TT 34: Correlated Electrons: f-Electron Systems and Heavy Fermions 1

Time: Wednesday 9:30–13:00 Location: HSZ 204

TT 34.1 Wed 9:30 HSZ 204

Crystal-field wave function of $CeCu_2Si_2$ across T_c and T_K studied with linear polarized x-ray absorption — •Andrea Marino[1,2], Andrea Amorese[1], Martin Sundermann[2,3], Kai Chen[4], Gertrud Zwicknagl[5], Maurits Haverkort[6], Frank Steglich[1], Liu Hao Tjeng[1], and Andrea Severing[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Dipartimento di Fisica, Politecnico di Milano, Milano, Italy — [3]Institute of Physics II, University of Cologne, Cologne, Germany — [4]Helmholz Zentrum Berlin (HZB) BESSY, Berlin, Germany — [5]Institute for Mathematical Physics, Technical University Braunschweig, Braunschweig, Germany — [6]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

We have investigated the crystal-field wave functions of $CeCu_2Si_2$ in the temperature range between 250 mK and 300 K, i.e. from well below to well above the superconducting transition temperature $T_c = 0.6$ K and the Kondo temperature $T_K \approx 10$ K using Ce $M_{4,5}$ x-ray absorption spectroscopy (XAS). The experiments in the mK regime were performed with the new mK insert at the DEIMOS beamline at synchrotron SOLEIL in France. The overall temperature dependence of the linear dichroism in the XAS is well explained with the thermal occupation of excited crystal-field states. Small deviations are discussed in terms of hybridization of f-electrons and conduction bands, supported by the temperature dependence of the f^0 satellite in the isotropic XAS spectra.

TT 34.2 Wed 9:45 HSZ 204

Temperature and Momentum Dependences of the Kondo Peak in the Heavy-Fermion System $CeRh_2Si_2$ — •Georg Poelchen[1], Susanne Schulz[1], Monika Güttler[1], Max Mende[1], Alexander Generalov[2], Christoph Geibel[3], Cornelius Krellner[4], Steffen Danzenbächer[1], James W Allen[5], Clemens Laubschat[1], Yuri Kucherenko[6], and Denis V Vyalikh[7,8] — [1]IFMP, TU Dresden, Germany — [2]Max IV Laboratory, Lund, Sweden — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]Kristall- und Materiallabor, Goethe-Universität Frankfurt, Germany — [5]Randall Laboratory, University of Michigan, USA — [6]Institute for Metal Physics, National Academy of Science, Ukraine — [7]DIPC, San Sebastian, Spain — [8]IKERBASQUE, Bilbao, Spain

Ultra-violet angle-resolved photoemission spectroscopy (UV-ARPES) was used to explore the temperature dependences of different surface terminations of the antiferromagnetic Kondo lattice $CeRh_2Si_2$. Spectra were taken from Ce- and Si-terminated surfaces in a wide temperature range, and reveal characteristic $4f$ patterns for weakly (surface) and strongly (bulk) hybridized Ce, respectively. Surprisingly, the temperature dependence of the Fermi level peak points to a considerably larger effective Kondo temperature at the surface, likely due to a higher local-moment effective degeneracy.

Further, we derived the k-resolved dispersion of the Kondo peak which is also found to be distinct due to different sets of itinerant bands to which the $4f$ states couple, highlighting that the Kondo physics vary remarkably between surface and bulk of the Kondo lattice material.

TT 34.3 Wed 10:00 HSZ 204

$TbRh_2Si_2$ and $TbIr_2Si_2$: Single crystal growth and characterization — •Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

In the last decades, many studies on RT_2Si_2 (R = rare earth, T = transition metal) ternary silicides have been made. The compounds which crystallize in the bodycentered tetragonal $ThCr_2Si_2$ structure exhibit exceptional magnetic properties such as superconductivity, valence fluctuations or the Kondo effect. In recent years, we have started to systematically investigate the magnetic properties of RRh_2Si_2 compounds, which present exciting surface properties, strongly influenced by the 4f-magetism [1,2]. So far, the magnetism of $TbRh_2Si_2$ and $TbIr_2Si_2$ has been studied on polycrystalline samples [3,4]. These compounds show antiferromagnetic order below $T_N = 92$ K and $T_N = 84$ K respectively with a magnetic ordering vector k = (001). In this contribution, we present the details of the crystal growth of single crystals of these two compounds grown by Bridgman method from indium flux. We show the results of specific heat, specific resistivity and magnetization measurements, with the focus on the magnetic transition [5].

