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Electronic Structure of Ternary Antimonides YbPdSb

M. Hermanowicz[a], A. Jezierski[b], J. Kaczkowski[b] and D. Kaczorowski[c]

[a]Institute of Physics, Poznań University of Technology
Nieszawska 13A, 60-965 Poznań, Poland
[b]Institute of Molecular Physics, Polish Academy of Sciences
M. Smoluchowskiego 17, 60-179 Poznań, Poland
[c]Institute of Low Temperatures and Structure Research, Polish Academy of Sciences
50-950 Wrocław, Poland

In this paper we present the electronic structure and magnetic properties of YbPdSb in low-temperature MgAsAg-type structure and high-temperature TiNiSi-type structure. The calculations were performed by *ab initio* full-relativistic full potential local orbital method within the local spin density approximation. *Ab initio* calculations showed the metallic character of YbPdSb compound in both structures. The density of states at the Fermi level is greater in high-temperature than in low-temperature structure.

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1. Introduction

The electronic, magnetic and transport properties of the rare-earth-based Heusler (RPdZ; R = Y, Ho, Er, Nd, Dy, Z = Sb, Bi) compounds have been investigated experimentally and theoretically in the last years [1, 2]. These compounds are atractive materials for thermoelectrical applications. In this paper we have studied the electronic structure of YbPdSb Heusler compound using the local spin density (LSD) approximation implemented in the full potential local orbital (FPLO 7.00) method [3–6]. YbPdSb compound crystallizes in TiNiSi-type structure (*Pnma*, No. 62) (high-temperature HT phase) (Fig. 1) and in MgAgAs-type structure ($F\bar{4}3m$, No. 216) (low-temperature LT phase) (Fig. 2). The band calculations were performed for two phases for the experimetal lattice

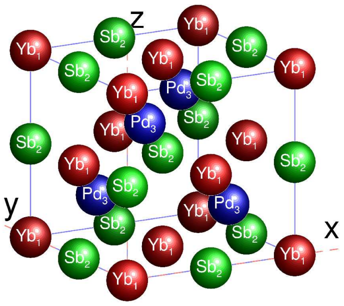

Fig. 1. Crystal structure of LT phase.

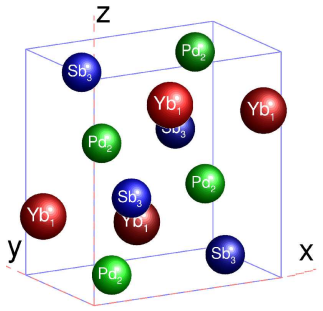

Fig. 2. Crystal structure of HT phase.

TABLE I

Lattice parameters for LT and HT YbPdSb compounds.

Compound	*a* [Å]	*b* [Å]	*c* [Å]
HT-YbPdSb	7.2562	4.6831	7.8542
LT-YbPdSb	6.45585	6.45585	6.45585

TABLE II

Atomic coordinates for both HT and LT phases of YbPdSb, *Pnma* and $F\bar{4}3m$ space groups, respectively.

Atom (HT)	Wyckoff position	x	y	z
Yb	4c	0.9969(3)	0.25	0.7067(2)
Pd	4c	0.1859(4)	0.25	0.0785(4)
Sb	4c	0.2922(3)	0.25	0.4059(3)
Atom (LT)	Wyckoff position	x	y	z
Yb	4c	0.0	0.0	0.0
Sb	4c	0.5	0.5	0.5
Pd	4c	0.75	0.75	0.75

parameters [2] (Table I). The high-temperature phase was observed while quenching of the YbPdSb sample from high temperature [2]. The positions of atom in the unit cell in both structures are listed in Table II. The half-Heusler YbTSb (T = Ni, Pd, Pt, Cu, Ag, Au) compounds were widely considered as a very promising material for the thermoelectric conversion [1].

2. Method of calculations

The electronic densities of states (DOS) were calculated by using the FPLO-7 method within density functional theory (DFT) [7, 8]. The exchange-correlation potential was used in the form proposed by Perdew and Wang [9]. The full-relativistic self-consistent calculations were performed for 735 (1331) k-points in the irreducible Brillouin zone for LT and HT type structure, respectively [10]. We have calculated the electronic properties for scalar- and full-relativistic mode for the spin-unpolarized and spin-polarized systems.

3. Results and discussion

The electronic DOS of YbPdSb compounds obtained by full-relativistic FPLO method are plotted in Figs. 3 and 4 for HT and LT phase, respectively. Upper curve presents the total density of states per spin and formula unit. The lower figures give the contribution from Yb, Sb and Pd atoms to the total DOS. The peaks located near $E = 0$ and $E = -1.5$ eV give the contribution from $4f$ states of Yb. Two broad peaks located between -5 and -2 eV are connected to $4d$ states of Pd atom. The main contribution to the DOS at the Fermi level comes from ytterbium $4f$ states. The shape of the total DOS for LT and HT phase is quite similar, although we observe the modification of the position of peaks. The densities of states at the Fermi level $N(E_{\mathrm{F}})$ in [states /(eV f.u.)] for LT and HT phase are listed in Table III. In HT phase the density f states at the Fermi level is greater than for LT structure. In the scalar-relativistic calculations (not presented here) we observed only one peak at the Fermi level due to $4f$ states of Yb. In both type of structures HT and LT we observed the similar position of $4f$ peaks of Yb. The modifications of bands and the densities of states in the region of energy -5 eV $< E < -2$ eV can result from the different local environment of Yb atoms in both structures (see Fig. 1 and Fig. 2). *Ab initio* calculations have shown that in the both phases the number of $4f$ electrons of Yb was about 13.6 and only in the LT phase we observed the small magnetic moment on Yb ($m_{\mathrm{s}} = 0.11\ \mu_{\mathrm{B}}$ and $m_{\mathrm{orb}} = 0.30\ \mu_{\mathrm{B}}$). The plots of the band structure of LT and HT YbPdSb compound are presented in Figs. 5

