# TT 17: Heavy Fermions

Time: Wednesday 14:00–18:00

Antiferromagnetic groundstate in CeCu<sub>2</sub>(Si<sub>0.55</sub>Ge<sub>0.45</sub>)<sub>2</sub> with broken body center — •ENRICO FAULHABER<sup>1</sup>, OLIVER STOCKERT<sup>2</sup>, ASTRID SCHNEIDEWIND<sup>1,3</sup>, MICHA DEPPE<sup>2</sup>, CHRISTOPH GEIBEL<sup>2</sup>, FRANK STEGLICH<sup>2</sup>, and MICHAEL LOEWENHAUPT<sup>1</sup> — <sup>1</sup>TU Dresden; Institut für Festkörperphysik; Zellescher Weg 16; D-01062 Dresden — <sup>2</sup>Max-Planck-Institut CPfS; Nöthnitzer Str. 40; D-01187 Dresden — <sup>3</sup>Forschungsneutronenquelle Heinz Meier-Leibnitz; D-85747 Garching The heavy fermion system CeCu<sub>2</sub>(Si<sub>1-x</sub>Ge<sub>x</sub>)<sub>2</sub> allows to study the interplay between antiferromagnetism and superconductivity (for  $x \leq$ 

0.1). CeCu<sub>2</sub>(Si<sub>0.55</sub>Ge<sub>0.45</sub>)<sub>2</sub> is especially interesting, since its characteristic temperatures which are easier accessible than in CeCu<sub>2</sub>Si<sub>2</sub>, and the value of the ordered magnetic moment ( $\mu_{Ce} \approx 0.5 \ \mu_{B}$ ) [1] qualify it as a reference system for the magnetic structures within the system.

Recently, we performed an elastic neutron scattering experiment on the PANDA triple-axis-spectrometer at the FRM-II, tuned for high q resolution. Additional satellite peaks were observed below  $T_{\rm L} \approx 1.4 \pm 0.1$  K  $< T_{\rm N} \approx 3.1$  K consistent with the same incommensurate propagation vector  $\tau = (0.27 \ 0.27 \ 0.51)$  found above  $T_{\rm L}$ , but corresponding to a broken symmetry of the body centred ThCr<sub>2</sub>Si<sub>2</sub> structure (I4/mmm) and, therefore, a reduced Brillouin zone. Our findings can be modelled with two magnetic sublattices formed by counterrotating cycloids. The results will be discussed in comparison to previous measurements.

[1] E. Faulhaber et al., J. Magn. Magn. Mater. 272 (2004) 44.

### TT 17.2 Wed 14:15 H18

Pressure depending  $\mu$ SR measurements on CeCu<sub>2</sub>Si<sub>2</sub> — •ASTRID SCHNEIDEWIND<sup>1</sup>, OLIVER STOCKERT<sup>2</sup>, DANIEL ANDREICA<sup>3</sup>, ALEX AMATO<sup>3</sup>, JULIA ARNDT<sup>2</sup>, HIRALE S. JEEVAN<sup>2</sup>, CHRISTOPH GEIBEL<sup>2</sup>, and FRANK STEGLICH<sup>2</sup> — <sup>1</sup>Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — <sup>2</sup>MPI-CPfS, Nöthnitzer Str. 40, D-01178 Dresden, Germany — <sup>3</sup>Laboratory for Muon-Spin Spectroscopy, CH-5232 Villigen PSI, Switzerland

The heavy-fermion compound CeCu<sub>2</sub>Si<sub>2</sub> is located quite close to a quantum phase transition (QPT) at the disappearence of magnetic order. Applying pressure the QTP can be tuned without any change of the amount of disorder. We performed weak transverse-field  $\mu {\rm SR}$ measurements to investigate an A/S-type CeCu<sub>2</sub>Si<sub>2</sub> single crystal and to study how the antiferromagnetic order vanishes under pressure and gives way to superconductivity. With increasing pressure the Néel temperature decreases until the magnetic signal finally vanished. In the superconducting state the magnetic volume decreases with lowering temperature while superconducting volume increases as expected from ambient pressure measurements [1]. This can be related to phase separation into magnetically ordered and superconducting regions. Surprisingly, the temperature range, where magnetism and superconductivity are co-existing, becomes narrower with increasing pressure. In conclusion, applying pressure leads to a stabilization of superconductivity and supression of antiferromagnetism in CeCu<sub>2</sub>Si<sub>2</sub>. [1] Stockert et al., Physica B374-375 (2006) 415.

