

# Monday Afternoon, October 28, 2013

## Actinides and Rare Earths Focus Topic

Room: 102 C - Session AC+MI+SA+TF-MoA

### Actinides and Rare Earths: Theory and Electron Correlation

Moderator: L. Havela, Charles University, Czech Republic

2:00pm AC+MI+SA+TF-MoA1 **Structural and Electronic Relationships Between the Lanthanide and Actinide Elements, B. Johansson**, Uppsala University, Sweden **INVITED**

The similarity and difference between the solid state properties of the 4f and 5f transition

metals are pointed out. The heavier 5f elements show properties which have direct

correspondence to the early 4f transition metals, suggesting a localized behaviour of the

5f electrons for those metals. On the other hand, the fact that Pu metal has a 30% lower

volume than its neighbour heavier element, Am, suggests a tremendous difference in the

properties of the 5f electrons for this element relative to the heavier actinides. This change

in behaviour between Pu and Am can be viewed as a Mott transition within the 5f shell

as a function of the atomic number  $Z$ . On the metallic 5f side of the Mott transition (i.e.,

early actinides), the elements show most unusual crystal structures, the common feature

being their low symmetry. An analogous behaviour for the lanthanides is found in cerium

metal under compression, where structures typical for the light actinides have been observed

experimentally. A generalized phase diagram for the actinides is shown to contain features

comparable to the individual phase diagram of Ce metal. The crystal structure behaviour of

the lanthanides and heavier actinides is determined by the number of 5d (or 6d) electrons

in the metallic state, since for these elements the  $f$  electrons are localized and nonbonding.

For the earlier actinide metals electronic structure calculations – where the 5f orbitals

are treated as part of the valence bands – account very well for the observed ground state

crystal structures. The distorted structures can be understood as Peierls distortions away

from the symmetric bcc structure and originate from strongly bonding 5f electrons occupying

relatively narrow 5f states.

2:40pm AC+MI+SA+TF-MoA3 **Signature of Strong Correlations in Actinides and its Compounds: A Dynamical Mean Field Theory Perspective, G. Kotliar**, Rutgers University **INVITED**

Plutonium is a unique element, poised at the edge of a localization delocalization transition. Its compounds exhibit

remarkable phenomena, ranging from insulating behavior with a topologically non trivial band structure in PuB<sub>6</sub> [1]

to high temperature superconductivity PuCoGa<sub>5</sub> [2].

In the last decade a new paradigm for understanding, modeling and predicting physical properties of these materials

has emerged based on realistic implementations of dynamical mean field theory (DMFT) concepts [3][8] [9]. This theory

treats the wave (band-like) and the (particle-like) multiconfigurational aspects of the  $f$ -electrons on the same

footing. This theory accounts for the volume of  $\delta$  Pu in a paramagnetic configuration [6] and predicted its phonon

spectra [7].

In DMFT, an underlying self consistent impurity model can be used to reconstruct local observables of a material.

An illustrative example is the valence histogram, describing the weight of each atomic configuration in the ground

state of the solid. This important concept, and the resulting prediction for Pu can now be probed experimentally

using resonant XES [5] and neutron form factor measurements [11].

There are now many applications by many groups which have extended the reach of this approach to many actinide

based compounds. We will review the basis of the DMFT approach and compare some results with selected experiments

on 5f electron system. We will conclude with some new directions to face the challenge for material design in this

field [10].

[1] XY Deng, K. Haule and G. Kotliar preprint(2013).

[2] J. L. Sarrao et al., Nature 420, 297 (2002)

[3] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. of Mod. Phys. 68, 13-125 (1996).

[4] Per Soderlind, G. Kotliar, K. Haule, P. Oppeneer and D. Guillaumont, MRS Bulletin vol 35, 883, (2010).

[5] C.H. Booth, Y. Jiang, D.L.Wang, J.N. Mitchell, P.H. Tobash, E.D. Bauer, M.A.Wall, P.G. Allen, D. Sokaras, D. Nordlund,

T.-C. Weng, M.A. Torrez, and J.L. Sarrao PNAS 109, 10205-10209 (2012)

[6] J. H. Shim, K. Haule, and G. Kotliar, Science 318, 1615- 1617 (2007).

