

Site preference and electronic structure of Mn_2RhZ ($\text{Z} = \text{Al, Ga, In, Si, Ge, Sn, Sb}$): a theoretical study

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The electronic structure and magnetism of Mn_2RhZ ($\text{Z} = \text{Al, Ga, In, Si, Ge, Sn, Sb}$) Heusler alloys have been studied by using first-principles calculations. Three half-metallic ferromagnets, namely, Mn_2RhAl , Mn_2RhGe and Mn_2RhSb have been considered. The calculated equilibrium lattice constant increases with increasing atomic number of Z atoms lying in same column of periodic table. The calculated total magnetic moments M_{tot} are 2 $\mu_B/\text{f.u.}$ for Mn_2RhAl and Mn_2RhGa , 3 $\mu_B/\text{f.u.}$ for Mn_2RhSi , Mn_2RhGe and Mn_2RhSn , and 4 $\mu_B/\text{f.u.}$ for Mn_2RhSb , which agrees with the Slater-Pauling curve quite well. In all these compounds, except for Mn_2RhSb , the moments of Mn (A) and Mn (B) are antiparallel to each other. The total magnetic moments of the three considered half-metals assume integral values in a wide range of equilibrium lattice parameters.

Keywords: Heusler alloy; electronic structure; h-metal; site preference

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1. Introduction

In recent years, Mn-based Heusler alloys have attracted much attention due to their physical properties as half-metallic materials and potential applications [1–3] in the fields of magnetic actuators and spintronics devices. The so-called half-metallic materials have an energy gap in one spin direction at the Fermi level E_F whereas the other spin band is strongly metallic. As a result, a 100 % spin polarization can be obtained [4] and half-metals can be used as spin injectors for magnetic random access memories and other spin-dependent devices [5]. Many Mn-based Heusler alloys have been studied experimentally for their half-metallic band structure and high Curie temperatures. At the same time, many Mn-based Heusler alloys have been theoretically predicted to be half-metals, and experiments have been carried out to establish their half-metallic band structure and magnetic properties, which make them suitable for technical applications [6–12].

Since the time when de Groot et al. predicted NiMnSb to be a half-metal as well as half-Heusler

alloy, much attention has been paid to the Heusler alloy family for their unique character [4]. Among these materials, Mn_2 -based Heusler alloy with half-metallicity attracted much attention. Among Mn_2YZ alloys, Mn_2VAl was the first half-metal predicted by the band theory calculation in Mn-based Heusler alloys [13]. Later Mn_2CoZ ($\text{Z} = \text{Al, Si, Ge, Sn, Sb}$) [14–16], Mn_2FeZ ($\text{Z} = \text{Al, Sb}$) [17] and Mn_2CrZ ($\text{Z} = \text{Al, Sb}$) [18] also attracted much attention due to their half-metallicity. Recently, Mn_2CuZ ($\text{Z} = \text{Si, Sb, Ge}$) [19–21] alloys have been reported to exhibit half-metallic character in their electronic structures. These Mn_2YZ alloys (where Y denotes 3d elements) have been thoroughly investigated. However, the electronic structure as well as half-metallicity of Heusler alloys containing 4d or 5d elements is not very clear. Recently, Abada et al. [22] have found Mn_2ZrZ ($\text{Z} = \text{Si, Ge}$) alloy exhibiting half-metallicity in theory, and Endo et al. [23] have synthesized a new Heusler alloy Mn_2RuSn , which besides Mn contained a 4d-element Ru, indicating the possibility to find new functional materials in Heusler alloys consisting of 4d elements in theory and experiment.

In this paper, we studied the site preference in Mn_2RhZ ($\text{Z} = \text{Al, Ga, In, Si, Ge, Sn, Sb}$)

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by first-principles calculations. The electronic structure and the magnetic properties of the compounds were investigated in details. Three half-metals, namely, Mn_2RhAl , Mn_2RhGe and Mn_2RhSb , were predicted. For all these alloys, except Mn_2RhSb , the antiparallel alignment between the large local moments of the Mn atoms is observed. The total magnetic moments of the three half-metals with Z atoms lying in the same columns assume integral values for a wide range of equilibrium lattice parameters. Furthermore, we also explored the influence of tetragonal distortion on the half-metallicity property of Mn_2RhAl as an example for the subsequent research.

