ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF Ce_5CuPb_3 BASED ON $AB-INITIO$ CALCULATIONS

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9.7 cm

Ce_5CuPb_3 crystallizes in the hexagonal Hf_5CuSn_3-type structure (sp. group $P6_3/mcm$) with two different cerium sites: 4d and 6g positions. To give insight into electronic and magnetic structures of Ce_5CuPb_3 system we employed the full potential local orbital (FPLO [1]) and full potential linear augmented plane wave (FP LAPW [2]) methods. The calculations were performed with and without spin polarization. Starting from the generalized gradient approximation (GGA), we additionally tested either an orbital polarization (OP) correction [3] and the GGA+U approach [4] with Coulomb repulsion energies U varied from 0 to 6 eV within the Ce 4f electron shell.

References:

[1] K. Koepernik, H. Eschrig, Phys. Rev. B 59 (1999) 1743.

[2] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, *Wien2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties* (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2.

[3] O. Eriksson et al., J. Phys. Condens. Matter 1 (1989) 4005.

[4] V.I. Anisimov et al., Phys. Rev. B 48 (1993) 16929.

13.4 cm

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