Electronic, Elastic and X-ray spectroscopic properties of direct and inverse full Heusler compounds: DFT+U study

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Half-metallicity, low magnetic damping and high curie temperature (Tc) are crucial for application in spintronics and full Heusler alloys in this regard exhibit remarkable properties. Herein, we have considered Co2FeAl (CFA) and Fe2CoAl (FCA) as a representative of direct and indirect full Heusler compounds which crystallizes in L21 and C14 phases, respectively. The theory of L21 type Heusler alloys has been well established, however the fundamental understanding of Fe2CoAl is still under developed. In this paper, we have employed density functional theory (DFT) to study the electronic, elastic and X-ray spectroscopic properties of Co2FeAl and Fe2CoAl. The electron exchange correlation were treated within a generalized gradient approximation (GGA) as PBE-scheme. Inorder to include the impact of valence electrons an onsite Coulomb potential is added to GGA as GGA+U. Within both GGA and GGA+U, CFA shows a half-metallic behaviour but FCA is metallic. The calculated values of magnetic moment and Tc are in close agreement with the experimental data.

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I. INTRODUCTION

The recent challenges for the material scientists and material engineers is to develop a new and eco-friendly material for the advancement of smart devices. Material science is an open field to accept the new approaches for the technological development. The conventional semiconductor electronic devices works on the basis of electron charge transfer that accomplished by high level of energy consumption. Alternatively, the usage of electron spin-based innovation called spintronics1–6 which utilizes the spin degrees of freedom, can give extra functionality and new capabilities, including faster switching time and lower power consumption. The spintronics devices solely rely on the spin polarization at the Fermi energy (EF) of the material7–14. Researchers believed that the future spin based electronic devices outclass the customary charge-based electronic devices in terms of low power consumption, ecologically and efficiency. The spin functionality of electron was successfully implemented in a device as giant-magneto-resistance (GMR) in 198815. One of the potential competitors is transition based Heusler compounds due to the presence of d-orbitals which play an important role in determining the multi-functional properties and their application in diverse field16. The transition metal based Heusler alloys show high magnetic moment in the absence of applied magnetic field15–20. The other fascinating feature is their high Curie temperature TC which is an important criteria for technological application and can be well fabricated in devices preserving the ferromagnetism above the room temperature (RT). The theoretical TC of some of the well known Co-based Heusler compounds calculated from atomistic spherical wave approximation (ASW)21 are Co2VGa(TC=368 K), Co2CrGa(TC=362 K), Co2MnAl(TC=609 K), Co2MnSi(TC=990 K), Co2MnSn(TC=899 K) and Co2FeSi(TC=1183 K). While the experimental22–25 values of TC for the aforementioned compounds are 352 K, 495 K26, 697 K, 985 K, 1100 K, respectively. Majority of Heusler compounds show high spin polarization at Fermi level (EF), due to the presence of conducting electrons that gives dispersed bands around the EF at one of the spin channels whereas other spin channel is semiconducting with a band gap. The Half-metallic characteristics in Heusler compound is attributed to the hybridization between the d−d orbitals of the transition elements27. The half-metallic Heusler compounds are superior interms of their technological application as compared to other class of half metals like oxides (CrO2, Fe3O4)28, manganites La0.7Sr0.3MnO329,30, perovskite Sr2FeReO629,30, pyrites CoS231, chalcogenides CrS32, pnictides CrAs32 etc., due to higher value of Tc and high magnetic moment. The above discussed diverse properties of Heusler compound are highly plausible for the advancement of new spin-based technology33,34. However, the understanding of complex magnetization due to the presence of d-electrons and the distribution of magnetic moments in atomistic-scale is crucial. An insight of the intrinsic magnetic properties can be achieved by using magneto-optical spectroscopy, e.g. the X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD)35–38. The magneto-optical analysis provide a quantitative information about the local spin and orbital magnetic moments of the 3d atoms in the form of 2p1/2,3/2 → 3d transitions as L2,3 absorption edges. The transition metal based Heusler compound constituted strongly correlated electrons which are not accounted within a conventional density functional theory (DFT). Hence, the information obtained are inaccurate and inadequate. In this paper we have implemented DFT+U (Coulomb potential) approach to integrate the impact of the valence electrons(strongly correlated d-electrons) to procure precision in the outcomes.

