



TECHNISCHE
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ANGEWANDTE PHYSIK
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IAP-SEMINAR

ANNOUNCEMENT

Date: **Tuesday, 3.5.2016**
Time: **16:00 p.m.**
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**
yellow tower „B“, 5th floor, Sem.R. DB gelb 05 B (room number
DB05L03), 1040 Wien, Wiedner Hauptstraße 8-10

Lecturer: **A.B. Shick**
Institute of Physics, ASCR, Prague/Czech Republic

Subject: **Role of atomic multiplets in intermediate valence SmB₆ and PuB₆**

Abstract: The electronic structure of SmB₆ and PuB₆ was investigated making use of a combination of the density functional theory, and the exact diagonalization (ED) of an effective discrete Anderson impurity model [1]. Intermediate valence ground state with the f-shell occupation $n_{4f}=5.6$ is found for the Sm atom in SmB₆. This ground state is a singlet, and the first excited triplet state ~3 meV higher in the energy. SmB₆ is a narrow band insulator already in DFT, with the direct band gap of ~10 meV. The electron correlations increase the band gap, which now becomes indirect supporting the idea of "topological Kondo insulator".
For PuB₆, an intermediate valence ground state with the f-shell occupation $n_{5f}=5.5$ for the Pu atom is calculated. This ground state is a non-magnetic singlet with all angular momenta of the 5f-bath cluster equal to zero. The 5f-shell magnetic moment is completely compensated by the moment carried by the electrons in the conduction band. Already in DFT, PuB₆ is an insulator with a small amount of holes near the X-point, and the indirect band gap of 60 meV. This band gap becomes direct in DFT+ED calculations. Connection between the electronic structure of PuB₆, d-Pu and PuCoGa₅ is established. We propose that these materials belong to a new class of the intermediate valence "Racah" materials with the multi-orbital "Kondo-like" singlet ground-state.

[1] A. B. Shick, L. Havela, A. I. Lichtenstein, M. I. Katsnelson, Scientific Reports 5, 15429 (2015).

*All interested colleagues are welcome to this seminar lecture
(45 minutes presentation followed by discussion).*

P. Mohn e.h.
(Seminar-Chairperson)

H. Störi e.h.
(LVA-Leiter)