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Electronic and Magnetic Properties of Half Metallic Heusler Alloy Co_2mnsi: A First-Principles Study

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Abstract : *Heusler alloys have been of great interest because of their application in the field of modern technological word. Electronic and magnetic properties of Co, Mn, Si and the Heusler alloy Co_2MnSi have been studied using Density functional theory based Tight Binding Linear Muffin Tin Orbital with Atomic Sphere Approximation (TB-LMTO-ASA) approach. From the calculation lattice parameter of optimized structure of Co, Mn, Si and Co2MnSi are found to be 2.52A0 , 3.49A0 , 5.50A0 , 5.53A0 respectively. Band structure calculations show that Co and Mn are metallic, Si as semi-conducting while the Heusler alloy Co_2MnSi as half-metallic in nature with band gap 0.29eV. The charge density plot indicates major bonds in Co_2MnSi are ionic in nature. Magnetic property has been studied using the density of states (DOS), indicating that Co and Co_2MnSi are magnetic with magnetic moment 2.85μ_B and 4.91μ_B respectively. The contribution of orbitals in band, DOS and magnetic moment are due to d-orbitals of Co and Mn and little from s and p-orbital of Si in Co_2MnSi.*

Key Words: TB-LMTO-ASA, Band structure, DOS, Half-Metallic, Heusler Alloy, Charge Density

1. INTRODUCTION

Heusler compounds in ferromagnetic state are highly relevant for spintronic applications because of their predicted half- metallic behavior, that is, 100% spin polarization at the Fermi energy[1]. Heusler alloys was named after a German mining engineer and chemist Friedrich Heusler in 1903[2]. It is also important because surface property of it is quite distinct from the corresponding bulk which is ultimately depend upon the electrical behavior of the bulk. Surface reconstruction has been an active area in the field of semi conductors[3]. The basic thing of the electronics devices is to inject the spin polarized electrical current in semiconductors[4]. Ferromagnetic material with full spin polarization at Fermi level will be the most applicable for the spin injecting[5] purpose which is mostly used in the field of the spintronics[6]. Half metals are those materials whose spin up channel has no gap in the Fermi level where as spin down channel has gap in the Fermi level, showing metallic character in the spin up region and non-metallic nature in spin down region in the Fermi level, which in combine gives the definition of half-metals. Present system shows the half-metallic nature. In half metallic ferromagnetism, majority of spin band is metallic and the minority of spin band is semiconducting. Co based Heusler shows more than 70% spin polarization, some of them shows 100% polarization, which makes the system applicable for the developing field of spintronics. It was first studied by de Groot et al.[7]. The main purpose of present study is to go more insight into the band structure and DOS and to find out the origin of magnetic moment. In our previous communication we have performed electronic and magnetic properties of binary and ternary alloys in their ordered [8, 9, 10] as well as disordered [11, 12, 13] structures including perovskite [14] indicating that TBLMTO approach, one of the effective model for the electronic structure problems. The other aim of present study to use this approach for the analysis of electronic and magnetic behavior of full- Hustler alloy.

The rest of the work is organized as follows: in section II we present the computational details used for the calculation. The results and discussion are presented in section III where as section IV provides the conclusions of the present study and finally references used in the present study are listed at the end of the paper after the acknowledgment.

2. COMPUTATIONAL DETAILS

All the systems considered are studied using Tight Binding Linear Muffin Tin Orbital with Atomic Sphere Approximation (TB-LMTO-ASA) approach. The results

are derived from self-consistence calculation based on the density function theory in local density approximation LDA[15,16,17,18]. Throughout the calculation, we use the exchange correlation potential [19]. According to the spirit of the TB-LMTO-ASA procedure only the energetically higher-lying valance state have been included in the self-consistence calculation of the effective crystal potential[20, 21, 22]. The calculations were treated to self-consistence with an accuracy in total energy less than 10^{-6} Rydberg.