II. COMPUTATIONAL DETAIL

In general, the full Heusler alloy (FHA) is expressed as X2YZ, where X and Y are transition elements and Z species is p-elements. There are two types of full-Heusler; direct
and inverse depending on the arrangement of atoms according to their electronegativity. The direct FHA crystallizes in L2\(_1\) structure, consisting of four inter-penetrating FCC lattices with space group 225(\(Fm\overline{3}m\))\(^{39}\). Inverse FHA crystallizes in C1\(_b\) type structure having space group 216(\(F\overline{4}3m\)) where the electronegativities of X and Y are just the reverse as compared to direct one [Fig.1(a,b)]. In this work, we have used an efficient and globally adopted an open source DFT-package called Quantum Espresso\(^{40}\). The relaxed structure at its ground state has been achieved by optimizing the lattice parameters based on Murnaghan’s equation of states (EOS)\(^{41}\). For further confirmation of thermodynamical stability we have also calculated the frequency dependent phonon dispersion based on linear response method\(^{42}\) in combination with the density functional perturbation theory (DFPT) as program in Quantum Espresso\(^{43}\). Quantum Espresso works on the basis of projected augmented wave (PAW) method that rely on the ultrsoft pseudopotential functional\(^{44}\). All electrons are treated by using a generalised gradient approximation (GGA) within Perdew-Burke-Ernzerhof (PBE) functional\(^{45}\). A cut-off energy of 50 eV has been considered within a plane wave basis set. The k-points correspond to the electronic wave functions are integrated within a first Brillouin Zone (BZ) by Monkhorst-pack 8×8×8\(^{46}\). For the accurate and efficient treatment of the electron-electron interaction among the strongly correlated d-electrons, we have also deployed Hubbard on-site Coulomb interaction (U) within the DFT formalism as GGA+U. The respective U values\(^{47}\) of Co and Fe are \(U_{Co}=3.89\) eV and \(U_{Fe}=3.82\) eV, have been adopted for our calculation. We have also computed the X-ray Absorption Spectra (XAS) and X-ray Magnetic Circular Dichroism (XMCD) using the spin-polarized, relativistic Korringa-Kohn-Rostoker method (SPR-KKR)\(^{48,49}\).

III. RESULTS AND DISCUSSION

The optimized lattice constants \(a_0\) of Co\(_2\)Fe\(_2\)Al calculated from GGA and GGA+U are 5.044Å and 5.703Å respectively. Also, the respective values of lattice constants for Fe\(_2\)Co\(_2\)Al within GGA and GGA+U are 5.70Å and 5.73Å. The calculated lattice parameters in comparison with the previously reported theoretical and experimental data are presented in Table I. Our calculated lattice parameters are in qualitative and in close agreement with the previous results.

| Compounds    | B\(_1\) (GPa) | B\(_2\) (GPa) | \(a\) (Å) | \(a_{exp}^{\text{Lam}}\) (Å) | \(a_{exp}^{\text{Th}}\) (Å) |
|--------------|---------------|---------------|----------|--------------------------|--------------------------|
| CFA-GGA      | 193.7         | 209.27        | 5.704    | 5.69\(^{55}\), 5.70\(^{53}\), 5.74\(^{51}\) |
| CFA-GGA+U    | 110.4         |               |          | 5.746                    |
| FCA-GGA      | 187.2         | 208.67        | 5.703    | 5.71\(^{55}\), 5.67\(^{34}\), 5.766\(^{34}\) |
| FCA-GGA+U    | 325.0         |               |          | 5.733                    |

TABLE I. Calculated Lattice Constant \(a\) (Å) in comparison with the reported data and the Bulk Modulus (where B\(_1\) based on Murnaghan’s equation\(^{41}\) and B\(_2\) from Elastic code\(^{50}\))

FIG. 1. Conventional and primitive cell of (a) L2\(_1\)-type Co\(_2\)Fe\(_2\)Al, (b) C1\(_b\)-type Fe\(_2\)Co\(_2\)Al structure and (c) Total density of states (DOS) of Co\(_2\)Fe\(_2\)Al and Fe\(_2\)Co\(_2\)Al calculated from GGA and GGA+U.

