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REVIEW

First-Principle Study of Structural, Elastic, Electronic and Magnetic Properties of the Quaternary Heusler CoZrFeP

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Abstract

Many studies nowadays are available to predict the half-metallic behaviour of Heusler's quaternary compounds. Using the first principle study of the quaternary Heusler CoZrFeP, we examined its structural, electronic and magnetic properties with the full-potential linearized augmented plane wave (FP-LAPW) method within the generalized gradient approximation (GGA) and the generalized modified potential plus Becke-Johnson approximation (GGA-mBJ). Our quaternary Heusler CoZrFeP compound has shown a half-metallic ferromagnetism character with a small band gap in the minority spin which makes it an excellent candidate for the development of new devices in spintronic and magnetoelectronic. In order to know whether our Heusler quaternary CoZrFeP compound can be experimentally synthesized, we studied its mechanical stability by calculating its formation energy, cohesion energy and elastic constants.

Keywords Quaternary Heusler compound · First-principle calculations · Half-metallic properties

1 Introduction

Since the calculations of the first principles were used to predict the half-Heusler NiMnSb by de Groot and collaborators in 1983 [1], and with the development of computer science, numerous theoretical and experimental studies have been performed to demonstrate the half-metallic ferromagnetism character of Heusler compounds [2, 3], by calculating their structural, elastic, electronic, magnetic and optical properties, for the development of spintronic devices [4, 5], because they are semiconductors in minority spin (majority spin) and metallic in majority spin (minority spin).

Many theoretical studies on quaternary Heusler alloys with 4d transition elements have demonstrated their half-metallic character, as seen in the works of Kundu and collaborators [6, 7], on alloys with Co bases a high Curie temperature. The quaternary Heusler alloys

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Table 1 The three possible atomic occupations of quaternary Heusler compound CoZrFeP

	4a (0,0,0)	4c (1/4,1/4,1/4)	4b (1/2,1/2,1/2)	4d (3/4,3/4,3/4)
Y-type (I)	P	Co	Zr	Fe
Y-type (II)	P	Co	Fe	Zr
Y-type (III)	p	Zr	Co	Fe

crystallize in the LiMgPdSb-type crystal structure with F-43m space group [8, 9] and have the chemical formula *XX′YZ* where *X*, *X′* and *Y* are transition metals, and *Z* is from the III, IV or V group element [10, 11, 12].

In the present work, we compared the structural, elastic, electronic and magnetic properties of the quaternary Heusler CoZrFeP composed of 4d transition metal elements based on Co, using the full-potential linearized augmented plane wave (FP-LAPW) method within the generalized gradient approximation (GGA) [15, 16] and the generalized modified potential plus Becke-Johnson approximation (GGA-mBJ) [17]. In addition, we also discussed the stability of this alloy by calculating the formation energy and the cohesion energy.

2 Computational Details

The different properties were studied using the full-potential linearized augmented plane wave (FP-LAPW) method [13, 14], and the results of two approaches were compared; the generalized gradient approximation (GGA) [15, 16] and the generalized gradient approximation plus the modified Becke-Johnson potential (GGA-mBJ) [17] all of which were implemented in the WIEN2k package [18, 19].

We have chosen the muffin-tin radii (MT) to be 2.30 (a.u) for the transition metal elements Co, Zr and Fe, and to be 2.16 (a.u) for non-metal elements P. We used $R_{MT}.k_{max} = 9$ which determines matrix size (convergence), and the value of $G_{max} = 12$, where G_{max} is defined as the magnitude of the largest vector in the charge density Fourier expansion. The energy and the charge convergence values have been set to 0.0001 Ry and 0.001 e, respectively.

3 Results and Discussion

3.1 Structural Properties and Phase Stability

Generally quaternary Heusler alloys have a formula *XX′YZ*, in which *X*, *X′* and *Y* are transition elements and *Z* is III, IV or V group elements, crystallized in a cubic structure with LiMgPdSn type structure (Y-type structure) having space group F-43m (216) [8, 9]. According to the symmetry, there are three possible structures, as shown in Table 1 and in Fig. 1. The calculated total energy could fit as a function of the volumes for all three *Y*-types, by the Murnaghan's equation of state [20], for the ferromagnetic (FM) and the non-magnetic (NM) states. Figure 1 shows that the FM state of CoZrFeP with *Y*-type (I) structure always has the lowest energy, indicating that the FM state of CoZrFeP with *Y*-type (I) is the most stable one of the three structures for both the FM and the NM states.

