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Ab-initio study of electronic properties of Co_2MnAl and Co_2MnSi

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Abstract

The electronic properties of Co_2MnAl and Co_2MnSi are investigated using the Korringa-Kohn-Rostoker method within the generalized gradient approximation (GGA). This is implemented in SPRKKR code. The full potential spin-polarized case is used to obtain the Density of States of the electron. Here we obtained that both the systems were found to be half-metallic ferromagnetic alloys. The Density of States (DOS) and bandstructure are studied in detail.

Keywords: *Multiple Scattering Theory, Density Functional Theory, Half-metallic Ferromagnets, Density of States and Bandstructures.*

1. Introduction

Heusler alloys are studied extensively due to their high spin polarization at the Fermi level. Many of the Heusler alloys exhibit a property known as half-metallicity. In these compounds, conduction electrons are 100% spin polarized at T = 0 due to a gap at the Fermi level at the minority channel and a finite density of states in the majority channel [1]. The spin polarization ratio P is computationally as given in equation 1 [2].The first material to be identified as half-metal was the half-Heusler alloy NiMnSb which was studied by de Groot et al. [3] in 1983 by using first-principle calculation based on density functional theory. Recently rapid development of magneto-electronics intensified the research on ferromagnetic materials that are suitable for spin injection into a semiconductor [4]. The full Heusler compounds X_2YZ crystallize in the cubic space group no. 225 with $Fm\bar{3}m$ symmetry; where X is a high-valence transition or noble metal atom, Y a low-valence transition metal atom and Z; an sp element [5]. Here we present a theoretical study on the full Heusler alloys Co_2MnAl and Co_2MnSi using the Korringa-Kohn-Rostoker method of Multiple Scattering Theory (MST).

2. Computational details

The calculations were performed using the Spin-Polarized Relativistic Korringa Kohn Rostoker (SPRKKR) package [6]. Our calculations are performed taking into account the full potential of the system. The lattice parameter were taken to be 5.7261 Å for Co_2MnAl [7] and 5.678 Å for Co_2MnSi [8] as previously calculated. The full-potential spin polarized scalar relativistic mode with an angular momentum cutoff of l_{max} = 4 within the generalized gradient approximation of Perdew, Burke, and Ernzerhof [9] was used for the calculation.

3. Results and Discussions

3.1 Density of States

In the sytems considered ie Co_2MnAl and Co_2MnSi we found from the total DOS that a gap is obtained at the minority spin channel at the Fermi level E_F on both the systems as shown in Fig 1(a) and Fig 1(b) respectively. Inspecting the the majority spin channel we saw that the density of electrons overlap at the Fermi level E_F. Thus the spin up region has a metallic character. From the plots we saw that the Al atom in Co_2MnAl and the Si atom in Co_2MnSi have small contributions when compared with the contributions by Co and Mn atoms for both systems and therefore can be neglected. In this study we found both the systems to be half-metallic ferromagnets. On closer inspection of the partial DOS, in both alloys, we found that the *3d* states of the Co atom has maximum contribution in the valence band and considerable contribution in the conduction band as shown in Figures 2(a) and 2(b) respectively. Studying the partial DOS for Mn we found that *3d* states of Mn has the maximum contribution in the conduction region as obtained from the DOS plots in Figures 3(a) and 3(b).

3.2 Bandstructures

Upon inspection of the bandstructure, we conclude the same results as what was obtained in the case for DOS. In this study we plot the dispersion relation along five symmetry directions namely X, Γ, L, W, K. For the case of Co_2MnAl we found that the gap is an indirect band gap between Γ and X along Δ direction of about 0.6 eV as shown in Figure 4. For Co_2MnSi we found that the gap in the spin down channel is an indirect band gap between Γ and X along Δ direction of about 0.8 eV as shown in

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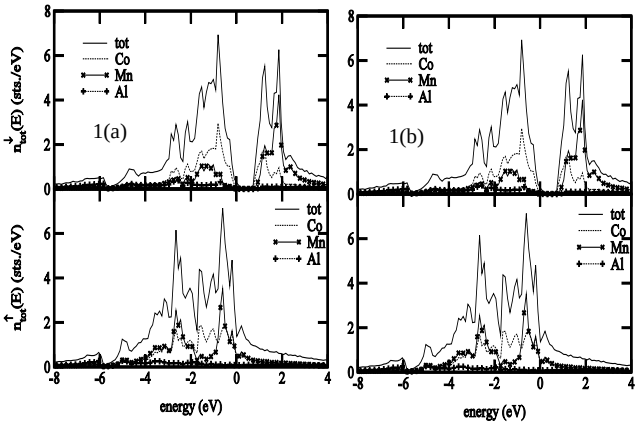
Figure 5. We can also see that in the spin up channel for both casesthe density of states of the electrons overlap.