#### TT 17.3 Wed 14:30 H18

Polarization dependent Ce- $M_{45}$  x-ray spectroscopy on CeCu<sub>2</sub>Si<sub>2</sub> and CePd<sub>2</sub>Si<sub>2</sub>: a new approach to determine the symmetry of the lowest crystal field states — •P. HANSMANN<sup>1</sup>, A. SEVERING<sup>1</sup>, Z. HU<sup>1</sup>, C.F. CHANG<sup>1</sup>, S. KLEIN<sup>1</sup>, H.J. LIN<sup>2</sup>, C.T. CHEN<sup>2</sup>, B. FAK<sup>3</sup>, C. GEIBEL<sup>4</sup>, F. STEGLICH<sup>4</sup>, and L.H. TJENG<sup>1</sup> — <sup>1</sup>II. Phys. Inst., Univ. Köln, Cologne — <sup>2</sup>NSRRC Hsinchu, Taiwan — <sup>3</sup>CEA, SPSMS, Grenoble, France — <sup>4</sup>MPI CPFS, Dresden

In the past neutron scattering as the standard technique has given confusing and often contrary results about the symmetry of the lowest crystal field states of correlated RE compounds, particularly on CeCu<sub>2</sub>Si<sub>2</sub> [1,2] and CePd<sub>2</sub>Si<sub>2</sub> [3,4,5]. The knowledge about these lowest states is crucial for the understanding of the magnetic properties and also provides an important ansatz for a proper description of the low energy electronic structure including the Fermi surface. We will present results obtained with a different technique, namely soft-x-ray absorption spectroscopy (XAS) at the Ce- $M_{45}$  edges. This technique is known to be sensitive to the symmetry of the initial state and through the polarization dependence we obtain direct spectroscopic information about the  $|J_z\rangle$  admixtures of the ground state. XAS used in this

# Location: H18

manner should be a powerful new tool, complementary to neutrons, in determining the symmetry of crystal field ground states in RE.

 S. Horn et al. PRB 23 (1981) 3171 [2] E.A. Gorimychkin et al. PRB 47 (1993) 14280 [3] A. Severing et al. PRB 39 (1989) 2557 [4]
R.A. Steemann et al. J. Appl. Phys. 67 (1990) 5203 [5] N.H. van Dijk et al. PRB 61 (2000) 8922

TT 17.4 Wed 14:45 H18 Study of a smeared ferromagnetic quantum phase transition in CePd<sub>1-x</sub>Rh<sub>x</sub> single crystals — •MICHA DEPPE<sup>1</sup>, TANJA WESTERKAMP<sup>1</sup>, ADAM PIKUL<sup>1</sup>, NUBIA CAROCA-CANALES<sup>1</sup>, CHRISTOPH GEIBEL<sup>1</sup>, ROBERT KÜCHLER<sup>1</sup>, PHILIPP GEGENWART<sup>1</sup>, and JULIAN SERENI<sup>2</sup> — <sup>1</sup>Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — <sup>2</sup>Lab. Bajas Temperaturas, Centro Atómico Bariloche (CNEA), 8400 S.C. de Bariloche, Argentina

Appropriate Cerium based compounds for the study of a ferromagnetic (quantum) critical point are extremely scarce. On the other hand the orthorhombic alloy  $CePd_{1-x}Rh_x$  shows a continuous decrease of the ferromagnetic transition temperature  $T_C(x)$  from 6.6 K for x =0 to 0.025 K at x = 0.87. Detailed low temperature measurements of  $CePd_{1-x}Rh_x$  polycrystalline samples showed an extended range of non-Fermi liquid behavior between  $0.85 \le x \le 0.9$ , suggesting a smeared ferromagnetic quantum phase transition near  $x_{cr} \approx 0.87$ . We extended our studies on  $CePd_{1-x}Rh_x$  single crystals, which allow to include anisotropy effects in the study and analysis of this system. The anisotrophy is quite strong for  $x \leq 0.6$  with the easy axis along the c-direction, but decreases rapidly for  $x \ge 0.7$ . Furthermore the ferromagnetic signal in the ac-susceptibility becomes frequency dependent at  $x \ge 0.72$  supporting a suppression of long-range magnetic order. We explain the unusual magnetic behavior of  $CePd_{1-x}Rh_x$  with a distribution of local Kondo temperatures near  $x_{cr}$  due to disorder introduced by  $Pd \rightarrow Rh$  exchange and the formation of a "Kondo -Cluster glass".