2. Computational methods

The electronic structure calculations were carried out by using the CASTEP code based on pseudopotential method with a plane-wave basis set [24, 25]. The electronic exchange-correlation energy was treated under the local-density approximation (LDA) [26, 27]. The interactions between the atomic core and the valence electrons were described by the ultrasoft pseudopotential [28]. We considered two cases of initial spin moments of Mn (A) and Mn (B) atoms: antiparallel and parallel, and set the spins as -1 , $+2$ and $+2$, $+2$, respectively. The plane wave basis set cut-off was used as 500 eV for all the cases. A mesh of $15 \times 15 \times 15$ k-points was employed for Brillouin zone integrations for all the cases. The convergence tolerance for the calculations was selected as a difference of total energy within 1×10^{-6} eV/atom. These parameters ensured good convergence for total energy and the calculations were based on the theoretical equilibrium lattice parameters.

3. Results and discussion

3.1. Lattice parameter

Heusler alloy has a structure of four interpenetrating face-center-cubic (fcc) lattices and a stoichiometric composition of X_2YZ , where X and Y atoms are transition metal elements, and Z atom is an element of group III, IV or V.

Generally, Heusler alloy has two possible structures: Hg_2CuTi -type and Cu_2MnAl -type. In Hg_2CuTi -type structure, the X atoms occupy the A (0, 0, 0) and B ($1/4$, $1/4$, $1/4$) sites, and the Y atom enters the C ($1/2$, $1/2$, $1/2$) site, with Z atom located at the D ($3/4$, $3/4$, $3/4$) site in the Wyckoff coordinates. While in Cu_2MnAl -type structure, the X atoms occupy the A and C sites, Y atom enters the B site, leaving the D site to Z atom.

For 3d transition metal elements, the preference of transition metal elements is determined by the number of their valence electrons. And the elements with less electrons prefer to occupy the B sites, while others prefer to enter the (A, C) sites [29]. According to the previous studies on Mn_2RhZ ($Z = \text{Al, Ga, Sn}$), Felser et al. studied the tetragonal distortion based on the cubic Heusler alloys in Hg_2CuTi -type structure [30]. Thus, we considered Mn_2RhZ ($Z = \text{Al, Ga, In, Si, Ge, Sn}$ and Sb) with Hg_2CuTi -type structure in this paper, and performed calculations for two cases of different initial spin moments for Mn atoms: antiparallel and parallel.

All these calculations concerning total energy as a function of lattice parameters, except for Mn_2RhIn alloy, are completely identical in both cases, and the calculated equilibrium lattice constants are listed in Table 1. In Table 1, the equilibrium lattice constants increase with increasing atomic number of Z atoms from the same column of the periodic table. The theoretical lattice constant of Mn_2RhAl is smaller than that of Mn_2RhGa because the Al atoms have a smaller atomic radius than Ga atoms. The radius of In atom is much larger than those of Al and Ga atoms. Thus, the lattice constant of Mn_2RhIn is the largest in the series of Mn_2RhZ ($Z = \text{Al, Ga}$ and In). Similarly, Mn_2RhSn has the largest lattice constant among Mn_2RhZ ($Z = \text{Si, Ge}$ and Sn) compounds and the lattice constants increase with the rising of the atomic number of $\text{Si} \rightarrow \text{Ge} \rightarrow \text{Sn}$.

3.2. Electronic structure and magnetic properties

The electronic structure of the Mn_2RhZ ($Z = \text{Al, Ga, In, Si, Ge, Sn, Sb}$) alloys has been

studied by first-principles calculations. The calculated total and partial densities of states (DOSs) of Mn_2RhZ are shown in Fig. 1. In Fig. 1, we chose the majority-spin states as positive values and the minority-spin states as negative values. The states between -5 eV and -6 eV are mainly from the p electrons of Z atoms in the occupied valence states, which hybridize with the d electrons of Mn and Rh atoms and determine the degree of occupation of the p-d orbitals. The total DOSs of -4 eV to $+2$ eV arise from d states of transition metal atoms. The widely spread d states are mainly from covalent hybridization between Mn and Rh atoms. The covalent hybridization between the lower-energy d states of the higher-valence transition metal atom, like Rh, and the higher-energy d states of the lower-valence transition metal atom, like Mn, can be strong and lead to the formation of bonding and antibonding bands [31].

