TT 43: Correlated Electrons: f-Electron & Heavy Fermion Systems

Time: Wednesday 9:30–13:00 Location: H20

TT 43.1 Wed 9:30 H20

Quantitative study of the f-occupation in CeMIn$_5$ and other cerium compounds with hard x-ray core level photo emission — •Martin Sundermann[1], Fabio Strigari[1], Thomas Willers[1], Jonas Weinen[2], Yen-Fa Liao[3], Ku-Ding Tsuei[3], Eric D. Bauer[4], John L. Sarrao[4], Joe D. Thompson[4], Pascal Lejay[5], Arata Tanaka[6], Liu Hao Tjeng[2], and Andrea Severing[1] — [1]University of Cologne, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]Los Alamos National Laboratory, Los Alamos, US — [5]Institut NEEL, CNRS, Grenoble, France — [6]Hiroshima University, Higashi-Hiroshima, Japan

Bulk-sensitive hard x-ray photoelectron spectroscopy (HAXPES) data of the Ce3d core levels of the CeMIn$_5$ family with M = Co, Rh, and Ir will be presented. The data analysis combines a full multiplet and configuration interaction model so that the strong plasmons intensities can be corrected for. This way spectral f^n weights can be extracted and the configuration interaction model yields quantitative values for the initial state f-occupation of the CeMIn$_5$. The results are compared with HAXPES data of other heavy Ce compounds of very different hybridization strength. A systematic decrease of the hybridization strength V_{eff} from $CePd_3$ to $CeRh_3B_2$ to $CeRu_2Si_2$ is observed, and it is smallest for the three CeMIn$_5$ compounds. The f-occupation increases in the same sequence and is close to one for the CeMIn$_5$ family.

TT 43.2 Wed 9:45 H20

Combined crystal field - phonon excitations in non-centrosymmetric heavy fermion $CeAuAl_3$ — •Petr Čermák[1], Astrid Schneidewind[1], Christian Franz[2,3], Rudolf Schönmann[2], Oleg Sobolev[3,4], and Christian Pfleiderer[2] — [1]Jülich Centre for Neutron Science, MLZ, Garching, DE — [2]Physik-Department, Technische Universität München, Garching, DE — [3]FRM II, Technische Universität München, Garching, DE — [4]Institute for Physical Chemistry, Georg-August-University, Göttingen, DE

Hybridized excitations that comprise of well-understood collective modes have received increasing interest as the possible origin of unconventional materials properties. In strongly correlated systems the effects of electron-phonon interactions are typically neglected, being deemed not important for the overall understanding. Recently, neutron experiment on $CeCuAl_3$ has provided putative evidence for a combined crystal field - phonon excitation [1]. In turn, an important question concerns to what extent these modes are a generic property, say, at least of the entire series of CeTAl$_3$ compounds (T: transition metal element) or even f-electron systems in a more general sense.

Our triple axis neutron measurement on single-crystal $CeAuAl_3$ revealed a new weakly dispersive excitation in contrast with earlier reports on polycrystals [2], suggesting rather generic phenomena. We have further proven, that this excitation is magnetically driven and is strongly connected with localized optical acoustic modes.

[1] D.T. Adroja et al., Phys. Rev. Lett. **108**, 216402 (2012)
[2] D.T. Adroja et al., Phys. Rev. B **91**, 134425 (2015)

TT 43.3 Wed 10:00 H20

Magnetic field dependence of spin fluctuations in CeB_6 — •P. Y. Portnichenko[1], A. V. Semeno[2], H. Ohta[3], A. S. Cameron[1], M. A. Surmach[1], H. Jang[4,5], G. Friemel[4], A. V. Dukhnenko[6], N. Yu. Shitsevalova[6], V. B. Filipov[6], A. Schneidewind[7], J. Ollivier[8], A. Podlesnyak[9], S. V. Demishev[2], and D. S. Inosov[1,4] — [1]TU Dresden, Germany — [2]GPI of RAS, Moscow, Russia — [3]Kobe University, Japan — [4]MPI Stuttgart, Germany — [5]SLAC, Stanford, USA — [6]IMPS, Kiev, Ukraine — [7]JCNS, Jülich, Germany — [8]ILL, Grenoble, France — [9]SNS, Oak Ridge, USA