TT 17.5 Wed 15:00 H18 Larmor diffraction study of the thermal expansion of URu<sub>2</sub>Si<sub>2</sub> under high pressure — •PHILIPP NIKLOWITZ<sup>1</sup>, CHRIS-TIAN PFLEIDERER<sup>1</sup>, THOMAS KELLER<sup>2,3</sup>, and JOHN MYDOSH<sup>4</sup> — <sup>1</sup>Physik Department E21, Technische Universität München, 85748 Garching, Germany — <sup>2</sup>Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — <sup>3</sup>ZWE FRMII, Technische Universität München, 85748 Garching, Germany — <sup>4</sup>II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

The metallic rare-earth system URu<sub>2</sub>Si<sub>2</sub> shows two transitions at zero pressure: at  $T_0 \approx 17.5$  K a strong peak in the heat capacity indicates the transition to an unknown so-called hidden order (HO) state; the HO state might be relevant to explain the occurance of a superconducting state at  $T_s \approx 1.4$  K. A key to the HO state might be the large-moment AF state, to which the HO state is transformed under pressure. The pressure dependence of  $T_0$  is surprisingly weak across the pressure induced phase change and it is interesting to follow the pressure evolution of thermodynamic quantities.

We have studied the pressure evolution of the thermal expansion from zero pressure to 20 kbar and in a wide temperature range down to 3 K. Larmor diffraction experiments have been performed on a high quality single crystal of stoichiometric URu<sub>2</sub>Si<sub>2</sub>. In particular, we present in detail the pressure evolution of the signature of  $T_0$  in the thermal expansion of the *a*- and *c*-axis. Here, Larmor diffraction proves to be a very reliable technique for high precision measurements of the lattice constants.

#### TT 17.6 Wed 15:15 H18

**Pressure-temperature phase diagram of URu<sub>2</sub>Si<sub>2</sub> by resistivity measurements** — •ELENA HASSINGER<sup>1,2</sup>, GEORG KNEBEL<sup>2</sup>, BERNARD SALCE<sup>2</sup>, JACQUES FLOUQUET<sup>2</sup>, and PASCAL LEJAY<sup>3</sup> — <sup>1</sup>KIP, Universität Heidelberg, Germany — <sup>2</sup>DRFMC, SPSMS, CEA Grenoble, France — <sup>3</sup>CRTBT, CNRS Grenoble, France

At ambient pressure URu<sub>2</sub>Si<sub>2</sub> undergoes a transition at T<sub>0</sub> = 17.5 K to so called hidden order phase and a second transition to superconducting ground state at T<sub>SC</sub> = 1.5 K. We measured the resistivity of a small single crystal in highly hydrostatic pressure up to 2.5 GPa in a diamond anvil pressure cell with Argon as pressure transmitting

medium. At the critical pressure  $p_c = 0.5 \ GPa$  a large moment antiferromagnetic phase develops and can be seen as a small anomaly in the resistivity curves  $\rho(T)$  at constant pressure. In these measurements the superconducting transition can be seen up to 1.3 GPa. In the vicinity of  $p_c$  the resistivity curves in the normal state at low temperature follow a power law with an exponent smaller than 2 indicating non Fermi liquid behavior.

# TT 17.7 Wed 15:30 H18

Study of energy scales in  $Lu_{1-x}Yb_xRh_2Si_2 - \bullet ULRIKE$ KÖHLER<sup>1</sup>, SAMUEL MAQUILON<sup>2</sup>, CORNELIUS KRELLNER<sup>1</sup>, NIELS OESCHLER<sup>1</sup>, CHRISTOPH GEIBEL<sup>1</sup>, VELJKO ZLATIĆ<sup>3</sup>, ZACHARY FISK<sup>4</sup>, and FRANK STEGLICH<sup>1</sup> - <sup>1</sup>MPI for Chemical Physics of Solids, Dresden, Germany - <sup>2</sup>University of California, Davis, USA - <sup>3</sup>Institute of Physics, Zagreb, Croatia - <sup>4</sup>University of California, Irvine, USA In strongly correlated *f*-electron systems, Kondo interaction and crys-

tal electric field (CEF) excitations often give rise to large anomalies in the thermopower. Thermopower investigations are therefore known to be a useful tool to determine the Kondo and CEF energy scales.