3 RESULTS AND DISCUSSION

The calculation of lattice parameters of optimized crystal structures, electronic band structure, DOS and magnetic properties of Co, Mn, Si and alloy Co_2MnSi with charge density distributions are explained in this section as follows,

A. Lattice parameter of Co, Mn, Si and Co_2MnSi

We have optimized the structure of Co, Mn, Si and Co_2MnSi through energy minimization process using experimental data[23] as base. The value of lattice parameters for optimized structures are found to be $2.52A^0$, $3.49A^0$, $5.50A^0$, $5.53A^0$ for Co, Mn, Si and Co_2MnSi respectively . The energy vs lattice parameters curves are shown in Fig. (1) as,

The calculated lattice parameters are closely agree(within 1% deviations) with the experiments as well as previously calculated results [24, 25, 26]. Now these parameters are used for the further calculations.

B. Band structure , Density of states and magnetic properties

The following figure shows the band structure and density of states of Co, Mn, Si and alloy Co_2MnSi. From the band structure of Co, we observed 22 bands such that valance and conduction band overlapping with each other near the region of Fermi level, shows that it is metallic in nature as in fig(2)

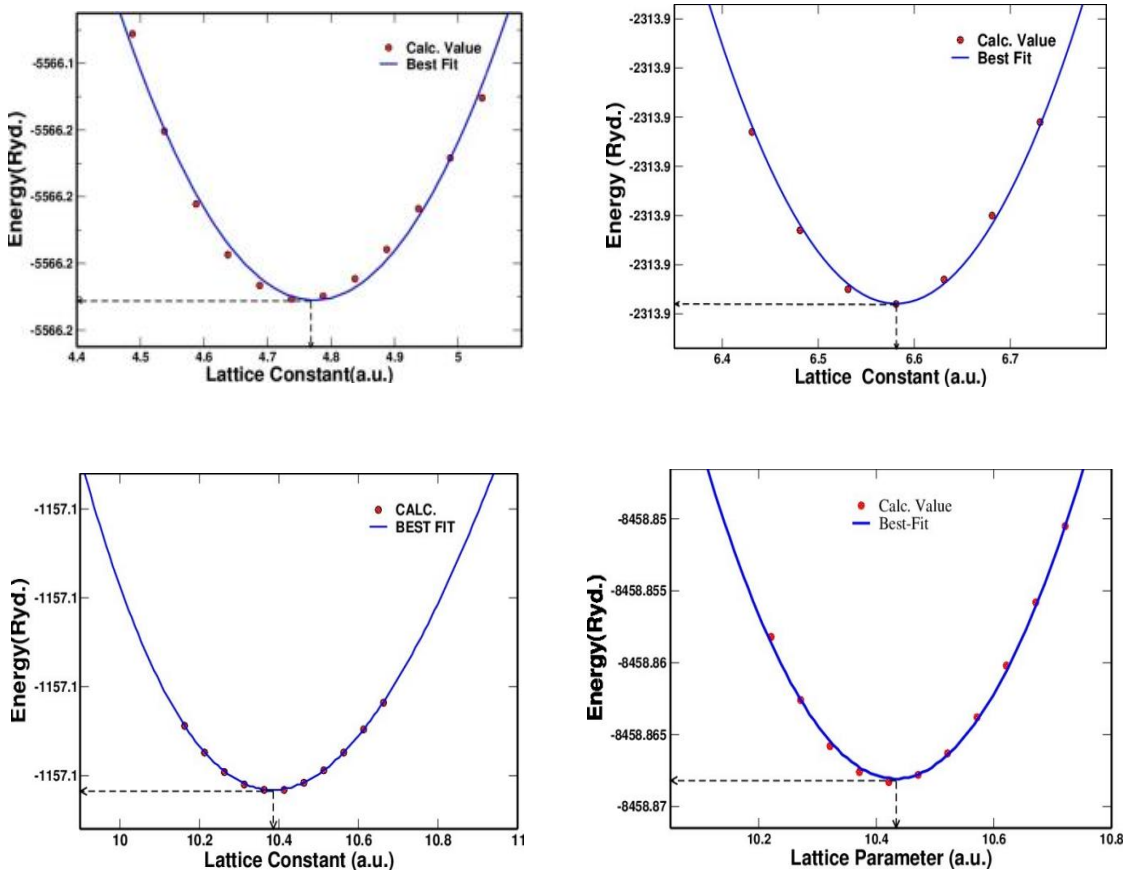

Fig.1.: (color online) Plot of energy vs lattice constant for (a) (up) Co and Mn, and (b) (down) Si and Co2MnSi

