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MAGNETIC PROPERTIES AND ELECTRONIC STRUCTURE OF HALF-HEUSLER ALLOYS $FeRhSb_{1-x}Z_x$ (Z = P, As, Sn, Si, Ge, Ga, In, Al)

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The electronic structure and magnetic properties of $FeRhSb_{1-x}Z_x$ (x = 0, 0,25, 0,5, 0,75, 1) alloys with Z = P, As, Sn, Si, Ge, Ga, In, Al are studied by first-principles methods. For all compounds, three cubic phases with different atomic arrangement (α, β, and γ) are considered. It is shown that the β-phase is energetically favorable for $FeRhSb_{1-x}P_x$(x = 0,75, 1), FeRhAs and FeRhSi alloys. For the remaining 29 alloys, the γ phase is more energetically stable. The values of equilibrium lattice parameters and magnetic moments of stoichiometric ternary alloys are in good agreement with the literature values collected from other theoretical studies. The half-metallic ferromagnetic behavior is predicted for $FeRhSb_{0,25}Sn_{0,75}$, FeRhGe, FeRhSn, and $FeRhSb_{0,5}Al_{0,5}$. It has been found that the replacement of the Z element with another *sp* element allows for the creation of new four-component alloys that exhibit 100 % spin polarization.

Keywords: Heusler alloys; density of electronic states; half-metallic ferromagnets; density functional theory.

Introduction

Heusler alloys are represented by the general formula X_2YZ, and they constitute a large family of materials that exhibit diverse properties. These alloys are of interest due to the possibility of their practical application in various fields as thermoelectrics, shape memory alloys, magnetocaloric and spintronic materials etc. [1–3]. Half-Heusler alloys are also of great interest due to the fact that among these alloys there are many semimetallic ferromagnets. These alloys are described by the formula XYZ, where X and Y are typically transition metals and Z is a main group element and have a $C1_b$ structure.

Heusler-based half metals have attracted significant interest for spintronics applications [4, 5]. In particular, the density functional theory (DFT) study of half-metallicity in Fe-Rh based alloys can be found in Refs [6–10]. Ahmad et al [6], studied RhVZ alloys (Z = P, As, Sb) and reported that all compounds are half-metals. Bennani et al [7] studied the structural, electronic, magnetic and thermoelectric properties of RhFeX (X = Ge, Sn) alloys. Both compounds are stable half-metallic ferromagnets and can be potential candidates for use as thermoelectrics at low temperatures. Ma et al performed systematical study of 378 half-Heusler alloys XYZ (X = Cr, Mn, Fe, Co, Ni, Ru, Rh; Y = Ti, V, Cr, Mn, Fe, Ni; Z = Al, Ga, In , Si, Ge, Sn, P, As, Sb) and discussed their phase stability within ab initio calculations [5]. It was found that 45 alloys have a negative formation energy being the half-metals. Meenakshi et al [8] considered the optical, structural, magnetic and transport properties of RhFeZ alloys (Z = P, As, Sb, Sn, Si, Ge, Ga, In, Al). It is

shown that RhFeZ alloys (Z = Sb, Sn, Ge, Ga, In and Al) are stable in the γ phase, while RhFeZ alloys (Z= P, As and Si) are stable in the β phase. It was found that the alloys RhFeSn and RhFeGe are half-metals and can find potential application in spintronic devices. Zhanga [9] applied a Gaussian process regression model to calculate the structural parameters of half-Heusler compounds. Due to the need to search for new materials with high spin polarization values, the attention of researchers is aimed at finding the possibility of increasing the spin polarization values. Ahmad et al [10] studied the effect of pressure on the structural, thermal, magnetic and electronic properties of RhMnSb alloy. It was found that the RhMnSb alloy retains its properties up to a pressure of 38 GPa. In the absence of pressure, the spin polarization in the alloy is 25 %. The RhMnSb half-Heusler alloy makes a phase transition from metallic to half-metallic when the external hydrostatic pressure exceeds 21 GPa. As a result, it can be concluded that the properties of alloys containing Fe and Rh atoms are of great interest [7–12].

Our interest in this problem was stimulated by recent findings on RhFeSb discussed above. Within the context of this study, it should be emphasized that the spin polarization in RhFeSb can be adjusted by partially substituting the Sb atom with another sp element. In this work, the electronic structure and magnetic properties of compounds $FeRhSb_{1-x}Z_x$ (x = 0, 0,25, 0,5, 0,75, 1) with Z = P, As, Sn, Si, Ge, Ga, In, Al were studied using DFT calculations.

