TT 25: f-Electron Systems

Time: Tuesday 9:30–12:30 Location: HSZ/0101

TT 25.1 Tue 9:30 HSZ/0101

Strong correlations in rare earth intermetallic compounds — •Payel Shee[1], Chia Jung Yang[2], Tanaya Halder[1], Nainish Tickoo[1], Shishir Kumar Pandey[3], Ashis Kumar Nandy[1], Ruta Kulkarni[4], Arumugam Thamizhavel[4], Manfred Fiebig[2], Anamitra Mukherjee[1], and Shovon Pal[1] — [1]National Institute of Science Education and Research, Bhubaneswar, India — [2]ETH Zurich, Zurich, Switzerland — [3]Artificial Intelligence for Science Institute, Beijing, China — [4]Tata Institute of Fundamental Research, Mumbai, India

In rare-earth intermetallic compounds, the strong correlations between magnetic ordering and the crystal electric field (CEF) are essential to understand their many-body ground states. The CEF excitations at a low energy scale becomes crucial to study as it leaves its fingerprints on the exotic magnetic behaviour in rare-earth intermetallics. Using THz time-domain spectroscopy, we have directly probed the underlying CEF states in two distinct material system: a prototype Kondo lattice system ($CeAg_2Ge_2$) and a metallic ferromagnet (PrSi). In $CeAg_2Ge_2$, we elucidate the low lying CEF state to strongly couple with the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, evidenced by a distinct blueshift in the transition frequency [1]. However, in PrSi, we identify a prominent increase in the population of the higher CEF state at the curie temperature, showcasing an intricate interplay between CEF and magnetic ordering in these strongly correlated systems[2].

[1] P. Shee et al., Phys. Rev. B 109, 075133 (2024)
[2] P. Shee et al. manuscript submitted to Advanced Science.

TT 25.2 Tue 9:45 HSZ/0101

Rare-earth nitrides: nitrogen stoichiometry, 4*f* valence, and the role of the rare-earth 5*d* states in SmN — Anna Meléndez-Sans[1], Vanda M. Pereira[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,2,3], Chien-Te Chen[2], Liu Hao Tjeng[1], and •Simone G. Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

We report on the influence of nitrogen stoichiometry on the electronic structure of epitaxial rare-earth nitride (REN) thin films grown by molecular beam epitaxy under ultra-high vacuum base conditions using moderate growth conditions, i.e., slow deposition rates, and moderate temperatures and pressures. The systematic variation of the growth parameters enables precise control of the nitrogen content and the preparation of near-stoichiometric, well-ordered REN thin films [1,2]. Using samarium nitride as a critical model system, we present a combined x-ray photoelectron spectroscopy and x-ray absorption spectroscopy study that reveals the dependence of the rare-earth valence and electronic structure on the nitrogen content. Our findings suggest that the RE 5*d* states may play a crucial role in the nitrogen-deficient samples, as the empty states can stabilize the RE 4*f* valence by hosting the extra electrons.

[1] V. M. Pereira *et al.*, Phys. Rev. Mater. 7, 124405 (2023)
[2] A. Meléndez-Sans *et al.*, Phys. Rev. B 110, 045120 (2024)

TT 25.3 Tue 10:00 HSZ/0101

Terahertz Signatures of Coupled Topological and Heavy-Fermion States in SmB_6 — •Zekai Chen, Debankit Priyadarshi, Erik W. de Vos, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland.

We present a THz time-domain spectroscopy study that resonantly probes the conducting surface state of the topological Kondo insulator samarium hexaboride (SmB_6). Previous work on Kondo insulators has shown that the Kondo quasiparticles disintegrate near a quantum critical point (QCP) following THz radiation, leading to a delayed echo-pulse-like signal in the time domain [1]. In contrast to these materials, SmB_6 exhibits an additional in-gap state that is hypothesized to be related to its topological surface conductivity. In the presented experiment, this in-gap state is resonantly probed with THz radiation. Our results show the aforementioned echo-like signal at 3 ps, which matches the theoretical surface Kondo temperature [2]. The link between the topological surface state and the Kondo effect is corroborated by the observation of a transition towards negative optical conductivity of the instantaneous THz reflection, which emerges on the same temperature scale as the echo-response. Our results provide insight into the emergence of a coupling between the in-gap surface state and the underlying correlated Kondo physics in SmB_6.

