1. Introduction

The Heusler class of materials are well known for their plenty of applications ranging from spintronics to thermoelectric due to their wide range of material properties that can be engineered. These Heusler compounds seem to be the material of choice for many applications because of their tunable electronic structure properties. This helps in the design of materials with desirable properties from half-metallic ferromagnet \[1, 2\] over completely ferrimagnet \[3\] to non-magnetic semiconductors \[4, 5\]. In the present days, the search of new materials for spintronics applications was growing within the Heusler class of compounds which was started before 30 years \[1\]. These materials have passionate applications in spintronics \[2, 6, 7\], optoelectronics \[8\], as shape memory \[9\] alloys \[10, 11\]. Over the past few decades, new areas of applications emerged comprising the environmental technologies such as thermoelectric \[12, 13\] and solar cell applications \[8\]. Recently, a new trend in the material properties which belong to new quantum state of matter is observed \[14, 15\]. These materials are named as topological insulators and are having technological importance due to the conduction of electrons being extremely high because of its surface states and might attract application in high performance electronic systems. This could be one of the future research perspectives of Heusler compounds enabling them to be more productive.

Ternary intermetallic Heusler compounds can be represented with general formula \text{XYZ} (known as Half-Heusler)
or \( X_2YZ \), where \( X \) and \( Y \) elements generally belong to transition metals (having \( d \) states) and \( Z \) belongs to main group element. In 1903 Fritz Heusler [16, 17] discovered these class of materials. The important feature of these compounds is, the properties of the total system are completely different from the properties of the individual elements contained in this type of compounds. For example, if we consider the compound \( Cu_2MnAl \), which is reported as magnetic none of its constitutional elements possess magnetic order independently [16, 17]. Similarly, in another compound \( TiNiSn \), which is reported to have semiconducting nature all its constitutional elements possess metallic character [18]. The count on the number of these type of compounds is endless and can be prepared by mixing all the elements in the periodic table and leading to several applications and need to be explored.

By doping in Heusler compounds, the Fermi level can be adjusted and half metallicity can be increase as in the case of \( Co_2MnGe_{1-x}Ga_{x} \) [19]. The co-doping effect of \( Co^+\) on nearly half-metallic Heusler compound \( NiFeMnSn \) has been seen and shown that by doping it becomes perfectly half-metallic [20]. The more \( d \)-electrons doping effect has been seen in \( Ti_2CoAl \) by Chen et al [21], it was shown how \( V/Nb \) doping is more energetically favourable on different site of \( Ti \). Effect of Fe substitution by Co on off-stoichiometric \( Ni–Fe–Co–Mn–Sn \) Heusler alloy ribs has been seen and it was predicted that Ce substitution by Co creates change in the magnetic behaviour [22].

Considerable attention had paid in the quaternary Heusler compounds like \( CoFeMnAl, CoFeMnSi, CoFeMnGa, CoFeMnGe, CoFeScSb, CoFeTiSb, NiFeMnGa \) and \( NiCoMnGa \). There are two types of half-metallic materials: the complete half-metals with 100% spin polarization at the Fermi-level and the near half-metals where there is some small density of states at the Fermi level so that the spin polarization is less than 100% [25]. The compounds like \( CoFeMnSi, CoFeMnAs \) and \( CoFeTiSb \) [24] are belongs to the 100% spin polarization category. But \( CoFeMnSb \) have only 85% spin polarization [26] and \( CoFeScSb \) is reported to be nearly half metallic [23]. It is, therefore, worth to investigate the possibility of 100% spin polarization in \( CoFeMnSb \) by means of fractional alloying. The study of mechanical, structural, electronic, magnetic and thermoelectric properties of \( CoFeMnSb \) ternary Heusler alloy has already been done by spin polarized density functional and semiclassical Boltzmann transport theory [27]. It was found, \( CoFeMnSb \) is more thermodynamically stable in ferromagnetic phase [27].

