TT 9: f-Electron Systems and Heavy Fermions II

Time: Monday 15:00–17:00 Location: HSZ 201

TT 9.1 Mon 15:00 HSZ 201

Quantum oscillations in heavy-fermion ferromagnet $YbNi_4P_2$ over many Zeeman induced Lifshitz transitions — •William Broad[1], Sven Friedemann[1], Owen Moulding[1], Takaki Muramatsu[1], Kristin Kliemt[2], and Cornelius Krellner[2] — [1]University of Bristol, Bristol, United Kingdom — [2]Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is a heavy-fermion metal situated near a very rare ferromagnetic quantum critical point (FM QCP). Understanding the nature of this ferromagnetism requires knowledge of the Fermi surface; it has been speculated that this FM QCP is enabled by a quasi-1D Fermi surface. At the same time, the strongly renormalised band structure is readily modified by relatively small magnetic fields, with nine Lifshitz transitions below 20 T due to Zeeman splitting. Here, we present Shubnikov–de Haas oscillations up to 35T, including detailed rotation and mass studies. We present analysis over several of these Lifshitz transitions, observing frequency changes and appearances/disappearances. We model the band structure with DFT calculations of the local 4f reference compound $LuNi_4P_2$ and use rigid-band shifts to approximate the effect of the Kondo hybridisation. At highest fields, the Fermi surface is well modelled with a small shift to increase the Fermi volume. As the field is reduced, we find better agreement with a larger shift corresponding to stronger hybridisation of 4f electrons. Finally, we present models for the topology of the Lifshitz transitions.

TT 9.2 Mon 15:15 HSZ 201

Exploring the effect of different substitutions on the valence transition in $YbInCu_4$ single crystals — •Michelle Ocker, Bereket Ghebretinsae, Bernd Wolf, Kristin Kliemt, Michael Lang, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

At ambient pressure the compound $YbInCu_4$ undergoes a 1^{st} order valence transition at $T_v = 42$ K by changing the temperature [1]. Thus, ytterbium in the compound is present in the $Yb^{2.9+}$ state at high temperatures and as $Yb^{2.7+}$ at low temperatures [2]. In analogy to Eu compounds, the line of first order valence transitions might end in a second order critical endpoint [3]. In order to study the nature of the phase transition in more detail, single crystal samples can be prepared in In-Cu flux which are substituted with silver and gold [4]. With increasing substitution level, negative chemical pressure within the crystal is increased and the characteristics of the valence transition changes significantly. Here, we report on the single crystal growth with different substitution levels and the results of our structural, chemical and physical characterization.

[1] I. Felner et al., Phys. Rev. B 35, (1987) 6956
[2] H. Sato et al., Physica B 351, (2004) 298
[3] Y. Ōnuki et al., J. Phys. Soc. Jap. 89, (2020) 102001
[4] J. L. Sarrao et al., Phys. Rev. B 54, (1996) 12207.

TT 9.3 Mon 15:30 HSZ 201

Impact of Fe substitution on the electronic structure of URu_2Si_2 — •Andrea Marino[1], Denise S. Christovam[1], Chun-Fu Chang[1], Johannes Falke[1], Chang-Yang Kuo[2], Chi-Nan Wu[2], Martin Sundermann[1,3], Andrea Amorese[1,3], Hlynur Gretarsson[4,5], Camilla Moir[6], M. Brian Maple[6], Peter Thalmeier[1], Liu Hao Tjeng[1], and Andrea Severing[3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]University of Cologne, Cologne, Germany — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany — [5]PETRA III, DESY, Hamburg, Germany — [6]University of California, San Diego, USA

