ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF Ce₅CuPb₃ BASED ON AB-INITIO CALCULATIONS

M. Stasiakᵃ, M. Werwińskiᵇ, A. Szajekᵇ, P. Leśniakᵇ, W.L. Malinowskiᵇ

ᵃFaculty of Technical Physics, Poznań University of Technology, Nieszawska 13a, 60-965 Poznań, Poland
ᵇInstitute of Molecular Physics, PAS, Smoluchowskiego 17, 60-179 Poznań, Poland

Ce₅CuPb₃ crystallizes in the hexagonal Hf₅CuSn₃-type structure (sp. group P6₃/mcm) with two different cerium sites: 4d and 6g positions. To give insight into electronic and magnetic structures of Ce₅CuPb₃ 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:

Subject category:
3. Magnetic Structure and Dynamics

Presentation mode:
poster

Corresponding author:
M. Stasiak

Address for correspondence:
Faculty of Technical Physics, Poznań University of Technology, Nieszawska 13a, 60-965 Poznań, Poland

Email address:
maciej.stasiak1234@gmail.com