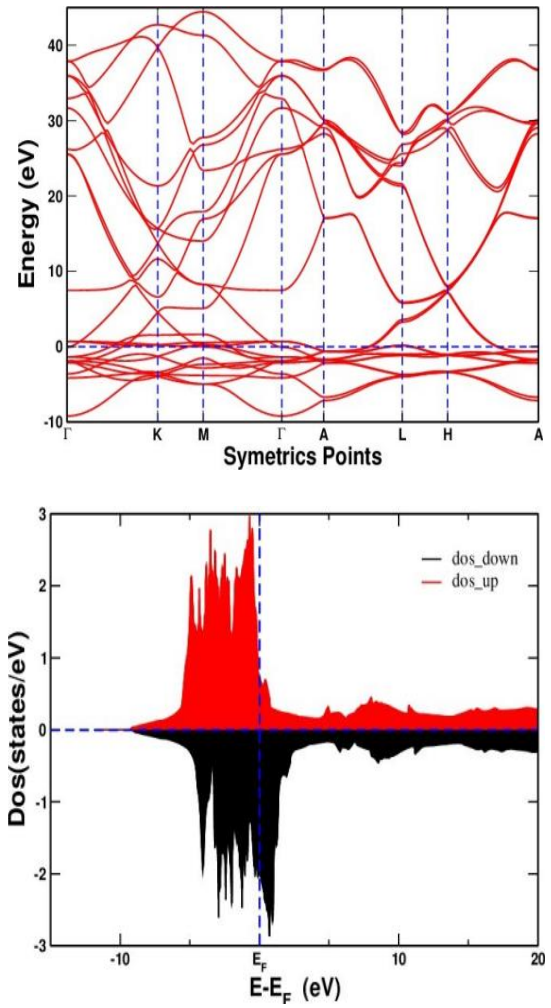

Fig. 2. (color online) Band structure and total DOS of Cobalt

To know the exact contributions of orbitals we used fat band calculations. From this it can be said that s and p orbital have minor contribution in the band structure. This may be due to filled s and p orbitals where as most of the regions around the Fermi levels are occupied by the electrons from d-orbitals (e_g and t_{2g}), indicating that d orbitals have the the major contribution. This contributions can easily be seen through density of states curve. The asymmetric nature of up and down spin DOS indicates that it is magnetic in nature. The magnetic moments of Cobalt is found to be $2.85\mu_B$ which is due to assymetric nature of d orbitals in up and down spin channels.

Manganese is the most complex of the elements from crystallographic point of view. It is the d-block element with the electronics configuration [Ar] $3d^5\,4s^2$. We have chosen fcc crystal of Mn. There are 9 bands altogether overlapping with each other above and beneath the Fermi level, shows it is metallic in nature. The main contribution in the band structure by orbitals can be observed via fat band. From the calculations we found the contribution of s and p-orbitals are totally dominated by contributions of d orbitals.