A. Electronic and Magnetic properties

By using the optimized lattice constant, the electronic and magnetic properties were calculated. The vivid description of the electronic properties of crystalline material is directly related to density of states (DOS) and band structures. Hence, the total DoS of Co\(_2\)Fe\(_2\)Al and Fe\(_2\)Co\(_2\)Al calculated from GGA and GGA+U are shown in Fig.1(c). We have found that the total DoS of Co\(_2\)Fe\(_2\)Al and Fe\(_2\)Co\(_2\)Al are not comparable despite of having similar chemical composition, due to the differences in their crystallization (space group). In case of Fe\(_2\)Co\(_2\)Al the Fermi energy (\(E_F\)) is completely shifted to the valence region, whereas in Co\(_2\)Fe\(_2\)Al we can see \(E_F\) falling exactly in the band gap in the spin down channel within both GGA and GGA+U approximation. The former exhibits a pure metallic behaviour on the other hand the later gives the half-metallic characteristics. The half metallicity is basically due to the presence of metallic state at one of the spin channels whereas other channel is semiconducting\(^{55}\). In Co\(_2\)Fe\(_2\)Al, Co-\(d(↑)\) (\(d-x↑+d-\)
FIG. 2. Calculated partial DoS of Co$_2$FeAl: (a) GGA, (b) GGA+U and Fe$_2$CoAl: (c) GGA, (d) GGA+U

FIG. 3. Calculated band structures of Co$_2$FeAl: (a) GGA, (b) GGA+U and Fe$_2$CoAl: (a) GGA, (b) GGA+U
$t_{2g}$) states are dispersed around the $E_F$ and Fe-d($\uparrow$) states are located at around -4.0 eV to -6.0 eV in spin up channel, and a presence of clear band gap at the spin down channel gives all the credulity to its half-metallic behaviour. [Fig.2(a, b)]. The formation of band gap in the spin down channel of Co$_2$FeAl ascribed to the hybridization between the $d$-orbitals of transition metal atoms [Fig. 2(a,b)]. The $d-d$ hybridization in L2$_1$ type structure has already been discussed somewhere else$^{[7]}$. The $d-d$ hybridization gives bonding (occupied) and anti-bonding (unoccupied) states where bonding states are stable with low energy and shifted below the $E_F$. The energy difference between the bonding and anti-bonding states is a measure of half-metallic band gap ($E_g$). The calculated band gap of Co$_2$FeAl along K-point from GGA and GGA+U are 0.2 eV and 0.51 eV respectively [see Fig. 3(a,b)]. However, the GGA band gap of Co$_2$FeAl is slightly narrower than that of GGA+U. The degenerated band gap is due to fact that GGA is insufficient in deriving the free electrons efficiently. Rather, the free electrons in the interstitial region are treated as impurities which induced extra states at the edge of the band gap. As a consequence of metal-semiconductor hybrids the $E_F$ lies within the band gap, thus Co$_2$FeAl exhibit 100% spin polarization. The empirical formula to estimate the degree of spin polarization at $E_F$ is$^{[28]}$ given by Eq. (1)

$$P = \frac{N_\uparrow(E_F) - N_\downarrow(E_F)}{N_\uparrow(E_F) + N_\downarrow(E_F)} \quad (1)$$

where $N_\uparrow(E_F)$ and $N_\downarrow(E_F)$ are the number of density of states at $E_F$ for spin-up and spin-down channels respectively. The partial DoS of Fe$_2$CoAl is shown in Fig.2(c,d) which predict its metallic characteristic. The band gap in the spin-down channel is located above the Fermi level. As one can see the $E_F$ is passing through the dispersed DoS in both the spin channels, also cross checked from Fig.3(c,d). The total magnetic moment of L2$_1$ and C1$_b$ type Heusler compound is based on the Slater-Pauling (SP) rule$^{[56]}$. Full-Heusler compound follows the rule of 24; $M_t=Z_t-24 (\mu_B)$, where $M_t$ and $Z_t$ are the total magnetic moment and total valence electrons, respectively. The integer value of $M_t$ is another important factor to determine the half-metallic behaviour. The respective values of $Z_t$ for Co$_2$FeAl and for Fe$_2$CoAl are 29 and 28. So the expected values of $M_t$ for Co$_2$FeAl and Fe$_2$CoAl are 5 ($\mu_B$) and 4 ($\mu_B$), respectively. The calculated $M_t=5.00 \mu_B$ for Co$_2$FeAl, exactly an integer value that falls within the SP-rule but $M_t=5.12 \mu_B$ for Fe$_2$CoAl deviates abruptly. This is because there are 11.5 electrons instead of 12 in the spin down band and in the majority band there 16.5 electrons instead of 16. This leads to $M_t=16.5-15.5=5.00 \mu_B$ instead of 4.00$\mu_B$ in Fe$_2$CoAl. To restore half metallicity the variation of lattice constant may works well. This will shift the $E_F$ into the band gap and the perfect half-metal with $M_t=4.00 \mu_B$ may be possible. The calculated $M_t$ values of Co$_2$FeAl and Fe$_2$CoAl are presented in Table II along with the previous reports. Our results are in good agreement with the available data. Another interesting feature is high value of Curie temperature ($T_C$) exhibited by majority of the Heusler compounds. The Curie temperatures ($T_C$) are calculated from the following Eq. (2)$^{[57,58]}