1. Computational Details

The DFT calculations were performed using the Vienna ab initio simulation package (VASP) [13, 14] with the Perdew, Burke and Ernzerhof generalized gradient approximation (PBE-GGA) [15] and projector augmented wave (PAW) potentials. The cutoff energy of plane waves was 500 eV. The number of k-points in the first Brillouin zone was $7 \times 7 \times 7$, obtained using a uniform grid centered at Γ point.

A half-Heusler compound XYZ crystallize in the face-centered cubic structure ($C1_b$) with one formula unit per primitive fcc unit cell and space group $F\overline{4}3m$ (No. 216). Three atomic configurations, labeled as α, β, and γ phases, are possible [8] (Fig. 1). In a case of α phase, Fe, Rh, and Sb (Z) atoms are located at 4c (1/4, 1/4, 1/4), 4b (1/2, 1/2, 1/2), and 4a (0, 0, 0) sites, respectively. For β phase, Fe, Rh, and Sb (Z) atoms were placed at 4a (0, 0, 0), 4b (1/2, 1/2, 1/2), and 4c (1/4, 1/4, 1/4) sites, respectively. In a case of γ phase, Fe, Rh, and Sb (Z) atoms were located at 4b (1/2, 1/2, 1/2), 4c (1/4, 1 /4, 1/4), and 4a (0, 0, 0) sites, respectively. The structural optimization and energetic calculations were carried out using the 12-atomic supercell for the ferromagnetic order of Fe and Rh atoms. To create the off-stoichiometric compounds $FeRhSb_{1-x}Z_x$ (x = 0, 0,25, 0,5, 0,75, 1), the Sb sublattice was successively replaced by P, As, Sn, Si, Ge, Ga, In, and Al. Thus, 33 compounds with as α, β, and γ phases were considered in the calculations.

For the calculation of electronic density of states (DOS), denser k-mesh grid of 21 × 21 × 21 was used for all compounds under study. The degree of spin polarization at the Fermi level was defined by the equation:

$$P = \frac{N^{\uparrow}_{E_F} - N^{\downarrow}_{E_F}}{N^{\uparrow}_{E_F} + N^{\downarrow}_{E_F}} \times 100\ \%, \tag{1}$$

here $N^{\uparrow}_{E_F}$ and $N^{\downarrow}_{E_F}$ are the DOS at E_F of spin-up and spin-down electrons, respectively.

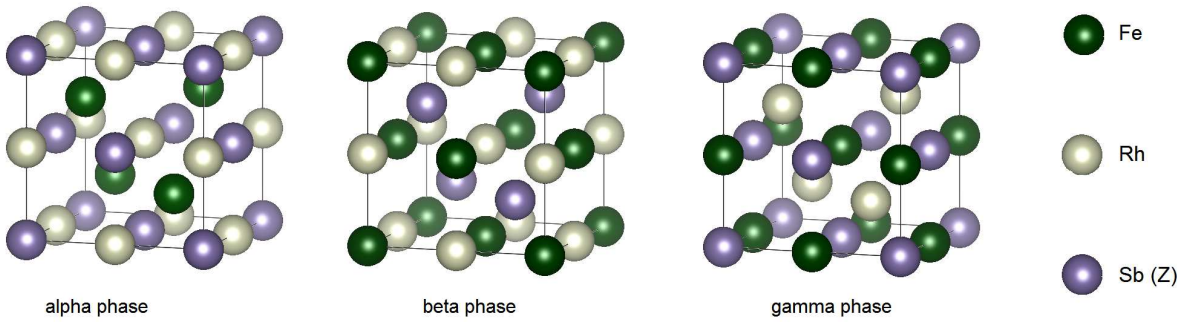
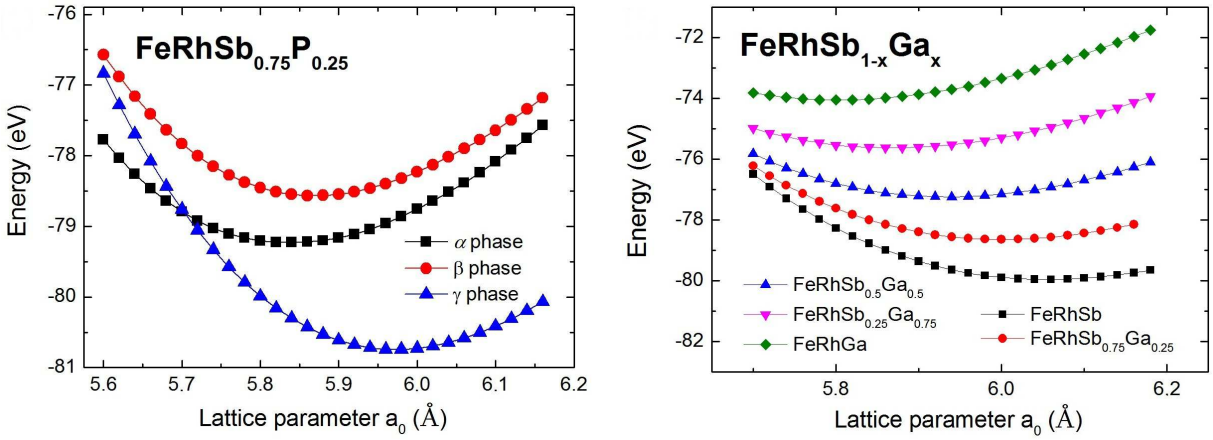