Calculation of formation energy plays a key role in identifying the thermodynamic stability of a predicted or alloyed compound. The negative value of formation energy indicates that at zero temperature the compound is more stable than its constituent elements. By using the formation energy criteria Ma et al discovered 45 half-metals and 34 nearly half metals by identifying the negative formation energies [28]. Understanding the nature of bonding is another important task, which can be performed by analysing the crystal orbital Hamilton population (COHP) scheme [30] in which partitioning of the energies allows to extract chemical bindings between the atoms from the electronic structure calculations.

This can be done with LOBSTER package [31] which is, in general, used to extract chemical bonding from plane-wave based density functional theory.

In this article, we have theoretically investigated the alloying element effect of transition metal (TM) (TM = Sc, Ti, V, Cr, Ni, Cu, Zn) on \( CoFeMnSb \) ternary Heusler alloy by using density functional theory (DFT) and see how half metallicity of \( CoFeMnSb \) changes with the alloying element. Thermodynamic stability of these new alloys is a major part of our study. It was found Sc and Ti alloying is more effective and change nearly half-metallic nature of \( CoFeMnSb \) to completely half-metallic. The paper is organized as follows: section 2 presents computational details of the first-principles calculations. The results and discussions of the pristine \( CoFeMnSb \) ground state, electronic structure, formation energy calculations and electronic structure details of alloyed \( CoFeMnSb \) are presented in section 3. Finally, conclusions are presented in section 4.

2. Computational details

All the ground state and electronic structure calculations are performed by using Vienna \textit{Ab initio} Simulation Package (VASP) [32, 33]. Firstly, structural optimizations for both pristine and alloyed \( CoFeMnSb \) structures were performed to obtain the minimum energy structure using the Perdew–Burke–Ernzerhof (PBE) functional [34], which is specifically customized for solids, that has been shown to yield structural data in agreement with experiment. The PBE pseudopotential was used with an energy cut-off of 600 eV. The Brillouin zone has been sampled using an \( 8 \times 8 \times 8 \) \( \Gamma \)-centred grid. The criteria for energy convergence between the two successive self consistent loop is taken \( 10^{-6} \) eV/cell. We have used tetrahedron method with Blöchl correction [35], along with \( 8 \times 8 \times 8 \) K-point mesh for the density of states calculations. There is full relaxation of atomic structures and volume by using
the conjugate gradient algorithm. Forces are converged to 0.01 eV Å⁻¹. For the study of alloying in CoFeMnSb, a supercell of $2 \times 2 \times 2$ has been designed from the primitive cell which contains eight atoms of each kind. To see, the impact of on-site Coulomb interaction of localized d electrons on electronic structure, PBE+U calculation has been performed. The PBE+U method, proposed by Dudarev et al [36] (a rotationally invariant approach) is used in our calculation. In this approach, the PBE+U energy takes the form

$$E_{\text{PBE}+\text{U}} = E_{\text{PBE}} + \frac{U}{2} \sum_\sigma \left[ \text{Tr}(\rho^\sigma) - \text{Tr}(\rho^\sigma \rho^\sigma) \right].$$

(1)

Where $U$ and $J$ are the spherically averaged matrix elements of the screened Coulomb electron–electron interaction and $\rho^\sigma$ is the atomic orbital occupation matrix. In the next section, we have discussed the effects of TM alloying in CoFeMnSb on Co, Fe, Mn sites and how these alloying elements affect half-metallicity and magnetism.

