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High-Pressure-Induced Transition from Ferromagnetic Semiconductor to Spin Gapless Semiconductor in Quaternary Heusler Alloy VFeScZ (Z = Sb, As, P)

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Received: 29 May 2019; Accepted: 13 July 2019; Published: 18 July 2019

Abstract: In this paper, the structure and the electronic and magnetic properties of VFeScZ (Z = Sb, As, P) series alloys are systematically studied based on the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) calculation within the first-principles density functional theory. The results showed that VFeScSb and VFeScP are ferromagnetic semiconductors and VFeScAs exhibits half-metallic ferromagnetism under zero pressure. As the pressure increases, the narrow indirect gap of VFeScZ (Z = Sb, As, P) alloy gradually decreases, and gets close to zero, leading to spin gapless semiconductor (SGS) transition. The pressure phase transition point of VFeScSb, VFeScAs, and VFeScP alloy is 132 GPa, 58 GPa, and 32 GPa, respectively. As a result, the pressure effect provides an opportunity to tune the electronic properties of the alloys by external pressure. The present findings provide a technical method for us to actually use the Heusler alloy SGS.

Keywords: Heusler alloy; spin gapless semiconductor; magnetism; pressure

1. Introduction

Spin gapless semiconductor shows a “zero” gap at the Fermi level in one of the spin channels, and a semiconductor band gap in the other spin channel from its electronic structure [1]. In Figure 1, several densities of states (DOSs) of the spin gapless semiconductor (SGS) are dramatically described. Both direct (Figure 1c) and indirect (Figure 1d) zero band gap existed in real SGS material. For SGS materials, in the past few years, many novel electronic and thermophysical properties have deeply attracted researchers’ attention and are expected to be applied in future spintronic devices [2]. The mobility of carriers, which includes full spin-polarized electrons and holes [3], is higher than that of the classical semiconductors or half-metallic ferromagnetisms (HMFs) [4]. Owing to this “ideal” spin-polarized electrons and holes, SGS can create a spontaneous transition of electrons from the valence band to the conduction band without any threshold energy [5]. Furthermore, the SGS can also retain high resistance and high Curie temperature simultaneously [6]; moreover, its electrical conductivity is seldom affected by temperature, electric field, electromagnetic radiation, or impurities, and the spin-polarized carriers of n-type and p-type can be switched by applying a gate voltage [7].

Figure 1. Schematic density of states of (a) semiconductor, (b) half-metal, and (c,d) spin gapless semiconductor. “↑” and “↓” indicate spin-up and spin-down channel, respectively.

In 2008, SGS was first predicted in diluted magnetic semiconductors (DMS) PbPdO_2 by X. L. Wang’s group [8]. Thereafter, graphene nanotubes [9], double perovskite $\text{La}_2\text{CrFeO}_6$ [10], and many Heusler alloys with SGS properties were detected. Especially for Heusler alloys, the previous results show that many Heusler alloys are (or nearly) spin gapless semiconductors in their ground states at low temperature. In 2013, five ternary Heusler alloys Ti_2MnAl , Ti_2CoSi , Ti_2VAs , Cr_2ZnSi , Mn_2CoAl and one binary Heusler alloy V_3Al were first detected and predicated as potential SGSs from the first-principle calculations [11]. In the experiment, the polycrystalline Heusler alloy Mn_2CoAl were also prepared and identified as an SGS [12]. According to Slater–Pauling rule [13–15], if the magnetic moment per primitive cell is agreeable well with $Z_t - 24$ for full-Heusler alloys and few quaternary Heusler alloys or $Z_t - 18$ for inverse-Heusler alloys and most of the quaternary Heusler alloys, where Z_t is the number of valence electrons in a primitive cell, Heusler alloys will present nonmagnetic states. Among those nonmagnetic Heusler alloys, there are more chances of finding new SGSs. Thus, in the past five years, a lot of SGSs have been found additionally in ternary Hg_2CuTi -type or LiMgPbSn -type quaternary Heusler alloys, such as Zr-based Heusler alloys including ZrCoVIn , ZrFeVGe , ZrCoFeP , ZrCoCrBe and ZrFeCrZ ($Z = \text{In}$ and Ga), and Zr_2MnGa [15], Ti-based Heusler alloy Ti_2CoAs [16], Ti_2MnAl [17], and Ti_2CrSi [18], as well as other quaternary Heusler alloy VCoHfGa , CrFeHfGa [19], and CoFeMnSi [1].