Fig. 1. Crystal structure of FeRh-based half-Heusler alloys with α, β, and γ phases

2. Results and Discussions

Let us firstly discuss the ground state energies of considered compounds $FeRhSb_{1-x}Z_x$ (Z= P, As, Sn, Si, Ge, Ga, In, Al) with α, β, and γ phases. Among the studied half-Heusler alloys, only for $FeRhSb_{1-x}P_x$ (x = 0,75, 1), FeRhAs, and FeRhSi, the β phase is energetically favorable. For the remain 29 compounds, the γ phase is predicted to be the ground state. As an example, Fig. 2a) shows the dependences of the ground state energy on the lattice parameter for the α, β, and γ phases of $FeRhSb_{0,75}P_{0,25}$. As can be seen from the figure, the energy of γ phase takes the lowest values and reveals a global minimum around 5.97 A as compared to the α and β phases. Meenakshi et al [8] have reported that the γ phase is energetically favorable for the FeRhZ (Z = Sn, Ge, Ga, In, Al), whereas the β phase is energetically favorable for the FeRhZ (Z = P, As, Si) alloys, which corresponds to the results of present work.



a) b)

Fig. 2. The total energy curves for a) $FeRhSb_{0,75}P_{0,25}$ with α, β, and γ cubic structures and b) γ-$FeRhSb_{1-x}Ga_x$ (x = 0, 0,25, 0,5, 0,75, 1) as functions of the lattice parameter

Table 1 shows the energetically favorable phases, total and partial magnetic moments and the values of the optimized lattice parameters of all compounds under study. As can be seen from Table 1, the optimized lattice parameters decrease with increasing content of atoms of the fourth element for $FeRhSb_{1-x}Z_x$ (Z = P, As, Si, Ge, Ga, Al) alloys, which is

due to the smaller atomic radius of Z compared to that of Sb. An example of this behavior can be obvious in Fig. 2b), displaying the total energy of $FeRhSb_{1-x}Ga_x$ (x = 0, 0,25, 0,5, 0,75, 1) in the γ phase as a function of the lattice constant.

The atomic radius of Ga is smaller than that of Sb, as a consequence, the energy minimum shifts towards lower values of lattice constant with increasing Ga content. The trend discussed above is accompanied by decrease in the total magnetic moment for $FeRhSb_{1-x}Z_x$ (Z = P, As, Si, Ge, Ga, Al). The largest change in magnetization of about 2.5 times was found between the β, and γ phases of FeRh(Sb,P), FeRh(Sb,As), and FeRh(Sb,Si) due to the significantly smaller magnetic moment of the γ phase. On the other hand, partial substitution of Sn or In for Sb has a little effect on the lattice parameter and the total magnetic moment. In general, the calculated values of optimized lattice constants and magnetizations of stoichiometric FeRhZ compounds are in a good agreement with the data reported previously [5, 7, 8, 16].