The results of the structural optimization are described in Table 2 for the FM and the NM states, and only the quaternary Heusler alloy CoZrFeP in *Y*-type (I) structure for the FM state is discussed for the remainder of our work.

Without experimental and theoretical data to be compared with our results for CoZrFeP, the quaternary Heusler, we calculated their cohesion and formation energies in order to check the stability of our compound [21, 22], by the following equation:

$$E_{coh} = \left(E_{Co}^{iso} + E_{Zr}^{iso} + E_{Fe}^{iso} + E_{P}^{iso}\right) - E_{Total}^{CoZrFeP} \quad (1)$$

$$E_f = E_{Total}^{CoZrFeP} - \left(E_{Co}^{bulk} + E_{Zr}^{bulk} + E_{Fe}^{bulk} + E_{P}^{bulk}\right) \quad (2)$$

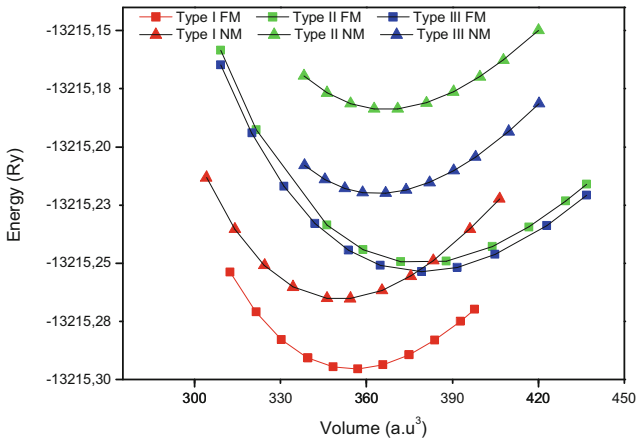

Fig. 1 Calculated total energy as a function of volume for type I, type II and type III of CoZrFeP alloy for non-magnetic (NM) and ferromagnetic (FM) states

Table 2 Calculated lattice constants a_0 (Å), total energies E_{tot} (Ry) per formula unit, the corresponding bulk modulus B_0 (GPa) and its pressure derivate B', formation energy E_f and cohesive energies E_{coh} of CoZrFeP in NM and FM states

Type	State	a_0 (Å)	B_0 (GPa)	B'	E_{tot} (Ry)	E_f (eV)	E_{coh} (eV)
Type I	NM	5.923	189.240	4.841	− 13215.265452	-	-
Type I	FM	5.950	184.579	4.793	− 13215.295505	− 1.34	22.8
Type II	NM	6.013	164.808	4.449	− 13215.183921	-	-
Type II	FM	6.080	144.925	4.278	− 13215.250010	-	-
Type III	NM	5.998	171.068	4.665	− 13215.219978	-	-
Type III	FM	6.080	140.284	4.290	− 13215.253632	-	-

where E_{coh} is the total energy of the CoZrFeP and E_{Co}^{iso}, E_{Zr}^{iso}, E_{Fe}^{iso} and E_{P}^{iso} are the energies of isolated constituent atoms in each alloy, The value of E_{coh} is 22.8 eV, Such high cohesion energy indicates that the alloy should be stable [23, 24].

The E_{Co}^{bulk}, E_{Zr}^{bulk}, E_{Fe}^{bulk} and E_{P}^{bulk} are the total energy per atom for bulk Co, Zr, Fe and P jointly. The calculated values of formation energy E_f are − 1.34 eV. This negative value of formation energy indicates the stability of the compound and implies that it can be experimentally synthesized.

3.2 Mechanical Properties

For the mechanical stability of the compound, we will be interested in the mechanical properties of CoZrFeP compound by calculating these elastic constants for cubic crystal C_{11}, C_{12} and C_{44} [23]. We have been able to verify that the quaternary CoZrFeP Heusler alloy is mechanically stable in the cubic phase, since it satisfies the traditional mechanical criteria for stability in cubic crystal [24] (Born stability criteria) expressed as:

$$C_{11}-C_{12} > 0, \quad C_{44} > 0, \qquad (C_{11} + 2C_{12}) > 0$$

We listed in Table 3 the three elastic constants, the constant shear modulus (G), Young's modulus (Y), Poisson's ratio (υ), ratio of B/G, elastic anisotropy factor (A), Cauchy pressure ($C_{12}-C_{44}$), sound wave velocities (υ_t, υ_l, υ_m), density (ρ) and Debye temperature (θ_D) for quaternary Heusler CoZrFeP compound.

