European XFEL

THEORY GROUP MEETING

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16:00

AER 19 Seminar Room 4.14

Role of atomic multiplets in intermediate valence SmB_6 and PuB_6

by

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The electronic structure of SmB_6 and PuB_6 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 SmB_6. This ground state is a singlet, and the first excited triplet state ~3 meV higher in the energy. SmB_6 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 PuB_6, 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, PuB_6 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 PuB_6, δ-Pu and $PuCoGa_5$ 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).