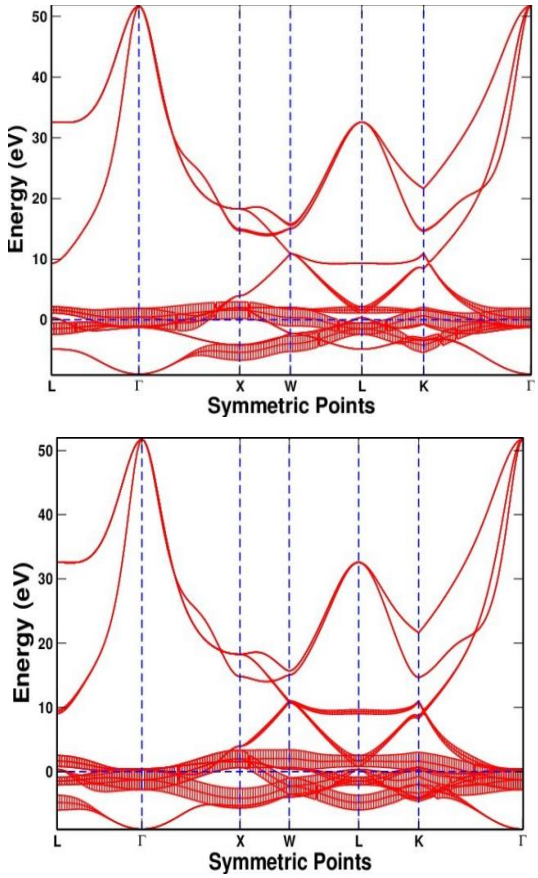

Fig. 3. (color online) Band structure of Magnese indicating e_g-orbital (left) and t_{2g}-orbital (right) .

The d-orbital is further splitted as eg and t2g-orbitals. Fat bands of these orbitals are shown in figure (3), the flat nature of band is in the Fermi level of both the orbitals, clearly seen that major contribution is from d-orbitals in the band structure of Mn. It also has symmetric types of DOS it is due to the effect that Mn is anti ferromagnetic in nature, such behviour is not deduce by LMTO-ASA. However, from total DOS as in figure(4), it is clear that contribution of d-band is maximum in the case of Mn.

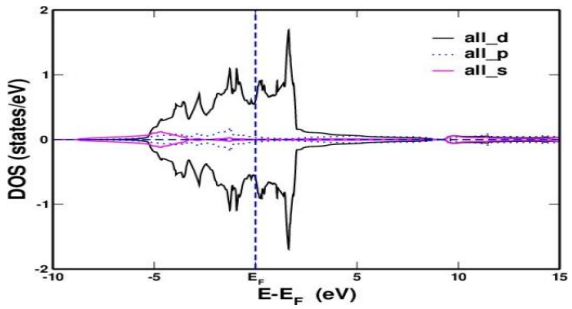

Fig. 4. (color online) Density of states of Mn showing contribution of d band dominates others

Similarly Silicon is p-block element with electronic configuration [Ne] $3s^2 3p^2$ with face centered cubic structure. The most widely used element in the field of electronic, and is widely used in field of research. It shows that there are 10 bands altogether, not overlapping with each other in the conduction and valance band indicating that it is non-metallic in nature, i.e. semi-conducting. The symmetric nature of up and down spin channel shows nonmagnetic nature of Si. The DOS plot equally resembles with the properties defined by band structure calculations.