Table 1

Energetically favorable phases, equilibrium lattice parameters (a_0), total (μ_{tot}) and partial magnetic moments (μ_{Fe}, μ_{Rh}) of $FeRhSb_{1-x}Z_x$ alloys. The literature values [5, 7, 8], calculated within DFT, are collected for stoichiometric FeRhZ compounds

	phase	a_0, A	μ_{tot}, μ_B/f.u.	μ_{Fe}, μ_B/atom	μ_{Rh}, μ_B/atom
FeRhSb	γ γ [8]	6,0548 6,0618[8]	3,465 3,6197 [8]	3,084 3,04456 [8]	0,400 0,42574 [8]
$FeRSb_{0,75}P_{0,25}$	γ	5,977	3,338	3,076	0,396
$FeRhSb_{0,5}P_{0,5}$	γ	5,882	3,422	3,075	0,39
$FeRhSb_{0,25}P_{0,75}$	β	5,577	1,422	1,539	−0,068
FeRhP	β β [8]	5,402 5,412 [8]	1,139 1,213 [8]	1,215 1,26244 [8]	−0,043 −0,02878 [8]
$FeRSb_{0,75}As_{0,25}$	γ	6,004	3,454	3,076	0,396
$FeRhSb_{0,5}As_{0,5}$	γ	5,946	3,439	3,061	0,397
$FeRhSb_{0,25}As_{0,75}$	γ	5,884	3,441	3,055	0,405
FeRhAs	β β[8]	5,630 5,633 [8]	1,448 1,492 [8]	1,634 1,60116 [8]	−0,087 −0,06669 [8]
$FeRSb_{0,75}Sn_{0,25}$	γ	6,06	3,491	3,118	0,406
$FeRhSb_{0,5}Sn_{0,5}$	γ	6,06	3,417	3,066	0,369
$FeRhSb_{0,25}Sn_{0,75}$	γ	6,054	3,240	3,04	0,303
FeRhSn	γ γ[8]	6,047 6,052 [8] 6,05 [5, 16] 6,057 [7]	3,01 3,001 [8] 3,0 [5]	2,958 2,978 [5] 2,89064 [8]	0,185 0,192 [5] 0,2412 [8]
$FeRSb_{0,75}Si_{0,25}$	γ	5,98	3,44	3,077	0,385
$FeRhSb_{0,5}Si_{0,5}$	γ	5,890	3,371	3,048	0,354
$FeRhSb_{0,25}Si$,75	γ	5,789	3,19	2,941	0,294
FeRhSi	β β [8]	5,53753 5,6813 [8]	2,217 2,211 [8]	2,165	0,129
$FeRSb_{0,75}Ge_{0,25}$	γ	6,002	3,462	3,092	0,393
$FeRhSb_{0,5}Ge_{0,5}$	γ	5,939	3,401	3,072	0,364

Table 1 (end)

	phase	a_0, A	μ_{tot}, μ_B/f.u.	μ_{Fe}, μ_B/atom	μ_{Rh}, μ_B/atom
$FeRhSb_{0,25}Ge_{0,75}$	γ	5,867	3,234	2,993	0,297
FeRhGe	γ γ [8]	5,782 5,786 [8] 5,78 [5, 16] 5,7978 [7]	3,030 3,001 [8] 3,0 [5]	2,882 2,82828 [8] 2,908 [5]	0,225 0,2506[8] 0,201 [5]
$FeRSb_{0,75}Ga_{0,25}$	γ	6,003	3,386	3,066	0,353
$FeRhSb_{0,5}Ga_{0,5}$	γ	5,937	3,05	2,901	0,224
$FeRhSb_{0,25}Ga_{0,75}$	γ	5,867	2,854	2,78	0,160
FeRhGa	γ γ [8]	5,798 5,799 [8]	2,921 2,820 [8]	2,759	0,232
$FeRSb_{0,75}In_{0,25}$	γ	6,060	3,419	3,092	0,361
$FeRhSb_{0,5}In_{0,5}$	γ	6,062	3,098	2,96	0,209
$FeRhSb_{0,25}In_{0,75}$	γ	6,063	3,066	2,91	0,216
FeRhIn	γ γ [8]	6,080 6,079 [8]	3,177 3,0951 [8]	2,959 2,87643 [8]	0,287 0,29895 [8]
$FeRSb_{0,75}Al_{0,25}$	γ	6,000	3,385	3,058	0,353
$FeRhSb_{0,5}Al_{0,5}$	γ	5,929	3,09	2,91	0,237
$FeRhSb_{0,25}$Al,75	γ	5,853	2,9	2,766	0,185
FeRhAl	γ γ [8]	5,782 5,784 [8]	2,976 2,836 [8]	2,747 2,66873 [8]	0,265 0,28496 [8]

