TT 4: f-Electron Systems

Time: Monday 9:30–13:00 Location: H 3005

Invited Talk TT 4.1 Mon 9:30 H 3005

Hyperfine interactions and nuclear-electronic quantum criticality in $PrOs_4Sb_{12}$ — •Alix McCollam — School of Physics, University College Cork, Ireland

Many strongly correlated electron systems develop ordered phases at low temperatures that can be well understood in terms of an electronic order parameter. At ultra-low temperatures, however, the hyperfine interaction becomes increasingly important, and we must consider how this affects ordered phases and phase transitions near $T = 0$.

$PrOs_4Sb_{12}$ is a superconductor below $T_C = 1.85$ K and $H_{C_2} = 2.2$ T, and develops antiferroquadrupolar (AFQ) order in magnetic fields between ~ 4 T and 14 T. The hyperfine constant of Pr is relatively large at 52 mK, and influences the Pr crystal electric field levels that are closely involved in both the superconducting and AFQ phases.

To explore this influence, we performed magnetic susceptibility measurements as a function of temperature and magnetic field to temperatures as low as 1 mK. We find that the phase boundaries in $PrOs_4Sb_{12}$ show anomalous behaviour down to ~ 5 mK: AFQ order is enhanced at low temperature, whereas superconductivity is suppressed.

We explain our results in terms of a ground state composed of hybrid nuclear-electronic states with novel low energy excitations. The low temperature quadrupole excitations develop from these nuclear-electronic states, and are considerably modified compared to their higher temperature counterparts. Our results indicate a novel type of nuclear-electronic quantum critical point at the AFQ transition.

TT 4.2 Mon 10:00 H 3005

Inelastic neutron scattering of single-crystal ErB_2 — Michal Stekiel[1], •Christoph Resch[2], Andreas Bauer[2], Karin Schmalzl[3], Jakob Lass[4], Astrid Schneidewind[1], and Christian Pfleiderer[2,5,6,7] — [1]Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85747 Garching, Germany — [2]TUM School of Natural Sciences, Physik Department 85748 Garching, Germany — [3]Institut Laue-Langevin, 38042 Grenoble Cedex 9, France — [4]Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [5]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, D-85748 Garching, Germany — [6]Zentrum für Quantum Engineering (ZQE), Technische Universität München, D-85748 Garching, Germany — [7]Munich Center for Quantum Science and Technology (MCQST), Technische Universität München, D-85748 Garching, Germany

We present inelastic neutron scattering data on the hexagonal rare-earth diboride ErB_2. Previous neutron Laue and single-crystal diffraction together with measurements of the magnetic and electrical bulk properties consistently established the magnetic ground state to be an easy-plane ferromagnet with strong magnetocrystalline anisotropies [1]. We studied the magnetic excitation spectrum as a function of magnetic field by means of multiplexing triple-axis spectroscopy. We interpret the observed spectra to be consistent with a strong easy-plane ferromagnet. Additional anomalous features may be explained in the context of strong magnon-phonon-coupling.

[1] C. Resch, unpublished

TT 4.3 Mon 10:15 H 3005

Electronic structure, transport and magnetic properties of ErB_2 — •André Deyerling[1], Christoph Resch[1], Michal Stekiel[2], Christian Pfleiderer[1,3,4,5], and Marc A. Wilde[1,3] — [1]Physik Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Germany — [3]Zentrum für Quantum Engineering (ZQE), Technische Universität München, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), Technische Universität München, Germany — [5]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Germany

ErB_2 is a hexagonal easy plane ferromagnet exhibiting a large field-dependent anomalous Hall effect for magnetic fields along the hard axis. The magnetic excitation spectrum has features reminiscent of strong single-ion anisotropy and magnon-phonon coupling. We present density functional theory calculations of the magnetic anisotropy energies in and out of the hexagonal plane and calculate the Heisenberg exchange coupling constants via the spin spiral method. Further, we report the Berry curvature contribution of the electronic structure to the anomalous Hall effect when rotating the magnetization from the easy-plane to the hard axis.

