Competition of L2$_1$ and XA ordering in Fe$_2$CoAl Heusler alloy: a first-principles study

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Abstract. The physical properties of Fe$_2$CoAl (FCA) Heusler alloy are systematically investigated using the first-principles calculations within generalized gradient approximation (GGA) and GGA+U. The influence of atomic ordering with respect to the Wyckoff sites on the phase stability, magnetism and half-metallicity in both the conventional L2$_1$ and XA phases of FCA is focused in this study. Various possible hypothetical structures viz., L2$_1$, XA-I, and XA-II are prepared by altering atomic occupancies at their Wyckoff sites. At first, we have determined the stable phase of FCA considering various non-magnetic (or paramagnetic), ferromagnetic (FM) and antiferromagnetic (AFM) configurations. Out of these, the ferromagnetic (FM) XA-I structure is found to be energetically most stable. The total magnetic moments per cell are not in agreement with the Slater-Pauling (SP) rule in any phase; therefore, the half-metallicity is not observed in any configurations. However, FM ordered XA-I type FCA shows 78% spin polarization at the Fermi Energy (E$_F$). Interestingly, the results of XA-I type FCA are closely matched with the experimental results.

1 Introduction

Traditional electronic devices, which are mostly based on semiconductors, work on the electronic charge flow and lead to the consumption of higher power. The spin degree of freedom along with the charge of electrons could be exploited as an alternative in the existing semiconductors to minimize power consumption, maximize the speed of operation and add the non-volatility in the electronic devices [1,2]. As a thumb rule, materials with high spin polarization are required in spin-based electronics called spintronics [1,3–7]. Many full-Heusler alloys (HAs) of type X$_2$YZ (where X and Y are transition metal elements, and Z is an s-p element) exhibit half-metallicity, which means that one of the spin channels is gapless at the Fermi energy (E$_F$), while the other one possesses a semiconducting or insulating band gap. Thus, the half-metallic HAs would be 100% spin-polarized. It is widely known that the high spin polarization (P) plays a key role in the performance of spintronics devices such as magnetic tunnel junction (MTJ) or spin valves [7]. The inclusion of Fe$_2$CoAl Heusler alloy may enhance the giant magnetoresistance or tunneling magnetoresistance as compared with normal ferromagnetic transition metals, where spin polarization (P) is about 30–40%. The half-metallicity is ascribed to the strong hybridization between the d orbitals of the two transition metals [8]. The other features of those materials are of high Curie temperature around 1000 °C and a high magnetic moment up to 6.5 $\mu_B$/f.u. [9], both of which are important for device applications. Since the last decades, more and more Heusler alloys have been explored to search for the property of half-metallicity. Among them, Fe$_2$-based Heusler alloys such as Fe$_2$CoZ (Z = Ge, Ga) [10], Fe$_2$CrZ (Z = Bi, Sb, As, P) [11], Fe$_2$YP (Y = Zr, Mn, and Ti) [12–14], Fe$_2$YAl (Y = Sc, Cr) [15], Fe$_2$YAl (Y = Ni, Mn, Cr) [16], Fe$_2$YGa (Y = Mn, Cr, V) [17], Fe$_2$YSi (Y = Co, Cr, Mn) [18–20], and Fe$_2$TiZ (Z = Sb, Sn, In, As, Ge and Ga) [21], have been extensively investigated by means of first-principles calculations. It is progressively being known that the physical properties of HAs are dependent on their structural order [22]. The site preference rule (SPR) has been widely used in the theoretical design of the full-Heusler (of type X$_2$YZ) alloys. This rule sets a demarcation between the formation of the L2$_1$ and XA phases of the full Heusler alloys. The detail description of the SPR will be presented in the results and discussions section of this paper. Some of the XA type full-Heusler alloys such as Mn$_2$CoAl [23], Ti$_2$MnAl [24], and Ti$_2$CoSi [25] have been predicted to be a spin-gapless semiconductor using SPR. On the other hand, some of them e.g. X$_2$CuAl (X = V, Ti, Cr, Sc, Mn, Zr, Hf), are found to be a perfect half-metals [26]. Interestingly, some counter-examples such as Ti$_2$FeZ (Z = Ga, Al) [27], and our