The total DOSs of Mn_2RhZ ($Z = Al, Ga, In, Si, Ge, Sn, Sb$) shown in Fig. 2 can be divided into three groups according to valence electrons of Z atoms: Al, Ga and In alloys belonging to the first group, Si, Ge and Sn alloys attributed to the second group, and Mn_2RhSb as the third group. All total DOSs of the three-group compounds are similar in shape. The low energy states are mainly contributed by s electrons of Z atoms, and the s states are separated from the d states by a gap in the DOSs in both spin directions. Thus, we have ignored the effect of s electrons on the d-d interaction and have not presented s states in Fig. 1. Similar behavior has also been observed in Mn_2FeZ ($Z = Al, Ga, Si, Ge, Sb$) [32] alloys.

In order to clarify the variation trend of the DOSs of the three groups, we analyzed the DOSs of Mn_2RhIn , Mn_2RhSn and Mn_2RhSb alloys, which are shown in the Fig. 2 (the 3rd, 6th and 7th panel). The DOSs obviously move to the lower energy as the number of valence electrons increases. Sn atom has one more p state valence electron in comparison to In atom, and Mn_2RhSb also has an extra valence electron compared with Mn_2RhSn . The p electrons of the main group element hybridize with the d states of Mn and Rh, determining the degree of occupation of p-d orbitals and influencing the

position of the majority spin states relative to the Fermi level due to the extra electrons from Z atoms filling in only majority spin states [33]. The majority states move to a lower energy as Z element is varying from In to Sn. The Fermi level locates at a deep DOS valley in the Mn_2RhSi , and moves to a large DOS peak in Mn_2RhSn . However, the change in minority states is not so obvious. The minority states are slightly shifted to a lower energy with respect to the Fermi level. Similar results have also been found in Mn_2FeAl and Mn_2FeSi alloys [32]. In the same way, the majority states of Mn_2RhSb shift to a lower energy with respect to the Fermi level. Meanwhile, the extra charge leads to a change in their spin moments. Mn (A) has four Z atoms as nearest neighbors, so the hybridization between Mn (A) and Z is strong. Thus, Mn (A) spin moment increases intensely.

It is worth noting that Sb atom has the largest number of valence electrons among the main group atoms Z ($Z = Al, Ga, In, Si, Ge, Sn, Sb$), and the majority DOS of Mn_2RhSb moves to a lower energy relative to the other Mn_2RhZ ($Z = Al, Ga, In, Si, Ge, Sn$) due to the extra electrons filling in only majority spin states. Mn (A) is the nearest neighbor atom of Sb atom, and the magnetic moment of Mn (A) reveals the most obvious change in Table 1. The moments of Mn (A) and Mn (B) for Mn_2RhSb are parallel instead of antiparallel ones for the other Mn_2RhZ ($Z = Al, Ga, In, Si, Ge, Sn$). Thus, the magnetic structure of Mn_2RhSb is ferromagnetic.

The total DOS of Mn_2RhAl compound is shown in Fig. 1a. A three-peak structure is in the majority spin states. The peak above E_F is mainly composed of the antibonding peak of Mn (A) and the occupied bonding peak results from the d states of Rh atom. It was reported that the bonding hybrids are localized mainly at the higher-valence transition metal atom site, such as Rh, and the unoccupied antibonding states are mainly from the lower-valence transition metal atom site, such as Mn [31]. A two-peak structure (bonding and antibonding peak), which is separated by an energy gap at the E_F , can be observed in the minority spin states. The PDOS shapes of Mn (A) and Mn (B) are opposite to each other. In the majority states of