We note the importance of the values of the Bulk modulus B of CoZrFeP, obtained from the Murnaghan's equation of state which is too close to the Bulk modulus calculated using the elastic constants because it represents the resistance to volume variations under external stress.

The elastic parameters obtained informed us about the ductile or brittle nature of this compound. These parameters identify this compound as a ductile material.

The ductility of our Heusler is deduced by checking the three following factors:

- Pugh's ratio [25] B/G must be greater than the critical value 1.75 (brittle < 1.75 < ductile); this ratio B/G = 3.23 > 1.75.
- Poisson's ratio must be greater than 0.26. According to the rule of Frantsevich [26], Poisson's ratio (υ) is equal to 0.36.
- The Cauchy pressure (C_{12}–C_{44}) must have a positive value, and this pressure is equal to 889,751 > 0.

Also, to deduce if this material has a low probability of developing structural defects or micro-cracks during its

Table 3 The three elastic constants (C_{11}, C_{12}, C_{44}) (GPa), the constant shear modulus (G) (GPa), Young's modulus (Y) (GPa), Poisson's ratio (υ), ratio of B/G, elastic anisotropy factor (A), Cauchy pressure ($C_{12}-C_{44}$) (GPa), sound wave velocities (υ_t, υ_l, υ_m) (m/s), density (ρ) (g/cm^3) and Debye temperature θ_D (K) for CoZrFeP alloy

Properties	CoZrFeP
C_{11}	218.5068
C_{12}	166.4821
C_{44}	77.5070
G	56.908
Y	154.754
μ	0.359
B/G	3.23
A	2.87
$C_{12}-C_{44}$	88.9751
υ_t	2588.48
υ_l	5790.25
υ_m	2920.22
ρ	7.576
θ_D	368.233

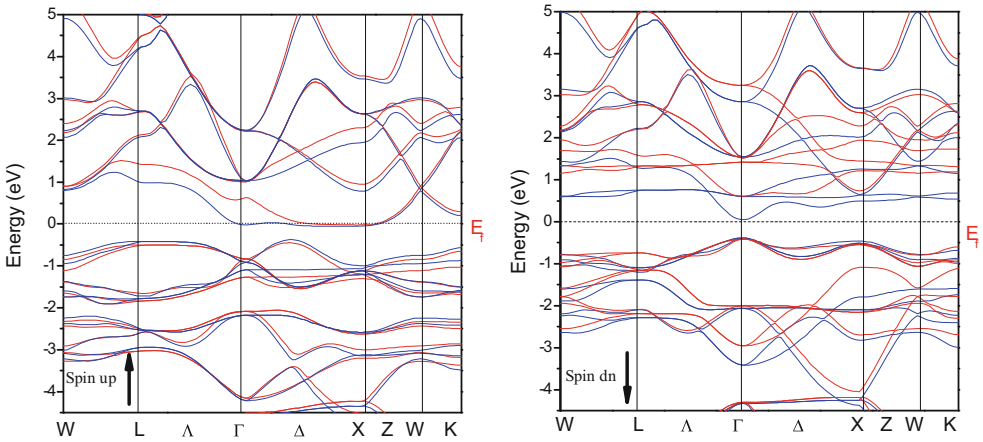

Fig. 2 Spin polarized band structure of half-Heusler CoZrFeP at their predicted equilibrium lattice constant (Blue (Red), GGA (GGA-mBJ))

growth, it must be shown that it is an anisotropic material; since it is sufficient that the value of the anisotropic elastic factor (A) is different from 1, and since the anisotropic parameter A obtained is 2.87, we can say that our compound is an anisotropic material.

3.3 Electronic and Magnetic Properties

In this subsection, for the calculations of the electronic and magnetic properties of this quaternary Heusler alloy, we will use the GGA and GGA-mBJ approximations, with the *Y*-type (I) structure, the most stable structure, with the lowest total energy.

We calculated band structures of majority and minority spin states for the compound as shown in Fig. 2. The majority spin exhibits a metallic behaviour due to the downward and upward shifts of the maximum of the valence band (VBM) and the minimum of the conduction band (CBM) for both the approximation GGA and GGA-mBJ.

