ELECTRONIC STRUCTURE OF TERNARY ANTIMONIDES PdYbSb

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The electronic and magnetic properties of the ternary PdYbSb and Pd₂YbSb Heusler alloys have been studied experimentally and theoretically in the last years. The structural analysis [1] has shown that YbPdSb has a low temperature (LT) MgAgAs-type structure and high temperature (HT) TiNiSi-type structure. In this work we present the electronic structure of YbPd_{2-x}Sb compounds calculated by ab-initio method. We applied relativistic full potential FPLO7 method [2] in the local spin density approxmation (LSDA). The calculations were performed for two types of crystal structures LT and HT for the experimental values of lattice parameters. We have also studied the influence of dilution on the electronic structure of Pd_{2-x}YbSb for 1 < x < 2.

[1] R.Mishra et al., Z.Naturforsch 57b (2002) 1215.

[2] K.Koepernik, H.Eschrig, Phys, Rev. B.59 (1999) 1743.:http://www.fplo.de

[3] K.Koepernik, B.Velicky, R.Hayn and H.Eschrig, Phys.Rev.B 55 (1997) 5717.

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