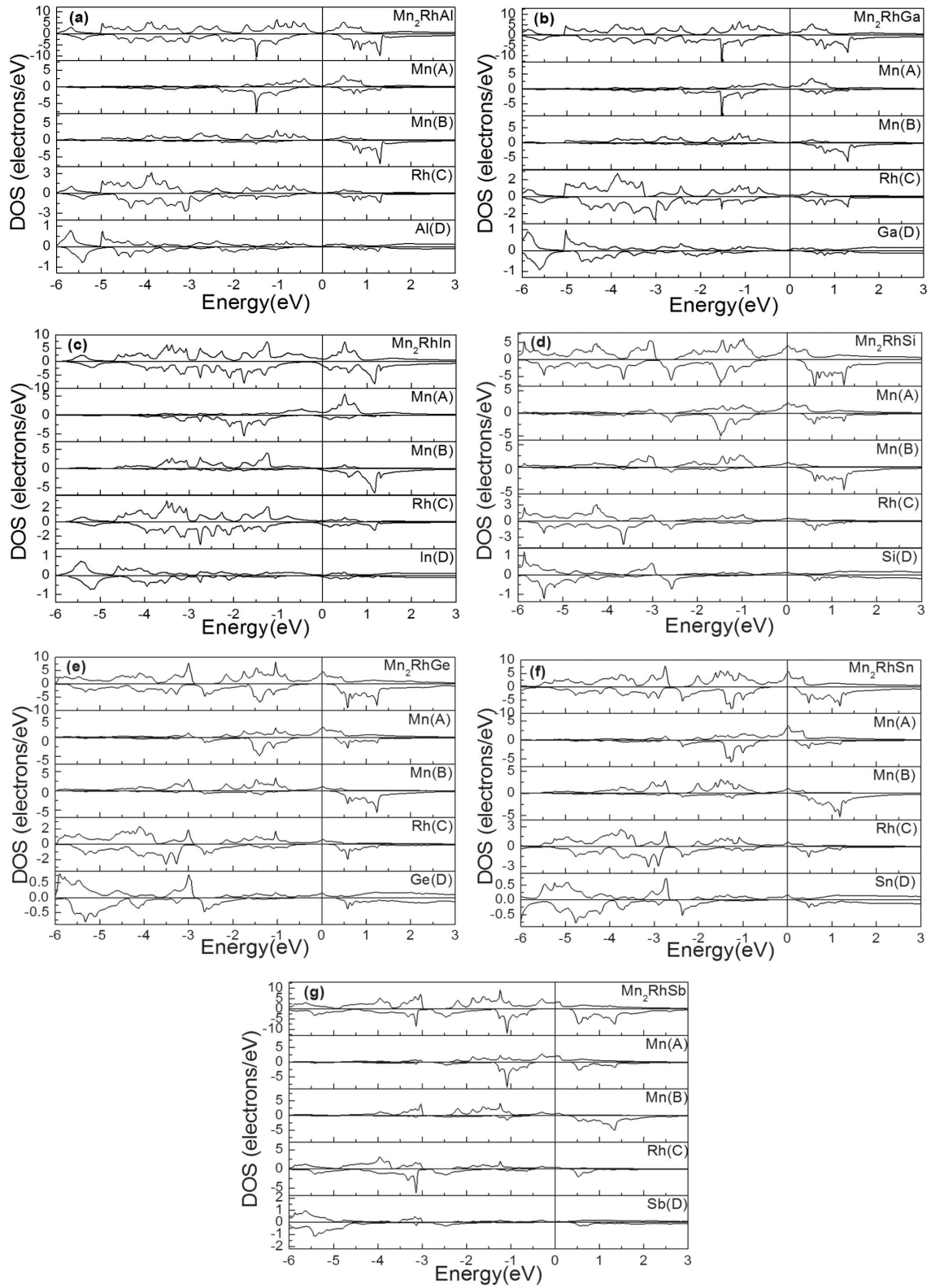


Fig. 1. The calculated spin-projected total and partial DOS plots for (a) Mn₂RhAl, (b) Mn₂RhGa, (c) Mn₂RhIn, (d) Mn₂RhSi, (e) Mn₂RhGe, (f) Mn₂RhSn, and (g) Mn₂RhSb.

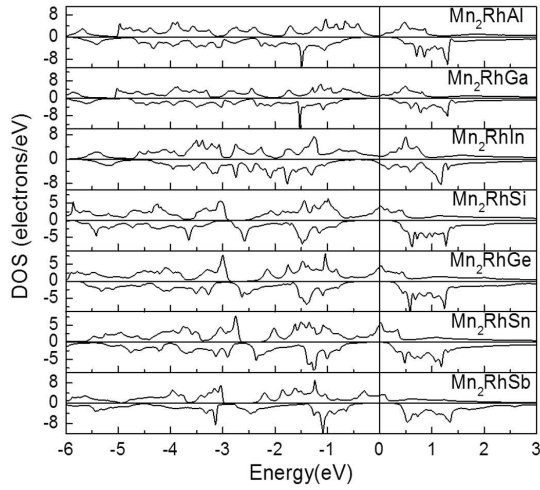


Fig. 2. The calculated total DOS of Mn_2RhZ ($Z = \text{Al, Ga, In, Si, Ge, Sn, Sb}$).