From GGA calculations, CoZrFeP exhibits a half-metallic behaviour in the spin-down channel with an energy band gap equal to 0.436 eV, and we observed that our compound CoZrFeP retains its half-metallic behaviour with an energy band gap equal to 1.016 eV using GGA-mBJ approximation; the Band structure diagram indicates a direct band-gap in the minority spin at the Γ point for CoZrFeP with both the GGA and GGA-mBJ approximations.

In order to better understand and to confirm the nature of the band structure of our compound, we calculated the total and the partial density of states, as can be seen in Fig. 3. We observed in the total density of states (TDOS) that there is a small overlap of the band around the Fermi level without any band crossing describing a metallic behaviour in the majority spin and semiconductor behaviour in the minority spin, where we remark a large space and the Fermi level is in this space.

From the calculated partial density of states (PDOS) in Fig. 4, for a better understanding of the origin of the half-metallic behaviour of CoZrFeP, it is noted in Fig. 4 that the main contribution to the density of states around the Fermi level comes from the orbitals 3d of the atoms of Co and Fe, while the contribution of the atoms Zr and P is very small, deducing that the half-metallic behaviour is influenced by the heavy hybridization of the states Co-3d and Fe-3d, in agreement with the results of [27–29].

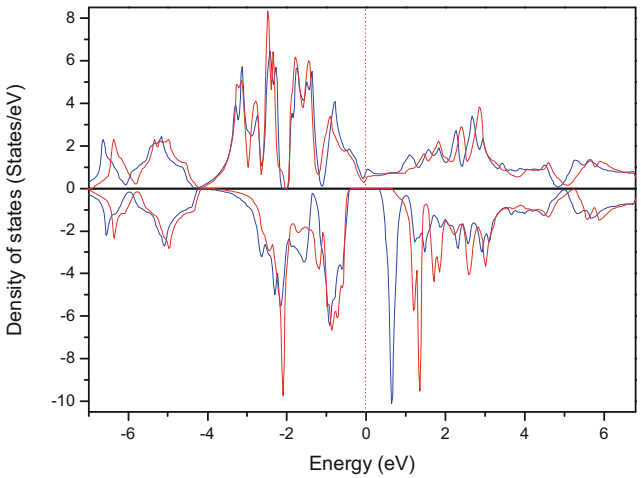

Fig. 3 The calculated total density of states (TDOS) of CoZrFeP (Blue (Red), GGA (GGA-mBJ))

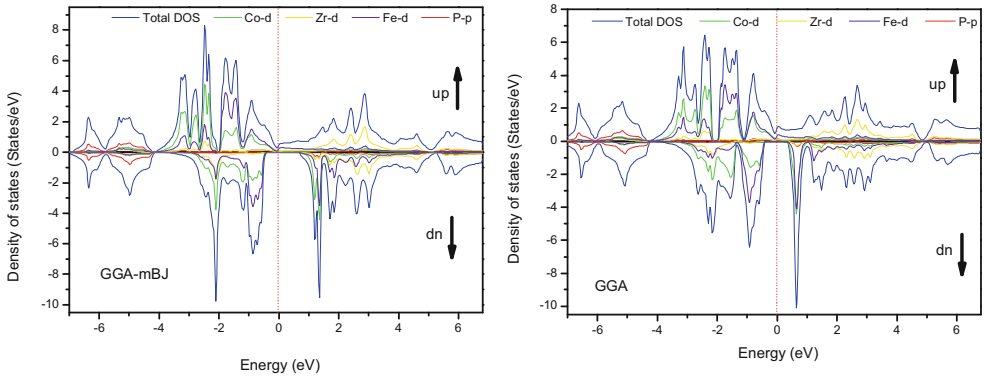

Fig. 4 The calculated partial density of states (PDOS) of CoZrFeP

To understand the origin of the minority band gap, Fig. 5 shows a possible hybridization state of CoZrFeP. We can see that the s, p states and $2e_g$ state, $3t_{2g}$ state and $3t_{1u}$ state of CoZrFeP can accommodate 24 valance electrons, and as the total number of valance electrons of CoZrFeP is 26 [30, 31], so there are still 2 valence electrons which occupy the $2e_u$ state of the majority spin state. Hence, as is evident from Fig. 5, the Fermi level is located between the orbital of $3t_{1u}$ and $2e_u$, in the minority spin direction, and the band gap is due to the Co–Fe interaction [31–33].