In fact, in those SGS candidates by theoretical prediction, it is hard to select an “ideal” SGS for promising application experimentally owing to the sensitive and flimsy “zero” gap, which can be easily damaged by the crystal structure, surface or interface interaction, and other external factors. A slight adjustment of band gap can sharply decrease the initial spin polarization and weaken the transport properties of the carriers. To solve this problem, the optimal method is to manipulate the band width by means of the external field, controllably. Assuredly, the pressure as a force field is one of the appropriate choices. Thus, the dependence of SGS properties on pressure is focused in our present work. Since Sc_2FeSi or Sc_2FeGe is a nonmagnetic inverse-Heusler semiconductor [20] and ZrFeVGe shows typical SGS behavior [16], we, therefore, deduce that quaternary Heusler alloy VFeScZ ($Z = \text{Sb}$, As , P) is nearly an SGS or a semiconductor.

In the present work, the structure and magnetic and electronic properties of VFeScZ ($Z = \text{Sb}$, As , P) bulk are first detected. Next, the variation of band gap and spin-polarization ratio of VFeScZ as the pressure changes are focused. In the end, the physical mechanism is discussed.

2. Structures and Calculation Methods

In Wyckoff coordinates, LiMnPbSn -type quaternary Heusler alloy VFeScZ possibly has three different structures: Type-I, V atom is located at (0, 0, 0), Fe atom is at (0.5, 0.5, 0.5), Sc atom is at (0.75, 0.75, 0.75), and Z ($Z = \text{Sb}$, As , P) is at (0.25, 0.25, 0.25); type-II, the coordinates of the V and Sc atoms are swapped; and type-III, the coordinates of the Fe and Sc atoms are swapped based on the

type-I configuration. In our calculations, the initial crystal constant of 6.0 Å in VFeScZ is adopted by comparing with the structure of Heusler alloy CoFeCrZ (Z = Sb, As, P) [14]. After geometry optimization, the lowest-energy type-I, -II, and -III structures of VFeScZ are obtained. In the lowest-energy state, the structure, magnetism, and DOS are detected. To reveal the pressure effect in VFeScZ alloy, the geometry optimization is implemented once for every 5 or 10 GPa additional pressures until the alloy becomes an ordinary nonmagnetic metal. Usually, more pressure detection is done near the transformation point in VFeScZ for accurately describing the electronic transition behavior.

All tasks are done by using the CASTEP code within the density functional theory (DFT). PBE GGA functional is adopted to describe the exchange-correlation interaction [21]. In all calculations, the Vanderbilt-type ultrasoft pseudopotentials [22] and the valence electron configurations of V ($3d^3 4s^2$), Fe ($3d^6 4s^2$), Sc ($3d^1 4s^2$), P ($3s^2 3p^3$), As ($4s^2 4p^3$), and Sb ($5s^2 5p^3$) are used. In geometry optimization of VFeScZ bulks, the ferromagnetic states in all alloys are initially assumed and the options of the spin-polarization are checked. In the self-consistent field (SCF) task, the $6 \times 6 \times 6$ mesh of special k -points in the Brillouin zone, the SCF convergence criterion of 1×10^{-6} eV/atom, and energy cutoff of 380 eV is applied, respectively. To satisfy the criterion of total energy convergence, the maximal force convergence criterion of 0.02 eV/Å is chosen when the positions of atoms are relaxed. The total energy convergence criterion of 1×10^{-5} is used for all calculations. In our work, all technical parameters were tested carefully to ensure the accuracy of the results. By GGA + PBE scheme, quaternary Heusler alloy CoFeMnSi was tested. The crystal constant and the magnetic and electronic properties are in accordance with the results from Ref. [7]. So we think the GGA + PBE scheme adopted in the present work is reasonable for dealing with the VFeScZ system.

