TT 5: f-Electron Systems and Heavy Fermions I

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

TT 5.1 Mon 9:30 H 3005

X-ray absorption study of Sn and Cd substituted $CeCoIn_5$ — Kai Chen[1,6], Fabio Strigari[1], Martin Sundermann[1,2,3], Stefano Agrestini[2], Zhiwei Hu[2], Davide Betto[4], Kurt Kummer[4], Javier Herrero[5], Steffen Wirth[2], and •Andrea Severing[1,2] — [1]University of Cologne, Institute of Physics II, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]PETRA III, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [5]ALBA Synchrotron, Barcelona, Spain — [6]present address: SOLEIL Synchrotron, Saclay, France

In a previous soft x-ray absorption investigation of the crystal-electric field wave function of the $CeRh_{1-x}Ir_xIn_5$ substitution series we showed that changes in the cerium wave function correlate with the phase diagram while these changes anticorrelate with the lattice anisotropy. Here we will present the crystal-electric field wave functions for two other related substitution series: $CeCo(In_{1-x}Cd_x)_5$ and $CeCo(In_{1-y}Sn_y)_5$. The parent compound $CeCoIn_5$ is an unconventional superconductor (T_c=2.3 K) with a field-induced antiferromagnetic quantum critical point inside the superconducting dome. The substitution of tiny amounts of In by Cd or Sn suppresses superconductivity. Sakai *et al.* suspected that Cd and Sn doping has a different impact on hybridization. Our soft x-ray absorption results strongly support this conjecture and show that M-edge XAS is a very sensitive probe of the direction dependence of hybridization.

TT 5.2 Mon 9:45 H 3005

Magnetic field dependence of the zone-center excitation in the heavy-fermion metal CeB_6 — •P. Y. Portnichenko[1], S. E. Nikitin[1,2], S. V. Demishev[3], A. V. Semeno[3], H. Ohta[4], A. V. Dukhnenko[5], N. Yu. Shitsevalova[5], V. B. Filipov[5], Z. Huesges[6], Z. Lu[6], A. Schneidewind[7], and D. S. Inosov[1] — [1]TU Dresden, Germany — [2]MPI-CPfS Dresden, Germany — [3]GPI of RAS, Moscow, Russia — [4]Kobe University, Japan — [5]IMPS, Kiev, Ukraine — [6]HZB, Berlin, Germany — [7]JCNS, Jülich, Germany

The heavy-fermion metal CeB_6 with a simple cubic crystal structure is characterized by a rich magnetic-field – temperature phase diagram. Neutron scattering experiments showed an intense ferromagnetic collective mode that dominates the magnetic excitation spectrum. ESR measurements revealed a significant anisotropy of the g-factor as a function of the applied field direction. The g-factor remains temperature independent and isotropic for field directions like [110] or [111], but shows a noticeable anomaly for $\mathbf{B} \parallel [100]$. Knowing that the energy of the ESR resonance matches perfectly with that of the field-induced INS excitation, we expected a corresponding softening of the zone-center mode in field parallel to [100]. However, our results show absolutely no temperature effect on the g-factor at high fields. We observe significant difference of the resonance energy upon change of the field direction. Observed difference of the resonance energy can be explained either by anisotropy or by redistribution of the spectral weight between two collective magnetic modes, which we perceive as a change of the resonance energy.

TT 5.3 Mon 10:00 H 3005

Doping-induced redistribution of magnetic spectral weight in substituted hexaborides $Ce_{1-x}La_xB_6$ and $Ce_{0.7}Nd_{0.3}B_6$ — •S. E. Nikitin[1,2], P. Y. Portnichenko[2], A. V. Dukhnenko[3], N. Yu. Shitsevalova[3], V. B. Filipov[3], Y. Qiu[4], J. A. Rodriguez-Rivera[4,5], J. Ollivier[6], and D. S. Inosov[2] — [1]MPI CPfS, Dresden, Germany — [2]TU Dresden, Germany — [3]I.M. Frantsevich Inst. for Problems of Materials Sci. of NAS, Kiev, Ukraine — [4]NIST Center for Neutron Research, Maryland, USA — [5]University of Maryland, USA — [6]ILL, Grenoble, France