$$T_C = 23 + 181 \times M_t \quad (2)$$

$T_C$ is strongly related to the total magnetic moment ($M_t$) thus we can get a linear relation between $T_C$ and $M_t$ (mimic $y = mx + c$) which shows that higher value of $M_t$ gives high $T_C$. We have also estimated the strength of the magnetic inter-

![FIG. 4. Calculated exchange coupling $J_{ij}$ parameter of: (a) Co$_2$FeAl at Co center within LDA (b) Co$_2$FeAl at Co center within LDA+U, (c) Fe$_2$CoAl at Fe center within LDA and (d) Fe$_2$CoAl at Fe center within LDA+U](image-url)
approximation (MFA) by using Eq. (4).

\[ k_B T_C \langle s_i \rangle = \frac{2}{3} c \sum_{j, r \neq 0} J_{ij}^{s,r} \langle s_j \rangle \]  

(4)

where \( c \) is the concentration of impurities and \( k_B \) is the Boltzmann constant, \( \langle s_j \rangle \) is the average \( j \) component of the unit vector \( s_j \) along the direction of magnetization. The calculated \( T_C^{\text{MFA}} \) are tabulated in Table II and overestimated because of the inadequate description of the magnetic percolation effect \(^{6,61} \).

IV. X-RAY ABSORPTION SPECTRA (XAS) AND X-RAY MAGNETIC CIRCULAR DICHIROMBS (XMCD)

A theoretical study of XAS and XMCD have been performed based on the sum rule within the frame work of DFT+U in an absence of external applied field. Fig. 5(a,b) shows the calculated XAS and XMCD spectra of Co and Fe at L\(_{2,3}\) edges for Co\(_2\)FeAl and Fe\(_2\)CoAl. The XAS of Co atoms in Co\(_2\)FeAl are more sharp with high intensity as compared to Fe atoms. On the other hand the XAS of Fe atoms in Fe\(_2\)CoAl shows more intense peaks. The L\(_3\) and L\(_2\) edges are denoted as peak 1 and peak 2 in Fig. 5(a,b). The ratio of intensities of XAS, between L\(_3\) and L\(_2\) edges in Co is 2:1 and Fe is 2:4:1 for Co\(_2\)FeAl, in good agreement with the experiment \(^{62} \). Moreover, the ratio of L\(_3\) and L\(_2\) in Fe\(_2\)CoAl is 3:1 for Co and 2:6:1 for Fe atom. The similar result of deviation of branching ratio from standard 2:1 as in later case has also been reported in all one-electron approach \(^{63,64} \). This discrepancy may be because of the implementation of inaccurate Coulomb potential \((U_C/U_{\text{Fermi}})\) for electron core-hole exchange correlation in Fe\(_2\)CoAl. The L\(_{3,2}\)-XAS of Co and Fe are related to the unoccupied d-states near \( E_F \). The L\(_3\) edges in Fig. 5(a, b) are derived from the spin-resolved unoccupied Co-d \( t_{2g}(\uparrow) \) and Fe- \( t_{2g}(\uparrow) \) states for Co\(_2\)FeAl and Fe\(_2\)CoAl, respectively [see Fig.2 (b,d)]. These results are in good agreement with the experimental one calculated from the ultra-high vacuum magnetron sputtering by applying pressure below \( 8 \times 10^{-10} \) Torr \(^{65} \). The absorption peaks at 2 eV and 18 eV are due to the transition of \( 2p_{3/2} \rightarrow 3d \) and \( 2p_{1/2} \rightarrow 3d \) which corresponds to L\(_3\) and L\(_2\) edges, respectively. The XMCD spectra are calculated corresponds to XAS. The first XMCD spectra of Co and Fe atoms occur at 0.5 eV but in the second XMCD spectra Co edg eout Fe by \( \sim 3.0 \) eV [Fig. 5(a)]. The occurrence of XMCD Co-L\(_{2,3}\) and Fe-L\(_{2,3}\) peaks are in a direct relation to ferromagnetic ordering of Co\(_2\)FeAl, which has also been reported earlier \(^{62,65} \). The similar explanation may follows for Fe\(_2\)CoAl as well [Fig.5(b)].