[1] Nature Physics 14, 1103 (2018)
[2] Physical Review Letters, 114, 177202 (2015)

TT 25.4 Tue 10:15 HSZ/0101

Observation of 5f valence fluctuations in UPd_2Cd_{20} by high-resolution XAS — •Jindřich Kolorenč — Institute of Physics (FZU), Czech Academy of Sciences, Prague, Czech Republic

The regime of valence fluctuations, known from anomalous rare-earth systems, has not yet been identified by microscopic techniques in any uranium compound. It was only suggested in a few of them on the basis of thermodynamic measurements (such as the magnetic susceptibility) and their similarity to the behavior of rare-earth valence fluctuators. Such arguments, however, are hardly unequivocal. We present uranium L_3 and M_4 x-ray absorption spectra taken on UPd_2Cd_{20}, which is a heavy-fermion *antiferromagnet*. Although it has only one type of uranium site in its primitive cell, the spectra obtained in the high-energy-resolution fluorescence-detection mode display two edges, each associated with a different valence state, $5f^2$ and $5f^3$. Moreover, the shape of the M_4 spectrum is well approximated by a combination of UCl_3 ($5f^3$) and UCl_4 ($5f^2$) spectra. This suggests $5f^2 \leftrightarrow 5f^3$ fluctuations on a timescale longer than the characteristic time of the spectroscopy technique. Unlike 4f systems, in which such fluctuations typically lead to a *destruction of magnetism* due to one of the involved $4f^n$ configurations being non-magnetic, the $5f^2$ and $5f^3$ states are both magnetic, allowing for a magnetic ordering in the fluctuating state.

This contribution is a result of a collaboration between Niigata University, Japan Atomic Energy Agency, Kyushu University, Japan Synchrotron Radiation Research Institute, Helmholtz-Zentrum Dresden-Rossendorf, ESRF in Grenoble, and Charles University in Prague.

TT 25.5 Tue 10:30 HSZ/0101

Stoichiometry control of the magnetic structure and crystalline electric field effects in the Kondo lattice CeAlGe — •Soohyeon Shin and Yixi Su — Juelich Center for Neutron Sciense at MLZ, Lichtenbergstrasse 1, Garching 85748, Germany

CeAlGe crystallizes in the LaAlSi-type tetragonal structure, where spatial inversion symmetry is broken. This system is expected to host Weyl fermions near a Fermi surface that becomes more stable when time-reversal symmetry is broken. The magnetic ground state and associated topological properties of CeAlGe are known to depend sensitively on chemical stoichiometry. For instance, crystals grown by the flux method typically contain 5-15% excess Al on the Ge site and exhibit commensurate antiferromagnetic order below T=5.1 K. In contrast, crystals prepared by the floating-zone method under 30 bar of Ar gas yield stoichiometric compositions and display incommensurate order below T=4.4 K, where topological Hall effects are induced by external magnetic fields.

In this presentation, we report recent neutron-scattering experiments. Small-angle scattering reveals the emergence of additional incommensurate magnetic ordering associated with Al substitution. Furthermore, time-of-flight measurements suggest the presence of a magnetoelastic bound state between the first excited crystal-field level and an optical phonon mode near 17 meV. We will discuss the implications of this magnetoelastic bound state for the magnetic structures in CeAlGe.

TT 25.6 Tue 10:45 HSZ/0101

Acoustic signatures of field-induced electronic topological transitions in $YbNi_4P_2$ — •Jérémy Sourd[1], E.O. Eljaouhari[2], B.V. Schwarze[1], K. Kliemt[3], C. Krellner[3], F. Husstedt[1,4], J. Wosnitza[1,4], S. Zherlitsyn[1], and G. Zwicknagl[2,5] — [1]Dresden High Magnetic Field Laboratory (HLDEMFL), HZDR, Germany — [2]Institut für Mathematische Physik, TU Braunschweig — [3]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main — [4]Institut für Festkörper- und Materialphysik, TU Dresden — [5]Max Planck Institute for Chemical Physics of Solids, Dresden

The Fermi surface is a central concept to elaborate the physical properties of correlated electron systems. While resulting from the pre-

cise chemistry of a given material through its crystal and electronic structures, the Fermi-surface shape and topology can evolve drastically upon varying a control parameter leading to an electronic-topological transition (ETT). In heavy-fermion systems the strong electronic correlations generate renormalized flat bands close to the Fermi level, leading to effective Fermi energies of the order of 10 T. Thus, in these systems the Zeeman energy from moderate magnetic field is enough to induce an ETT, as observed for example in $YbNi_4P_2$. We used acoustic waves in order to probe the sequence of ETT in $YbNi_4P_2$, by performing ultrasound experiments at low temperature. By comparing the observed anomalies of the sound velocity for different acoustic modes, we show how ultrasound permits to better explore the reciprocal space structure of the ETTs in $YbNi_4P_2$.