Table 2 presents the values of spin polarization (P) calculated from DOS profiles at the Fermi level for $FeRhSb_{1-x}Z_x$. For the parent compound, the value of P is found to be 72 %, which is in a good agreement with Ref. [8] (P = 66,8 %). It was found that among the studied half-Heusler alloys, only $FeRhSb_{0,25}Sn_{0,75}$, FeRhGe, FeRhSn, $FeRhSb_{0,5}Al_{0,5}$ exhibit ferromagnetic half-metallic behavior. High values of spin polarization are predicted for FeRhSi (P = 76 %), FeRhIn (P = 77 %) and $FeRhSb_{0,5}Ga_{0,5}$ (P = 87 %) alloys. Fig. 3 shows the DOSs profiles with 100 % spin polarization in the minority channel for $FeRhSb_{0,25}Sn_{0,75}$, FeRhGe, FeRhSn, and $FeRhSb_{0,5}Al_{0,5}$. It can be seen that the main contribution to the total DOS profile results from the d states of Fe.

Conclusion

In conclusion, this work investigates half-Heusler FeRhSb alloys with off-stoichiometry, which have been doped with the main group elements using first-principles calculations. Herein, the structural, electronic and magnetic properties were examined for 33 compounds in the α, β, and γ cubic phases, which differ in the occupation of tetrahedral sites. $FeRhSb_{1-x}P_x$ (x = 0,75, 1), FeRhAs, and FeRhSi are the only investigated half-Heusler alloys with an energetically advantageous β phase. For the remaining 29 compounds, the γ phase is expected to be the ground state. It is shown that high spin polarization values are expected for FeRhSi (P = 76 %), FeRhIn (P = 77 %), and $FeRhSb_{0,5}Ga_{0,5}$ alloys (P = 87 %), whereas $FeRhSb_{0,25}Sn_{0,75}$, FeRhGe, FeRhSn, and $FeRhSb_{0,5}Al_{0,5}$ exhibit half-metallicity and can be used for spintronic applications with 100 % spin polarization at the Fermi level. Our findings on nonstoichiometric half-Heusler alloys give insight and direction for future theoretical and experimental investigation.

Table 2

Spin polarization (P) of conduction electrons for the $FeRhSb_{1-x}Z_x$ alloys. The literature values [5, 8], calculated within DFT, are collected for stoichiometric $FeRhZ$ compounds

	P, %	phase
$FeRSb_{0,75}P_{0,25}$	64	γ
$FeRhSb_{0,5}P_{0,5}$	72	γ
$FeRhSb_{0,25}P_{0,75}$	69	β
FeRhP	52 58.99 [8]	β β [8]
$FeRSb_{0,75}As_{0,25}$	40	γ
$FeRhSb_{0,5}As_{0,5}$	68	γ
$FeRhSb_{0,25}As_{0,75}$	60	γ
FeRhAs	74 72.36 [8]	β β [8]
$FeRSb_{0,75}Sn_{0,25}$	14	γ
$FeRhSb_{0,5}Sn_{0,5}$	60	γ
$FeRhSb_{0,25}Sn_{0,75}$	100	γ
FeRhSn	100 100 [5, 8]	γ γ [8]
$FeRSb_{0,75}Si_{0,25}$	24	γ
$FeRhSb_{0,5}Si_{0,5}$	7	γ
$FeRhSb_{0,25}Si.75$	27	γ
FeRhSi	76 85.41 [8]	β β [8]

	P, %	phase
$FeRSb_{0,75}Ge_{0,25}$	40	γ
$FeRhSb_{0,5}Ge_{0,5}$	36	γ
$FeRhSb_{0,25}Ge_{0,75}$	70	γ
FeRhGe	100 100 [5, 8]	γ γ [8]
$FeRSb_{0,75}Ga_{0,25}$	1	γ
$FeRhSb_{0,5}Ga_{0,5}$	87	γ
$FeRhSb_{0,25}Ga_{0,75}$	46	γ
FeRhGa	66 69.56 [8]	γ γ [8]
$FeRSb_{0,75}In_{0,25}$	28	γ
$FeRhSb_{0,5}In_{0,5}$	45	γ
$FeRhSb_{0,25}In_{0,75}$	70	γ
FeRhIn	77 72.36 [8]	γ γ [8]
$FeRSb_{0,75}Al_{0,25}$	11	γ
$FeRhSb_{0,5}Al_{0,5}$	100	γ
$FeRhSb_{0,25}Al.75$	41	γ
FeRhAl	73 72.36 [8]	γ γ [8]