CeB_6 is a model example of intriguing heavy-fermion physics. At zero field it exhibits a complex magnetic phase diagram with antiferromagnetic (AFM) and "hidden order" phases, which is associated with the ordering of Ce^{3+} antiferroquadrupolar (AFQ) moments. Our recent ARPES and INS measurements have shown that both propagation vectors of AFQ and AFM phases are dictated by the nesting instability of the Fermi-surface. In this work we have extended this approach to probe the evolution of the electronic properties cerium hexaboride upon La and Nd substitutions. We observe that strong diffuse peak at the corner of the Brillouin zone, which coincides with the propagation vector of the elusive AFQ order in CeB_6, is rapidly suppressed by both La and Nd doping, like the AFQ order itself and the corresponding spectral weight is transferred to the $X(\frac{1}{2}00)$ point. Our results provide direct evidence that the complex magnetic phase diagrams of substituted hexaborides are dictated by the evolution of the Fermi-surface upon effective "hole"-like doping.

TT 5.4 Mon 10:15 H 3005

Investigation of the surface properties of SmB_6 by STM — •Lin Jiao[1], Sahana Rössler[1], Priscila F. S. Rosa[2,3], LiuHao Tjeng[1], Zachary Fisk[2], Frank Steglich[1], and Steffen Wirth[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, University of California, Irvine, California, USA — [3]Los Alamos National Laboratory, Los Alamos, New Mexico, USA

We present scanning tunneling microscopy and spectroscopy measurements on SmB_6, which is a candidate material for a topological Kondo insulator. The measurements were conducted on non-reconstructed (001) surfaces [1,2] at temperatures down to 0.35 K. At these low temperatures, we observe several well-resolved states within the hybridization gap of SmB_6. The temperature evolution of the tunneling spectra indicates two energy scales, in line with bulk and surface Kondo effect, respectively [3]. Moreover, we can put our results into perspective with the predicted existence of topologically protected surface states. In this respect, we will also present spectroscopic as well as resistivity results on substituted samples $(Sm_{1-x}R_x)B_6$ for R = Gd, Y, Yb and, in particular, discuss the influence of magnetic substituents on the topological surface states.

[1] S. Rößler *et al.*, Proc. Natl. Acad. Sci. USA **111**, 4798 (2014).
[2] S. Rößler *et al.*, Phil. Mag. **96**, 3262 (2016).
[3] L. Jiao *et al.*, Nat. Commun. **7**, 13762 (2016).

TT 5.5 Mon 10:30 H 3005

DFT+DMFT simulations of rare-earth hexaborides — •Florian Sohn[1], Steffen Backes[4], Salvatore R. Manmana[1], Roser Valentí[3], and Peter E. Blöchl[1,2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Institut für theoretische Physik, Technische Universität Clausthal, Germany — [3]Institut für theoretische Physik, Goethe-Universität Frankfurt am Main, Germany — [4]Centre de Physique Théorique, École polytechnique, Palaiseau, France

Rare-earth hexaborides (REB_6) are strongly correlated materials, where the strong Coulomb interaction between electrons in the rare earth's f-electron shell influence the electronic properties of the whole material decisively. REB_6 exhibit a variety of low-temperature phenomena, including antiferromagnetic ordering for most partially filled f-shells, ferromagnetic ordering in EuB_6, superconductivity for LuB_6, topological insulating behavior in SmB_6 and a complex phase diagram with Kondo behavior in CeB_6. We present results of DFT+DMFT simulations performed on selected REB_6, in particular for the spectral function. For the DFT calculations, the Wien2k code is applied, while for the DMFT we employ the continuous-time hybridization expansion quantum Monte Carlo (CT-HYB) matrix code of the ALPSCore project. Our goal is to compare with ARPES experiments.

We gratefully acknowledge financial support by the DFG project PR298/19-1.

TT 5.6 Mon 10:45 H 3005

Magnetic anisotropy in $YbRh_6Si_4$ single crystals — •Sebastian Witt, Doan-My Tran, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, D-60438 Frankfurt

Recently, researchers have started to investigate the structural properties of rhodium-rich silicides $RERh_6Si_4$ (RE = rare earth) [1]. The new interest in these hexagonal and non-centrosymmetric compounds derives from the suppression of a ferromagnetic transition to a quantum critical point in Si-doped $CeRh_6Ge_4$. Recently, a magnetic transition at 4.5K in $YbRh_6Si_4$ polycrystals was reported.