3. Results and Discussion

3.1. Bulk Properties of VFeScZ (Z = Sb, As, P)

In Figure 2, the type-I structure of VFeScZ alloy is shown dramatically. We can also construct two other structures, which are stipulated as type-II and -III, using the atomic exchange method discussed above. The three types of structures were optimized in the zero-pressure environment, and the recorded results are shown in Table 1. We found that the type-I structure of VFeScZ has the lowest energy among the three types of structures, so it can be judged as the ground state configuration. We also found that the ground state energy difference between the two structures of VFeScAs and VFeScP is 0.03–0.05 eV/primitive-cell, while the ground state energy difference between the two structures of VFeScSb is about 0.5 eV/primitive-cell by contrast. Therefore, the energy of type-II is quite different from that of type-I and -III structures. Based on the above analysis, we can preliminarily judge that the ground state alloys of type-I VFeScAs and VFeScP are not stable enough and may change to type-III structure. So the probability of Fe–Sc atomic disorder occurring in these two alloys is relatively high. But, the type-I VFeScSb has better structural stability, so the atomic exchange disorder rate of Fe–Sc and Fe–V is significantly lower than that of the other two alloys. We present in detail the relationship between the energies and lattice constant changes of VFeScZ (Z = Sb, As, P) system in order to analyze the structural stability of VFeScZ with the three structures in Figure 3. It can be obviously seen that VFeScSb in the ground state has good stability. The energy difference of type-I and -III structure will continue to narrow only when the lattice constant keeps increasing, but, such difference will continue to increase as the lattice constant shrinks. Meanwhile, it was found in both VFeScAs and VFeScP, which is different from VFeScSb, that the energy of type-I and type-III alloys cross with the function diagram of the lattice constant when the lattice constant becomes larger, indicating that VFeScAs and VFeScP alloys are more inclined to form type-III structure with the increase of the lattice constant. But, we can see that the ground state energy difference between type-I, -III, and even -II structures will increase as the lattice constant decreases, which is consistent with the behavior of VFeScSb.

Figure 2. Type-I structure of the quaternary alloy VFeScZ (Z = Sb, As, P).

Table 1. Ground state energy (E , eV), lattice constant (L , Å), and magnetic moment (M , μ_B) of type-I, -II, and -III structures of VFeScZ (Z = Sb, As, P).

Structure	Type	E	L	M_V	M_{Fe}	M_{Sc}	M_{Sb}	M_{Total}
VFeScSb	I	−4270.94176	6.34	3.18	−0.12	0.16	−0.20	3.02
	II	−4269.79299	6.38	2.08	0.48	0.54	−0.12	2.98
	III	−4270.39456	6.44	0.96	2.32	−0.34	0.06	3.00
VFeScAs	I	−4292.08041	6.08	2.96	0.08	0.14	−0.18	3.00
	II	−4291.1535	6.14	2.32	0.02	0.60	−0.14	2.80
	III	−4292.05693	6.19	−0.16	2.34	−0.18	0.18	2.18
VFeScP	I	−4299.87526	5.93	2.82	0.22	0.10	−0.16	2.98
	II	−4298.93401	5.96	1.32	0.36	0.38	−0.04	2.02
	III	−4299.84489	6.05	−0.04	2.22	−0.14	0.12	2.16

Figure 3. Total energy as a function of lattice constant in the Heusler alloy (a) VFeScSb, (b) VFeScAs, and (c) VFeScP with type-I, -II, and -III structures.

In Table 1, the total magnetic moment per primitive cell and the atomic magnetic moment in VFeScZ are also listed. A few results as the following can be deduced, respectively: First, the VFeScSb alloy is focused. In all of the structures, the total magnetic moment is (or is very close to) $3.02 \mu_B$, which is very close to the value of the Slater–Pauling rule, $M_t = Z_t - 18$. The total magnetic moment in primitive cell mainly comes from V for type-I and -II structure, while the magnetism is mainly contributed by the Fe atom for type-III structure. Second, as far as VFeScAs is concerned, the total magnetic moment is $3.00 \mu_B$ in a primitive cell and conforms to the Slater–Pauling rule well only in the type-I structures of VFeScAs. For the type-II and -III structures, the total magnetic moments of about $2.80 \mu_B$ and $2.18 \mu_B$, respectively, significantly deviated from the Slater–Pauling rule. It is worth noting that in the type-I structure the contribution of V atom to the total magnetic moment is about $2.96 \mu_B$, which is about 98% of the magnetism of VFeScAs. Third, in the VFeScP alloy, it can be

found that the total magnetic moment of the type-I alloy is $2.98 \mu_B$ and close to $3 \mu_B$, which abides by the Slater–Pauling rule. In type-II and -III structures, the total magnetic moments are $2.02 \mu_B$ and $2.16 \mu_B$, respectively, which is obviously a deviation from the Slater–Pauling rule and behave like the VFeScAs alloy.

