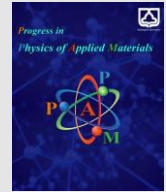




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Structural, electronic, and magnetic properties of Fe₂TiP full-Heusler compound: A first-principles study

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ARTICLE INFO

Article history:

Received: 12 May 2024

Revised: 27 September 2024

Accepted: 2 October 2024

Keywords:

Magnetic intermetallic
Density functional theory
Half-metallic
Band structure

ABSTRACT

This study examined the electronic, magnetic, and structural properties of Fe₂TiP full-Heusler compound, using the pseudo-potential plane wave (PP-PW) formalism based on density functional theory (DFT). Energetically, the AlCu₂Mn-type structure of Fe₂TiP had greater stability in comparison with the CuHg₂Ti-type structure and showed the half-metallic (HF) ferrimagnetic behavior. Based on the results at the lattice constant of 5.65 Å, the total magnetic moment (M_{tot}) was 1 μ_B /unit cell; this finding is consistent with the Slater-Pauling (SP) rule. The minority spin band exhibited a semiconductor behavior (spin-flip gap of 0.21 eV; gap of 0.35 eV), whereas the majority spin band was metallic. The origin of half-metallicity and appearance of the minority band gap were discussed using the band structure calculations and density of states (DOS). In addition, dependence of magnetic properties on the lattice constant was evaluated. In the lattice constant range of 5.55-5.85 Å, the Fe₂TiP compound can retain the half-metallicity. Therefore, the half-metallic feature was not influenced by the lattice distortion, and this material seems to have potential applications in future spintronics devices.

1. Introduction

Given their potential use in spin-dependent electronic devices, more attention is being paid to half-metallic (HM) materials [1-5]. Among different HM materials, Heusler alloys may be suitable compounds given their high Curie temperature and compatibility with semiconductors. The chemical formula of full-Heusler alloys, as ternary intermetallic compounds, is X₂YZ (X and Y denote transition metals, and Z indicates the main group element). These compounds are crystallized in both AlCu₂Mn (L2₁, space group Fm3m) and CuHg₂Ti (space group F43m) prototypes [6, 7].

So far, various reports based on the first-principles methods have suggested full-Heusler compounds as half-metals. These compounds include Ti₂-based [8-10], Mn₂-based [11-13], Co₂-based [14-16], and Fe₂-based [17-19] alloys. In a study, Canko et al. [20] measured the electronic structure of Fe₂ZrP Heusler alloy using the first-principles full-potential linearized augmented plane wave (FP-LAPW) method and reported its HM behaviors in the AlCu₂Mn-type structure. In another research, Kervan et al. [21] studied the electronic structure of the Fe₂TiP Heusler compound as

an isomeric compound of Fe₂ZrP, using the generalized gradient approximation (GGA) scheme within the FP-LAPW method, as it is implemented in the Wien2k package. Based on their results, Fe₂TiP is predicted to be a half-metallic ferrimagnet with a magnetic moment of 1 μ_B /f.u. and a minority-spin indirect band gap of 0.38 eV. However, they did not explain in details the origin of the half-metallicity and appearance of the minority band gap in this compound. For this reason, the motive of the present study is to re-examine the magnetic, electronic, and structural features of Fe₂TiP full-Heusler compound using the pseudo-potential plane wave (PP-PW) scheme and understand the origin of half-metallicity in this material. Since there are no experimental data available in the literature to describe the physical properties of Fe₂TiP, results of our study and relevant research [21] will promote future experimental analysis of this compound as a potential candidate for spintronic applications.

2. Computational Details

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Cite this article as:

Sarhaddi, R., 2024. Structural, electronic, and magnetic properties of Fe₂TiP full-Heusler compound: A first-principles study. *Progress in Physics of Applied Materials*, 4(2), pp 183-188. DOI: [10.22075/PPAM.2024.34112.1101](https://doi.org/10.22075/PPAM.2024.34112.1101)

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For the calculations, the PWscf code was used in the Quantum ESPRESSO software suite [22, 23]. The generalized gradient approximation (GGA) by Perdew and Wang was applied to treat the exchange-correlation potential [24]. The interactions between valence and core electrons were described with the Vanderbilt-type ultrasoft pseudopotentials [25]. For ensuring an acceptable convergence for total energy, the kinetic cutoff energy was selected to be 800 eV in the plane-wave basis set. The integration of k space in the irreducible Brillouin zone consists of a $20 \times 20 \times 20$ k -mesh, based on the Monkhorst-Pack scheme [26]. The self-consistent convergence threshold was set to 1×10^{-8} Ry as well as the conjugate gradient (CG) algorithm during all calculations.