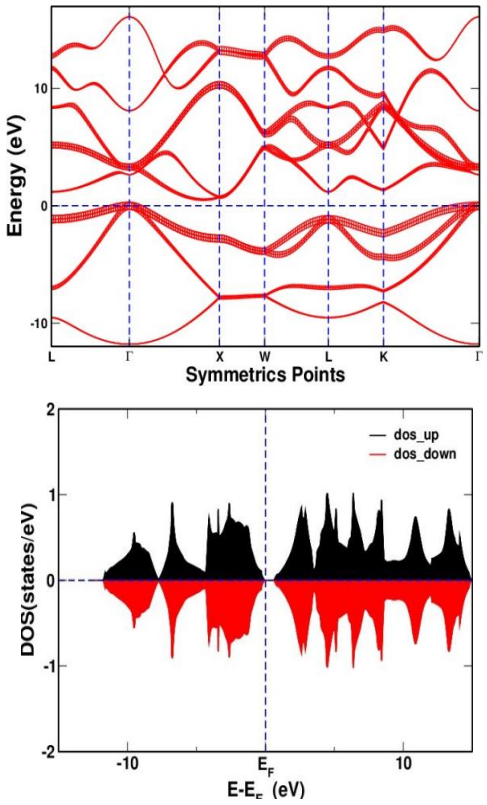

Fig. 5.(color online) Band structure and total DOS of Silicon

In case of Co_2MnSi, which is a Heusler alloy showing 100% spin polarization, widely used in the spintronics. The crystal structure is simple cubic with the position of Co (.25, .25, .25), Mn (.5, .5, .5) and Si as (0, 0, 0) [23]. We used optimized value of lattice constant, obtained from energy minimization ($5.53A^0$) for the calculation of band structure and density of states. The band structure calculation of Co_2MnSi alloy shows half metallic nature , the structure of up spin channel and down spin chanel is shown in the figure (6). From the figure it is observed that some of the bands are overlapping crossing near the fermi level for up-spin channel. However, some band gap is observed in down spin channel i. e. about 0.29eV. This feature indicates that Co_2MnSi posses half-metalic properties.

The DOS plot shows the same nature with gap at down spin channel with full of number of states per energy range indicating that it has 100% polarisation. From the fat band study, the main contribution for band structure and DOS comes from the d-orbitals of Co and Mn as shown in figure. The contributions of d orbitals clearly reflects same from the plot of DOS as well.

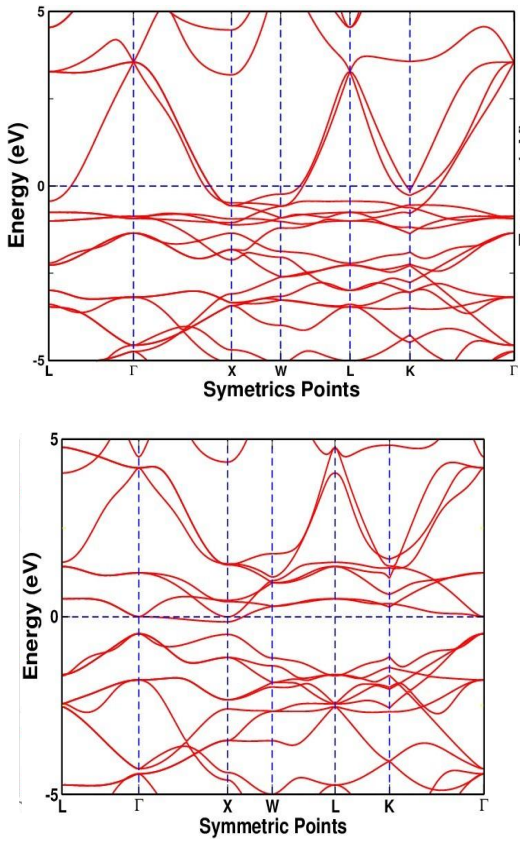

Fig.6.: (color online) Plot of up band (up) and down band (down) of Co_2MnSi.