4. Figures and Equations



4.1 Figures

Fig 1(a): Total DOS for Co_2MnAl

Fig 1(b): Total DOS for Co_2MnSi

Fig 2(a): Partial DOS of Co for Co_2MnAl

Fig 2(b): Partial DOS of Co for Co_2MnSi

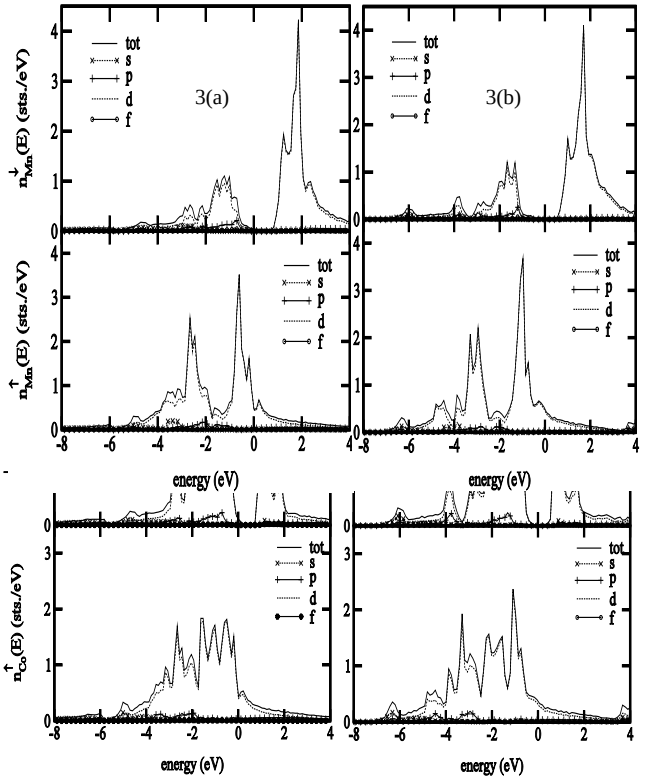


Fig 3(a): Partial DOS of Mn for Co_2MnAl

Fig 3(b): Partial DOS of Mn for Co_2MnSi

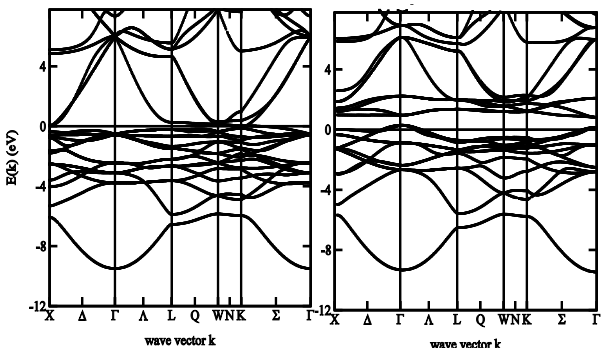


Figure 4: Bandstructure for spin up (left) and spin down (right) cases of Co_2MnAl.

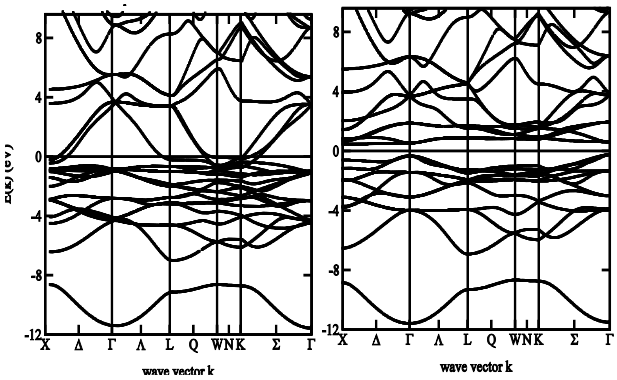


Figure 5: Bandstructure for spin up (left) and spin down (right) cases of Co_2MnSi.

4.2 Equations

$$P(\%) = \left|\frac{N_\uparrow(E_F) - N_\downarrow(E_F)}{N_\uparrow(E_F) + N_\downarrow(E_F)}\right| \times 100 \qquad (1)$$

where $N_\uparrow(E_F)$ and $N_\downarrow(E_F)$ denote the density of states (DOSs) at the Fermi energy E_F of the majority spin state and the minority spin state, respectively.

5. Conclusions

We can conclude from this study that the observed systems Co_2MnAl and Co_2MnSi are both half-metallic ferromagnets which have great potential to be used as spintronic devices. We found the Fermi level for Co_2MnAl at 9.878 eV and for Co_2MnSi at 10.799 eV. On inspection of the electronic properties we found that the spin polarization is higher in the case of Co_2MnSi when compared to Co_2MnAl. The band gap were found to be 0.6

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eV for Co2MnAl which is in close agreement with the results obtained by Rai *et al.* [7] and 0.8 eV for Co2MnSi which also come close to the results obtained by Rai *et al.* [10] and Kandpal *et al.* [11].

Acknowledgments

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