3. Results and Discussion

3.1. Structural Properties

For structural optimization in nonmagnetic (NM) and ferromagnetic (FM) states, we calculated the Fe_2TiP total energy (E) in CuHg_2Ti and AlCu_2Mn -type structures as a function of the lattice constant or unit cell volume (V). Following that, the universal Murnaghan equation of state [27] was applied for the $E(V)$ data, as shown in Figure 1.

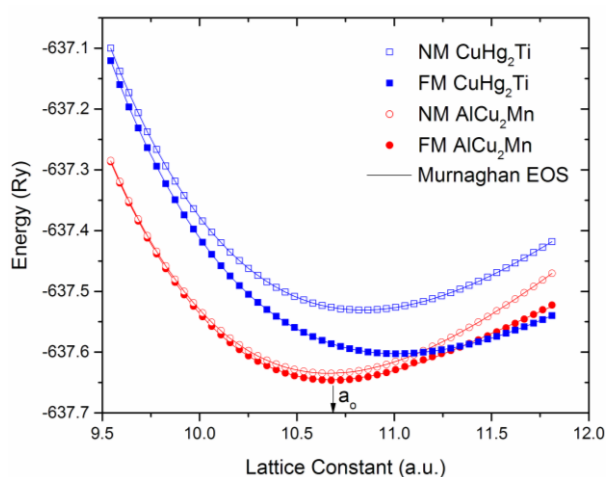


Fig. 1. Total energy of Fe_2TiP with AlCu_2Mn and CuHg_2Ti -type structures in the NM and FM states.

As the lattice volume increases (i.e., decreasing pressure) for both crystalline structures, the energy difference increases between FM and NM phases. Moreover, a structural phase transition from AlCu_2Mn to CuHg_2Ti can occur as the lattice expands. Energetically, the AlCu_2Mn -type structure in the magnetic state is found to be the most favorable structure which in good agreement with previous report [21]; therefore, from now on, we only presented the data in the FM state for this structure. The equilibrium structural parameters, i.e., lattice constant (a_0), bulk modulus (B_0), and pressure derivative of bulk modulus (B'_0), are presented in Table 1. To our knowledge, no experimental data could be found for comparison. Nonetheless, the other theoretical data calculated by WIEN2k package based on FP-LAPW approach and also, theoretical data reported for Fe_2ZrP as the isomeric compound of Fe_2TiP are given in Table 1. It can be seen that

our results, especially lattice constant, agree well with the other theoretical data [21]. However, our calculated bulk modulus and also first pressure derivative of bulk modulus underestimate their data which may be due to the different approach used in PP-PW and FP-LAPW calculations.

On the other hand, the lattice constant for Fe_2TiP in this study was 4.15% smaller than that of Fe_2ZrP , as reported by Canko et al. [20], which may be related to the greater atomic radius of Zr versus Ti ($r_{\text{Ti}} = 1.462 \text{ \AA}$, $r_{\text{Zr}} = 1.603 \text{ \AA}$) [28]. Besides, the bulk modulus of Fe_2TiP was compared with that of Fe_2ZrP ; the latter showed a smaller bulk modulus, which is consistent with the relationship between the lattice constant and bulk modulus ($B_0 \propto V^{-1}$; V , unit cell volume). Therefore, a lower bulk modulus is reported in compounds with a higher lattice constant. In addition, Fe_2TiP may be relatively harder than Fe_2ZrP , since bulk modulus is indicative of mechanical resistance to hydrostatic pressure. This result reflects the weaker bonding of Fe_2ZrP compared to Fe_2TiP which should be also investigated in terms of thermal stability analysis.

3.2. Thermal Stability

The enthalpy of formation (ΔH) can be used for determining the thermal stability of a Heusler compound. For the Fe_2TiP compound, ΔH is calculated considering the difference between the total energy of this compound and sum of total energies related to solid constituents (i.e., Fe, Ti, and P) at specific ground states. The following formula was used to determine ΔH :

$$\Delta H = E(\text{Fe}_2\text{TiP}) - [2E(\text{Fe}) + E(\text{Ti}) + E(\text{P})] \quad (1)$$

Table 1 presents the ΔH value for Fe_2TiP , as well as other theoretical data. The negative value of ΔH shows that the composition of Fe_2TiP is stable thermodynamically and can be experimentally formed. In addition, the Fe_2TiP compound had a significantly larger absolute ΔH (higher stability), compared to Fe_2ZrP . This finding, besides the bulk modulus data, can be evaluated considering the electronegativity difference of titanium/zirconium with iron and phosphorus atoms ($\chi_{\text{Ti}} = 1.54$, $\chi_{\text{Zr}} = 1.33$, $\chi_{\text{Fe}} = 1.83$, $\chi_{\text{P}} = 2.19$) [29]. The greater difference in electronegativity of a compound results in stronger bonds [30]; therefore, a more negative ΔH is associated with a larger bulk modulus.