The application of pressure as well as the substitution of Ru with Fe in the hidden order (HO) compound URu_2Si_2 lead to the formation of the large moment antiferromagnetic phase (LMAFM), with the respective phase diagrams bearing similarities for low Fe content (<0.3). For higher Fe content (>1) $URu_{(2-x)}Fe_{(x)}Si_2$ adopts the Pauli paramagnetic ground state of UFe_2Si_2. However, the question remains open what causes the suppression of HO in favour of the LMAFM phase. We investigate the $URu_{(2-x)}Fe_{(x)}Si_2$ series with $4f$ core-level photoelectron spectroscopy. The $4f$ satellite features are enhanced at low Fe content ($x<0.4$) and suppressed as x increases, following the trend shown by the ordered moment. We discuss this in terms of the variation of the filling of the $5f$ shell. Implications for the exchange interaction in a Doniach phase diagram picture are then also considered.

TT 9.4 Mon 15:45 HSZ 201

High-resolution tender x-ray RIXS at the example of UGa_2 — •Martin Sundermann[1,2], Andrea Marino[1], Denise Christovam[1], Andrea Amorese[1,3], Ladislav Havela[4], Bernhard Keimer[5], Hlynur Gretarsson[1,2,5], Peter Thalmeier[1], Liu Hao Tjeng[1], and Andrea Severing[1,3] — [1]MPI-CPfS, Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Institute of Physics II, University of Cologne, Germany — [4]Condensed Matter Physics, Karls-Universität, Prag, Czech — [5]MPI-FKF, Stuttgart, Germany

The nature of the $5f$ electrons in U intermetallic compounds, usually thought to be on the verge between localization and itinerant states, still challenges the reach of well-established condensed matter physics' techniques. Yet, it is not uncommon that U-based compounds show no inelastic neutron scattering excitations, and the question remains, if these compounds are fully delocalized or if multiplet states are present but not observable. Cutting-edge instrumental developments enables us to perform tender x-ray high-resolution (150 meV) resonant inelastic X-ray scattering (RIXS) experiments at the strong U $M_{4,5}$ absorption edges. We demonstrate the potential of this technique at the example of the intermetallic high T_C ferromagnet UGa_2. We observe mutliplet excitations that are well reproduced with a full multiplet calculation that includes the crystal-electron field splitting and is based on an U $5f^2$ configuration. Further we show that, although crystal-field splittings are too small to be resolved, the directional dependence of the scattering cross-section gives access to the ground-state symmetry.

TT 9.5 Mon 16:00 HSZ 201

Electronic structure of UO_2 studied by high-resolution tender-x-ray RIXS — •Denise S. Christovam[1], Martin Sundermann[1,2], Andrea Marino[1], Daisuke Takegami[1], Andrea Amorese[1,3], Hlynur Gretarsson[2,4], Bernhard Keimer[4], Philipp Raison[5], Robertro Caciuffo[5], Andrea Severing[1,3], and Liu Hao Tjeng[1] — [1]MPI-CPfS, Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Institute of Physics II, University of Cologne, Germany — [4]MPI-FKF, Stuttgart, Germany — [5]Joint Research Centre, Euorpean Commission, Karlsruhe, Germany

The investigation of the $5f$ electronic states in uranium-based compounds is a great challenge for x-ray instrumentation. Recent instrumental developments in the tender x-ray regime enable us to carry out resonant inelastic x-ray scattering (RIXS) experiments at the strong U $M_{4,5}$ absorption edge with an experimental resolution of 150 meV. In this work, we studied the electronic structure of UO_2. We observe the excitations the U^{4+} $5f^2$ ionic multiplet states as well as the excitations involving the O $2p$ to U $5f$ charge transfer satellites. Detailed insight in the many-body nature of the ground state and excited states of UO_2 is obtained by analysing the data with full-multiplet cluster calculations which also take into account crystal field and hybridization effects.