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recent work on Co$_2$FeAl Heusler alloy [28] don’t follow the site preference rule (SPR). Moreover, Dahmane et al. [29] studied the L2$_1$ (Cu$_2$MnAl prototype) and XA (Hg$_2$CuTi prototype) ordering effect on the phase stability of Fe$_2$XAl (X= Cr, Mn, Ni) Heusler compounds. They found that L2$_1$ phase of Fe$_2$CrAl and Fe$_2$MnAl are more stable as compared with XA phase at the equilibrium volume. Wang et al. [30], studied the L2$_1$ and XA ordering effect on Hafnium-based full-Heusler alloys and found that all of them were likely to exhibit the L2$_1$-type structure instead of the XA one. We also reported L2$_1$ and XA ordering effects on Co$_2$FeAl [28], and found that XA (or indirect) ordered structure is much more stable than the L2$_1$ (direct) structure. Further, we have shown that the physical properties were not only dependent on L2$_1$ and XA ordering of atoms at their Wyckoff sites, but also strongly dependent on the exchange-correlation potential (U).

Siakeng et al. recently reported that Fe$_2$CoAl alloy in C1$_b$ (or XA) phase [31], while the calculated electronic structures were not able to address the site preferences of atoms in their respective structures under different symmetries viz., L2$_1$ (space group (SG): Fm$ar{3}$m) and XA (SG: F$ar{4}$3m). Additionally, which magnetic state (paramagnetic, ferromagnetic or antiferromagnetic) will be the ground state of FCA need to be explored to understand the complete electronic behavior of Fe$_2$CoAl alloy.

The present systematic study addresses some important features, which may hinder the device compatibility and performance:

1. Comprehensive reports are available for Co$_2$FeAl (CFA) full Heusler alloys (see Ref. [28], and references therein) where all literature says that CFA alloy tends to form L2$_1$ structure; however, our recent comparative study of L2$_1$ and XA ordering effect on the phase stability of CFA reveals that XA phase is a ground state of CFA, not the L2$_1$. A very few reports are available on Fe$_2$CoAl alloy and all of them are based on the XA (indirect/inverse) phase of CFA. Hence, we systematically studied the phase stability of CFA alloy under different cubic symmetries: L2$_1$ (SG: Fm$ar{3}$m) and XA (SG: F$ar{4}$3m). Additionally, we consider the stability of magnetic states, which are not addressed before.

2. For decades, the Slater Pauling rule is commonly used to predict the half-metallic ferromagnets. Here we explore whether it has one to one relationship with the electronic properties of FCA. We also examine whether the site preference rule (SPR) is also suitable for Fe$_2$CoAl.

3. It is widely known that only generalized gradient approximation (GGA) is not sufficient to describe the complete electronic behavior of the systems having 3d electrons, therefore, we also focus on the exchange and correlation (U) effects on electronic and magnetic properties of FCA.

Our results reveal that the physical properties are highly dependent on L2$_1$ and XA ordering of atoms at their Wyckoff sites. Furthermore, electronic structure is significantly affected by the presence of Coulomb potential (U). We found that XA-I type FCA alloy is energetically most stable and exhibit $\sim$78% spin polarization at the Fermi energy ($E_F$) as compared with other structures. The site preference rule is also valid in Fe$_2$CoAl alloy. Hence it is proficient for spintronics application. The present theoretical study will guide the synthesis of efficient Fe$_2$CoAl based alloy.

