW Dresden, Dresden, Germany — [5]MPI for Solid State Research, Stuttgart, Germany

We have investigated the electronic structure of iridates in the double perovskite crystal structure containing either $Ir^{4+}$ or $Ir^{5+}$ using HAXPES. The experimental valence band spectra can be well reproduced using tight binding calculations including only the Ir 5*d*, O 2*p* and O 2*s* orbitals with parameters based on the down-folding of the DFT band structure results. We found that regardless the A and B cations, the $A_2BIrO_6$ iridates have essentially zero O 2*p* to Ir 5*d* charge transfer energies. They are extremely covalent systems with the consequence is that the magnetic exchange interactions become very long-ranged, thereby hampering the materialization of the Kitaev model. Nevertheless, it still would be possible to realize a spin-liquid system using the iridates with a proper tuning of the competing exchange interactions.

MA 31.10 Wed 12:15 HSZ 304

**Magnetization density distribution of $Sr_2IrO_4$: Deviation from a *local* $j_{\mathrm{eff}} = 1/2$ picture** — Jaehong Jeong[1], •Benjamin Lenz[2,3], Arsen Gukasov[1], Xavier Fabreges[1], Andrew Sazonov[4], Vladimir Hutanu[4], Alex Louat[5], Cyril Martins[6], Silke Biermann[3,7], Veronique Brouet[5], Yvan Sidis[1], and Philippe Bourges[1] — [1]Laboratoire Léon Brillouin, CEA Saclay, Gif-sur-Yvette, France — [2]IMPMC, Sorbonne Université, Paris, France — [3]CPHT, Ecole Polytechnique, Palaiseau, France — [4]Institute of Crystallography, RWTH Aachen, Germany — [5]LPS, Université Paris-Saclay, Orsay, France — [6]LCPQ, Université Paul Sabatier, Toulouse, France — [7]Collège de France, Paris, France

5*d* iridium oxides are of huge interest due to the potential for new quantum states driven by strong spin-orbit coupling. The $j_{\mathrm{eff}} = 1/2$ state of $Sr_2IrO_4$ is such a state and consists of a quantum superposition of the three $t_{2g}$ orbitals with nearly equal population, which stabilizes an unconventional Mott insulating state.

Here, we report an anisotropic and aspherical magnetization density distribution measured by polarized neutron diffraction in a magnetic field up to 5T at 4K, which strongly deviates from a *local* $j_{\mathrm{eff}} = 1/2$ picture. Theoretical considerations based on a momentum-dependent composition of the $j_{\mathrm{eff}} = 1/2$ orbital and an estimation of the different contributions to the magnetization density casts the applicability of an effective one-orbital $j_{\mathrm{eff}} = 1/2$ Hubbard model into doubt.

The analogy to the superconducting copper oxide systems might thus be weaker than commonly thought.

MA 31.11 Wed 12:30 HSZ 304

**Magnetodielectric and magnetoelastic coupling in the frustrated fcc antiferromagnet $(NH_4)_2IrCl_6$** — •Nazir Khan and Alexander A. Tsirlin — Experimental Physics VI, University of Augsburg, 86135 Augsburg, Germany

Magnetodielectric and magnetoelastic phenomena in the fcc antifluorite $(NH_4)_2IrCl_6$ single crystal have been investigated using thermodynamic, dielectric and magnetostriction measurements. The compound is an antiferromagnetic Mott insulator with the charge gap $\Delta$=0.9 eV and Néel temperature $T_N$=2.2 K. The antiferromagnetic ordering leads to a decrease in temperature-dependent dielectric constant at zero applied field. Further, in the magnetically ordered state the dielectric constant and macroscopic sample length show a strong magnetic field dependence. The dielectric constant increases monotonically with increasing field without any saturation up to a field 14 T where it exhibits a magnetocapacitance of about 0.6%. The magentodielectric phenomenon in the present system is believed to be due to the magnetostrictive effects and spin-phonon coupling. The magnetostrictive effects are evident from the temperature and field dependence of the macroscopic length change. Spin-phonon coupling results when the energy scale of a soft phonon mode associated with the rotation of $IrCl_6$ octahedra becomes comparable with that of a magnetic interaction or magnetic field.

[1] T. Katsufuji *et al.*, Phys. Rev. B **64**, 054415 (2001)
[2] Jaye K. Harada *et al.*, Phys. Rev. B **93**, 104404 (2016)

MA 31.12 Wed 12:45 HSZ 304

**$MgIrO_3$ and $ZnIrO_3$: new hyperhoneycomb iridates** — •Alexander O. Zubtsovskii and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Iridates with edge-sharing $IrO_6$ octahedra host Kitaev interactions and show unusual magnetic behavior triggered by the exchange anisotropy and frustration. Here, we report two new compounds, $MgIrO_3$ and $ZnIrO_3$, obtained by the ionic substitution into the hyperhoneycomb beta-$Li_2IrO_3$. Crystal structures studied by synchrotron x-ray diffraction and high-resolution electron microscopy show lower symmetry than the parent compound, because $Mg^{2+}$ and $Zn^{2+}$ as divalent cations occupy different positions than $Li^+$. Magnetic behavior is characterized using magnetization and heat capacity measurements as well as muon spin relaxation.