Here, we present the single crystal growth of $YbRh_6Si_4$ with indium flux. In first measurements (susceptibility, resistivity and specific heat) we have investigated the magnetic transition around 4.5K in needle-

shaped single crystals. In susceptibility and resistivity data the magnetic anisotropy for field along and perpendicular to the c-direction will be presented.
[1] D. Voßwinkel et al., Z. Naturforschung B, **72**, 11 (2017).

TT 5.7 Mon 11:00 H 3005

A Study of the Ferromagnetic and Lifshitz Phase Transitions in the Heavy-Fermion Metal $YbNi_4P_2$ by Ultrasonic Measurements — •Yeekin Tsui, Lars Postulka, Bernd Wolf, Ulrich Tutsch, Kristin Kliemt, Cornelius Krellner, and Michael Lang — Goethe-Univeristät, Physikalisches Institut SFB/TR49, D-60438 Frankfurt(M),Germany

$YbNi_4P_2$ is a stoichiometric heavy-fermion Kondo-lattice system with a Kondo temperature of 8 K [1]. This system is situated in the close vicinity of a ferromagnetic (FM) quantum-critical point (QCP) and can be tuned to the FM QCP by substituting a small amount of phosphorous by arsenic [1]. Recently, nine field-induced Lifshitz transitions (LTs) have been proposed in $YbNi_4P_2$ [2] from the results of the transport and thermodynamic measurements, revealing a complicated electronic band structure of the system. We have performed ultrasonic measurements on single crystals of $YbNi_4P_2$ to deepen the understanding of these phase transitions. We found clear features in the ultrasound velocity (v) and the attenuation (α) corresponding to crystal-electric-field and Kondo effects. However, we detected no or very small anomalies in v or α at the expected FM phase transition in the longitudinal c33 mode, reflecting a weak coupling of the corresponding symmetry strain to the magnetic structure. On the other hand, pronounced features were identified at the proposed Lifshitz transitions at roughly 0.4, 6 and 7 T clearly demonstrating the different character of these transitions.
[1] A. Steppke et al., Science 339 (2013) 933.
[2] H. Pfau et al., Physical Review Letters 119 (2017) 126402.

15 min. break.

Invited Talk TT 5.8 Mon 11:30 H 3005

Superconductivity in $YbRh_2Si_2$ — •Erwin Schuberth — Technische Universität München

Our recent experiments on $YbRh_2Si_2$ showed - aside from the well known antiferromagnetic transition at 70 mK - two new phases below 10 mK and 2 mK respectively[1]. The latter is practically coinciding with superconductivity. Evidence for these findings came from magnetic susceptibility measurements, dc as well as ac, performed at the Walther-Meissner Institut in Garching. The 2mK A-phase transition is a hybrid electronic-nuclear spin transition and it extends to fields of 23 mT where it is suppressed to below our detection limit of 800 μK. In addition, specific heat data show, that at this transition a large entropy is involved coming from the nuclear spins of the Yb isotopes. Here we present additional, unpublished results around and below this temperature up to the Quantum Critical Point at 60 mT. Also, we reanalyzed previous data on the magnetic susceptibility of $CeCu_6$ taken in Garching and Cornell in 1994 [2]. The results are very similar to those of $YbRh_2Si_2$ and it is very likely that the same mechanism holds in both systems.
[1] E. Schuberth et al., Science 351, 485 (2016)
[2] C. Jin et al., Physica B 194-196, 207-208 (1994)

TT 5.9 Mon 12:00 H 3005

Crystal field scheme of the topologically non-trivial Kondo insulator $CeRu_4Sn_6$ determined by RIXS — •Andrea Amorese[1,2], Kurt Kummer[3], Oliver Stockert[2], Andrey Prokofiev[4], Silke Paschen[4], Maurits Haverkort[5], and Andrea Severing[1,2] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [4]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [5]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Rare earth Kondo insulators have the potential for being strongly correlated topological insulators and $CeRu_4Sn_6$ is one of the promising candidates. Unfortunately, in the presence of correlations the models employed for describing the topological insulating properties lack reliability so that information about the electronic structure must be determined experimentally. In particular, the degeneracy of the the Ce^{3+} Hund's rule ground multiplet is lifted in $CeRu_4Sn_6$ by the crystal electric field (CEF), but the CEF potential was up to now only partially characterized, due to limitations of the traditional neutron-based techniques. Resonant inelastic soft x-ray scattering (RIXS) has been recently shown to be a very powerful tool to overcome these limitations. With RIXS the ground state and excited Hund's rule multiplet are accessible and due to the resonant process the electronic excitations are pure and not overshadowed by e.g. phonons. With soft RIXS we have fully determined the CEF scheme of $CeRu_4Sn_6$.