2 Computational methods

All calculations were performed using Wien2k code [32] based on the full-potential linearized augmented plane wave method [33]. Band-gap underestimation was known to occur with the consideration of the semi-local exchange-correlation function, and hence a generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was employed in the calculations to overcome it [34]. The effect of on-site Coulomb interaction (U) was also included in our calculations. The maximum l value ($l_{\text{max}}$) for the expansion of the wave function in spherical harmonics inside the atomic sphere was restricted to $l_{\text{max}} = 10$. The wave function in the interstitial region was expanded in plane waves with a cutoff of $R_{\text{MT}}K_{\text{max}} = 7$, where $R_{\text{MT}}$ represents the atomic radii of the smallest sphere and $K_{\text{max}}$ is the largest k vector. The charge density in the interstitial region was expanded up to $G_{\text{max}} = 12$ a.u.$^{-1}$. A grid of $15 \times 15 \times 15$ k-points was taken for the computations. The electronic and magnetic properties were studied at optimized lattice constants.

3 Results and discussions

3.1 L2$_1$ and XA ordering competition in Fe$_2$CoAl Heusler alloy

The ground state of Fe$_2$CoAl Heusler alloy is found, performing the lattice optimization calculation for different atomic occupations (as listed in Table S1 in Supplementary material) in L2$_1$ and XA phases with various magnetic configurations viz., non-magnetic or paramagnetic (NM/PM), ferromagnetic (FM) and antiferromagnetic (AFM). The X$_2$YZ type Heusler compounds such as Fe$_2$CoAl may crystallize in conventional L2$_1$ (Cu$_2$MnAl) and inverse XA (Hg$_2$CuTi) structures under space group of Fm$ar{3}$m (space group number 225), and F$ar{4}$3m (space group number 216), respectively. A detailed description/definition of the difference in L2$_1$ and XA structures can be found in our previous paper [28]. There are four available Wyckoff sites: A (0, 0, 0), B (0.25, 0.25, 0.25), C (0.5, 0.5, 0.5), and D (0.75, 0.75, 0.75) along the body diagonal as shown in Figures 1a and 1b. In L2$_1$ (or direct) structure, Fe atoms occupy B (0.25, 0.25, 0.25) and D (0.75, 0.75, 0.75) sites, and Co/Al atoms occupy A (0, 0, 0) and C (0.5, 0.5, 0.5) sites, respectively. On the other hand, in XA (or inverse) structure, two inequivalent atoms of Fe (as labelled Fe1 and Fe2) occupy A (0, 0, 0) and D (0.75, 0.75, 0.75) sites, and Co and Al atoms occupy C (0.5, 0.5, 0.5) and B (0.25, 0.25, 0.25) sites, respectively (see Fig. 1). Generally, X$_2$YZ compounds prefer XA (Hg$_2$CuTi) prototype structure if the Y atom has a larger
Fig. 1. Crystal structure of Fe$_2$CoAl (FCA) alloy in (a) L$_2$\textsubscript{1} (Cu$_2$MnAl prototype), and (b) XA (Hg$_2$CuTi prototype); (c, d) shows the arrangement of Co/Fe magnetic moments for ferromagnetic (FM) and antiferromagnetic (AFM) configuration, respectively. All crystal structures are generated using XCrysDen software [36].

atomic number than the X (from the same period) atom [35].

The geometrical frustration is always present in the FCC lattice. To achieve antiferromagnetic (AFM) ordering, structural distortion is required and it can be one of the three types: (i) distortion is along the [001] direction (tetragonal distortion) that is seen in our case; (ii) distortion is along the [011] direction (orthorhombic distortion) and (iii) distortion is along [111] direction (rhombohedral distortion). The tetragonal distortion is usually observed in Heusler alloys [37]. A ferromagnetic arrangement is shown in Figure 1c. To obtain an AFM structure, we construct a supercell of FCA which takes the space group Pmmm (space group number 47) as shown in Figure 1d. Here, the ferromagnetic planes of Co spins (up/down) are alternatively arranged in a specific direction [001]. Similarly, ferromagnetic planes of Fe spins (up/down) are also arranged [38]. The non-magnetic (or paramagnetic) state means that all the constituents atoms of Fe$_2$CoAl alloy have zero spin polarization (P) at Fermi energy (E$_F$).