[1] M. Güttler et al., Sci. Rep. 6, 24254 (2016)
[2] A. Generalov et al., Nano Lett. 17, 811 (2017).
[3] S. Quezel et al., Solid State Commun. 49, 7 (1984)
[4] T. Shigeoka et al., Physics Procedia, 75, 837-844 (2015)
[5] K. Kliemt et al., Cryst Res. Technol. 1900116 (2019)

TT 34.4 Wed 10:15 HSZ 204

Superconductivity and heavy-fermion behavior in locally non-centrosymmetric $Ln\mathbf{Ir_2As_2}$ (Ln = La and Ce) — •Seunghyun Khim, Markus König, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Compounds containing atoms with a large atomic number are considered a candidate for the realization of unconventional phenomena induced by spin-orbit splitting of degenerated bands and orbitals. In combination with a non-centrosymmetric crystal structure, the resulting asymmetric spin-orbit coupling (ASOC) gives rise to spin-momentum coupled electronic structures. Appearance of superconductivity or strong electronic correlations within these electronic structures could lead to nontrivial phases. Accordingly, $Ln\mathrm{Ir_2As_2}$ (Ln = La and Ce) in the $CaBe_2Ge_2$-type structure are promising systems because of the presence of the 5d-orbital element as well as of the lack of local inversion symmetry on each sublayer in the unit cell. Here, we present studies on single crystals of $LaIr_2As_2$ and $CeIr_2As_2$. We discover superconductivity in $LaIr_2As_2$ with a transition temperature T_c = 1.5 K. The Sommerfeld coefficient is $\gamma_0 \sim 9$ mJ/mol-K^2, implying weak electronic correlations. $CeIr_2As_2$, on the other hand, shows enhanced effective mass due to the Kondo interactions between the Ce^{3+} magnetic moments and itinerant electrons. Below 5 K, the specific-heat C/T increases with decreasing T to reach ~ 350 mJ/mol-K^2 at 0.5 K, revealing non-Fermi liquid character. We discuss the physical properties of these compounds in detail, in view of the possible ASOC.

TT 34.5 Wed 10:30 HSZ 204

Quasiparticle bands in the locally non-centrosymmetric heavy-fermion $CeRh_2As_2$ — •Évrard-Ouicem Eljaouhari[1,2], Sébastien Burdin[2], and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany — [2]LOMA, Université de Bordeaux, France

In the study of heavy-fermion materials, non-centrosymmetric ones have gained much interest in the past decade. Indeed, their lack of inversion symmetry in combination with strong spin-orbit coupling (SOC) and magnetic interactions can lead to the emergence of novel phenomena such as unvoncentional superconductivity and quantum phase transitions.

Of particular significance is the new non-centrosymmetric heavy-fermion $CeRh_2As_2$ for which some interesting properties have been reported. For example, measurements have shown the existence of a quasi-quartet crystal electric field (CEF) ground state which would normally not be expected in a tetragonal system. Also and as for other non-centrosymmetric superconductors, a Rashba-type SOC which leads to the splitting of the Fermi surface into two and to the possibility of mixing singlet-triplet superconducting states is expected.

In order to get deeper understanding of this compound and its properties, a realistic modeling of its electronic structure is needed. In this talk we present our results on the quasiparticle bands of $CeRh_2As_2$ which have been calculated thanks to the Renormalised Band method which proceeds from a relativistic description of the electronic structure and accounts for CEF effects and for the mass renormalisation.