3.3. Electronic Structure

For determining the electronic and HM features of Fe_2TiP , the band structure of AlCu_2Mn -type structure was calculated for the minority and majority spins, as indicated in Fig. 2. In the majority spin state, the Fermi level passed the energy bands, indicating its metallic nature. On the contrary, a semiconducting band gap was clearly observed near the Fermi level in the minority spin state, confirming HM character of Fe_2TiP compound with the AlCu_2Mn -type structure.

Table 1. The equilibrium lattice constant (a_0), bulk modulus (B_0), first pressure derivative of bulk modulus (B'_0), and enthalpy of formation (ΔH) in the FM phase of Fe_2TiP compound with the AlCu_2Mn -type structure. The other theoretical data of Fe_2TiP and also Fe_2ZrP compound with similar crystal structure are also presented for comparison.

Compound	a_0 (Å)	B_0 (GPa)	B'_0	ΔH (kJ/mol)	Refs.
Fe_2TiP	5.655	228.8	4.27	-176.57	This work
Fe_2TiP	5.65	236.98	4.66	-180.43	[21]
Fe_2ZrP	5.9	202.4	4.64	-121.34	[20]

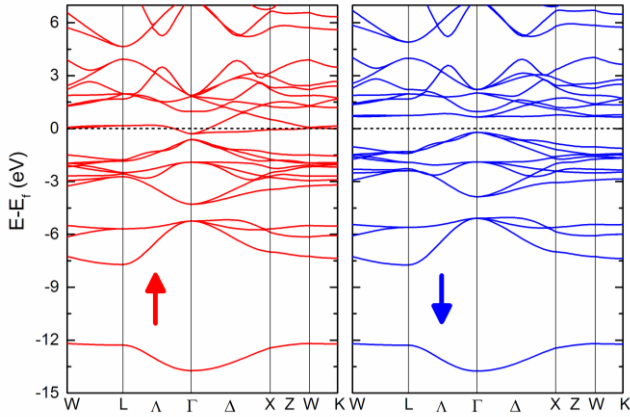


Fig. 2. The spin-polarized band structure of the Fe_2TiP compound with the AlCu_2Mn -type at the equilibrium lattice constant for the spin-up and spin-down channels. The dashed line presents the Fermi energy (E_F) at 0 eV.

The energy gap width was nearly 0.35 eV near the high symmetry direction Γ , which can be determined in the minority-spin channel based on the highest occupied and lowest unoccupied bands. This band gap value is in quite good agreement with 0.38 eV reported in the Kervan et al. [21] literature. However, the type of band gap observed for this compound is different: direct (Γ - Γ) and indirect (Γ -X) band gap, respectively for PP-PW and FP-LAPW approaches. Besides, valence band maximum (VBM) for minority spins is separated from Fermi level by an energy gap of 0.21 eV, i.e. the minority spin-flip gap, which marks the minimum energy required to reverse the spin of minority electrons. Since the spin-flip gap has a non-zero value, therefore, the Fe_2TiP compound with structure of AlCu_2Mn -type can be regarded as a “true” HM ferrimagnet (HMF).

The total and partial density of states (TDOS and PDOS, respectively) of the Fe_2TiP compound were calculated to find the origin of the minority band gap, as presented in Fig. 3. In the spin-down channel, near E_F , no PDOS was found for atoms, while the spin-up states crossed the Fermi level. Based on the spin polarization (P) formula:

$$P = \frac{N_{up}(E_F) - N_{dw}(E_F)}{N_{up}(E_F) + N_{dw}(E_F)} \quad (2)$$

where N_{up} and N_{dw} respectively refer to the spin-up and spin-down density of states at the Fermi level), the Fe_2TiP compound exhibited spin polarization of 100% at E_F , confirming its HM feature in the equilibrium state. As a result, it can be used to produce perfect spin-polarized currents in spintronic devices.

According to Figure 3, the main contributions in energy regions between -14 and -4.5 eV originate from the s and p states of phosphorus atoms, while small contributions arise from Fe-4d and Ti-3d states. However, PDOS in the energy

range $-4.5 < E$ (eV) < 5 mostly consists of Fe-4d and Ti-3d states. In addition, TDOS of compound at Fermi energy E_F for spin-up channel are mainly attributed to Fe-d electrons.