The total energies (E$_{\text{tot}}$) have been calculated for both L$_2$\textsubscript{1} and XA phases for the different volumes of the cell and the energy difference (E$_{\text{tot}}$-E$_0$) curves as a function of the unit cell volume are shown in Figure 2. It is noted that the total energy difference versus volume (E$_{\text{tot}}$-E$_0$) vs. $V$ curves are obtained after fitting with Birch-Murnaghan equation [39] and the fitted ground state parameters such as optimized lattice constants “a$_0$”, equilibrium volume $V_0$, bulk modulus $B$ and its pressure derivative $B'$ are shown in Table S2 (in Supplementary material). From Figure 2, it is seen that Fe$_2$CoAl alloy energetically prefers to crystallize in XA phase, but not in L$_2$\textsubscript{1} phase. More specifically, it crystallizes in the XA-I phase with ferromagnetic ordering as expected from the site preferences rule (SPR) [18,40,41]. The results reveal that the element with a higher number of valence electrons prefers C (0.5, 0.5, 0.5) site and the element with a lower number of valence electrons tend to enter at A (0, 0, 0) and D (0.75, 0.75, 0.75) Wyckoff sites, whereas the main group element Al usually prefers B (0.25, 0.25, 0.25) site. Hence, XA-I structure follows the site preference rule. A similar theoretical study was carried out on Fe$_2$CoGa alloy, which has the same valence as Fe$_2$CoAl, and it was predicted that the inverse XA (Hg$_2$CuTi prototype) structure was preferable [42]. Similar results also reported by our group elsewhere [28]. However, these results are contrary to other’s reports [30], where they predicted that the L$_2$\textsubscript{1} phase is much more stable than the XA one. Therefore a comparative study of phase stability is crucial and should be addressed properly.

From data of Table S2, it is clear that the optimized value of lattice constant “a$_0$” of XA-I (Hg$_2$CuTi prototype) structure is found to be 5.70 Å, which is much closer to the experimental one compared to the other structures. In the next sections, we shall focus on in-depth studies on electronic structures of ferromagnetic XA-I (most stable) structure.

3.2 Electronic properties of L$_2$\textsubscript{1} and XA types Fe$_2$CoAl within GGA

It is progressively being known from the theoretical electronic structures [43–45] that the physical properties of the Heusler alloys are strongly dependent on the atomic occupancies at their available Wyckoff sites in the unit cell.
and hence need to be explored. Therefore, in this section, we discuss the electronic behavior and magnetism of the L2₁ and XA types FCA. The spin polarization \( P \), at Fermi energy (\( E_F \)) is defined by the following equation (1).

\[
P = \frac{D \uparrow (E_F) - D \downarrow (E_F)}{D \uparrow (E_F) + D \downarrow (E_F)}
\]  

(1)

where \( D \uparrow (E_F) \) and \( D \downarrow (E_F) \) represent the density of states at Fermi energy (\( E_F \)) for up and down spin channels, respectively. It displays a finite value for ferromagnetic materials and vanishes for paramagnetic and antiferromagnetic materials below Curie temperature \( [18] \). Half-metallic materials exhibit 100% spin polarization only when \( D \uparrow (E_F) \) or \( D \downarrow (E_F) \) equals to zero at \( E_F \).

