ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE $UCoAs_2$ COMPOUND

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9.7 cm

The $UCoAs_2$ compound crystallizes in the tetragonal $HfCuSi_2$ type structure with space group $P4/nmm$ [1]. The compound orders ferromagnetically at 150K with a spontaneous magnetic moment of about 1.8 μ_B per formula unit. It exhibits a giant magnetic anisotropy alike in the ordered and the paramagnetic region, which has been interpreted as being caused predominantly by strong f-d hybridization and a pronounced crystal field effect [1].
We present results of fully relativistic band structure calculations based on the Full-Potential Local-Orbital Minimum-Basis Scheme (FPLO-5.10-20) [2]. An interesting problem is the magnetic behavior of the Co atoms. In this paper we compare magnetic moments obtained from calculations with and without orbital polarization correction [3].

[1] D. Kaczorowski, H. Noël, M. Potel, J. Alloys Compd. **302** (2000) 1
[2] FPLO code by K. Kopernik and H. Eschrig, Phys. Rev. B **59** (1999) 1743;
http://www.fplo.de
[3] O. Eriksson, M.S.S. Brooks, B. Johansson, Phys. Rev. B **41** (1990) 7311

13.4 cm

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