Mn (B), the two peaks are occupied and lie below the Fermi level. In the minority of PDOS, the exchange splitting moves the antibonding peak high above E_F , resulting in a large local moment of Mn (B). Large Mn moment has also been observed in other Heusler alloys, such as Mn_2FeZ ($Z = \text{Al, Ga, Si, Ge, Sb}$) [32]. In contrast, the partial DOS of Mn (A) lies below E_F in the minority spin states, and above E_F in the majority spin states. Therefore, the contributions to the total DOS from Mn (A) and Mn (B) are opposite to each other, indicating an antiparallel configuration of their spin moments [34]. With the help of the calculated total and partial magnetic moments in Table 1, it can be inferred that the spin splitting of Mn (B) is large, resulting in a large local moment of Mn (B). The atomic energy level $E_{(A,C)} < E_{(B)}$ has been reported by Bansil et al. [34]. They stated that the spin down bonding states preferentially reside at Rh (C) site and produce a negative spin density in the occupied states, resulting in strong bonding states in the minority spin states of Rh and causing a small exchange splitting. As a result, Rh shows only a small magnetic moment. The total moment of Mn_2RhAl is $2.00 \mu_B$, which is mainly determined by the antiparallel aligned Mn (A) and Mn (B) spin moments.

The DOSs of Mn_2RhGa and Mn_2RhIn are shown in Fig. 1b and Fig. 1c, and are similar

in shape to the one of Mn_2RhAl . The two-peak structures are in the minority spin states and are separated by the energy gaps around E_F . In the majority spin states, the Fermi level falls in a pseudo-gap, dividing the majority states into bonding and antibonding parts. The PDOSs of Mn (A) and Mn (B) contribute to both the bonding and antibonding parts in the total DOS. Mn atoms show spin splitting in both sites, and a different trend in their PDOS is observed. In Fig. 2, we gathered the calculated total DOS of Mn_2RhZ ($Z = \text{Al, Ga, In, Si, Ge, Sn, Sb}$). Mn(A) is the nearest neighbor atom of the main group atoms (Al, Ga, In), thus, the influence of $\text{Al} \rightarrow \text{In}$ on the Mn(A) atom is the largest. The DOSs of Mn_2RhZ ($Z = \text{Al, Ga, In}$) move to a lower energy as Z is varying from Al to In because of the p-d hybridization between Z and Mn (A) atoms. From the total DOSs of Mn_2RhZ ($Z = \text{Si, Ge, Sn}$) in Fig. 1d, Fig. 1e and Fig. 1f, an energy gap is in the minority states at the E_F . And in the majority spin states, the antibonding peak mainly from Mn (A), is just located at the Fermi level. The energy gap variation trend, which is shown in Fig. 2 (the 4th to 6th panel), is similar to the trend in Mn_2RhAl , Mn_2RhGa and Mn_2RhIn . The DOS moves to a lower energy as Z varies from Si to Sn, and the E_F falls throughout the energy gap. In contrast, the bonding peak in the majority states moves to a higher energy with the increase in atomic number of $\text{Si} \rightarrow \text{Ge} \rightarrow \text{Sn}$. The Z atom plays an important role in Heusler alloys, which causes s-p states to hybridize with d electrons and determines the degree of the p-d orbital occupation [31]. The splitting of Z atom p states electrons occurs at higher energy when Z varies from Si to Sn (-2.9 eV for Si, -2.8 eV for Ge and -2.5 eV for Sn). Thus, the bonding hybridization between p and d electrons can be observed at the higher energy. The total magnetic moment of the Mn_2RhZ ($Z = \text{Si, Ge, Sn}$) alloys is $3.00 \mu_B$, which is in line with the s-p rule of $M_t = Z_t - 24$. Mn (B) spin moment is large and increases with increasing atomic number of Z atoms. Mn (A) and Rh atom moments are small and contribute little to the total moment.

The calculated total and partial DOS for Mn_2RhSb is shown in Fig. 1g. There are

Table 1. The calculated equilibrium lattice constants, gap width, the calculated total and partial magnetic moments for the Mn_2CrZ ($Z = \text{Al, Ga, In, Si, Ge, Sn}$ and Sb) alloys.

Compound	a [Å]	Gap width [eV]	m_{total} [μ_B]	$m_{\text{Mn(A)}}$ [μ_B]	$m_{\text{Mn(B)}}$ [μ_B]	m_{Rh} [μ_B]	m_Z [μ_B]
Mn_2RhAl	5.80	0.20	2.00	−1.56	3.18	0.38	0.00
Mn_2RhGa	5.82	–	2.02	−1.64	3.30	0.36	0.00
Mn_2RhIn	6.10	–	1.61	−2.62	3.84	0.38	0.04
Mn_2RhSi	5.73	0.17	3.00	−0.50	3.16	0.32	0.02
Mn_2RhGe	5.79	0.16	3.00	−0.58	3.24	0.34	0.00
Mn_2RhSn	6.01	0.11	3.00	−0.80	3.46	0.32	0.00
Mn_2RhSb	6.02	0.41	4.00	0.14	3.52	0.36	0.00

