Electronic band structure, XPS and bulk physical properties of UCoGe

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9.7 cm

The electronic structure as well as bulk physical properties of orthorhombic TiNiSi-type UCoGe have been investigated. The results of band structure calculations, employing the modern full-potential local-orbital (FPLO) code [1], are compared with experimental data of x-ray photoelectron spectroscopy (XPS), transport and magnetic properties, obtained for single crystalline samples. Based on measurements on polycrystalline samples, Huy et al. [2] have interpreted the ground state of this compound as weak itinerant ferromagnetism ($T_C = 3$ K) coexisting with superconductivity ($T_{SC} = 0.8$ K). In contrast, our sample does not confirm their findings but turns out to be paramagnetic and non-superconducting down to the lowest values of temperature. A ferromagnetic phase is, however, close in energy to the non-magnetic phase according to our spin- and orbital-polarized calculations. Good agreement between results of non-magnetic calculations and XPS experimental data is achieved mainly for the U 5f electrons but not as much for the Co contributions. This indicates that the real electronic structure could be different from the predicted one.

[1] FPLO 3 and 5 [improved version of the original FPLO code by K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999)]; www.FPLO.de;

N.T. Huy et. al, Phys. Rev. Lett. 99, 067006 (2007);

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