The heavy fermion metal CeB_6 with a simple cubic crystal structure is characterized by a rich magnetic-field – temperature phase diagram. The zero-field antiferromagnetic ground state can be suppressed by an external field of only 1.7 T, above which an antiferroquadrupolar phase II is stabilized, resulting in a field-induced quantum critical point (QCP). Our recent inelastic neutron scattering (INS) studies have revealed a complex spectrum of low-energy collective excitations with intensity maxima at the Γ and R points. We have followed the magnetic field dependence of the excitation spectrum across the QCP. Our data reveal a nonmonotonic behavior of the strong ferromagnon mode at the Γ point, as it initially gets suppressed and becomes quasielastic, but then develops into a collective mode within phase II. At high fields, it follows the same linear behavior as one of the recently discovered electron-spin resonances, proving the common origin of these excitations. An even more complex field dependence was also observed at the R point, where a second low-energy mode emerges in phase II.

TT 43.4 Wed 10:15 H20

Quantum Oscillations without a Fermi Surface – the Anomalous de Haas-van Alphen Effect and relation to SmB_6 — •Johannes Knolle and Nigel Cooper — T.C.M. Group, Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

The de Haas-van Alphen effect (dHvAE), describing oscillations of the magnetization as a function of magnetic field, is commonly assumed to be a definite sign for the presence of a Fermi surface (FS). Indeed, the effect forms the basis of a well-established experimental procedure for accurately measuring FS topology and geometry of metallic systems, with parameters commonly extracted by fitting to the Lifshitz-Kosevich (LK) theory based on Fermi liquid theory. Here we show that, in contrast to this canonical situation, there can be quantum oscillations even for band insulators of certain types. We provide simple analytic formulas describing the temperature dependence of the quantum oscillations in this setting, showing strong deviations from LK theory. We draw connections to recent experiments on the tentative topological Kondo insulator SmB_6.

TT 43.5 Wed 10:30 H20

Valence fluctuations in the boride $Eu_4Pd_{29+x}B_8$ — •Roman Gumeniuk[1], Walter Schnelle[2], Mahmoud Ahmida[3], Mohsen Abd-Elmeguid[3], Kristina Kvashnina[4], Alexander Tsirlin[2], Andreas Leithe-Jasper[2], and Christoph Geibel[2] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany — [3]Universität zu Köln, II. Physikalisches Institut, Zülpicher Str. 77, 50937 Köln, Germany — [4]ESRF, 71, Avenue des Martyrs, Grenoble France

We synthesized a high quality sample of the boride $Eu_4Pd_{29+x}B_8$ (x = 0.76) and studied its structural and physical properties. Its tetragonal structure was solved by direct methods and confirmed to belong to the $Eu_4Pd_{29}B_8$ type. All studied physical properties indicate a valence fluctuating Eu state, with a valence decreasing continuously from about 2.9 at 5 K to 2.7 at 300 K. Maxima in the T dependence of the susceptibility and thermopower at around 135 K and 120 K, respectively, indicate a valence fluctuation energy scale on the order of 300 K. Analysis of the susceptibility evidences some inconsistencies when using the ionic interconfigurational fluctuation (ICF) model, thus suggesting a stronger relevance of hybridization between $4f$ and valence electrons compared to standard valence-fluctuating Eu systems.

TT 43.6 Wed 10:45 H20

Coexistence of magnetic order and valence fluctuations in a heavy fermion system $Ce_2Rh_3Sn_5$. — •Monika Gamza[1,2,4], Roman Gumeniuk[3,2], Walter Schnelle[2], Ulrich Burkhardt[2], Andrzej Ślebarski[4], and Helge Rosner[2] — [1]Jeremiah Horrocks Institute, University of Central Lancashire, Preston, UK — [2]MPI CPfS, Dresden, Germany — [3]Institute of Experimental Physics, Freiberg University of Mining and Technology, Freiberg, Germany — [4]Institute of Physics, University of Silesia, Katowice, Poland

While most Ce-based intermetallics contain either trivalent or intermediate-valent Ce ions, only for a few compounds a coexistence of both species has been reported. Here, we present a combined experimental and theoretical study based on thermodynamic measurements and spectroscopic data together with ab-initio electronic structure calculations aiming at exploring magnetic properties of Ce ions in two nonequivalent sites in $Ce_2Rh_3Sn_5$. Ce L_{III} XAS spectra give direct evidence for valence fluctuations. Magnetization measurements show an onset of an antiferromagnetic order at $T_N \approx 2.5$ K. The electronic structure calculations suggest that the magnetic ordering is related only to one Ce sublattice. This is in-line with a small entropy asso-

ciated with the magnetic transition $S_{\mathrm{mag}} \approx 0.35$ R ln2 per Ce atom as revealed by the specific heat measurement. Furthermore, the temperature dependence of the magnetic susceptibility can be well described assuming that there are fluctuating moments of Ce^{3+} ions in one sublattice, whereas Ce atoms from the second sublattice are in a nonmagnetic intermediate valence state.