three-peak structures in both spin directions. The bonding peak around -3.2 eV in the minority spin states is mainly determined by the Rh atom. And in the majority spin states, the bonding peak around -3 eV mainly arises from the hybridization of Mn and Rh atoms. The majority states are similar to the one of Mn_2RhSi , the Fermi level is also located on the antibonding part. In this paper, Mn_2RhSb is a ferromagnet with a small positive magnetic moment at the Mn (A) site, different from the ferromagnet of the others. The magnet moment strongly depends on the atomic order of the nearest neighbor shell. The moment of Mn (B) is nearly constant because the Mn (A) and Rh atoms are the nearest atoms to Mn (B). In contrast, the moment of Mn (A) atom changes considerably as the nearest atom of Sb provides p electrons to hybridize with d states and determines the degree of p-d orbital occupation [30]. The PDOS of Mn (A) moves to a lower energy, resulting in the spin moment parallel to that of Mn (B).

3.3. Half-metallicity

In the total DOSs of Mn_2RhZ , the energy gap can be obtained in the minority spin around the Fermi level. However, in the majority states, the DOSs are quite large, indicating a high spin polarization at the E_F . The spin polarization ratios of Mn_2RhZ ($Z = \text{Al, Ge, Sb}$) are 100 % due to the fact that the alloys do not have DOSs at E_F in the minority gap. Here, the spin polarization ratio is calculated as the value of $(N_{\uparrow} - N_{\downarrow})/(N_{\uparrow} + N_{\downarrow})$, where $N_{\uparrow}$ and $N_{\downarrow}$ are the majority-spin and minority-spin DOSs at the E_F , respectively. So, Mn_2RhAl , Mn_2RhGe and Mn_2RhSb are “true” half-metals.

With the help of the band structure, the majority-spin and minority-spin band structures under the theoretical equilibrium lattice parameters, 5.80 Å for Mn_2RhAl , 5.79 Å for Mn_2RhGe and 6.02 Å for Mn_2RhSb , are shown in Fig. 3. In the majority-spin states, the top of valence band overlaps with the E_F , exhibiting metallic character at the E_F . However, the minority-spin states exhibit an indirect G-X gap, and the E_F is exactly located in the band gap, indicating semiconducting nature. The values of the band gap are shown in Table 1. In summary, Mn_2RhAl , Mn_2RhGe and Mn_2RhSb alloys have an ideal half-metallic band structure.

In the half-metallic Heusler alloys, the total moments M_t are integral values and follow the Slater-Pauling rule of $M_t = Z_t - 24$, where Z_t is the number of valence electrons [33]. Mn_2RhAl , Mn_2RhGe and Mn_2RhSb have 26, 27 and 28 valence electrons, respectively. The total magnetic moment should be 2.00 μ_B , 3.00 μ_B and 4.00 μ_B , respectively, which agrees with our results in Table 1 quite well.

The calculations for all the cases have been performed under their theoretical equilibrium lattice constants and Mn_2RhZ ($Z = \text{Al, Ge, Sb}$) alloys exhibit half-metallic characters. However, a small change in the lattice parameter may shift the E_F with respect to the minority gap, which obviously affects the half-metallic character [35]. In experimental studies, such as melt spinning or ball milling, the strain may be quite large and will make the lattice constant deviate from the ideal one. Furthermore, the growth of thin film materials becomes possible by modern techniques. The lattice constant of the thin films is strongly influenced by

