Band Structure of ternary antimonides YbPdSb compounds by ab-initio methods

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9.7 cm

The physical properties of the ternary equiatomic antimonides YbPdSb and $YbPd_2Sb$ have been investigated in the recent years [1]. The structural analysis [1] has shown that YbPdSb has two type of structure: low temperature (LT) (MgAgAs type) F43m No.216) and high temperature (HT) (TiNiSi-type) Pnma No.62). In this work we present the electronic structure of YbPdSb. The ab-initio calculations are performed for two types of crystallographic structures. We applied fully relativistic full potential FPLO method [2]. The calculations the 4f states of Yb are treated as valence as well as semicore states. The band structure is also calculated by ASW method [3].

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