Here, in order to understand the relationship between the electronic structure and the geometric structure we carefully analyzed the DOS of VFeScZ ($Z = \text{Sb, As, P}$) type-I, -II, and -III structures after geometric optimization. As shown in Figure 4a for the VFeScSb alloy when it has type-I structure, two band gaps (spin-up and spin-down) can be clearly seen and the Fermi surface is located in the middle of the band gap, which is a typical semiconductor behavior. It can be basically judged as a typical ferromagnetic semiconductor combined with the previous magnetic analysis. For the type-II structure, although the spin-down band gap still exists, the spin-up state crosses the Fermi surface, which is a typical half-metallic property. And for the type-III structure, the spin-up and -down bands of the state density cross the Fermi surface, which is a general ferromagnetic alloy. In Figure 4b, when the alloy VFeScAs is in type-I structure, we found that it has a relatively wide spin-up gap. The Fermi level just locates at the edge of the spin-down gap, which can only be roughly judged as a semiconductor or half-metal. For the type-II and -III structures, the spin-up and -down bands cross the Fermi level, respectively, and are therefore ferromagnetic metals. In the VFeScP system, see Figure 4c, it is similar to the VFeScAs. The alloy with type-I structure is a narrow-band gap semiconductor, while with type-II or -III structure it is a common ferromagnetic alloy.

Figure 4. Density of states of the Heusler alloy (a) VFeScSb, (b) VFeScAs, and (c) VFeScP with type-I, -II, and -III structures.

The electronic properties of VFeScZ alloy need to be discussed in detail, which because of the type-I structure is the ground state configuration of the VFeScZ alloy. Figure 5 shows the total DOS and partial density of states (PDOS) of VFeScZ ($Z = \text{Sb, As, P}$). It can be found that the total DOS of VFeScZ in the low energy region from -6 eV to -3 eV is mainly contributed from the 2p electrons of Z atom and partially from the 3d electrons of V and Sc atom. In the high energy region from -3 eV to 0 eV , the total DOS mainly comes from the 3d electrons of Fe atom, V atom, and Sc atom. At and near the Fermi surface, the contribution of V and Fe atoms is prominent. Moreover, the magnetic exchange among the transition metals plays an important role in semiconductor or half-metallic gap in VFeScZ ($Z = \text{Sb, As, P}$). The split peaks near the Fermi level are mainly contributed by V, Fe, and Sc atoms. To further analyze the electronic behavior of VFeScZ, especially the behavior near the Fermi surface of VFeScZ with type-I structure, the energy band diagram of type-I structure VFeScZ is shown in Figure 6. It can be further confirmed from the figure that the VFeScSb of type-I structure is an indirect semiconductor

with a gap width of about 0.372 eV. The VFeScAs is approximately half-metallic because a small peak in the spin-up band gap just crosses the Fermi surface. For the VFeScP, it can be judged as an indirectly narrow-band gap semiconductor with a band gap width of only 0.172 eV.

Figure 5. Partial density of states of (a) VFeScSb, (b) VFeScAs, and (c) VFeScP with type-I structure.

Figure 6. Cont.

Figure 6. Energy band diagram of (a) VFeScSb, (b) VFeScAs, and (c) VFeScP with type-I structure.

3.2. Pressure Effect of VFeScZ ($Z = \text{Sb, As, P}$)

Based on the above analysis and discussion, we can find that the VFeScSb and VFeScP are typical ferromagnetic semiconductors with band gap widths of about 0.372 eV and 0.172 eV, respectively, when they stay in the ground state. However, the VFeScAs is predicted to be a half-metal, because the Fermi level of VFeScAs is at the edge of the spin-up gap and the spin-down semiconductor gap is slightly damaged. The detection from the structure indicates that the stability of the alloy with type-I structure will be further enhanced with the decrease of the lattice constant. Generally, external pressure on the alloy system is a possible way to decreasing lattice. Therefore, in this subsection, we conduct a specific discussion to detailly reveal the pressure effect on electrons and magnetism in the type-I VFeScZ ($Z = \text{Sb, As, P}$) alloy.