V. PHONON PROPERTIES

We have also presented the GGA calculation of lattice dynamics for Co\(_2\)FeAl and Fe\(_2\)CoAl with the relaxed structure. The graphical representation of the phonon dispersion curve within first Brillouin zone and the phonon density of states are shown in Fig.6 (a,b). Due to the presence of four atoms in a primitive cell, we can have twelve vibrational modes of phonon at any \( q \)-point, it consists of three acoustic modes and nine optical modes. The detail information about the dynamical stability of Co\(_2\)FeAl and Fe\(_2\)CoAl structure has been confirmed due to the absence of imaginary phonon frequencies[see Fig.6(a, b)]. For Co\(_2\)FeAl, the optical branches are located at 120.258 cm\(^{-1}\), 215.194 cm\(^{-1}\) and 258.68 cm\(^{-1}\) at the \( \Gamma \)-point. For Fe\(_2\)CoAl, the optical branches are observed at 211.134 cm\(^{-1}\), 228.466 cm\(^{-1}\) and 286.239 cm\(^{-1}\) along the \( \Gamma – point \) [Fig.6(b)]. However, we do not have sufficient data to compare our results for the same compounds, therefore we are compelled to compare with that of the analogous compounds Ru\(_2\)FeX (X=Si, Ge) \(^{70} \). The reported value of optical branches \(^{70} \) at \( \Gamma – point \) for Ru\(_2\)FeSi are 248.319 cm\(^{-1}\), 253.221 cm\(^{-1}\), 273.829 cm\(^{-1}\), 289.636 cm\(^{-1}\) and 365.966 cm\(^{-1}\) and for Ru\(_2\)FeGe are 205.147 cm\(^{-1}\), 215.651 cm\(^{-1}\), 221.954 cm\(^{-1}\), 232.458 cm\(^{-1}\) and 300.210 cm\(^{-1}\). In
TABLE II. Calculated partial magnetic moment of Co (M\(\mu\)Co), Fe (M\(\mu\)Fe) and Total Magnetic moment (M\(\mu\)) in \(\mu\)B in comparison with the reported data (M\(\mu\)exp) and Slater-Pauling rule (M\(\mu\)SP), Curie temperatures calculated from Eq.2 (T\(C\)) and Mean field approximation (T\(C\)MFA) in K, *denote other work (\(a\), \(b\), \(c\), \(d\), \(e\), \(f\), \(g\), \(h\))

\[
\begin{array}{|c|c|c|c|c|c|c|c|c|}
\hline
\text{Compd.} & \text{M\(\mu\)Co} & \text{M\(\mu\)Fe} & \text{M\(\mu\)SP} & \text{M\(\mu\)Co*} & \text{M\(\mu\)Fe*} & \text{M\(\mu\)exp} & \text{T\(C\)} & \text{T\(C\)MFA} \\
\hline
\text{CFA-GGA} & 1.236 & 2.757 & 4.99 & 1.2 & 2.8 & 5.08 & 5.0 & 1332.2 & 1000 \\
& & & & & & & & & \\
\text{CFA-GGA+U} & 1.290 & 2.952 & 5.33 & 1.64 & 2.5 & 5.14 & 4.0 & 937.05 & 1025.4 \\
& & & & & & & & & \\
\text{FCA-GGA} & 1.118 & 2.559 & 5.05 & 1.0 & 2.5 & 5.41 & 4.0 & 926.2 & 1332.2 \\
& & & & & & & & & \\
\text{FCA-GGA+U} & 0.888 & 2.759 & 5.33 & 1.6 & 2.8 & 5.08 & 4.0 & 987.73 & 1025.4 \\
\hline
\end{array}
\]