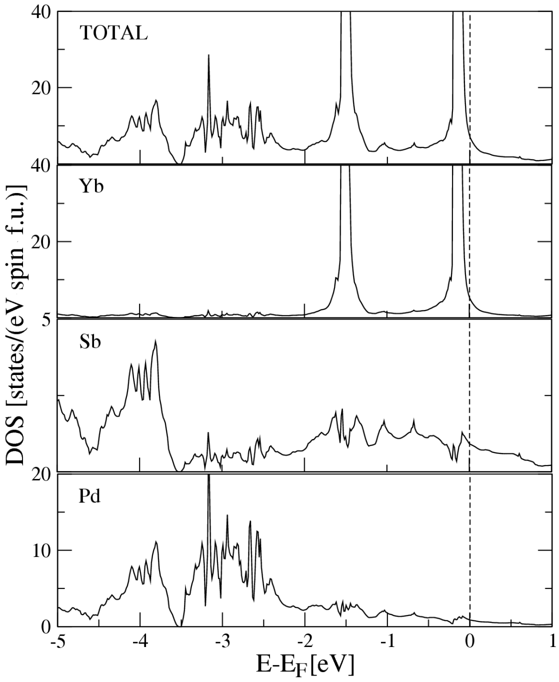

Fig. 3. Density of states for HT phase YbPdSb compound.

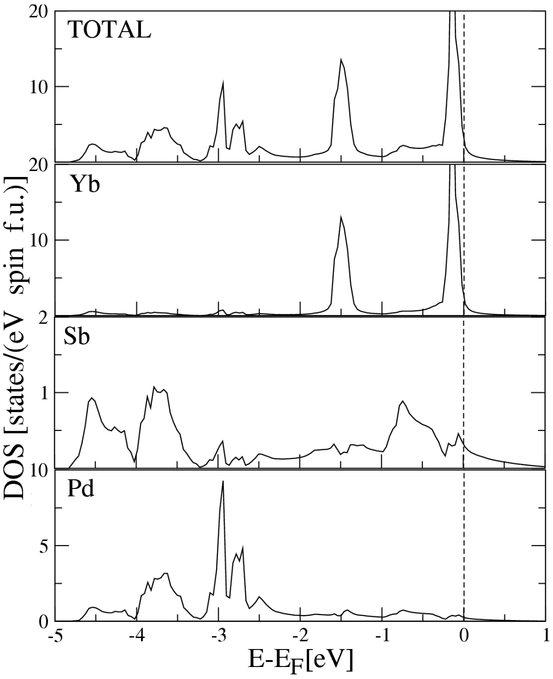

Fig. 4. Density of states for LT-YbPdSb half-Heusler compound.

TABLE III

The density of states at the Fermi level (states/(eV formula unit)).

Compound	$N(E_{\mathrm{F}})$
HT-YbPdSb	14.67
LT-YbPdSb	8.74

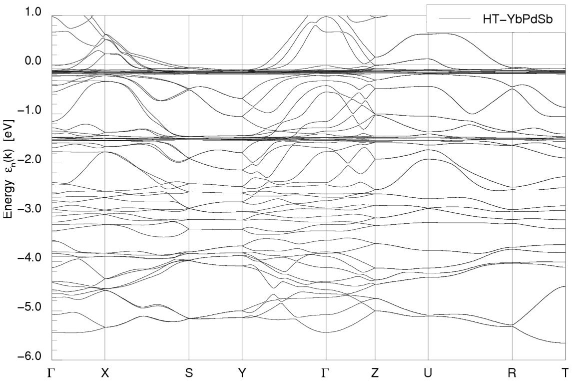

Fig. 5. Band structure of HT-YbPdSb half-Heusler compound.

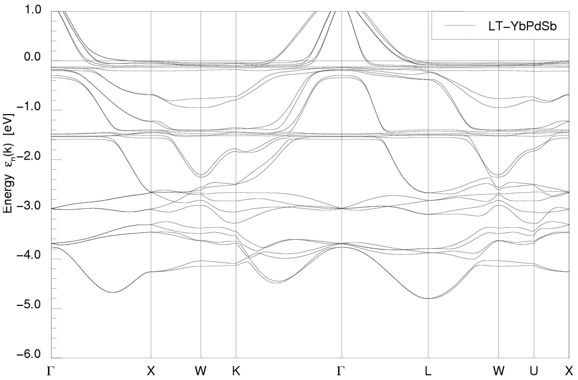

Fig. 6. Band structure of LT-YbPdSb half-Heusler compound.

and 6, respectively. In HT phase we observe the indirect gap in S–Y direction. The full-relativistic FPLO calculations indicate on metallic character of YbPdSb in both structures.

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