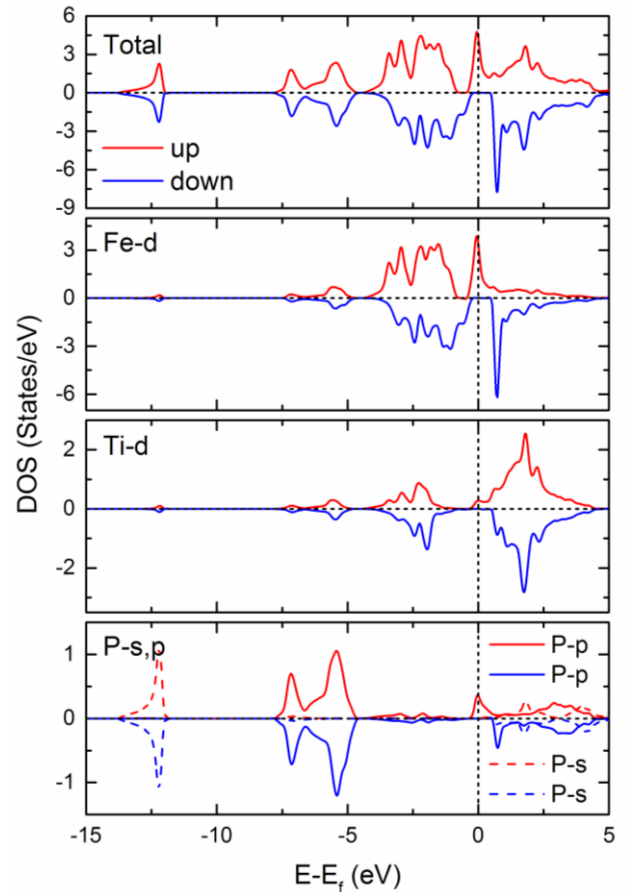


Fig. 3. TDOS and PDOS for the AlCu_2Mn -type structure of the Fe_2TiP compound at the equilibrium lattice constant (The zero energy indicates the Fermi level).

Although the results of the electronic structure calculations of this compound with two different pseudo- and full-potential based approaches are close together, however, the origin of the minority band gap of this compound has not been explored in the Kervan et al. [21] literature. Here, we discussed this issue in detail using the band structure calculations (Fig. 2) and density of states (Fig. 3). In both types of channels (spin-up and spin-down), the energy bands at -4.5 to 5 eV around E_F were mainly attributed to the d orbitals of iron (Fe) and titanium (Ti), hybridizing together. The three energy bands from -7.5 to -4.5 eV were mostly attributed to the p states of phosphorus (P) atom, whereas the energy band around -12 eV to the s orbitals of P atom. Therefore, among 12 minority occupied bands per unit cell for the Fe_2TiP Full-Heusler compound, one has s character, three p character, and eight d character. On the other hand, considering the PDOS of Fe_2TiP (Fig. 3), the energy gap observed in the spin-down

channel was attributed to hybridization between the 3d orbitals of Fe and Ti atoms which known as the “d-d band gap” [31]. The 3d electronic splitting of Fe atom exerted a major effect on the minority energy gap, as the gap of Fe PDOS was similar to that of TDOS of Fe_2TiP compound. Besides, the bonding states below the Fermi level were mainly from the d-states of high-valent Fe, whereas the unoccupied antibonding states were mostly in correspondence to the d-states of low-valent Ti atom. Therefore, low- and high-valent transition metal atoms showed a covalent hybridization, which resulting in an energy gap between the antibonding and bonding bands, also known as the “covalent band gap” [32]. Therefore, both d-d and covalent hybridizations were effective in the energy gap detected in the minority spin state of the Fe_2TiP compound.

3.4. Magnetic characteristics

The total (M_{tot}) and partial magnetic moments are presented in Table 2 at the equilibrium lattice constant for the AlCu_2Mn -type structure of the Fe_2TiP compound. Based on the findings, the M_{tot} of this compound was $1 \mu_B$ integer value per formula unit, which is in accordance with the Slater-Pauling rule [33]. Based on this rule, the M_{tot} of a full Heusler compound is presented as $N_V - 24$ (N_V denotes the total valence electron count in the unit cell of compound).