TT 9.6 Mon 16:15 HSZ 201

Strain-tuning of charge frustration in the heavy $3d$ fermion oxide LiV_2O_4 — •Ryosuke Oka[1,2], Dennis Huang[1], Minu Kim[1], Peter Wochner[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Physics, University of Tokyo, Tokyo, Japan — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany

The mixed-valent spinel LiV_2O_4 is the first discovered $3d$ electron system showing heavy fermion behavior without localized f moments, but its origin has remained a decades-old mystery. Amongst numerous scenarios proposed so far, including an analogy with a dense Kondo system, one of the leading scenarios is charge frustration inherent in the pyrochlore sublattice of the spinel. In this scenario, the ground state is composed of a macroscopic number of degenerate charge orderings (COs), and the frustration prevents the system from undergoing a metal-to-insulator transition, thereby enhancing the effective mass. By applying external perturbations that lift the degeneracy in different ways, various insulating COs can be selected out of the frustrated

metallic ground state. For example, hydrostatic pressure and biaxial tensile strain in the (001) plane stabilize distinct [111]- and [001]-oriented COs, respectively. We have grown LiV_2O_4 thin films on various substrates, in order to apply uniaxial strain in different directions. We used synchrotron x-ray diffraction to characterize the applied strain and transport measurements to probe how the heavy fermion phase in LiV_2O_4 moves toward possible distinct charge-ordered states.

TT 9.7 Mon 16:30 HSZ 201

Evolution of the 4f states in $TmSe_{1-x}Te_x$ from semimetals to semiconductors — •Chul Hee Min[1], Simon Müller[2], Michael Heber[3], Lenart Dudy[4], Hendrik Bentmann[3], Matthias Kalläne[1], Markus Scholz[3], Woojae Choi[5], Yong Seung Kwon[5], Friedrich Reinert[2], and Kai Rossnagel[1,3] — [1]IEAP, CAU Kiel, Germany — [2]EP7 and ct.qmat, University of Würzburg, Germany — [3]DESY, Hamburg, Germany — [4]Synchrotron SOLEIL, Saint-Aubin, France — [5]Dep. of EMS, DGIST, South Korea

Localized 4f states are often considered to become coherent states at low temperatures by hybridizing with itinerant conduction 5d states. In the standard Anderson model, only one type of interaction between the two states is taken into account, which is sufficient to describe Kondo physics. However, additional interaction has been suggested for the mixed valence regime to satisfy the Friedel sum rule when two charge states exist on a short time scale [1]. Here we present photoemission results of mixed-valent Thulium monochalcogenide $TmSe_{1-x}Te_x$. This system allows us to study the evolution of the localized 4f states between semimetallic and semiconducting phases without applying external pressure and disturbing the periodicity of Tm ions. Our results show two different interactions between 4f and 5d states across the phase transition.

[1] F. Haldane, Phys. Rev. B 15, 2477 (1976)
C. Varma, Phys. Rev. B 102, 155145 (2022)

TT 9.8 Mon 16:45 HSZ 201

Orbital-selective Mott transition and heavy-fermion physics in the van der Waals ferromagnet $Fe_{3-x}GeTe_2$ — •Frank Lechermann[1], Xiaojian Bai[2], Yaohua Liu[2], Yongqiang Cheng[2], Alexander I. Kolesnikov[2], Feng Ye[2], Travis J. Williams[2], Songxue Chi[2], Tao Hong[2], Garrett E. Granroth[2], Andrew F. May[3], and Stuart Calder[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [3]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The van der Waals ferromagnet $Fe_{3-x}GeTe_2$ is a fascinating material that attracts combined strong interest from magnetoelectronics as well as from strong correlation physics. While near room temperature, the possibilities to exfoliate conducting ferromagnetic layers is investigated, at temperatures below $T \sim 100\,\mathrm{K}$ the system displays surprising signatures of heavy-fermion physics. By means of first-principles many-body calculations, we here show that the latter temperature regime is governed by a rare orbital-selective Mott phase. This leads to emergent Kondo(-lattice) behavior in an unique transition-metal 3d compound, accompanied by antiferromagnetic fluctuations within the ferromagnetic phase. These fluctuations are experimentally revealed by neutron scattering.