[7] X. Dai, S. Y. Savrasov, G. Kotliar, A. Migliori, H. Ledbetter, and E. Abrahams, Science Mag. 300, 953-955 (2003).

[8] (2007) Advances in Physics, 56:6, 829 - 926 (2007)

[9] G. Kotliar, S. Savrasov, K. Haule, V. Oudovenko, O. Parcollet, and C. Marianetti, Rev. of Mod. Phys. 78, 000865 (2006).

[10] Z. P. Yin, Xiaoyu Deng, K. Basu, Q. Yin, G. Kotliar, arXiv:1303.3322 (2013).

[11] M. E. Pezzoli, K. Haule, and G. Kotliar, Phys. Rev. Lett. 106, 016403 (2011).

3:40pm AC+MI+SA+TF-MoA6 **Towards a Better Understanding of Low-Energy Excitations in Heavy-Fermion Systems, G. Zwirknagl**, Technische Universität Braunschweig, Germany **INVITED**

Metals containing lanthanide or actinide ions have been at the focus of interest in condensed matter physics during the past decades. The presence of the partially filled  $f$ -shells leads to unexpected "anomalous" behavior such as heavy fermions, unconventional superconductivity, unusual magnetism as well as their co-existence.

The  $f$ -electron systems lie at the intersection of a large number of long-standing problems in the physics of metals. In metals containing ions with partially filled inner shells, we immediately face the fundamental question which picture provides the better starting point for theoretical models, a delocalized description in terms of energy bands or a localized representation which accounts for the atomic properties. The answer to the question which of the above-mentioned pictures is the appropriate starting point seems to depend on the physical quantities under consideration. This fact is a consequence of electronic correlations which prevent to describe the influence of the  $f$ -states over the entire temperature and energy range in terms of a unique simple model. While the high-temperature (high-energy) properties of lanthanide compounds can be understood in terms of localized  $f$ -moments it is generally accepted by now that the  $f$ -electrons should also be described in within a band picture as delocalized states as far as the low-energy excitations are concerned.

Concerning the underlying microscopic picture, it is generally accepted that the formation of strongly renormalized 4f-bands in lanthanides is a consequence of the Kondo effect where the degrees of freedom of the 4f-shell form a collective singlet ground state with the conduction electrons. The Kondo model, however, does not apply to actinide compounds where the situation is more complex. In some compounds, experiments suggest the co-existence of both localized atomic-like 5f-degrees of freedom with itinerant 5f-band states at low temperatures/ low energies. Microscopic model calculations suggest that partial localization of 5f-electrons may result from the intra-atomic Hund's rule-type correlations.

In the present talk, I shall give an overview over our present understanding of the "Dual Nature" of  $f$ -electrons. I present recent results on the suppression of the Kondo state in YbRh<sub>2</sub>Si<sub>2</sub> [1]. I discuss microscopic

calculations for electron spectroscopies in actinide compounds emphasizing the consequences of strong intra-atomic correlations of the 5f -shell [2,3].

[1] H. Pfau et. al., arXiv:1302.6867

[2] Gertrud Zwicknagl, MRS Online Proceedings Library, Volume 1444, (2012)

[3] Gertrud Zwicknagl, Phys. Stat. Sol. B 250, 634 (2013)

4:20pm **AC+MI+SA+TF-MoA8 Electronic Structure of EuO under Pressure**, *L. Petit, D. Szotek, M. Lueders, W.M. Temmerman*, Daresbury Laboratory, UK, *A. Svane*, Aarhus University, Denmark

We present results of an ab-initio study of EuO under pressure. The calculations are based on a first-principles methodology that adequately describes the dual character of electrons, itinerant versus localized by correcting for the unphysical self-interaction that underpins the local spin density approximation. We find that EuO, which at ambient conditions crystallizes in the NaCl structure, undergoes an isostructural insulator to metal transition around 35 GPa. The transition is associated with a change in the ground state valency configuration from  $\text{Eu}^{2+}(f^7)$  to  $\text{Eu}^{3+}(f^6)$ . At even higher pressure we observe a transition to the CsCl structure. The ground state valency configuration remains  $\text{Eu}^{3+}$ , i.e. this latter transition is isovalent. We compare our results to a recent experimental investigation that postulates a reentrant valence transition to a nearly divalent  $\text{Eu}^{2+}$  configuration at high pressures.

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