### 3. Results and discussion

Present compound CoFeMnSb crystallizes in face centred cubic type with space group $F\bar{4}3m$ (216) and the unit cell occupied with the Wyckoff positions: Co (000), Fe (0.50.50.5), Mn (0.250.250.25) and Sb (0.750.750.75). We have created a $2 \times 2 \times 2$ supercell which is consisting of total 32 atoms, described in figure 1. We performed complete structural optimization for the supercell created in spin polarization case and the calculated equilibrium lattice constant is found to be 8.44 Å. The calculated total magnetic moment of the system is observed as 5.005 μB per primitive cell. The atom dependent magnetic moments are observed as 0.894 μB for Co, 1.071 μB for Fe, 3.077 μB for Mn and −0.037 μB for Sb. From this, it is observed that Mn, Fe and Co atoms are contributing positively to the total magnetic moment while Sb is providing a negative contribution. It is also observed that the primary contribution to the total magnetic moment arrives from the Mn and the secondary contribution is arriving from Fe and Co sites.

To know more about the electronic structure details, we have calculated total and atom projected electronic density of states and are described in figure 2. Multiple peaks are observed in the total density of states both in majority (up) and minority (down) spin cases. The peak around $-4.6$ eV in majority spin and $-4$ eV in minority spin is due to the hybridization of all elements. Particularly at $-4$ eV it is due to the Sb-p states. The peaks around $-3.0$ eV to $-2.5$ eV and $-1.4$ eV to $-1$ eV are mainly due to Mn atoms in the majority spin case. The states in the energy region from $-1.0$ eV to 0 eV in both majority and minority are highly dominated by Fe atom. For Mn atom, the split in the d states is more in comparison to Fe and Co, which causes for the high magnetic moment in Mn in compare to Fe and Co in the present system. From the overall plot, the system is found to nearly half metallic with a large density of states in majority spin case and very small value of density of states in minority spin case at Fermi level ($E_F$). So, it is quite informative to discuss about the system near the Fermi level. From the figure 2, at $E_F$, the decreasing trend in the density of states observed from the contribution of Fe, Mn, Co and Sb atoms respectively in majority spin case but in the minority spin case we have observed a small value of density of states which are arising mainly from Co and Fe atoms. As the present compound is almost having a half metallic nature it is worth to discuss about the spin polarization, $P$, in the present compound. The well known formula to calculate $P$ is $$P = \frac{\left[ N(E_F) \uparrow - N(E_F) \downarrow \right] / \left[ N(E_F) \uparrow + N(E_F) \downarrow \right]}{\times 100\%},$$ where $N(E_F) \uparrow$ is total density of states at $E_F$ in majority spin case and $N(E_F) \downarrow$ is total density of states at $E_F$ in minority spin case. The calculated value of $N(E_F) \uparrow$ is 13.69 states/eV and $N(E_F) \downarrow$ is 1.229 states/eV. From this, the estimated $P$ is 83.52% which is in good agreement with other studies.

![Figure 2](image-url)
(85%) [26]. As the present compound is found to nearly half metallic, it could be more useful if we can tune the Fermi level to get complete half metallic nature with 100% spin polarization. The best way to tune the Fermi level is fractional alloying with TM elements in the periodic table.

3.1 Proper selection of alloying element from the calculation of formation energies

In order to know the possibility to synthesize a compound, calculation of formation energy (\(\Delta E_f\)) is the best way [37]. The formation energy can be written as,

\[
\Delta E_f = E' - E - \sum n_i \mu_i,
\]

where \(E'\) is the total energy of the supercell containing the impurity atom, \(E\) represents the total energy of the perfect crystal using an equivalent supercell, integer \(n_i\) is the number of alloying element atoms, which has been subtracted (negative value) or added (positive value) to form the disorders and \(\mu_i\) represents the chemical potential of these species. The calculated value of \(\Delta E_f\) for the pristine CoFeMnSb is found to be \(-0.68\) eV f.u.\(^{-1}\) So, the alloyed compound should have the lower values of \(\Delta E_f\) in compare to pristine CoFeMnSb.