Measurements of the thermopower of the stoichiometric heavy fermion system YbRh<sub>2</sub>Si<sub>2</sub> revealed a single large minimum around 80 K which was attributed to both, Kondo interaction and CEF effects. From the obtained data no separation of Kondo and CEF energy scales was possible. We performed thermopower measurements on the diluted heavy fermion system Lu<sub>1-x</sub>Yb<sub>x</sub>Rh<sub>2</sub>Si<sub>2</sub>. For Yb concentrations of  $x \leq 0.5$  the pronounced thermopower minimum splits into 2 separate features. An extrapolation of the position of the low temperature shoulder allows to determine the Kondo temperature of pure YbRh<sub>2</sub>Si<sub>2</sub> ( $T_{\rm K} \approx 25$  K). Our data suggest a strong dependence of the minima on the Yb concentration x that may not be solely attributed to the extremely small unit cell volume change. We compare our results to theoretical calculations of the high temperature thermopower of Yb intermetallics including both, CEF splitting and charge fluctuations.

### TT 17.8 Wed 15:45 H18

Pressure dependence of the characteristic Kondo temperature of YbRh<sub>2</sub>Si<sub>2</sub> — •GABRIEL ALEJANDRO DIONICIO, HERIBERT WILHELM, JULIA FERSTL, CHRISTOPH GEIBEL, and FRANK STEGLICH — Max-Planck-Institute for Chemical Physics of Solids

Several anomalies were observed in the electrical resistivity of YbRh<sub>2</sub>Si<sub>2</sub> as a function of the pressure, namely,  $T_N$  and maxima at  $T_{max}$  and  $T_{max}^{low}$ . The engative logarithmic temperature dependence of the electrical resistivity  $\rho(T)$  for  $T > T_{max}$  and for  $T > T_{max}^{low}$  indicates that a combined incoherent Kondo scattering on the ground state and the excited CEF-levels are responsible for these anomalies. Therefore, we attempt to infer the pressure dependence of the characteristic Kondo temperature  $T_K(p)$  of YbRh<sub>2</sub>Si<sub>2</sub> by means of a simple model that considers the effect of the orbital degeneracy on a dense Kondo state and the pressure dependence of the Néel temperature  $T_N(p)$ , in particular in the pressure range 4 GPa < p < 9 GPa where  $T_N(p)$  shows a quasi-pressure independent behavior.

## 15 min. break

#### TT 17.9 Wed 16:15 H18

Ferromagnetism in the layered Kondo system CeRuPO — •CORNELIUS KRELLNER<sup>1</sup>, NAGESH KINI<sup>2</sup>, EVA MARIA BRUENING<sup>1</sup>, MICHAEL NICKLAS<sup>1</sup>, MICHAEL BAENITZ<sup>1</sup>, and CHRISTOPH GEIBEL<sup>1</sup> — <sup>1</sup>Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — <sup>2</sup>Department of Applied Chemistry, Hiroshima University, Higashis-Hiroshima 739-8527, Japan

Intermetallic Kondo lattice systems have attracted considerable attention in the last decades. While there exist many Ce-based compounds showing antiferromagnetic ground states, only very few systems are known which exhibit ferromagnetic order. On the way to find new Cebased Kondo lattices close to a ferromagnetic quantum phase transition, the CeTPO (T=transition metal) compound series attracted our interest, because of the rather unusual crystal structure with alternating layers of TP<sub>4</sub> and OCe<sub>4</sub> tetrahedra. In this contribution, we will present the first investigations of the physical properties of CeRuPO crystallizing with the tetragonal ZrCuSiAs type structure (P4/nmm). Measurements of the magnetic susceptibility reveal that Cerium is in a trivalent state with a ferromagnetic transition at  $T_C = 15$  K which is confirmed in the temperature dependence of specific heat. A pronounced decrease of the resistivity below 50 K and enhanced ther-

mopower  $S(10 \text{ K}) = 10 \ \mu\text{V/K}$  confirm the presence of Kondo interaction. Detailed study of <sup>31</sup>P NMR and results of the magnetization under pressure up to 2 GPa will be discussed. In addition, we show first investigations of the physical ground states of the isostructural compounds CeTPO (T = Os, Fe, Co).