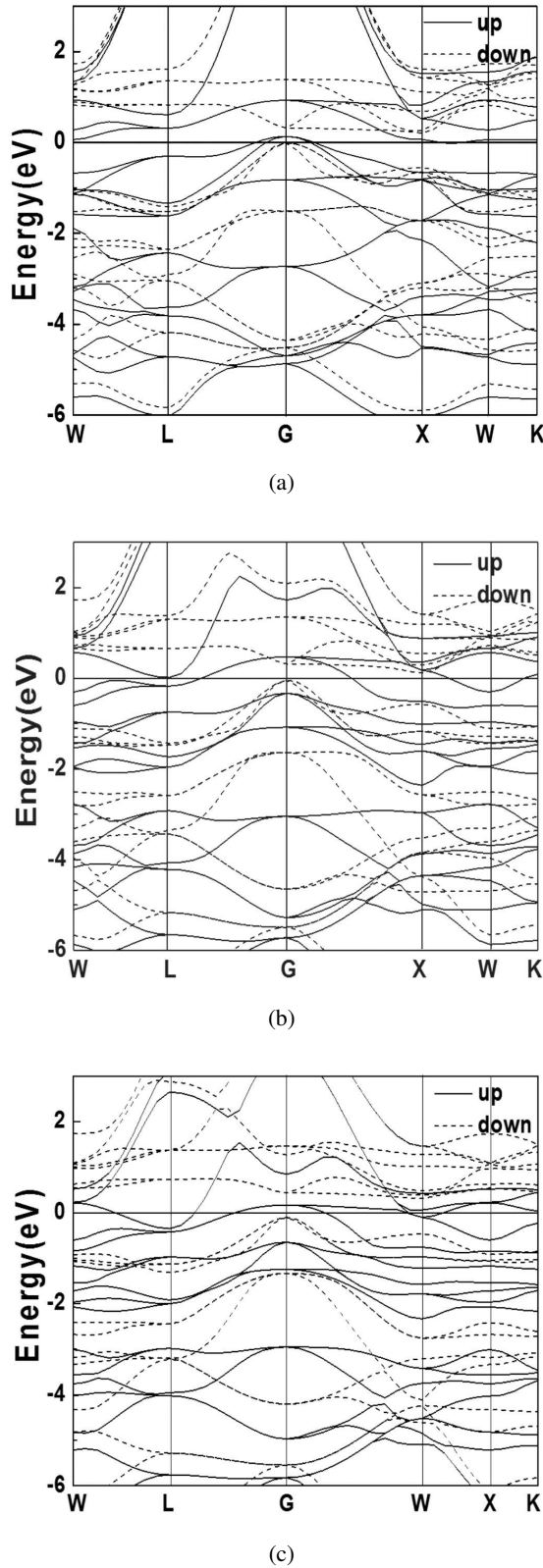


Fig. 3. The calculated band structure plots for (a) Mn_2RhAl , (b) Mn_2RhSi , and (c) Mn_2RhSb .

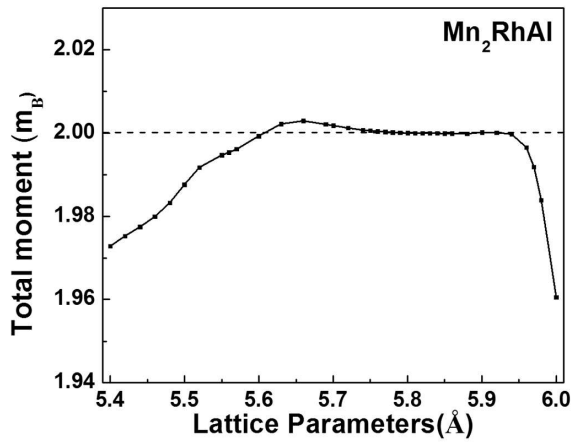
the relationship between the half-metallic character and the lattice constant for a given material from both theoretical and technical point of view. Therefore, it is meaningful to study the dependence of the magnetic properties and spin polarization on the lattice parameters for Mn_2RhAl , Mn_2RhGe and Mn_2RhSb .

Here, we have investigated the relationship between the dependence of the magnetic moments and lattice parameters for the three half-metals. The total magnetic moments as functions of the lattice parameter for Mn_2RhZ ($Z = \text{Al, Ge, Sb}$) are shown in Fig. 4. A moderate variation in the lattice parameter does not significantly change the total magnetic moments in these compounds as the movement of the Fermi level usually takes place within the minority gap. The half-metallic properties of Mn_2RhZ ($Z = \text{Al, Ge, Sb}$) can be obtained within the range of 5.56 Å to 5.96 Å, 5.69 Å to 6.06 Å, 5.81 Å to 6.49 Å, respectively. Thus, Mn_2RhAl , Mn_2RhGe and Mn_2RhSb can be considered as new candidates for spintronics applications.