TT 34.6 Wed 10:45 HSZ 204

$CeRu_2P_2$ and $CeCo_2P_2$: Single Crystal Growth Method and Magnetic Properties — •Fabian Feldmann, Marius Peters, Johannes Hellwig, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut Goethe Universität Frankfurt/Main

CeT_2P_2 (T = Co, Ru) are rare-earth ternary phosphides with tetragonal $ThCr_2Si_2$ -type crystal structure. $CeRu_2P_2$ is an intermediate valent system [1],[2] and $CeCo_2P_2$ is an antiferromagnet with a rather high Néel temperature $T_N = 440$ K [3], most likely due to an interplay of 3d and 4f magnetism, although Ce is close to a non-magnetic Ce^{4+}

state.

Here, we present the high-temperature metal-flux technique that was used to obtain millimeter-sized single crystals. Furthermore, we show magnetic measurements for both systems. $CeCo_2P_2$ shows anisotropic behavior above the ordering temperature, which is unexpected for itinerant 3d magnetism. $CeRu_2P_2$ as a reference system without the d magnetism of Co also shows anisotropic behavior and may indicate that $CeCo_2P_2$ also exhibits some remaining Ce 4f magnetism [4].

[1] A. Amorese et al., Phys. Rev. B **93**, 165134 (2016)
[2] T. Fujiwara et al., J. Phys.: Conf. Ser. **273**, 012112 (2011)
[3] Y. Tian et al., Physica B **512**, 75 (2017)
[4] K. Kliemt et al., Cryst. Res. Technol., 1900116 (2019)

TT 34.7 Wed 11:00 HSZ 204

Orientation of ground-state orbital in $CeCoIn_5$ and $CeRhIn_5$ — •Martin Sundermann[1,2], Andrea Amorese[1,2], Fabio Strigari[1], Brett Leedahl[2], Liu Hao Tjeng[2], Maurits W. Haverkort[3], Hlynur Gretarsson[4,2], Hasan Yavaş[4], Marco Moretti Sala[5], Eric D. Bauer[6], Priscila F. S. Rosa[6], Joe D. Thompson[6], and Andrea Severing[1,2] — [1]2. Physikalisches Institut, Universität zu Köln — [2]Max Planck Institut für Chemische Physik fester Stoffe, Dresden — [3]Institut für Theoretische Physik, Universität Heidelberg — [4]PETRA III, Deutsches Elektronen-Synchrotron (DESY), Hamburg — [5]European Synchrotron Radiation Facility (ESRF), Grenoble, Frankreich — [6]Los Alamos National Laboratory, New Mexico, USA

We present core-level non-resonant inelastic x-ray scattering (NIXS) data of the heavy fermion compounds $CeCoIn_5$ and $CeRhIn_5$ measured at the Ce $N_{4,5}$-edges. The higher than dipole transitions in NIXS allow determining the orientation of the Γ_7 crystal-field ground-state orbital within the unit cell. The crystal-field parameters of the $CeMIn_5$ compounds and related substitution phase diagrams have been investigated in great detail in the past; however, whether the ground-state wave function is the Γ_7^+ (x^2-y^2) or Γ_7^- (xy orientation) remained undetermined. We show that the Γ_7^- doublet with lobes along the (110) direction forms the ground state in $CeCoIn_5$ and $CeRhIn_5$. A comparison is made to the results of existing DFT+DMFT calculations.

15 min. break.

TT 34.8 Wed 11:30 HSZ 204

Investigation of Ce-based Materials with Multiple Inequivalent Kondo-sites. — Jardoslav Valenta[1], Petr Opletal[1], Jan Fikáček[1], Elen Duverger Nedellec[1], Jiří Pospíšil[1], Shinsaku Kambe[2], Hironori Sakai[2], Yo Tokunaga[2], Russel E Walstedt[3], Robert Küchler[4], Jacintha Banda[4], Manuel Brando[4], and •Jeroen Custers[1] — [1]Dept. of Condensed Matter Physics, Charles University, Ke Karlovu, 5, 121 16 Praha, Czech Republic — [2]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai-mura, Ibaraki 319-1195, Japan — [3]Physics Department, The University of Michigan, Ann Arbor, MI 48109, USA — [4]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, D-01187 Dresden, Germany