15 min. break

TT 25.7 Tue 11:15 HSZ/0101

Tuning quadrupolar order in $YbRu_2Ge_2$ using uniaxial stress — •Arindam Ghara[1], Caitlin I. O'Neil[1], Elena Gati[1,2], You-Sheng Li[3], Nubia Caroca-Canales[1], Christoph Geibel[1], Hilary Noad[1], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Goethe University Frankfurt, Germany — [3]National Taiwan University, Taiwan

Multipolar order has gained renewed attention due to its close connection with nematicity, altermagnetism, and quantum criticality. $YbRu_2Ge_2$ exhibits a ferroquadrupolar transition at $T_Q = 10.2\,\mathrm{K}$ accompanied by a tetragonal-to-orthorhombic structural distortion [1,2]. Experimental studies [2] have proposed a B_{1g} order parameter for the ferroquadrupolar ground state. According to theoretical work [3], a transverse field, such as a magnetic field along the c axis or a B_{2g} stress, can drive $YbRu_2Ge_2$ towards a quantum critical point. This makes $YbRu_2Ge_2$ a model system for studying quadrupolar fluctuations under symmetry-resolved tuning parameters.

We used these tuning parameters to map the phase diagram of $YbRu_2Ge_2$ via resistance and Young's modulus measurements. While the data under c-axis magnetic field behave as expected for a transverse field, the response to B_{2g} stress is unexpected: the resistivity anomaly broadens, whereas the Young's modulus anomaly stays sharp. This behaviour challenges the assumption that B_{2g} stress acts purely as a transverse field.

[1] Jeevan *et al.*, *Phys. Rev. B* **73**, 020407 (2006)
[2] Rosenberg *et al.*, *PNAS* **116**, 7232 (2019)
[3] Maharaj *et al.*, *PNAS* **114**, 13430 (2017)

TT 25.8 Tue 11:30 HSZ/0101

$Yb_5Rh_6Sn_{18}$: a valence fluctuating system with ultra-low thermal conductivity — •Oleksandr Bolielyi[1], Volodymyr Levytskyi[1], Kristina O. Kvashnina[2], Andreas Leithe-Jasper[3], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01314 Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

$Yb_5Rh_6Sn_{18}$ obtained by high-frequency melting of elemental metals crystallizes with an unique structural configuration closely related to the $Yb_3Rh_4Sn_{13}$ Remeika prototype. An important feature of this structure is that the small Sn1-atoms reside within enlarged Frank-Kasper polyhedra thus, possessing potential for a "rattling" motion. X-ray absorption spectra of $Yb_5Rh_6Sn_{18}$ indicate Yb-ions to be in the intermediate valence state (IVS), i.e. switching between the $4f^{13}$ (Yb^{3+}) and $4f^{14}$ (Yb^{2+}) configurations. In agreement with this finding temperature dependence of magnetic susceptibility reveals a well pronounced maximum. Both Hall and Seebeck coefficients indicate the change of charge carrier type from electrons to holes between 120 and 220 K. Together with electrical resistivity and theoretical DFT calculations these effects confirm $Yb_5Rh_6Sn_{18}$ to be a metal, which disobeys the free electron gas theory. The ultra-low thermal conductivity is attributed to the appearance of phonon resonance as well as to the "rattling" motion of Sn1 atoms in the studied structure.

TT 25.9 Tue 11:45 HSZ/0101

Antiferromagnetic order and spin excitations in $HoInCu_4$ — •O. Stockert[1], X. Boraley[2], J. Lass[2], R. Sibille[2], Ø. S. Fjellvåg[2,3], S. Moody[2], A. M. Läuchli[2,4], V. Fritsch[5], and D. G. Mazzone[2] — [1]Max-Planck-Institut CPfS, Dresden — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Institute for Energy Technology, Kjeller, Norway — [4]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [5]Universität Augsburg, Augsburg

Magnetic frustration quite often leads to novel quantum phases in condensed matter physics. Here, we focus on the intermetallic compound $HoInCu_4$ with a face-centered cubic structure being prone to frustration.