TT 17.10 Wed 16:30 H18 **Pressure Dependence of The Néel in CeRhIn**<sub>5-x</sub>**Sn**<sub>x</sub> **Stud iedby Thermal Expansion** — •J. GUIDO DONATH<sup>1</sup>, PHILIPP GEGENWART<sup>1,3</sup>, ERIC D. BAUER<sup>2</sup>, JOHN L. SARRAO<sup>2</sup>, and FRANK STEGLICH<sup>1</sup> — <sup>1</sup>Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — <sup>2</sup>Los Alamos National Laboratory, Los Alamos, New Mexico, 87545 USA — <sup>3</sup>I. Physikalisches Institut, Universitaet Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

We present low-temperature thermal expansion measurements on the Sn-substituted heavy fermion antiferromagnet CeRhIn<sub>5-x</sub>Sn<sub>x</sub> for  $0 \le x \le 0.48$  in which  $T_N(x)$  is linearly suppressed from 3.8 K at x = 0 to zero at  $x_c \approx 0.4$ . The application of the Ehrenfest relation allows to calculate the initial uniaxial and hydrostatic pressure dependences  $dT_N/dP$  at various x. The observed non-linear variation with x is interpreted in terms of the Doniach diagram by an increase of the 4f-conduction electron hybridization induced by Sn-doping. As no traces of superconductivity are observed close to  $x_c$ , this system is ideally suited for the study of the magnetic quantum critical point.

TT 17.11 Wed 16:45 H18 **Thin-film growth of the heavy-fermion superconductor CeCoIn**<sub>5</sub> — •OLEKSIY SOROKA and MICHAEL HUTH — Physicalisches Institut, J. W. Goete–Universität, Max-von-Laue-Str. 1, D-60438

Thin films of CeCoIn<sub>5</sub> were deposited on different substrates by using molecular beam epitaxy and found superconductive with transition temperatures about 2 K. Their transport properties are comparable with those of the bulk material and the resistivity shows typical heavy fermion behaviour. The growth characteristics were studied by means of x-ray diffraction and scanning tunneling microscopy and revealed (001)-oriented growth with pronounced island formation. Based on the chemical composition of the films obtained using energy dispersive x-ray analysis a ternary phase formation diagram was deduced. The heavy fermion compound CeCoIn<sub>5</sub> is a member of a recently discovered layered heavy fermion family with general formula CeMIn<sub>5</sub> (M=Co, Ir, Rh). These compounds exhibit many ground states that have been observed in f-electron systems, including paramagnetism, antiferromagnetism, exotic ambient-pressure and pressure induced superconductivity. There exists a relationship to the high- $T_c$  superconductors as well. The layered quasi-2D crystal structure of these materials and that of the high- $T_c$  cuprates share common features with regard to their spin-dependent electronic excitation spectrum. The most direct technique to investigate the spectrum of these excitations is tunneling spectroscopy which benefits strongly from well-defined surface as presented by epitaxial thin films.

### TT 17.12 Wed 17:00 H18

Paramagnetic moment in  $RFe_2Ge_2$  (R = Lu and Yb) — •JULIA FERSTL, HELGE ROSNER, and CHRISTOPH GEIBEL — Max Planck Institut für Chemische Physik fester Stoffe

We synthesised polycrystals and then grew single crystals of YbFe<sub>2</sub>Ge<sub>2</sub> and LuFe<sub>2</sub>Ge<sub>2</sub>. The analysis of their physical properties revealed the presence of a paramagnetic Fe-moment of  $3 \mu_B$ /Fe at high temperatures in both compounds, which strongly contrasts the well established non-magnetic behavior of Co and Fe in the RCo<sub>2</sub>Si<sub>2</sub>, RCo<sub>2</sub>Ge<sub>2</sub> and RFe<sub>2</sub>Si<sub>2</sub> compound series. Additionally a phase transition at T<sub>0</sub>  $\approx$  9 K appears in LuFe<sub>2</sub>Ge<sub>2</sub>, which likely corresponds to antiferromagnetic ordering of the Fe-moments. The observation of a paramagnetic Femoment is discussed in the context of results from LDA-calculations. Our results in YbFe<sub>2</sub>Ge<sub>2</sub> further indicate an intermediate valent Yb state with a comparatively low characteristic 4*f* energy of 80 K. This corresponds to a valence close to but less then 3. At low temperatures we observe a heavy Fermion behaviour with a moderately enhanced Sommerfeld coefficient  $\gamma = 200 \text{ mJ}\cdot\text{mol}^{-1}\text{K}^{-2}$ .