The calculated spin polarization values (\( P \)) for all types of ordered structures are shown in Table S3 (in Supplementary material). We have calculated the total and atomic specific spin-polarized density of states (DOS) per electron volt (eV) at their respective optimized lattice parameters “\( a_0 \)” under GGA approximation and shown in Figure 3. For L2₁, XA-I and XA-II types Fe₂CoAl, their density of states (DOS) exhibit a common ferromagnetic metallic nature at Fermi energy. The higher density peak at \( E_F \) is mainly due to the Co/Fe eg state, which can be easily seen in Figures 3a and 3c. These peaks are responsible for the instability of regular L2₁ and XA-II phases compared with the XA-I phase. In the case of XA-I, this peak is totally shifted to the valance region and hence attributed to energetically most stable XA-I structure which was also confirmed from the volume optimization curve (see Fig. 2). The site preferences of atoms under L2₁ and XA-II type structures do not affect the general shape of the total density of states excluding XA-I. Moreover, in XA-I, double pseudogap structures (in the spin-down channel) are observed just below (at about –0.8 eV) and above (at about 0.4 eV) the Fermi level (\( E_F \)), which imply the covalent bonding between the atoms \( [46] \). Similar pseudogap structures have also been reported for inverse XA structure: Fe₂CoGa and Fe₂CoZn \( [42] \). Half-metallicity is not observed in any possible structures as Fermi energy (\( E_F \)) has totally been shifted to the valance region and hence the spin polarization is reduced \( [47] \). This argument is further supported by the calculated spin-polarized band structures of the L2₁ and XA types FCA at their equilibrium lattice constants (\( a_0 \)) as shown in Figures 4a–4c.

The majority and minority bands of L2₁ and XA-II look similar and are in close agreement with the DOS plots shown in Figures 3a and 3c. The band structure of XA-I is highly affected by the influence of the atomic occupancies in the cell and that is why it shows quite different band structures than those of the L2₁ and XA-II. Although it exhibits a metallic nature since spin up and spin down bands are crossing at the Fermi level (\( E_F \)), however, a gap-like feature can be seen in the minority bands at X point.

### 3.3 Magnetic properties of L₂₁ and XA types Fe₂CoAl

Wurmehl et al. \( [48] \) studied many Co base full Heusler-alloys and made a linear relationship between the total magnetic moment per unit cell \( M_t (\mu_B/f.u.) \) and Curie temperature, \( T_c (K) \) as equation (2).

\[
T_c(K) = 23 + 181 \times M_t (\mu_B/f.u.).
\]

(2)

This equation gives the highest \( T_c \) for Half-metallic materials, which have a large magnetic moment. Using this equation, \( T_c \) of Co₂FeSi has been reported to be higher than 1000 K, which was consistent well with experimental results \( [48] \). A linear variation of \( T_c \) with magnetic
are consistent with recent DFT study too reported by Siakeng et al. [51]. From Table S3, it is clear that the net magnetic moment is contributed due to Fe and Co atoms and the contribution from Al is insignificant in all structures. Moreover, one can also see that the spin polarization and Curie temperature is high to those which have higher magnetic moments i.e. L2\textsubscript{1} and XA-II structures than the XA-I structure. Any structures don’t exhibit the integer magnetic moment and far away from the Slater-Pauling value [52], which is 4.0 µB in this case. In a search of half-metallic materials, we conclude that these two conditions will remain necessary to meet the criteria of exhibiting half-metallicity. The total and partial magnetic moments including spin polarization values and Curie temperatures are nearly equal for all structures excluding XA-I type. The experimental value of the total magnetic moment per cell, which is 4.9 µB/f.u. (see Tab. S3), is in close agreement with the XA-I (most stable) structure.

### 3.4 Effect of on-site Coulomb interaction (U)

Here the results of the electronic structure calculation of the most stable XA-I phase of Fe\textsubscript{2}CoAl alloy using GGA+U (Coulomb potential) are presented. Note that we have treated all possible structures under GGA+U, but did not get significant changes in the density of states (other data are not shown here). Typically, Heusler alloys are endorsed to exhibit localized moments; so electron correlation can play an important role [48]. The GGA+U scheme is used to calculate the electronic structure to understand whether the addition of correlation resolves the inconsistency between the theoretical and experimental magnetic moment. In Wien2k, the effective Coulomb-exchange interaction, $U_{\text{eff}} = U - J$, where $U$ and $J$ are the Coulomb and exchange parameter, is used to account for double counting corrections. In Figure 5, the spin-polarized total and partial density of states (DOS) are shown using the GGA+U method. The effective Coulomb-exchange parameters were set to $U_{\text{eff,Co}} = 4.22$ eV and $U_{\text{eff,Fe}} = 4.35$ eV [53] at the Co and Fe sites, respectively. As seen in Figure 6, a small energy gap of 0.87 eV is observed in the minority spin channel at about 0.5 eV above the $E_F$. The Fermi energy ($E_F$) cuts the minority bands below the gap is due to the region that the total magnetic moment per cell is too high than the predicted Slater-Pauling value and is not an integer, which is expected for a half-metal [48]. Additionally, a similar kind of gap-like structure has also been reported previously in references [31,48,54].