TT 43.7 Wed 11:00 H20

Exchange field effect in the crystal field ground state of CeMAl$_4$Si$_2$ — •Kai Chen[1], Fabio Strigari[1], Martin Sundermann[1], Stefano Agrestini[2], Eric D. Bauer[3], John L. Sarrao[3], Joe D. Thompson[3], Edwige Otero[4], Arata Tanaka[5], and Andrea Severing[1] — [1]University of Cologne, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Los Alamos National Laboratory, Los Alamos, US — [4]Synchrotron Soleil,Gif-sur-Yvette Cedex,France — [5]Hiroshima University, Higashi-Hiroshima,Japan

The crystal-field ground state wave functions of the tetragonal Kondo lattice materials CeMAl$_4$Si$_2$(M = Rh, Ir and Pt), as well as the crystal-field splittings, are determined with low temperature linear polarized soft x-ray absorption spectroscopy. Surprisingly, at T $<$ 20 K, which is far below the first excited crystal-field level at 200 K, a change in linear dichroism was observed that cannot be accounted for by population of crystal-field states. Adding an exchange field to the ionic full multiplet calculations below 20 K leads to a splitting to the ground state doublet and modification of J$_z$ admixture, thus accounting for the change in low temperature linear dichroism. The direction of the required exchange field is parallel along c-axis for the antiferromagnetic Rh and Ir compounds, and perpendicular to c-axis for ferromagnetic CePtAl$_4$Si$_2$.

15 min. break

TT 43.8 Wed 11:30 H20

Single crystal growth and low-temperature properties of Er$_3$Al$_2$ — •Christian Suttner, Georg Benka, Andreas Bauer, and Christian Pfleiderer — Physik Department, Technische Universität München, D-85748 Garching, Germany

In recent years, topologically non-trivial spin whirls in condensed matter systems attracted great scientific interest. Lattices of these objects, so-called magnetic skyrmion lattices, were mainly observed in Dzyaloshinskii-Moriya driven chiral magnets with the noncentrosymmetric cubic space group $P2_13$ [1,2]. Similar spin textures, however, may in principle also arise in a large number of further compounds. We report single-crystal growth of Er_3Al_2 crystallizing in the tetragonal space group $P4_2/mnm$ by means of optical float zoning under UHV-compatible conditions. We determined the magnetic phase diagram for fields applied along different crystallographic directions using magnetization, ac susceptibility, and specific heat measurements. Several phase pockets are observed below the Néel temperature $T_{\mathrm{N}} = 27$ K, consistent with earlier reports [3].

[1] S. Mühlbauer *et al.*, Science **323**, 915 (2009)
[2] N. Nagaosa and Y. Tokura, Nature Nanotech. **8**, 899 (2013)
[3] R. L. Davis *et al.*, Mater. Sci. Forum **27–28**, 249 (1988).

TT 43.9 Wed 11:45 H20

Synthesis and Characterisation of YbPdSb — •Charles R. S. Haines, Philip A. C. Brown, and Friedrich M. Grosche — Department of Physics, Cavendish Laboratory, University of Cambridge, UK

The intermetallic compound YbPdSb can form in two structures: the low temperature (LT) half-Heusler phase, in which the Yb atoms form a frustrated fcc structure, and the high temperature (HT) Pnma modification. We have prepared phase pure samples of both structures and report resistivity, magnetisation and heat capacity measurements on both. The LT phase is a Kondo lattice system [1] showing large-moment Curie-Weiss paramagnet behaviour without any phase transition anomalies down to the lowest temperatures measured. The resistivity is rather insensitive to temperature from room temperature down to ∼50K where it decreases steeply with further cooling. By contrast, in the HT phase the magnetic susceptibility displays weak temperature dependence and the resistivity falls with decreasing temperature in the way expected of a weakly correlated metal. These findings suggest that in contrast to the electronic state in the LT structure, the 4f-shell of Yb is completely filled in the HT structure of YbPdSb, presenting an interesting opportunity to study the interplay between lattice and electronic structure within the same compound.