The vast majority of heavy fermion compounds investigated in close proximity to a magnetic quantum phase transition exhibit only one crystallographic site for the Rare Earth or Actinide ion. Here we present results on ongoing research on several Ce–based compounds with multiple Ce-sites. Recent ^{115}In NQR/NMR results on Ce_3PtIn_{11} which has two inequivalent Ce-sites, show evidence for two quantum critical points. Each can be associated with a particular Ce-site. Our investigation on a series of $(Ce_{1-x}La_x)_3Al_{11}$ reveals that, up to $x = 0.25$, we substitute La for Ce on the Ce2 site only. As the parent compound Ce_3Al_{11} has 2 sites (Ce1: 2 atoms/f.u.; Ce2: 1 atom/f.u.) we thus can follow the evolution of removing one Kondo-site step by step. Finally we will present our first results on $Ce_3Rh_5Ge_7$. This novel compound harbors 3 inequivalent Ce-sites.

TT 34.9 Wed 11:45 HSZ 204

Valence effect in the thermopower of Eu systems — •Ulrike Stockert[1], Silvia Seiro[2,1], Nubia Caroca-Canales[1], Elena Hassinger[1], and Christoph Geibel[1] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Institute for Solid State Research, IFW, Dresden

$EuIr_2Si_2$ and $EuNi_2P_2$ have been classified as valence-fluctuating (VF) materials with a strongly temperature-dependent Eu valence. At low temperature T the effective charge carrier masses are significantly enhanced due to hybridization between the Eu 4f and the conduction electron states. The relative importance of hybridization and valence fluctuations in Eu-based VF systems is not yet clear and a topic of current interest.

We present thermal conductivity and thermopower data for $EuIr_2Si_2$ and $EuNi_2P_2$ in the temperature range beween 2 K and 300 K. The thermal conductivities of both materials are conventional with differences arising due to different crystal quality. By contrast, the thermopowers of $EuIr_2Si_2$ and $EuNi_2P_2$ exhibit large values and a characteristic T dependence that cannot be explained satisfactorily by simple hybridization models. Instead, we may describe the thermopower by taking into account the temperature-dependence of the Eu valence, which leads to additional thermopower contributions due to variations in the chemical potential. These findings corroborate the relevance of the valence fluctuations for understanding the properties of $EuIr_2Si_2$ and $EuNi_2P_2$ at intermediate temperatures.

TT 34.10 Wed 12:00 HSZ 204

Crystal growth of the valence fluctuating system $EuPd_2Si_2$ — •Marius Peters, Kristin Kliemt, Eunhyung Cho, Doan-My Tran, Franz Ritter, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt

The study of collective phenomena raising from enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both electronic and lattice-degrees of freedom. One system providing such a strongly coupled phase transition is $EuPd_2Si_2$ of the $ThCr_2Si_2$ structural type, showing a temperature induced valence transition of europium between the energetically vicinal valence states Eu^{2+} and Eu^{3+} at about 170K [1]. First reports on the synthesis of single crystals came up only recently [2], but a deep investigation of the valence transition in this compound is still missing.

We approached the ternary Eu-Pd-Si system using differential thermal analysis to map the local composition phase diagram. We used the Bridgman and the Czochralski method fort he successful growth of mm-sized single crystals of $EuPd_2Si_2$. In this contribution we will present chemical and structural characterization of these crystals and some preliminary physical measurements around the valence transition.

[1] E. V. Sampathkumaran et al., Journal of Physics C14, L237 (1981).
[2] Y. Onuki et al., Philosophical Magazine 97, 3399 (2017).

TT 34.11 Wed 12:15 HSZ 204

Crystal growth and characterization of isotope-pure $YbRh_2Si_2$ (^{171}Yb, ^{173}Yb, ^{174}Yb) — •Sebastian Witt[1], Susanna Rongstock[1], Thanh Duc Nguyen[1], Manuel Brando[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe University, Frankfurt, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

A central question in condensed matter research concerns the interplay between quantum criticality and unconventional superconductivity in strongly correlated electron systems such as heavy-electron systems. Recently, superconductivity was also discovered in the quantum-critical material $YbRh_2Si_2$ at 2mK [1]. So far the interplay between electronic and nuclear moments of Yb and its impact on the superconductivity is not settled. For that reason, it is essential to investigate $YbRh_2Si_2$ samples with a well-defined Yb nuclear spin.