TT 17.13 Wed 17:15 H18 Theory of magnetic excitons in the heavy-fermion superconductor  $UPd_2Al_3 - \bullet$ Jun CHANG<sup>1</sup>, ILYA EREMIN<sup>1,2</sup>, PE-TER THALMEIER<sup>3</sup>, and PETER FULDE<sup>1</sup> - <sup>1</sup>Max-Planck Institut für Physik komplexer Systeme, D-01187 Dresden, Germany - <sup>2</sup>Institute für Mathematische und Theoretische Physik, Technische Universität Carolo-Wilhelmina zu Braunschweig, 38106 Braunschweig, Germany — <sup>3</sup>Max-Planck Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany

We analyze the influence of unconventional superconductivity on the magnetic excitations in the heavy fermion compound UPd<sub>2</sub>Al<sub>3</sub>. We show that it leads to the formation of a bound state at energies well below  $2\Delta_0$  at the antiferromagnetic wave vector  $\mathbf{Q} = (0, 0, \pi/c)$ . Its signature is a resonance peak in the spectrum of magnetic excitations in good agreement with results from inelastic neutron scattering. Furthermore we investigate the influence of antiferromagnetic order on the formation of the resonance peak. We find that its intensity is enhanced due to intraband transitions induced by the reconstruction of Fermi surface sheets. We determine the dispersion of the resonance peak near  ${\bf Q}$  and show that it is dominated by the magnetic exciton dispersion associated with local moments. We demonstrate by a microscopic calculation that  $UPd_2Al_3$  is another example in which the unconventional nature of the superconducting order parameter can be probed by means of inelastic neutron scattering (INS) and determined unambiguously.

TT 17.14 Wed 17:30 H18 Magnetic Phase Diagram of the Doped 2D Kondo Lattice Model: a DCA calculation — •LEE C. MARTIN and FAKHER F. ASSAAD — Universität Würzburg, Germany

We apply an antiferromagnetic symmetry breaking implementation of the dynamical cluster approximation (DCA) to the two-dimensional hole-doped Kondo lattice model with hopping t and coupling J.

Precise calculations of single particle spectral functions compare well

with exact BSS results at the particle-hole symmetric point. However, our DCA version, combined with a QMC cluster solver, also allows simulations away from particle-hole symmetry and has enabled us to map out the magnetic phase diagram of the model as a function of doping, coupling J/t and band structure.

At half-filling, our results show that the linear behaviour of the quasi-particle gap at small values of J/t is a direct consequence of particle-hole symmetry, which leads to nesting of the Fermi surface. Breaking the symmetry, by inclusion of a diagonal hopping term, results in a greatly reduced gap which appears to follow a Kondo scale.

Upon doping the magnetic phase observed at half-filling survives and ultimately gives way to a paramagnetic phase. Across this magnetic order disorder transition, we track the topology of the Fermi surface.

#### TT 17.15 Wed 17:45 H18

Berechnung von Spektralfunktionen stark korrelierter 5f-Systeme – • MARTIN REESE und GERTRUD ZWICKNAGL – Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig

Es werden Aktinidsysteme mit stark korrelierten 5f-Elektronen mit orbitaler Entartung betrachtet. Der verwendete Ansatz kombiniert die Ergebnisse aus ab-initio Elektronenstrukturrechnungen mit Clusterstörungsrechnungen an zweidimensionalen Clustern. Dieses Vorgehen gestattet es, die komplexen Korrelationen angemessen zu berücksichtigen. Die berechneten Spektren zeigen sowohl dispersive Quasiteilchenbänder als auch inkohärente lokale Anregungen. Die Ergebnisse der Rechnungen sind in guter qualitativer Übereinstimmung mit experimentell gewonnenen Daten aus Photoemissionsspektroskopie.