As shown in Figure 7, we can find that in VFeScZ the lattice constant slowly decreases and the total energy linearly enhances with increasing pressure. This change is characterized by the linear decrease in the volume of the whole system because of pressure, which makes the bonding between the atoms shorter and the interaction between them stronger. As a result, the energy and lattice constant will linearly change in the alloy system until the novel phase change occurs. In Figure 7, the data is recorded within the pressure range from 0 GPa to the phase transformation point.

Figure 7. Lattice constant (L) and the energy change, (ΔE) in type-I (a) VFeScSb, (b) VFeScAs, and (c) VFeScP as a function of pressures. ΔE is the relative energy with respect to zero pressure.

The DOS and PDOS of VFeScZ under different pressures are shown in Figure 8. For the VFeScSb, see Figure 8a, when the pressure increases, the spin-down band gradually moves toward the low energy orientation and the spin-up band quickly shifts to the high energy region, which causes the indirect band gap width determined by the valence band top and the conduction band bottom to decrease. As the pressure increases to 50 GPa, the spin-down valence band moves near the Fermi level. With increasing pressure, the spin-up conduction band continues to move toward the high-energy region, while the spin-down valence band almost keeps still. When the pressure is increased to 132 GPa, in the type-I VFeScSb alloy, the semiconductor gap gets close to zero at the Fermi level. Therefore, we can judge that the type-I VFeScSb will be transformed from ferromagnetic semiconductor to SGS under external pressure of about 132 GPa. For the type-I VFeScAs alloy, see Figure 8b, along with the increase of pressure it was found that the position of the spin-down conducting band did not change with respect to the Fermi level, while the spin-up band moves rapidly toward the high energy region. This results in a remarkable shrink of the semiconductor gap. When the pressure is near 58 GPa, the gap width of the type-I VFeScAs system almost becomes zero, indicating the phase transition from ferromagnetic semiconductor to SGS. Similar behavior is seen in the type-I VFeScP alloy, as shown in Figure 8c. With the increase of pressure, the spin-up valence band moves toward the high energy region continuously, and the spin-down conduction band moves slightly toward the Fermi surface until it touches the Fermi level as the pressure continues to increase. Obviously, when the pressure reaches 32 GPa, the VFeScSb alloy system becomes a typical SGS.

Figure 8. Density of states of type-I (a) VFeScSb, (b) VFeScAs, and (c) VFeScP at various pressures.

In order to understand the mechanism of the band gap width changing with the increase of pressure, the indirect band gap of semiconductor at different pressures are detected and plotted in Figure 9. It is seen that the semiconductor gap decreases gradually and finally becomes 0 for type-I VFeScSb and VFeScP alloys. However, for type-I VFeScAs alloy we found that a band gap width increases to 0.175 eV at first and then decreases to 0 gradually because of a small peak appearing in the spin-up gap under zero pressure. And with the increase of pressure, the Fermi surface falls into the semiconductor gap because of the high-energy shift of the whole spin-up band. It is the reason for the anomalous gap phenomenon of VFeScAs.

Figure 9. Band gap of type-I (a) VFeScSb, (b) VFeScAs, and (c) VFeScP.

Pressure effect causes a novel electronic structural transition from semiconductor or half-metal to SGS in Heusler alloy VFeScZ (Z = Sb, As, P). The system with less s or p electrons of the Z atom has a relatively small pressure phase transition point. If the pressure is applied beyond the transition point, all of these alloys will eventually be transformed into ordinary non-magnetic alloys. The pressure dependence of the band gap width of the VFeScZ alloy provides an opportunity to tune the electronic properties by means of external pressure. By gradually applying pressure, a narrow gap in a semiconductor can be converted to zero, gradually. It can be an efficient way to get an “optimal” SGS material.

In addition, the pressure effect on the magnetism of the VFeScZ alloy is also discussed. In VFeScZ alloy, see Figure 10 for detail, with the increase of pressure from 0 to transition point 132 GPa, 58 GPa, and 32 GPa for VFeScSb, VFeScAs, and VFeScP, respectively, the magnetic moments of V and Sc atoms decrease gradually, while those of Fe and Z atoms increase gradually. But, the total magnetic moments of $3 \mu_B$ almost remained unchanged.