TT 4.4 Mon 10:30 H 3005

Direct observation of spin-split electronic structures in antiferromagnet NdBi by micro-focused laser SARPES — •Rikako Yamamoto[1,2], Takeru Motoyama[3], Takuma Iwata[1,3], Yukimi Nishioka[3], Kazumasa Ideura[3], Towa Kousa[3], Masashi Arita[4], Shinichiro Ideta[4], Kenya Shimada[4], Koji Miyamoto[4], Taichi Okuda[4], Akio Kimura[1,3], Takahiro Onimaru[3], and Kenta Kuroda[1,3] — [1]WPI-SKCM[2], Hiroshima University, Higashi-Hiroshima, Japan — [2]MPI-CPfS, Dresden, Germany — [3]AdSE, Hiroshima University, Higashi-Hiroshima, Japan — [4]HiSOR, Hiroshima University, Higashi-Hiroshima, Japan

Recently, rare-earth monopnictides RX (R: rare earth, X: N, P, As, Sb, and Bi) have received renewed interest due to the topological electronic structure in both paramagnetic and antiferromagnetic ordered states. The antiferromagnet NdBi has surface states and band splitting associated with the multi-q magnetic structure has been reported below $T_N = 24$ K and its topological origin has been discussed. However, the information on the spin of the electronic structure has not been experimentally determined.

In this study, we have performed spin- and angle-resolved photoemission spectroscopy (SARPES) experiments using a micro-focused 6.4 eV laser at the Synchrotron Radiation Center, Hiroshima University (T. Iwata *et al.*, Sci. Rep. in press). Our laser-SARPES separates spatially mixed magnetic domains and observes anisotropic surface band dispersions appearing in $T < T_N$. We unambiguously reveal the lifting of spin degeneracy in the surface electronic structures.

TT 4.5 Mon 10:45 H 3005

Quantum Phase Transitions in Ferromagnetic $CeAgSb_2$ under Pressure — •Christian de Podesta[1], Oliver Squire[1], Jiasheng Chen[1], David Graf[2], Stanley Tozer[2], Patricia Alireza[1], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]National High Magnetic Field Laboratory, Tallahassee, Florida, USA

The Kondo lattice system $CeAgSb_2$ is ferromagnetic below 10 K. Under pressure, $CeAgSb_2$ displays a complex phase diagram, incorporating quantum phase transitions of both the ambient pressure ferromagnetism and a high-pressure antiferromagnetic phase. Becuase of this, single crystals of $CeAgSb_2$ are ideal for studying the ferromagnetic quantum phase transition and the corresponding changes to the Fermi surface under pressure.

Here we present transport measurements of the high-pressure phase diagram up to 70 kbar, down to 100 mK and in high magnetic fields. We discuss these findings in relation to the new magnetic phases and tricritical wing structures which emerge at quantum phase transitions in itinerant ferromagnets. At ambient pressure we resolve the entire Fermi surface from Shubnikov de Haas oscillations and find heavy quasi-particles persisting to high fields and long mean free paths, documenting the high quality of our crystals. We present preliminary results of extending these measurements to higher pressures using the tunnel diode oscillator technique in a diamond anvil cell.

TT 4.6 Mon 11:00 H 3005

Nonlinear Transport and Fluctuation Spectroscopy in antiferromagnetic EuT_2P_2 at the CMR transition. — •Marvin Kopp[1], Charu Garg[1], Sarah Krebber[1], Kristin Kliemt[1], Cornelius Krellner[1], Sudhaman Balguri[2], Fazel Tafti[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany — [2]Departments of Physics, Boston College, USA

The colossal magnetoresistance (CMR) effect has been a focal point of extensive research for decades, owing to its pivotal role in the physics of correlated electron systems and its potential applications. Unlike typical CMR compounds characterized by mixed valence, double exchange in manganites, or structural Jahn-Teller distortion and ferromagnetic ordering, our focus lies on EuT_2P_2 (X = Cd, Zn), with both compounds exhibiting a strikingly large negative MR significantly preceding their antiferromagnetic ordering temperature. Initial reports

suggest that strong magnetic fluctuations could be responsible for the drastic change of resistance in the magnetic field [1]. In this work, we aim to investigate these fluctuations using higher harmonic resistance and resistance fluctuation (noise) spectroscopy. Higher harmonic measurements are sensitive to the small changes in magneto-electric coupling caused by the postulated forming of magnetic clusters (polarons), often hidden in standard resistance measurements. The dynamics of these magnetic clusters is studied using resistance noise spectroscopy as a function of temperature and magnetic field which can reveal further microscopic characteristics.
[1] Adv. Mat. 33 (2021) 2005755.