Our computed data of elastic constants strictly follows the above mentioned stability conditions(Eq.5). Therefore, both Co\(_2\)FeAl and Fe\(_2\)CoAl are Mechanically stable. The value of B/G=3.32 > 2.73 suggested that Co\(_2\)FeAl is more ductile as compared to Fe\(_2\)CoAl. Poisson’s ratio (\(\sigma\)) is an important parameter to describe the nature of atomic bonding in the crystal. The \(\sigma\) ∼ 0.1 refers to covalent bonding, moreover our calculated \(\sigma\)’s are 0.36 and 0.47 predict metallic bonding. The melting temperature of Fe\(_2\)CoAl is 1656.92±300 K higher than that of Co\(_2\)FeAl, 1390±300K. The hardness of a crystalline material is also a crucial factor in determining their practical applications and can be estimated from Young’s modulus (Y). Young’s modulus (Y) can also provide an information about the stiffness of a material, larger the Y values harder to deform. The results of direction dependences of Young modulus shows minima along the [100] axis (i.e., \(Y_1\)), [010] axis (i.e., \(Y_2\)), [001] axis (i.e., \(Y_3\)) and the maxima is located along [111] [see Fig.7(a,b)].
| Compounds    | C₁₁  | C₁₂  | C₄₄  | B   | G   | B/G  | Y    | σ    |
|-------------|------|------|------|-----|-----|-----|------|------|
| *Co₂FeAl    | 243.09 | 141.64 | 138.59 | 209.27 | 62.86 | 3.32 | 171.426 | 0.36 |
| *Fe₂CoAl    | 219.60 | 186.78 | 139.17 | 208.67 | 76.39 | 2.73 | 205.546 | 0.47 |
| Fe₂CrAl²    | 229.36 | 151.41 | 275.94 | 177.46 | 181.267 | 0.979 |
| CASTEP (GGA)³ | 289.75 | 156.75 | 153.07 | 201.08 | 106.617 | 1.886 |
| CASTEP (LDA)⁴ | 258.24 | 134.78 | 139.14 | 177.09 | 99.21 | 1.785 |
| Co₂CrAl²    | 355.82 | 314.69 | 417.86 | 328.40 | 258.99 | 1.268 |
| Fe₂ScAl²    | 280.14 | 51.03 | 120.03 | 127.40 | 117.854 | 1.081 |
| Co₂ScAl⁵    | 180.16 | 162.26 | 150.86 | 168.23 | 94.141 | 1.787 |
| Co₂FeAl⁶    | 250.25 | 171.38 | 148.10 | 197.67 | 87.50 | 2.259 | 113.17 |

TABLE III. Elastic constant (Cᵢⱼ), Bulk Modulus, Shear Modulus (G), Youngs’ modulus (Y) are in (GPa), B/G and Poisson’s ratio (σ) in comparison with the available reported data. Here, * denote our results, a⁷¹, b⁷², c⁷³.
VII. CONCLUSION

The electronic, magnetic, elastic and X-ray spectroscopic properties of Co$_2$FeAl and Fe$_2$CoAl have been computed from GGA and GGA+U functionals. Both L$_2$ and C$_1b$ structures are stabilized by calculating the minimum energy correspond to optimized lattice constants. The phonon dispersion relation as a function of frequency have been calculated to confirm their thermodynamical stability. The absence of imaginary phonon in the whole Brillouin zone of both L$_2$ and C$_1b$ structures is a concrete proof of dynamical stability. Both Co$_2$FeAl and Fe$_2$CoAl possess strongly correlated d-electrons which can be treated more efficiently by the implementation of onsite Hubbard Coulomb potential (U) as GGA+U functional. On careful investigation of electronic properties we have found the blende of conducting and semiconducting states, a finger print of typical half-metallicity in Co$_2$FeAl. Whereas Fe$_2$CoAl exhibit pure metallic behaviour with disperse Co-d and Fe d-states around the E$_F$. An integer value of total magnetic moment (5.0 $\mu_B$) is an additional testament of the half-metallicity in Co$_2$FeAl in accordance with the Slater-Pauling rule. However, for Fe$_2$CoAl the total magnetic moment deviate from the integer value defying the Slater-Pauling rule. We have found an enhanced band gap in Co$_2$FeAl with the application of GGA+U. Wide band gap half-metals with high value of $T_C$($\sim$1000 K) are critical factor for spintronic technology. The calculated values of $T_C$’s from Eq.2 are in close agreement with the experimental data where as the results from mean field approximation (MFA) are overestimated. The XAS and XMCD spectra are also calculated from LDA+U. Our result of XAS and XMCD spectra of Co$_2$FeAl are consistent with the available data. The L$_2$/L$_1$ ratio deviates from 2:1 branching ratio in Fe$_2$CoAl may be due to inaccurate choice of Coulomb potential (U). The elastic properties are highly crucial for the industrial application. The high value of $B/G > 2.0$, high $\sigma$ and high melting temperature are credentials for practical application in device fabrication at high temperature.

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