We performed extensive elastic and inelastic neutron scattering on $HoInCu_4$ to unravel the magnetic structure and to study the underlying exchange interactions [1,2]. Below 0.76 K $HoInCu_4$ orders in a type-III AF structure with a reduced ordered moment and partially disordered Ho spins. Enhanced spin fluctuations due to frustration are detected as a diffuse signal, even well inside the ordered state. In the magnetic field polarized state the spin excitations and the magnetic diffuse scattering can be well modeled using linear spin-wave theory yielding a consistent set of nearest and next-nearest neighbor interactions. In contrast, in zero magnetic field spin-wave theory fully fails to describe the overdamped spin excitations in the AF ordered state. All these findings emphasize the importance of frustration in $HoInCu_4$.

[1] O. Stockert et al., Phys. Rev. Res. 2, 013183 (2020).
[2] X. Boraley et al., Phys. Rev. Lett. 135, 046702 (2025).

TT 25.10 Tue 12:00 HSZ/0101

Single crystal growth and characterization of $EuMn_2Si_2$ and $EuMn_2Ge_2$ — •Janina Strahl[1], Tom Gerntke[1,2], Kristin Kliemt[1], Kurt Kummer[2], and Cornelius Krellner[1] — [1]Institute of Physics, Goethe-University, Frankfurt (Main), Germany — [2]European Synchrotron Radiation Facility (ESRF), F-38043 Grenoble Cedex, France

$EuMn_2Si_2$ exhibits a thermally driven valence transition of the europium ions from Eu^{3+} at low temperatures to $Eu^{2.5+}$ at high temperatures [1]. The isoelectronic and isostructural substitution of silicon with germanium leads to a stabilization of the divalent state of Eu in $EuMn_2Ge_2$ with reported ferromagnetic Eu ordering below 13 K [2]. Both rare earth intermetallic 122 compounds crystallize in the tetragonal $ThCr_2Si_2$ structure type and show antiferromagnetic ordering of the manganese sublattices above room temperature. In literature [1,2], additional Mn spin-reorientation transitions in polycrystalline $EuMn_2Si_2$ samples at low temperatures were observed. In this contribution, we present the single crystal growth and physical properties of both compounds. We found antiferromagnetic ordering of the Eu ions in single crystalline $EuMn_2Ge_2$ below 10.4 K. Furthermore, there is evidence that previously reported Mn reorientation transitions are absent in pure $EuMn_2Si_2$ single crystals, and a valence crossover occurs between 350-530 K.

[1] M. Hofmann et al., Phys. Rev. B 69, 174432 (2004)
[2] I. Nowik et al., Phys. Rev. B 55, 3033 (1997)

TT 25.11 Tue 12:15 HSZ/0101

Polaronic quasiparticles in the valence-transition compound $TmSe_{1-x}Te_x$ — •chul-hee min[1,2], simon müller[3], lenart dudy[4], michael heber[5], woojae choi[6], jonathan denligner[7], chang jong kang[8], matthias kalläne[2], nils wind[5], markus scholz[5], christoph schlueter[5], andrei gloskovskii[5], emile rienks[8], vladimir hinkov[3], hendrik bentmann[1], yong seung kwon[6], friedrich reinert[3], hyeong do kim[9], and kai rossnagel[2,5] — [1]FYI, NTNU, Norway — [2]IEAP, CAU Kiel, Germany — [3]Uni. Würzburg, Germany — [4]SOLEIL, France — [5]DESY, Germany — [6]DGIST, South Korea — [7]ALS, USA — [8]BESSY II, Germany — [9]PAL, South Korea

Exotic quasiparticle states have been proposed in mixed-valent compounds exhibiting valence transitions. However, clear spectroscopic evidence identifying these states has remained elusive. Using synchrotron-based photoemission spectroscopy, we have probed the Tm $3d$ and $4f$ emissions in $TmSe_{1-x}Te_x$, where a semimetal–insulator transition occurs. Our photoemission results reveal a novel quasiparticle excitation in the semimetallic phase: a Holstein polaron. This local lattice distortion, induced by $4f$ photohole, is surprising in a metallic system where efficient screening is expected. We interpret this observation as evidence that, in heavy fermion systems, the conduction electrons' screening response is slower than the characteristic atomic distortion. Our finding underscores the critical role of electron-phonon coupling, which necessitates an extension of the standard Periodic Anderson Model.

[1] Phys. Rev. Lett. 135, 186501 (2025)