15 min. break

TT 4.7 Mon 11:30 H 3005

Low-temperature physical properties of the $R_2Ni_5C_3$ (R = La-Nd, Sm, Gd, Tb) "interstitial" carbides — •Volodymyr Levytskyi[1], Volodymyr Babizhetskyy[2], Olivier Isnard[3], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, Freiberg 09596, Germany — [2]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodia Str. 6, Lviv 79005, Ukraine — [3]Université Grenoble Alpes, Institut Néel, CNRS, 25 rue des Martyrs, BP166, Grenoble, Cédex 9 38042, France

$R_2Ni_5C_3$ (R = La-Nd, Sm, Gd, Tb) represent a family of the interstitial carbides with a chemical composition in between those of the so-called carbometalates and metal-rich carbides [i.e., $R_xT_yC_z$ are in the range of $2 \leq (x+y)/z \leq 4$, with R staying for a rare earth and T as a 3*d*-metal]. The $La_2Ni_5C_3$ structure prototype is a two-layered structure (space group $P4/mbm$) combining structure fragments of $CaTiO_3$- and AlB_2-types. The structural stability of the $R_2Ni_5C_3$ series until R = Tb is confirmed by of crystal structure refinements and electronic structure calculations. The low-temperature (1.8–300 K) dependencies of magnetization, specific heat, and thermoelectric characteristics (electrical resistivity, thermal conductivity, and thermopower) have been studied. Respective physical properties of $R_2Ni_5C_3$ metallic systems will be discussed in details.
[1] V. Levytskyi, V. Babizhetskyy, O. Isnard, R. Gumeniuk, J. Alloys Compd. **969** (2023) 172411.

TT 4.8 Mon 11:45 H 3005

Searching for the critical endpoint in the valence-fluctuating $Eu(Rh_{1-x}Co_x)_2Si_2$-system — •Franziska Walther, Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

In ternary europium-based intermetallic compounds with the $ThCr_2Si_2$ structure valence fluctuations of the Eu ions and a coupling between lattice and electronic degrees of freedom lead to intriguing phenomena. Under variation of temperature and pressure, it is possible to enforce a valence transition from a magnetic Eu^{2+} to a non-magnetic Eu^{3+} state [1]. $EuRh_2Si_2$ orders antiferromagnetically below T_N= 24 K in a stable divalent state [2], whereas the isoelectronic compound $EuCo_2Si_2$ is nearly trivalent und indicates no magnetic ordering [1]. $EuRh_2Si_2$ can be shifted with pressure towards a first-order valence transition, which is expected to terminate in a second-order critical endpoint (CEP), where critical elasticity may occur [3]. In this study, we aim to approach the CEP by applying chemical pressure through substituting Rh with Co. It turned out, that the crystal growth process due to the high vapour pressure of europium is a real challenge, however, we successfully have grown first single crystals of this series. We report on the growth of $Eu(Rh_{1-x}Co_x)_2Si_2$ samples and investigated their physical properties.
[1] Y. Onuki et al., J. Phys. Soc. Jpn. **89**, 102001 (2020)
[2] S. Seiro, C. Geibel, J. Phys.: Condens. Matter **26**, 046002 (2014)
[3] F. Honda et al J. Phys. Soc. Jpn. **85**, 063701 (2016)

TT 4.9 Mon 12:00 H 3005

The valence and magnetism of Ce in $Mo_4Ce_4Al_7C_3$ nanolamellar ferromagnetic Kondo lattice — •Fabrice Wilhelm[1], Maxime Barbier[1,2], Thierry Ouisse[2], Daniel Braithwaite[3], Christine Opagiste[4], and Andrei Rogalev[1] — [1]ESRF, Grenoble, France — [2]LMGP, Grenoble, France — [3]IRIG-CEA, Grenoble, France — [4]CNRS, Grenoble, France

Rare-earth-based nanolaminates have attracted attention motivated by their potential as precursors for the synthesis of two-dimensional (2D) magnetic materials. Their intricate magnetism is governed by the strong interplay of the orbital and valence degrees of freedom that gives rise to a multitude of ground states. Herein we present the results of thorough study of the electronic and magnetic properties of $Mo_4Ce_4Al_7C_3$, exploiting X-ray absorption near edge spectroscopy and X-ray magnetic circular dichroism. This system orders ferromagnetically below 10.5 K [1] and allows for mechanical exfoliation being a derivative of the well-known MAX phases. The element-selective studies and magnetoresistance measurements under pressure evidenced that this mixed valent compound combines a Kondo lattice behavior with ferromagnetism [2]. We have shown that this unusual property is due to very different electronic and magnetic properties of the two non-equivalent Ce sites.
[1] Q. Tao et al., Phys. Rev. Mater. 2 (2018) 114401.
[2] M. Barbier et al., Phys. Rev. B 102 (2020) 155121