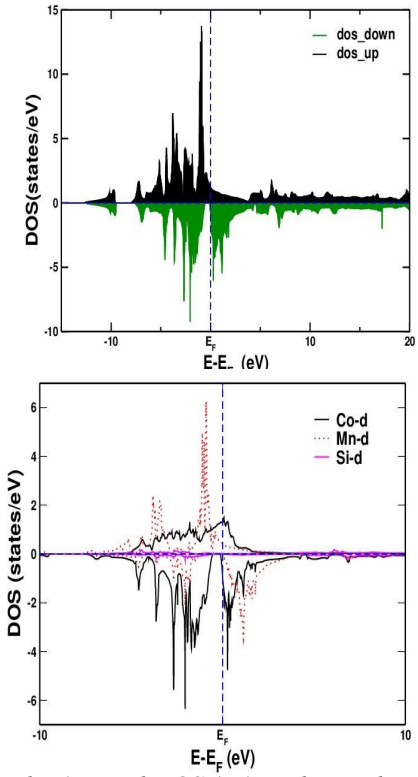

Fig.7.: (color online) Total DOS (up) and contributions of d due to Co, Mn and Si (down), on Co_2MnSi

The unsymmetric nature of DOS in the Fermi level gives magnetic moment of value $4.90\mu_B$ closely agrees with experiments[27, 28]. As in band the contribution of individual orbitals of Co, Mn, Si in Co_2MnSi can clearly observed via partial DOS plot.

The higher peak around the Fermi level is due to d-orbital of Co and Mn, indicates that the higher occupancy of electrons in d-orbital is of Co and Mn among all. From these results we can conclude that s and p-orbital of Si and d-orbitals of Mn and Co has major contribution in the band, DOS and Magnetic moment of Co_2MnSi.

We have studied the magnetic properties of our system by plotting the DOS and partial DOS. The magnetic moment of Co and Co_2MnSi was found to be $2.85\mu_B$ and $4.91\mu_B$ respectively, the magnetic moment of Mn and Si is found to be almost zero.

3.3 CHARGE DENSITY

The electrons accumulated around the atoms can be analyzed by charged density plot. If there is the large accumulation of charge between the two atoms then there is covalent bond, if the contour around the atoms is not symmetric then there is a complex type of interaction and become hard to analyze the bonding. The contour plot of the charged density of Co_2MnSi along the plane (100) and (110) is shown in the figure (7).

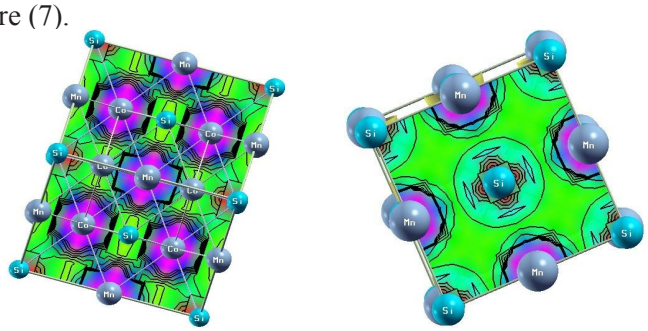

Fig 8:(color online) Plot of charge density of Co_2MnSi in lane 100(left) and lane110(right)

These plots shows that the contour around the atoms of Si as well as Co and Mn are distorted showing that bond between Mn-Si, Co-Si and Co-Mn are ionic within Co_2MnSi whee as Mn-Mn and Co-Co are metallic in nature.

4. CONCLUSIONS

In the present work, we performed the first principles calculation within local density approximation (LDA) in the basic hypothesis of density functional theory (DFT) using TB-LMTO-ASA approach to investigate the electronic and magnetic properties of Co_2MnSi . The optimized lattice parameter of Co, Mn, Si and Co_2MnSi are found to be $2.52A^0$, $3.49A^0$, $5.50A^0$, $5.53A^0$ respectively closely related to experimental results. Other calculations like band structure, DOS, magnetic property and charged density. From the calculation, the Co and Mn are found to be metallic and Si as semi-conducting and Co_2MnSi as half-metallic having band gap 0.29eV with Co and Co_2MnSi magnetic in nature. The magnetic moments of Co and Co_2MnSi found to be $2.85\mu_B$ and $4.90\mu_B$ respectively. The magnetic nature comes from the contributions of d orbitals of Co and Mn and p orbitals of Si. Orbitals' contribution was observed through fat band and partial DOS calculations.

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