On the other hand, as can be seen, Fe atoms have the largest contribution to M_{tot} , while P and Ti atoms only exhibit small magnetic moment in this compound; the difference can be examined with respect to PDOS (Fig. 3). In the spin-up channel of Fe, the antibonding peak was occupied below the Fermi level, while above the Fermi level, the antibonding peak moved in the spin-down channel due to exchange splitting; this produced different electron occupations in the spin channels, therefore Fe atoms showed a large magnetic moment. Moreover, the Ti atoms magnetic moment was anti-parallel to Fe atoms, thus specifying the magnetic composition of Fe_2TiP as a ferrimagnetic compound.

Table 2. The M_{tot} and partial magnetic moment of Fe_2TiP with the AlCu_2Mn -type structure at equilibrium lattice constant (a_0) of 5.655 Å. The other theoretical data is also listed for comparison.

M_{tot} (μ_B)	M_{Fe} (μ_B)	M_{Ti} (μ_B)	M_{P} (μ_B)	Refs.
1.00	0.639	-0.287	0.009	This work
1.00	0.633	-0.151	-0.003	[21]

The lattice constant was closely associated with the stability of half-metallic feature of Heusler compounds, as variations can influence the minority or majority band gap, as well as the Fermi level relative to the band gap [34, 35]. Accordingly, using the lattice constant, the magnetic property was measured (Fig. 4).

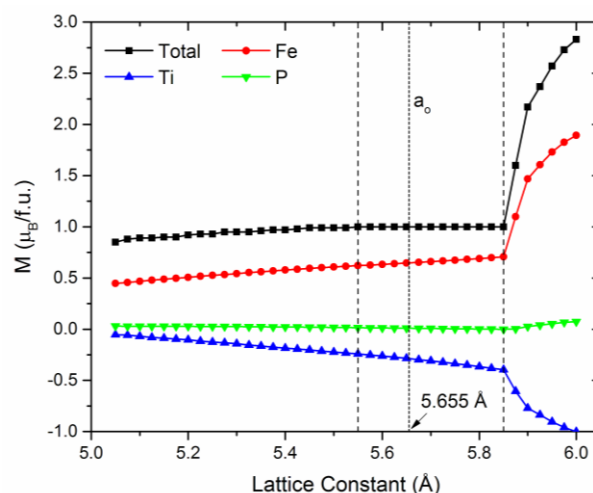


Fig. 4. The M_{tot} of Fe, Ti, and P atoms in relation to the lattice constant. The short and long vertical dashed lines represent the equilibrium lattice constant (a_0) and the half-metallicity range for Fe_2TiP , respectively.

Evidently, in a broad range of the lattice constant, the M_{tot} was $1 \mu_B$ integer value. Based on the findings, a moderate shift in the lattice constant cannot cause a significant change in M_{tot} . By reducing the lattice constant or improving pressure on the lattice, M_{tot} slowly reduced to $< 1 \mu_B$; therefore, the half-metallic property of Fe_2TiP disappeared. Nevertheless, the absolute partial magnetic moment of Fe and Ti atoms improved as the lattice constant increased, whereas the lattice distortion did not influence the magnetic moment of P. An explanation can be presented for this finding. Expansion of the lattice constant reduces the electron cloud overlap, thus deteriorating the hybridization of d states in transition metals, improving the exchange splitting in d states, and increasing the magnetic moment of Fe and Ti. With increasing lattice constants to values greater than 5.85 Å, hybridization between neighboring atoms decreases and the behavior of atoms tends toward isolated atoms which enhances their magnetization [36].

A similar behavior was reported by Kervan et al. [21] for Fe_2TiP and Canko et al. [20] for Fe_2ZrP compound. Moreover, the ferrimagnetic Fe_2TiP compound maintains its half-metallic characteristic at the lattice constant range of 5.55 to 5.85 Å. Considering this stability in a wide region, this material is useful for spintronic applications.

4. Conclusions

We employed the first-principles calculations, using the PWscf code in GGA-PW91 to examine the electronic structure, magnetic features, and stability of the Fe_2TiP compound. The results showed that the AlCu_2Mn -type structure was ferrimagnetic with half-metallic characteristics and at the Fermi level, it exhibited 100% spin polarization, while the CuHg_2Ti -type structure showed conventional ferromagnetic behaviors. The M_{tot} was $1.00 \mu_B/\text{f.u.}$ per unit cell, following the Slater-Pauling rule ($M_{\text{tot}} = N_V - 24$) for a broad range of the lattice constant. Based on the findings, the minority band gap may originate from the covalent and d-d hybridizations of Fe and Ti transition metals.

Acknowledgments

There is nothing to acknowledgement.

Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this article.

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