Selection of a proper alloying element is always a difficult task. It includes a lot of trails with different alloying elements along with different concentrations at different atomic sites. In the present case, we have selected several TM elements as alloying elements to alloy at Co, Fe and Mn sites. The selected TM elements are Sc, Ti, V, Cr, Ni, Cu and Zn. We have tested these alloying elements at Co, Fe and Mn sites with different alloying element concentrations, \(x = 0.125, 0.25, 0.375, 0.50, 0.75\) and \(1.00\) to check the site preference for a particular alloying element. For \(x = 0.75\) and \(1.00\), the calculated formation energy values are plotted in figure 3. From this, it is observed that Sc alloying element has lower formation energies in comparison to other elements with all alloying concentrations and all Co, Fe and Mn site preferences which confirm that Sc could be the best alloying element among the chosen elements. Along with Sc, Ti could be the second possible alloying element at Mn site with all alloying concentrations. These results are highlighted with a rectangular red coloured box for \(x\) concentrations at Mn site alloying figure 3. It is also observed that as the concentration of the alloying elements \(x\) increases from 0.125 to 0.375, the formation energy of CoFe(Mn\(_{1-x}\)TM\(_x\))Sb is approaching to the pristine CoFeMnSb formation energy value. At \(x = 0.500\) alloying concentration of Sc, the formation energy of CoFeMn\(_{0.50}\)TM\(_{0.50}\)Sb is lowering than the pristine CoFeMnSb indicating best choice of alloying concentration of Sc in the formation of alloy. As \(x\) concentration value increases further 0.75 and 1.00 both Sc and Ti alloyed CoFe(Mn\(_{1-x}\)TM\(_x\))Sb having lower \(\Delta E_f\) values in compare to pristine CoFeMnSb indicating Ti will be the
second possible element to synthesize CoFe(Mn$_{1-x}$TM$_x$)Sb alloy after Sc. To see effect of Coulomb interaction, PBE+U calculation has been performed (figure 2(a)) and it was found that half metallicity of CoFeMnSb is reducing (82.58%) after coming Coulomb interaction in the picture, earlier it was 83.52%. Therefore, Coulomb interaction is not affecting too much on half metallic nature of CoFeMnSb. The U value of Coulomb interaction is taken 2.33 eV for Co, 1.00 eV for Fe [38], 2.02 eV for Mn, 0.00 eV for Sb [39] and J value is considered equal to 0.

3.2. Alloyant effect on electronic structure and magnetic nature

To investigate the effect of alloying on the electronic structure of CoFeMnSb, we have calculated total electronic density of states for $x = 0.125$, 0.250, 0.375 and 0.500 concentrations alloyed with TM. In all the cases, majority spin states of CoFeMnSb in the presence various alloying elements has been stride over the Fermi level, describing typical metallic nature. On the other hand, the minority spin states, gradually decreases and becomes zero, describing half metallic nature of CoFeMnSb in presence various alloying elements along with alloying elements percentage. Even though we have observed half metallic nature with different alloying concentrations, their formation energies are not lower than the pristine CoFeMnSb. The alloys, which have half metallic nature but thermodynamically unstable is described in table 1. From the previous subsection, we have found only Sc and Ti are the two possible alloying elements, particularly at Mn site. Therefore, it is worth to discuss about only Sc and Ti alloying studies at Mn site. The calculated total density of states are plotted separately for Sc and Ti alloying elements only at Mn site with different alloying concentrations in figure 4, where we can observed complete half metallicity in CoFeMn$_{0.25}$Sb, CoFeMn$_{0.50}$Ti$_{0.25}$Sb, CoFeMn$_{0.625}$Ti$_{0.375}$Sb, CoFeMn$_{0.50}$Sb and CoFeTiSb. The calculated band structures are given in supplementary material figure S1 (available online at stackiop.org/JPhysCM/31/335702/mmedia) for the pristine CoFeMnSb, CoFeMn$_{0.25}$Sb, CoFeMn$_{0.50}$Ti$_{0.50}$Sb and CoFeTiSb to know the type of band gap in minority spin case. Calculated spin polarization values for Sc and Ti alloying element at Mn site are given in figure 5 along with different alloying concentrations. In Sc alloying at Mn site, the spin polarization value is found to increase with alloying concentration and observed a 100% spin polarization at $x = 0.75$. At the higher alloying concentrations of Sc greater than $x = 0.75$, spin polarization is found to decrease. From the literature, CoFeScSb is found to be nearly half-metallic [23] which is again confirmed from our calculations by complete replace of Mn with Sc. Here we can conclude one important point is that if we replace 0.25% of Sc with Mn in CoFeScSb we will get 100% spin polarization. In the case of Ti alloying at the same Mn site, 100% spin polarization is observed at $x = 0.25$ and above concentrations. From the literature, CoFeTiSb is found to have complete half-metallic [24] which is again confirmed from our calculations.