Figure 10. Magnetism changes of type-I (a) VFeScSb, (b) VFeScAs, and (c) VFeScP at various pressures.

4. Conclusions

In this paper, the structure and the electronic and magnetic properties of VFeScZ (Z = Sb, As, P) series alloys are systematically studied based on the GGA + PBE calculation within the first-principles density functional theory. The results show that VFeScSb and VFeScP alloys are ferromagnetic semiconductors and VFeScAs exhibits half-metallic ferromagnetism under zero pressure. As the pressure increases, the narrow indirect gap of VFeScZ (Z = Sb, As, P) alloy gradually decreases, and gets close to zero, leading to SGS transition. The pressure phase transition point of VFeScSb, VFeScAs, and VFeScP alloy is 132 GPa, 58 GPa, and 32 GPa, respectively. The pressure effect can provide an opportunity to tune the electronic properties of the alloys by external pressure. By gradually applying pressure, a narrow band gap semiconductor can be gradually transformed into a spin gapless semiconductor material. It provides a technical method for us to actually use the Heusler alloy SGS.

Author Contributions: Methodology, B.W.; software, K.Y. and T.Z.; data curation, X.Y.; writing—original draft preparation, K.Y. and W.Z.; writing—review and editing, B.W. and H.H.

Funding: This research was funded by the National Natural Science Foundation of China (Grant No. 11304410 and 11704426), Key Laboratory and Scientific Research Foundation of Zunyi City (SSKH[2015]55), Natural Science