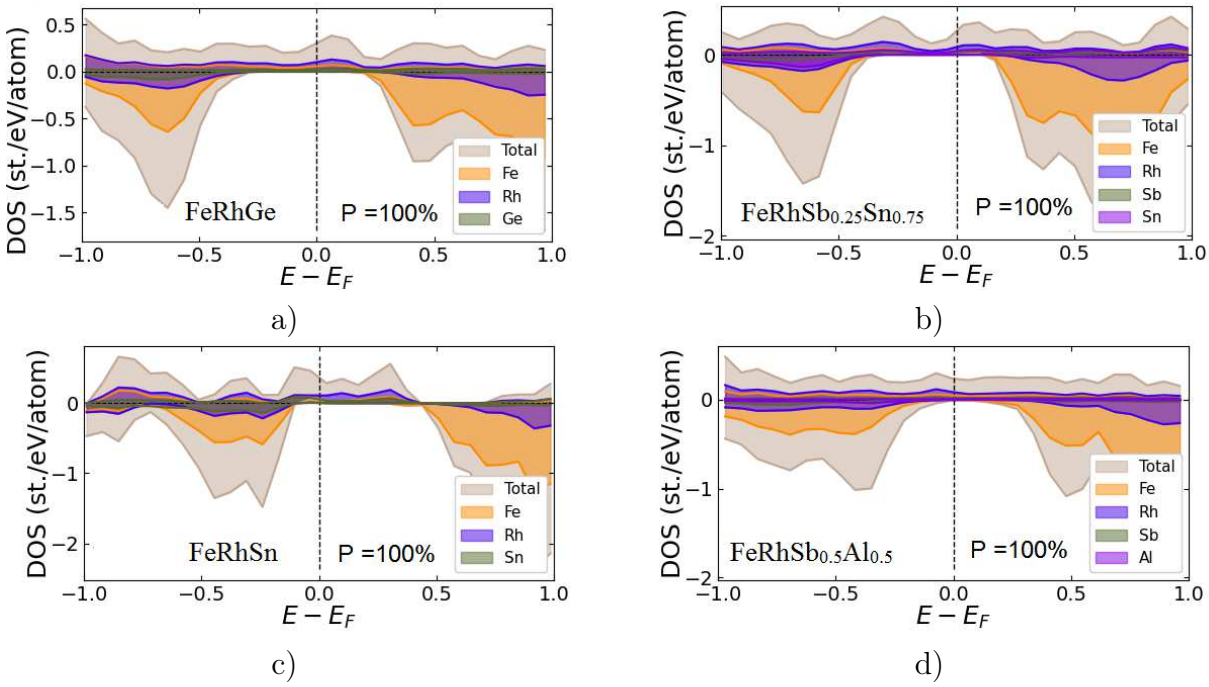


Fig. 3. Total and partial spin-resolved DOSs for a) FeRhGe; b) $FeRhSb_{0,25}Sn_{0,75}$; c) FeRhSn; d) $FeRhSb_{0,5}Al_{0,5}$ in the γ ground state phase

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МАГНИТНЫЕ СВОЙСТВА И ЭЛЕКТРОННАЯ СТРУКТУРА ПОЛОВИННЫХ СПЛАВОВ ГЕЙСЛЕРА $FeRhSb_{1-x}Z_x$ (Z = P, As, Sn, Si, Ge, Ga, In, Al)

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Первопринципными методами исследованы электронная структура и магнитные свойства сплавов $FeRhSb_{1-x}Z_x$ (x = 0, 0,25, 0,5, 0,75, 1) где Z = P, As, Sn, Si, Ge, Ga, In, Al. Для всех соединений рассмотрены три кубические фазы с различным расположением атомов (α, β и γ). Показано, что β фаза энергетически выгодна для сплавов $FeRhSb_{1-x}P_x$(x = 0,75, 1), FeRhAs и FeRhSi. Для остальных 29 сплавов энергетически выгодна γ фаза. Значения равновесных параметров решетки и магнитных моментов тройных сплавов хорошо согласуются с литературными данными, полученными из других теоретических исследований. Получено, что ряд сплавов является полуметаллическими ферромагнитиками: $FeRhSb_{0,25}Sn_{0,75}$, FeRhGe, FeRhSn и $FeRhSb_{0,5}Al_{0,5}$. Было показано, что замена элемента Z на другой *sp* элемент позволяет получить новые четырехкомпонентные сплавы, демонстрирующие 100 % спиновую поляризацию.

Ключевые слова: сплавы Гейслера; плотность электронных состояний; полуметаллические ферромагнитики; теория функционала плотности.

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