TT 4.10 Mon 12:15 H 3005

Valence-to-core RIXS at the uranium M_5 edge in UO_2 and UF_4 — •Ondrej Stejskal and Jindrich Kolorenc — Institute of Physics (FZU), Czech Academy of Sciences, Prague, Czech Republic

Motivated by a recent experimental study [1], we simulate the valence-to-core resonant inelastic x-ray scattering (RIXS) measured at the uranium M_5 edge in insulating compounds UO_2 and UF_4. To do so, we employ the Anderson impurity model from LDA+DMFT electronic-structure calculations [2]. We find that the feature experimentally observed at an energy loss of roughly 10 eV above the white line reflects the charge-transfer excitations from the uranium 5f to the ligand 2p states, in agreement with other closely related investigations [3]. We analyze how the intensity of this feature depends on the metal–ligand hybridization and discuss whether there is a direct link between the energy loss, at which the feature is observed, and the band gap as argued in [1].
[1] J. G. Tobin *et al.*, J. Phys.: Condens. Matter **34** (2022) 505601.
[2] J. Kolorenc, A. Shick, A. Lichtenstein, Phys. Rev. B **92** (2015) 085125.
[3] Kvashnina *et al.*, Chem. Commun. **54** (2018) 9757.

TT 4.11 Mon 12:30 H 3005

Signatures of hidden ocutpolar order from non-linear Hall effects — •Sopheak Sorn[1] and Adarsh S. Patri[2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Massachusetts Institute of Technology, Boston, USA

Multipolar moments are locally anisotropic distribution of charge and magnetization of electronic wave function. They commonly arise from a combined effect of crystal electric field and strong spin-orbit interactions. In a variety of d-electron and f-electron compounds, dipolar moments are quenched, and higher-rank multipolar moments emerge as the dominant features. Due to their tensorial nature and their uncommon symmetry properties, their long-ranged orders has been challenging to directly detect. In this talk, we theoretically propose a transport-based detection of a ferroic ordering of ocutpolar moments in a metallic system. Using a minimal electron model coupled to the order parameter, we demonstrate that the onset of the octupolar order enables a non-zero third-order Hall response–rise of a transverse Hall voltage which scales cubically with the applied current. Its dissipationlessness, its anisotropy and its unusual dependence on the order parameter will be discussed. Our work provides the first example of using nonlinear transports to investigate multipolar long-ranged orders.
[1] S. Sorn and A. S. Patri, arXiv:2311.03435 (2023)

TT 4.12 Mon 12:45 H 3005

Magnetic behaviour of UNi_4B in high magnetic fields — •Philip Schröder[1], Jannis Willwater[1], Stefan Süllow[1], Manfred Reehuis[2], Hiroshi Amitsuka[3], Bachir Ouladdiaf[4], Romain Sibille[5], Milan Klicpera[6], Michael Vališka[6], Jiří Pospíšil[6], and Vladimír Sechovský[6] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Helmholtz-Center Berlin for Materials and Energy, Berlin, Germany — [3]Department of Physics, Hokkaido University, Japan — [4]Institute Laue-Langevin, Grenoble, France — [5]Paul Scherrer Institut, Villingen, Switzerland — [6]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

UNi_4B is a rare example of an ising-like f-electron magnet with a highly unusual form of partial antiferromagnetic ordering at T_N = 19.5 K. Only two thirds of the U-ions participate in long-range magnetic order and form a vortex-like magnetic structure in the pseudo-hexagonal plane. Measurements of the elastic constants verified a complex and

highly anisotropic phase diagram, including a plethora of magnetic high field phases. Here we present a comprehensive study of the evolution of the ordered state of UNi_4B in its high field spin-reorienting phases III and III‘ on a microscopic level. We discuss the results of multiple elastic neutron scattering experiments on single crystalline UNi_4B in magnetic fields up to 10 T for H||b and in magnetic fields up to 12 T for H||c. This behaviour might indicate a spin-reorientation and a previously proposed quadrupolar contribution of the non ordering third of U-ions.