Hence, FCA alloy is still not a half-metal; however, spin polarization is as high as 78% which is very important for spintronics application. These values were underestimated when dealt with GGA approximation. The metallic nature of FCA alloy is further confirmed from the results of the spin-polarized band structures calculation shown in Figure 6. To achieve a half-metal, Fermi level could be tuned in the middle of the gap by varying the lattice constants “a” [31,48]. To explain the origin of the energy gap in the down spin channel, atomic resolved DOS has also been presented in Figure 5. We observed that the

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**Fig. 4.** Shown are the spin-polarized band-structures of Fe\textsubscript{2}CoAl alloy in (a) L2\textsubscript{1}, (b) XA-I and (c) XA-II phases. Fermi level EF has been shown by dotted lines, red and blue curves show the spin up and spin down bands within GGA, respectively.

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moment $M_{\text{tot}}$ was also reported by Kubler et al. [49] on the following compounds e.g., Co\textsubscript{2}TiAl, Co\textsubscript{2}VGa, Co\textsubscript{2}VSn, Co\textsubscript{2}CrGa, Co\textsubscript{2}CrAl, Co\textsubscript{2}MnAl, Co\textsubscript{2}MnSn, Co\textsubscript{2}MnSi, and Co\textsubscript{2}FeSi. The calculated Curie temperatures using equation (2) [48,50] are tabulated in Table S3 along with experimental results for comparison. These results
Fig. 5. Plots of spin-polarized total and atomic-resolved density of states of Fe$_2$CoAl (FCA) under GGA+U approximation.

Fig. 6. Spin-polarized band-structures of XA-I type Fe$_2$CoAl. Fermi level $E_F$ has been shown by dotted lines; red and blue curves show the spin up and spin down bands within the GGA+U.

bonding and antibonding states are formed due to the $d$-$d$ hybridization between the low valence Fe (A)/Fe (D) atoms having $d$ states in higher energy, and high valence Co (C) atoms with $d$ states in lower energy; hence attributed to the gap-like feature in the spin-down channel.

4 Conclusion

The effects of atomic ordering in their Wyckoff sites on phase stability, electronic structures and magnetic properties of conventional L2$_1$ and inverse XA type Fe$_2$CoAl alloy have been investigated and compared. FCA alloy energetically favored the inverse XA-I structure compared with the other structures, as expected from the site preference rule. Electronic, structural and magnetic properties were not much affected by atomic site preferences in ferromagnetic L2$_1$ and XA-II structures but significant changes have been observed in the case of XA-I structure. Moreover, only this structure has shown the possibility to achieve a half-metal because of having a finite spin-down energy gap within GGA+U. Atomic site preferences did not restore the half-metallicity in any structures of the Fe$_2$CoAl (FCA) alloy but the variation of lattice constants worked well. FCA alloy is a ferromagnetic (FM) metal under all kinds of possible structures and is found to be most stable in XA-I structure with a spin polarization value of around 78% at $E_F$. Hence, we conclude that FM-FCA alloy in XA-I ordering could be used as a highly spin-polarized material in spintronics devices.

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Author contribution statement

Aquil Ahmad performed all the calculations and manuscript writing under the supervision of Dr. A.K. Das and Dr. S.K. Srivastava.

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