To know the effect of magnetic nature with alloying, we have calculated total and atom dependent magnetic moments for both Sc and Ti alloying elements with different concentrations and are tabulated in table 2. It is observed that total and atom dependent magnetic moments are found to be decreased with increasing alloying concentration in the case of Sc at Mn site. The same scenario is observed with total, Sb and alloying element magnetic moments with Ti at Mn site but Co, Fe and Mn moments are found to increase a little with increasing Ti alloying concentration at Mn site.

Change in the electronic structure with alloying can be understood through the electronic density of states which are plotted in figure 6 for Sc with 75% alloying, Ti with 50% and
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100% alloying along with the pristine CoFeMnSb states. In all cases, the total density of states in minority spin case is found to be shifted towards the lower energies which causes a gap at the Fermi level in minority spin. The states near $E_F$ in minority spin case mainly belongs to $d$ states of Co and Fe in the pristine CoFeMnSb. These states are found to be shifted towards the lower energies and cause a 100% spin polarization with alloying. It is also observed a reduction in the height of peaks in Mn $d$ states after alloying with Sc or Ti. After alloying, the splitting of Sc and Ti $d$ states is very less as compare to Mn in the pristine CoFeMnSb which causes a decreasing trend in the total magnetic moment with alloying compare to the pristine CoFeMnSb value.

To obtain the Curie temperature, we have used the SPR-KKR-method [29], by which we have calculated the interatomic exchange constants. The Curie temperatures were calculated within the mean field approximation. It was found CoFeMnSb has Curie temperature ($T_c$) 923.1 K, which decreases by including alloying concentration at Mn site (described in table 2). CoFeMnSb and CoFeScSb are not a perfect half metal, have spin polarization 83.52% and 92% respectively. But CoFeMn$_{0.25}$Sc$_{0.75}$Sb has complete half metallic nature and Curie temperature 324.5 K i.e. more than room temperature. Therefore, CoFeMn$_{0.25}$Sc$_{0.75}$Sb is a perfect Heusler compound for spintronics application. The Curie temperature of CoFeMn$_{0.75}$Ti$_{0.25}$Sb is found 682 K, also has a possibility in spintronics application. This shows that we can engineer half-metallic compounds by alloying CoFeMnSb with Ti.

The above discussions intimate the importance of Co and Fe $d$ states, which are highly affected with alloying and reason for half metallic nature after alloying. So, it is very important to understand the bonding nature in between Co and Fe, and how it is affected with alloying. For this, we have computed Co–Fe COHPs [30]. COHP is the density of states weighted by the corresponding Hamiltonian matrix element. COHPs indicate the strength as well as the nature of interaction with bonding or antibonding interactions. These interactions being indicated by positive or negative values of COHP. Co–Fe

Table 2. Magnetic moments and Curie temperature for different alloying concentrations of Sc and Ti at Mn site.