Finally, in Table 4, the total and atomic magnetic moments of the CoZrFeP compound are presented using the GGA and the GGA-mBJ approximation. The total magnetic moment calculated M_{tot} for CoZrFeP of cell is an integer 2 μ_B, and the number of the total valence electrons is $Z_{tot} = 26$ [34, 35]. We can show that the quaternary CoZrFeP Heusler alloy obeys to the Slater-Pauling rule's $M_{tot} = (Z_{tot}\text{-}24)$ [36–38] where M_{tot} is the total magnetic moments per formula unit and Z_{tot} is the number of total valence electrons.

Our calculations demonstrate that Co, Fe and P have positive magnetic moments; however, Zr has a negative magnetic moment. We can deduce that the main contribution for the total magnetic moment is given by the magnetic moments of Fe and Co, while P contributes less to the magnetic moments. The negativity of the magnetic moments of Zr shows its ferrimagnetic character in the alloy.

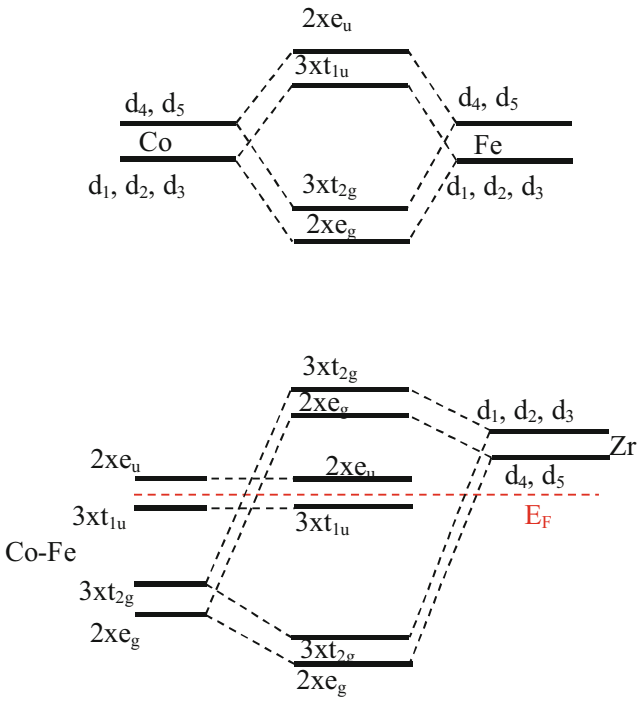

Fig. 5 Possible hybridizations of the origin of the gap in the minority band in CoZrFeP

4 Conclusions

Based on the first principles, the structural, electronic, magnetic and mechanical properties of the Heusler quaternary were calculated by the WIEN2k code, based on the functional density theory in the GGA and GGA-mBJ approximations. The results reveal that it is stable in YI-type ferromagnetic structure; the compounds exhibit a typical half-metallic characteristic with a band gap in the minority spin channel. The calculated elastic parameters indicate the ductile and anisotropic behaviour of these alloys. The total magnetic moment of this

Table 4 The partial magnetic moments (Co, Zr, Fe, P) (μ_B), magnetic moment in the interstitial region M_I (μ_B), the total magnetic moment M_{tot} (μ_B), valence band maximum VBM (eV), conduction band minimum CBM (eV) and the calculated band gap Eg (eV)

V_{xc}	M_{Co} (μ_B)	M_{Zr} (μ_B)	M_{Fe} (μ_B)	M_P (μ_B)	M_I (μ_B)	M_{tot} (μ_B)	VBM (eV)	CBM (eV)	Eg (eV)
GGA	1062	− 0.121	1147	0.051	− 0.138	2000	− 0.385	0.051	0.436
GGA-mBJ	1219	− 0.201	1197	0.053	− 0.268		− 0.407	0.609	1016

alloy is 2.00 μB, which matches well with the value predicted from the Slater-Pauling rules. We checked its stability by calculating its cohesion energy and formation energy in order to have the possibility to synthesize it by experiments. Our results show that if the quaternary Heusler CoZrFeP compound has a high Curie temperature, it makes it very promising and suitable for applications of devices based on magnetoelectronics and spintronics.

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