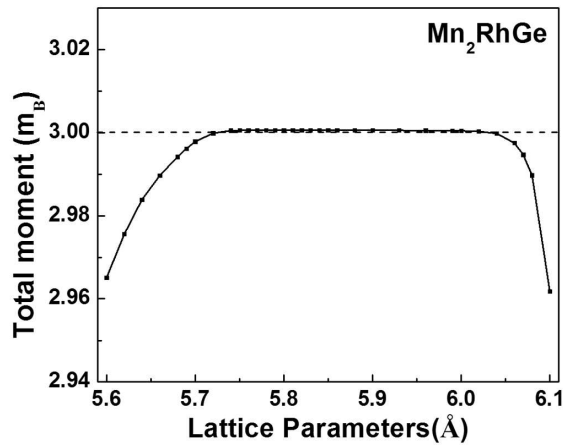
Furthermore, we have shown the influence of tetragonal distortion on the half-metallicity of Mn_2RhAl as an example of the later research of tetragonal distortion in the Mn_2RhZ . We have investigated the relative stability of the unit cell geometry by calculating the total energy as a function of the c/a ratio at a constant volume and the respective graph is shown in Fig. 5. The lowest total energy can be observed at the point of $c/a = 1$, indicating the stability of cubic phase in the structure.

4. Conclusions

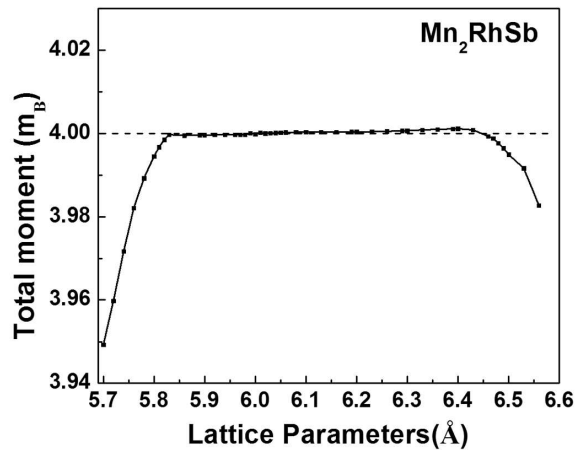
First-principles calculations were performed for the Mn_2RhZ ($Z = \text{Al, Ga, In, Si, Ge, Sn, Sb}$) Heusler alloys. We predicted three half-metallic ferromagnets, namely: Mn_2RhAl , Mn_2RhGe and Mn_2RhSb . The calculated equilibrium lattice constant increases with increasing atomic number of Z atoms lying in the same column of the periodic table. The calculated total magnetic moments M_{tot} are 2 $\mu_B/\text{f.u.}$ for Mn_2RhAl and Mn_2RhGa , 3 $\mu_B/\text{f.u.}$ for Mn_2RhSi , Mn_2RhGe and Mn_2RhSn ,



(a)



(b)



(c)

Fig. 4. The calculated total magnetic moments as functions of the Mn_2RhZ ($Z = \text{Al, Ge, Sb}$) Heusler alloys.

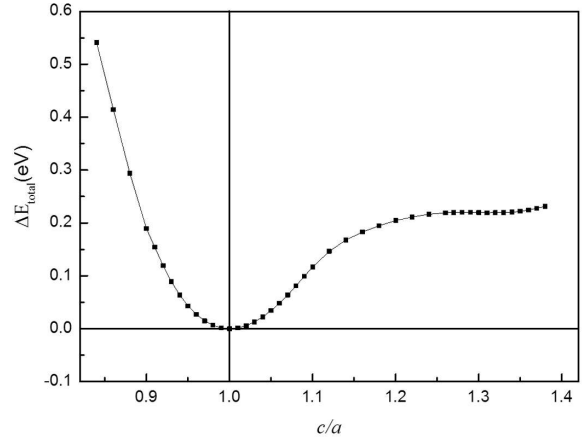


Fig. 5. Total energy difference $\Delta E_{\text{total}} = E_{\text{total}}(c/a) - E_{\text{total}}(c/a = 1)$ between cubic ($c/a = 1$) and tetragonally-distorted phases, calculated as a function of c/a ratio along the constant volume for Mn_2RhAl Heusler alloy.

and $4 \mu_B/\text{f.u.}$ for Mn_2RhSb , which agrees with the Slater-Pauling curve quite well. In all these compounds, except for Mn_2RhSb , the moments of Mn (A) and Mn (B) are antiparallel to each other. Mn_2RhSb is a ferrimagnet due to the influence of the extra valence electron filling in the majority spin states. It has been found that the total magnetic moments of Mn_2RhAl , Mn_2RhGe and Mn_2RhSb can assume an integral value within the range of $5.56 \text{ \AA}$ to $5.96 \text{ \AA}$, $5.69 \text{ \AA}$ to $6.06 \text{ \AA}$, $5.81 \text{ \AA}$ to $6.49 \text{ \AA}$, respectively. As an example, we also investigated the effect of tetragonal distortion on the half-metallicity of Mn_2RhAl and found that the structure of cubic phase is stable.

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