Foundation of Technology Department (QKHJZ-LKZS[2014]10, QJHJZ-LKZS[2012]03, and KHJZ[2014]2170), Youth Science Foundation of Education Ministry (QJHKZ[2012]084, QJHKY[2018]310) and the Regional First-class Discipline ([2018]216) of Guizhou Province of China.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Fu, H.; Li, Y.; Ma, L.; You, C.; Zhang, Q.; Tian, N. Structures, magnetism and transport properties of the potential spin-gapless semiconductor CoFeMnSi alloy. *J. Magn. Magn. Mater.* **2019**, *473*, 16–20. [\[CrossRef\]](#)
2. Ueda, K.; Hirose, S.; Asano, H. Ambipolar transport in Mn₂CoAl films by ionic liquid gating. *Appl. Phys. Lett.* **2017**, *110*, 202405. [\[CrossRef\]](#)
3. Wang, X. Proposal for a new class of materials: Spin gapless semiconductors. *Phys. Rev. Lett.* **2008**, *100*, 156404. [\[CrossRef\]](#) [\[PubMed\]](#)
4. Huang, H.; Jiang, Z.; Yang, J.; Xiong, Y.; He, Z.; Zhu, Z.; Laref, A. First principles study of RbVF₃: A spin gapless semiconductor under high pressure. *Chin. J. Phys.* **2019**, *58*, 132–136. [\[CrossRef\]](#)
5. Wang, X.-L. Dirac spin-gapless semiconductors: Promising platforms for massless and dissipationless spintronics and new (quantum) anomalous spin Hall effects. *Natl. Sci. Rev.* **2017**, *4*, 252–257. [\[CrossRef\]](#)
6. Patel, P.D.; Shinde, S.; Gupta, S.D.; Dabhi, S.D.; Jha, P.K. The first principle calculation of structural, electronic, magnetic, elastic, thermal and lattice dynamical properties of fully compensated ferrimagnetic spin-gapless heusler alloy Zr₂MnGa. *Comput. Condens. Matter* **2018**, *15*, 61–68. [\[CrossRef\]](#)
7. Deng, Y.-X.; Chen, S.-Z.; Zeng, Y.; Feng, Y.; Zhou, W.-X.; Tang, L.-M.; Chen, K.-Q. Spin gapless semiconductor and half-metal properties in magnetic penta-hexa-graphene nanotubes. *Org. Electron.* **2018**, *63*, 310–317. [\[CrossRef\]](#)
8. Wu, H.; Qian, Y.; Tan, W.; Kan, E.; Lu, R.; Deng, K. Vacancy-induced insulator–direct spin gapless semiconductor–half-metal transition in double perovskite La₂CrFeO₆: A first-principles study. *Phys. Lett. A* **2015**, *379*, 2897–2901. [\[CrossRef\]](#)
9. Skaftouros, S.; Özdoğan, K.; Şaşıoğlu, E.; Galanakis, I. Search for spin gapless semiconductors: The case of inverse Heusler compounds. *Appl. Phys. Lett.* **2013**, *102*, 022402. [\[CrossRef\]](#)
10. Ouardi, S.; Fecher, G.H.; Felser, C.; Kübler, J. Realization of Spin Gapless Semiconductors: The Heusler Compound Mn₂CoAl. *Phys. Rev. Lett.* **2013**, *110*, 100401. [\[CrossRef\]](#)
11. Galanakis, I.; Dederichs, P.; Papanikolaou, N. Slater-Pauling behavior and origin of the half-metallicity of the full-Heusler alloys. *Phys. Rev. B* **2002**, *66*, 174429. [\[CrossRef\]](#)
12. Galanakis, I.; Dederichs, P.; Papanikolaou, N. Origin and properties of the gap in the half-ferromagnetic Heusler alloys. *Phys. Rev. B* **2002**, *66*, 134428. [\[CrossRef\]](#)
13. Zhang, L.; Cheng, Z.; Wang, X.; Khenata, R.; Rozale, H. First-principles investigation of equiatomic quaternary heusler alloys NbVMnAl and NbFeCrAl and a discussion of the generalized electron-filling rule. *J. Supercond. Nov. Magn.* **2018**, *31*, 189–196. [\[CrossRef\]](#)
14. Bahnes, A.; Boukortt, A.; Abbassa, H.; Aimouch, D.; Hayn, R.; Zaoui, A. Half-metallic ferromagnets behavior of a new quaternary Heusler alloys CoFeCrZ (Z = P, As and Sb): Ab-initio study. *J. Alloys Compd.* **2018**, *731*, 1208–1213. [\[CrossRef\]](#)
15. Gao, Q.; Xie, H.-H.; Li, L.; Lei, G.; Deng, J.-B.; Hu, X.-R. First-principle study on some new spin-gapless semiconductors: The Zr-based quaternary Heusler alloys. *Superlattices Microstruct.* **2015**, *85*, 536–542. [\[CrossRef\]](#)
16. Osafile, O.; Adebambo, P.; Adebayo, G. Elastic constants and observed ferromagnetism in inverse Heusler alloy Ti₂CoAs using kjpaw pseudopotentials: A first-principles approach. *J. Alloys Compd.* **2017**, *722*, 207–211. [\[CrossRef\]](#)
17. Singh, M.; Kashyap, M.K.; Saini, H.S. Corroborating the Spin Gapless Character of Ti₂MnAl Inverse Heusler Alloy: A study of Strains Effect. *Mater. Today Proc.* **2018**, *5*, 15421–15425. [\[CrossRef\]](#)
18. Wang, L.; Jin, Y. A spin-gapless semiconductor of inverse Heusler Ti₂CrSi alloy: First-principles prediction. *J. Magn. Magn. Mater.* **2015**, *385*, 55–59. [\[CrossRef\]](#)
19. Yang, X.; Wu, X.; Wu, B.; Feng, Y.; Li, P.; Huang, H. First-principles calculated spin-gapless semiconducting behavior in quaternary VCoHfGa and CrFeHfGa Heusler compounds. *Mater. Sci. Eng. B* **2016**, *209*, 45–50. [\[CrossRef\]](#)

20. Li, J.; Yang, G.; Yang, Y.; Ma, H.; Zhang, Q.; Zhang, Z.; Fang, W.; Yin, F.; Li, J. Electronic and thermoelectric properties of nonmagnetic inverse Heusler semiconductors Sc_2FeSi and Sc_2FeGe . *J. Magn. Magn. Mater.* **2017**, *442*, 371–376. [[CrossRef](#)]
21. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865. [[CrossRef](#)] [[PubMed](#)]
22. Vanderbilt, D. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Phys. Rev. B* **1990**, *41*, 7892. [[CrossRef](#)] [[PubMed](#)]

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