The electronic and magnetic properties of $UNiAs_2$ and $UPdAs_2$ antiferromagnets

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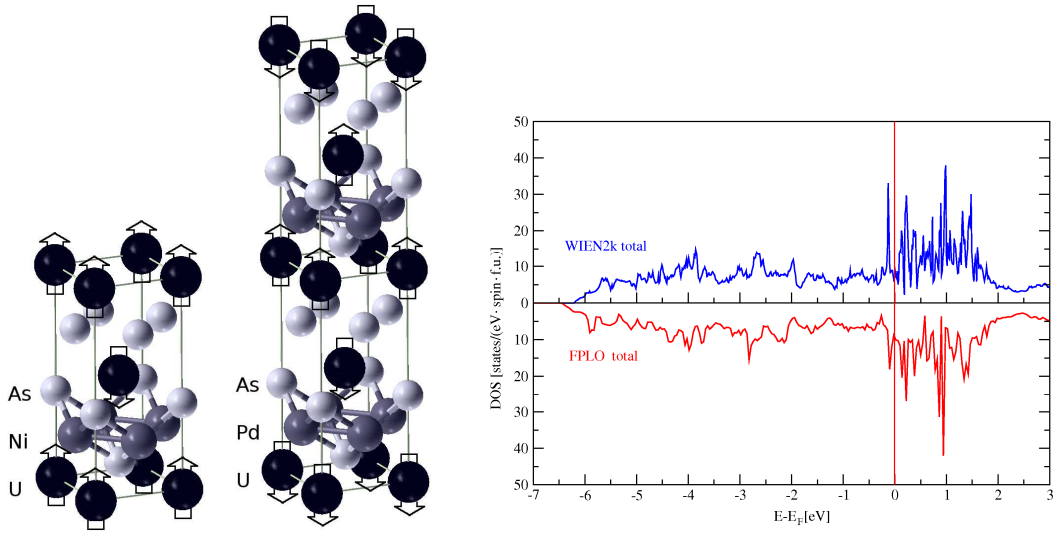
$UNiAs_2$ and $UPdAs_2$ compounds crystallize in the tetragonal structure type, P4/nmm space group [1,2]. The neutron diffraction indicates antiferromagnetic ordering below 195 and 240 K, respectively. Magnetic moments are oriented along the c direction and localized on uranium atoms. Experimental studies at 7.5 K amount to (1.85±0.06) μ_B for $UNiAs_2$ with sequence +-+- [1]. For $UPdAs_2$ magnetic reflections measured at 8.7 K could not be indexed based on single unit cell. The magnetic supercell is obtained by doubling chemical cell along c direction [Fig. 1.]. Magnetic moments are localized on uranium atoms with sequence ++-- [2,3] and amount to (1,69±0.05) μ_B.
Ab-initio calculations were performed based on two full-potential methods: WIEN2k [4] and FPLO[5]. Calculated magnetic moments confirm antiferromagnetic ground states and collinear magnetic sequences. WIEN2k and FPLO results are in agreement. The band structure has been calculated by using the local (spin) density approximation (L(S)DA). To improve spin-polarized calculation the orbital polarization correction were applied.



a) b)

Figure: a) crystallographic and magnetic structure of $UNiAs_2$ and $UPdAs_2$; b) total densities of states of $UPdAs_2$.
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[1] P. Fischer, A. Murasik, D. Kaczorowski, R. Troć, Physica B **156** (1989) 829-831
[2] A. Murasik, P. Fisher and D. Kaczorowski, J.Phys.:Condens. Matter **2** (1990) 3967-3972
[3] D. Kaczorowski et all., Phys. Rev. B **58** (1998), 9227
[4] P. Blaha et al., WIEN2k_7.3, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Karlheinz Schwarz, Techn. Universität Wien, Austria, 2007
[5] K. Koepernik and H. Eschrig, Phys. Rev. B **59** (1999), 1743