Electronic magnetic properties of $Ce_6Pd_{12}In_5$ and $La_6Pd_{12}In_5$ compounds based on *ab initio* calculations

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Recently the novel heavy fermion Kondo lattice $Ce_6Pd_{12}In_5$ and its non-magnetic isostructural counterpart $La_6Pd_{12}In_5$ has been investigated in the framework of crystal structure, magnetic, thermodynamic and transport properties [1]. Both compounds crystallize in the same hexagonal crystal structure (space group $P6_3/mcm$) with a unique location of the rare earth atom. The aim of this work is to give insight into the electronic and magnetic structure of the $Ce_6Pd_{12}In_5$ and $La_6Pd_{12}In_5$ compounds based on the modern *ab-initio* spin polarized band structure calculations. The band structure calculations were performed based on the *full potential local-orbital minimum-basis* code (FPLO [2], version 14.00-49 in the fully relativistic mode).

References:

[1] M. Falkowski, A.M. Strydom, J. Alloys Compd. **613** (2014) 204.
[2] K. Koepernik, H. Eschrig, Phys. Rev. B **59** (1999) 1743.