[1] H. Suzuki et al., Physica B: Condensed Matter **206-207**, 341 (1995).

TT 43.10 Wed 12:00 H20

Variational cluster approach to superconductivity in the Kondo lattice model — •Benjamin Lenz, Salvatore R. Manmana, and Thomas Pruschke — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

The variational cluster approximation (VCA) allows to study broken symmetry phases of various lattice models at zero temperature. However, most research has been done on electron systems without coupling to additional spins. Here, we investigate the Kondo lattice model (KLM) - a paradigmatic model for heavy fermion materials which contains interactions between electrons and localized spins. We first focus on the antiferromagnetic ground state in the half-filled KLM and compare our finite-size extrapolated VCA results to those of other established techniques, like quantum Monte Carlo. We further ask for the existence of superconductivity at finite doping in this model, motivated by findings for heavy fermion systems and dynamical mean-field theory (DMFT)[1]. We probe the system for s- and d-wave superconductivity and present an analysis of the different ground states which emerge on tuning the electron filling and exchange coupling strength J.

Financial support via DFG through FOR1807 is gratefully acknowledged.

[1] O. Bodensiek, R. Zitko, M. Vojta, M. Jarrell, and T. Pruschke, PRL **110**, 146406 (2013)

Invited Talk TT 43.11 Wed 12:15 H20

Rare-earth-like behavior of transition metals substituted in Li$_3$N — •Anton Jesche — EP 6, Electronic Correlations and Magnetism, University of Augsburg, Germany

Large magnetic anisotropy and coercivity are key properties of functional magnetic materials and are generally associated with rare-earth elements. The magnetic anisotropy of 3d transition metals, on the other hand, is usually considered to be weak. Main reason is the widely known paradigm of orbital quenching. However, a rare interplay of crystal electric field effects and spin-orbit coupling causes a large orbital contribution to the magnetic moment of the T = {Mn, Fe, Co and Ni} in Li$_2$(Li$_{1-x}T_x$)N. Accordingly, extremely large magnetic anisotropies have been found. Most notably, the magnetic anisotropy alternates as easy plane → easy axis → easy plane → easy axis when progressing from T = Mn → Fe → Co → Ni [1].

Furthermore, experimental evidence for a macroscopic quantum tunneling of the magnetization has been observed in diluted Li$_2$(Li$_{1-x}$Fe$_x$)N with $x \ll 1$. Steps in the hysteresis loops and relaxation phenomena in striking similarity to single-molecule magnets indicate the presence of nanoscale magnetic centers, which are likely built from single, isolated iron atoms [2]. Recent results are going to be discussed and contrasted with established molecular magnets, hard permanent magnets and rare-earth-based model systems.

[1] A. Jesche *et al.* Phys. Rev. B **91**, 180403(R) (2015)
[2] A. Jesche *et al.*, Nature Comm. **5**:3333
doi: 10.1038/ncomms4333 (2014)

TT 43.12 Wed 12:45 H20

Thin Film Fabrication and Transport Properties of the Heavy Fermion Oxide LiV$_2$O$_4$ — •Ulrike Niemann[1], Daigorou Hirai[2], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany

The spinel compound LiV_2O_4 is well-known for its heavy fermion behaviour, although it contains no f-electron bands [1],[2]. This unexpected behaviour has been a subject of several studies, but the origin of it is still not fully understood. In this study, we successfully fabricated single crystalline epitaxial thin film of LiV_2O_4 on $SrTiO_3$, LSAT and MgO substrates, using a pulsed laser deposition technique. By changing film thickness and substrate materials, dimensionality and epitaxial strain was controlled. The formation of an epitaxially grown LiV_2O_4 phase has been confirmed by X-ray diffraction measurements. LiV_2O_4 films on MgO were found to be strained, due to the small lattice mismatch, in contrast to fully relaxed films on $SrTiO_3$.The heavy fermion behaviour of bulk LiV_2O_4 at low temperatures is well reproduced in thick enough (≈ 7 nm) films on $SrTiO_3$ substrates. In contrast, an insulating phase was found in strained LiV_2O_4 thin films on MgO substrates, revealing the key role of the lattice in stabilising

the metallic ground state. In this presentation, we discuss the thin film fabrication and the effect of epitaxial strain on heavy fermion behaviour in LiV_2O_4.

[1] S. Kondo et al., PRL **78**, 3729 (1997)
[2] C. Urano et al., PRL **85**, 1052 (2000)