In this talk, we report the crystal growth with the entire range of nuclear spin number in the single crystals (^{171}Yb: I = 1/2, ^{173}Yb: I = 5/2, ^{174}Yb: I = 0). For the crystal growth we developed a new setup for small masses, especially for the metallothermic reduction of metallic Yb from Yb_2O_3. Besides the single crystal characterization (Laue, PXRD) we will present measurements of the resistivity and isotopic composition. To investigate the influence of nuclear spin on the electronic degrees of freedom, we will show the heat capacity around the antiferromagnetic transition at 70mK.

[1] E. Schuberth et al., Science, 351, 485-488 (2016).

TT 34.12 Wed 12:30 HSZ 204

Extremely weak magnetic exchange in metallic 4f-electron system leads to enormous magnetocaloric effect — •Thomas Gruner[1], Jiasheng Chen[1], Dongjin Jang[2], Jacintha Banda[3], Christoph Geibel[3], Manuel Brando[3], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]KRISS, Daejeon, Republic of Korea — [3]MPI CPfS, Dresden, Germany

Traditional cryogenic demagnetisation refrigerators for the temperature range 40 mK $< T <$ 2 K use hydrated paramagnetic salts as cooling

agents. This often imposes significant restrictions on equipment designs due to the weak thermal conductivity and the need for hermetic sealing of these insulating materials. Recently, we showed that certain Yb-based metallic materials provide attractive alternatives [1]. In a search for even more appropriate materials we investigated a number of Heusler- and half-Heusler compounds and studied their structural, magnetic, transport and magnetocaloric properties, enabling us to select a particularly promising Yb system.
Our measured data evidence metallic behaviour, the absence of superconductivity and a stable trivalent Yb^{3+} state, without any sign of a significant Kondo interaction. This new compound can be easily brought into shape, making the production of powerful cooling pills much simpler compared to commonly used paramagnetic salt or garnet refrigerants. By performing different demagnetisation tests, we demonstrated the feasibility of a simple, economical and durable alternative for traditional cooling devices for temperatures down to 120 mK.
[1] Jang, Gruner et al.; Nature Commun.; **6**, 8680 (2015)

TT 34.13 Wed 12:45 HSZ 204

Visualizing the Kondo lattice crossover in an Yb-based heavy fermion system with Compton scattering — •Monika Güttler[1], Kurt Kummer[2], Akihisa Koizumi[3], Kristin Kliemt[4], Cornelius Krellner[4], Clemens Laubschat[1], and Denis Vyalikh[5,6] — [1]IFMP, TU Dresden, Germany — [2]ESRF, Grenoble, France — [3]Graduate School of Material Science, University of Hyogo, Japan — [4]Kristall- und Materiallabor, Physikalisches Institut, Goethe-Universität Frankfurt, Germany — [5]DIPC, San Sebastian, Spain — [6]IKERBASQUE, Bilbao, Spain

With the breakdown of coherent Kondo scattering with rising temperature, the Fermi surface (FS) in rare earth Kondo lattices is expected to transition from the *large* FS counting the $4f$ moments, which form entangled quasiparticles with huge masses with the conduction states, to the *small* FS with decoupled and localized $4f$ moments. A direct observation of this transition with temperature has however remained elusive because conventional probes of the FS in Kondo lattices require high magnetic fields which might reconstruct the FS or cannot work reliably at elevated temperatures. Using high-resolution Compton scattering we overcome these limitations and show that the FS topology in the prototypical Kondo lattice $YbRh_2Si_2$ undergoes pronounced changes between 14 K and 300 K in zero magnetic field. We present clear evidence for a largely restored small FS at room temperature which could not be observed before. Our results set an upper bound for the relevant energy scale of the complex Kondo crossover phenomenon in $YbRh_2Si_2$.