TT 5.10 Mon 12:15 H 3005

Nuclear magnetic resonance investigation of the novel heavy fermion system $Ce_2CoAl_7Ge_4$ — •Adam P. Dioguardi[1,2], Pedro Guzman[2,3], Priscila F. S. Rosa[2], Nirmal J. Ghimire[2], Serena Eley[2], Stuart E. Brown[3], Joe D. Thompson[2], Eric D. Bauer[2], and Filip Ronning[2] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [3]Department of Physics and Astronomy, UCLA, Los Angeles, California 90095, USA

We present nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) measurements performed on single crystalline $Ce_2CoAl_7Ge_4$, a member of a recently discovered family of heavy fermion materials $Ce_2MAl_7Ge_4$ (M = Co, Ir, Ni, or Pd). A clear Knight shift anomaly ($K \not\propto \chi$) is observed at coherence temperatures $T^* \sim 17.5$ K for $H_0 \parallel \hat{c}$ and 10 K for $H_0 \parallel \hat{a}$ at the ^{59}Co site, and $T^* \sim 12.5$ K at the ^{27}Al(3) site for $H_0 \parallel \hat{a}$ characteristic of the heavy fermion nature of this compound. At high temperatures the ^{59}Co NMR spin-lattice relaxation rate T_1^{-1} is dominated by spin fluctuations of the 4-f local moments with a weak metallic background. Furthermore, we find $(T_1TK)^{-1} \propto T^{-1/2}$ at the ^{59}Co site as expected for a Kondo system for $T < T^*$ and $T < T_K$. ^{59}Co NQR T_1^{-1} measurements at low temperatures indicate slowing down of spin fluctuations above the magnetic ordering temperature $T_M \sim 1.8$ K. A weak ferromagnetic character of fluctuations around $\mathbf{q} = 0$ is evidenced by an increase of χT vs T above the magnetic ordering temperature.

TT 5.11 Mon 12:30 H 3005

Optical response of Cerium-based clathrates — Farzaneh Zamani[1], •Stefan Kirchner[2], and Silke Paschen[3] — [1]Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China — [3]Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

Clathrates are a class of caged compounds that display a wide range of physical properties as a function of host-guest composition. Cerium-based type-I clathrates are of particular interest due to their unusual thermoelectric properties with potential for application[1]. The origin of the observed thermopower enhancement at comparatively high temperature in $CeBa_7Au_6Si_{40}$, however, is still a matter of debate. While Kondo scattering does occur in the system, Curie-Weiss behavior prevails down to about 1K. In order to understand the role of the rattling modes in the thermopower enhancement we address the optical response of $CeBa_7Au_6Si_{40}$. In particular, we investigate if a model of phonon-enhanced Kondo scattering can explain the differences observed [2] in the optical conductivity of $CeBa_7Au_6Si_{40}$ and its rare-earth free reference compound.
[1] A. Prokofiev et al.,Nature Mat. **12**, 1096-1101 (2013).
[2] G. Johnstone et al., unpublished.

TT 5.12 Mon 12:45 H 3005

Crystalline electric field calculations for $CeIr_3Ge_7$ — •Jacintha Banda[1], Binod Rai[2], Emilia Morosan[2], Christoph Geibel[1], and Manuel Brando[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA

$CeIr_3Ge_7$ is a metallic antiferromagnet with an extremely low Néel temperature of 0.65 K despite the absence of Kondo effect and geometrical frustration. We have solved the crystalline electric field (CEF) scheme for the well localized Ce^{3+} moment which has a trigonal point symmetry. We compared our calculations with experimental data on single crystalline samples and found an excellent agreement with one possible solution. This yields a large positive B_2^0 CEF parameter, resulting in a large CEF splitting with the first and second excited CEF levels at 374 and 1398 K respectively. A large off diagonal B_4^3 parameter leads to a strong mixing of the $\left|\pm\frac{5}{2}\right\rangle$ function into the pre-

dominantly $\left|\pm\frac{1}{2}\right\rangle$ CEF ground state. As a result, the system shows a huge XY anisotropy. The overall CEF splitting in this compound is one of the largest ever observed in a Ce system. Comparison with other compounds suggest that such large CEF splitting might be connected with the presence of 5d ligands.