# ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE $UPdAs_2$ COMPOUND

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9.7 cm

The $UPdAs_2$ compound crystallizes in a tetragonal $HfCuSi_2$-type structure with the $P4/nmm$ space group [1]. $UPdAs_2$ orders antiferromagnetically below the Néel temperature of 240 K [1]. Magnetic moments localized on uranium atoms amount to 1,69±0.05 $\mu_B$ and are oriented along the c axis with sequence $++--$ [1,2].
The electronic band structure of $UPdAs_2$ is calculated using *FP-LAPW* method (Full Potential – Linearized Augmented Plane Wave) implemented in *WIEN2k* code[3]. *GGA*, *GGA+U*, *GGA+OP* (orbital polarization) approaches are studied. The Coulomb repulsion energy "$U$" applied to the uranium *5f* orbital is varying from 0 to 6 eV. Supercell doubled in c axis is built to reproduce magnetic moments sequence $++--$. Initial magnetic moments on uranium atoms are assumed to be opposite. The antiferromagnetic ground state is confirmed by total energies calculations for different magnetic configurations. Results of the *GGA+OP* approach are in the best agreement with the neutron scattering measurements of magnetic moments [1]. The total magnetic moment on uranium atoms is predicted to be 1.41 $\mu_B$ per atom.

[1] A. Murasik, P. Fisher and D. Kaczorowski, *J. Phys.:Condens. Matter* **2** (1990) 3967.
[2] D. Kaczorowski et al. *Phys. Rev. B* **58** (1998) 9227.
[3] P. Blaha et al., WIEN2k_7.3, Techn. Universität Wien, Austria, 2007.

13.4 cm

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