| Alloying elements | $x$ | $\mu_B$(Co) | $\mu_B$(alloying element) | $\mu_B$(Fe) | $\mu_B$(Mn) | $\mu_B$(Sb) | $\mu_B$(Total) | $T_c$(K) |
|------------------|----|--------------|--------------------------|-------------|-------------|-------------|---------------|---------|
| Sc               | 0.00 | 0.894 | 0.0 | 1.071 | 3.077 | −0.037 | 5.005 | 923.1 |
|                  | 0.125 | 0.869 | −0.194 | 1.018 | 3.054 | −0.031 | 4.504 | — |
|                  | 0.250 | 0.839 | −0.185 | 0.960 | 3.049 | −0.026 | 4.013 | — |
|                  | 0.375 | 0.815 | −0.168 | 0.889 | 3.048 | −0.020 | 3.526 | — |
|                  | 0.500 | 0.796 | −0.162 | 0.823 | 3.032 | −0.015 | 3.039 | — |
|                  | 0.750 | 0.719 | −0.153 | 0.768 | 2.792 | −0.006 | 2.064 | 324.5 |
|                  | 1.00 | 0.514 | −0.143 | 0.738 | 0.00 | −0.010 | 1.099 | 222.0 |
| Ti               | 0.00 | 0.894 | 0.0 | 1.071 | 3.077 | −0.037 | 5.005 | 923.1 |
|                  | 0.125 | 0.896 | −0.362 | 1.094 | 3.084 | −0.031 | 4.612 | — |
|                  | 0.250 | 0.898 | −0.330 | 1.110 | 3.114 | −0.025 | 4.236 | 682.0 |
|                  | 0.375 | 0.905 | −0.289 | 1.118 | 3.150 | −0.019 | 3.864 | — |
|                  | 0.500 | 0.908 | −0.246 | 1.137 | 3.166 | −0.012 | 3.493 | — |
|                  | 0.750 | 0.924 | −0.176 | 1.213 | 3.211 | −0.002 | 2.805 | — |
|                  | 1.00 | 1.017 | −0.203 | 1.204 | 0.00 | 0.009 | 2.027 | — |
COHPs are plotted in figure 7 for the pristine CoFeMnSb, CoFeMn0.25Sc0.75Sb, CoFeMn0.50Ti0.50Sb and CoFeTiSb. It is observed that bonding states in both spin cases at energies below around \(-1\) eV. From the energy range \(-1\) eV to \(0\) eV we have antibonding states in majority spin case for both pristine CoFeMnSb and new alloys. In the same energy range, the scenario is different in minority spin case, where we have observed bonding states in the pristine CoFeMnSb and Ti alloying but in Sc alloying, we have antibonding nature. At the \(E_F\), we have a small electronic density of states in minority spin case without alloying are belongs to Co and Fe. The inset of the figure indicates that these states are having bonding nature. This bonding nature still survived with Ti alloying but it changes to antibonding nature with Sc alloying.

4. Conclusions

We have investigated the TM element alloying effect on the electronic structure and magnetic properties of nearly half metallic CoFeMnSb by using first principles calculations.
within density functional theory. Calculations on the relative formation energy indicate Sc and Ti mono alloying is more favourable. The same calculations confirm the best site preference to alloy with Sc and Ti is at Mn-site. Therefore, the mono alloyed CoFe(Mn$_{1-x}$Sc$_x$)$_2$Sb and CoFe(Mn$_{1-x}$Ti$_x$)$_2$Sb alloys could be easily obtained. The calculated electronic structures reveals 100% spin polarization when alloying concentration, $x$, reaching to $x = 0.75$ with Sc and $x = 0.25, 0.375, 0.50, 0.75, 1.0$ with Ti at Mn site. CoFeMn$_{0.25}$Sc$_{0.75}$Sb and CoFeMn$_{0.75}$Ti$_{0.25}$Sb are perfectly half metallic with 100% spin polarization, have Curie temperature 324.5 K and 682 K, respectively. Therefore, both become good candidate in spintronics application. The density of states and COHP calculations confirms that both Co and Fe states are shifted towards to lower energy region and causes to open a gap at $E_F$ in the minority states.

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