Physical properties of isostructural Ga_2MnCo Heusler alloy : A first principles calculations and mean field approximation

E.M. Jalal[1,$], H. Kerrai[2]

$ Corresponding author (Email address): elmostafa.jalal@usms.ma

[1] LS2ME Laboratory, Polydisciplinary faculty of Khouribga, Sultan Moulay Slimane University, Beni Mellal, Morocco

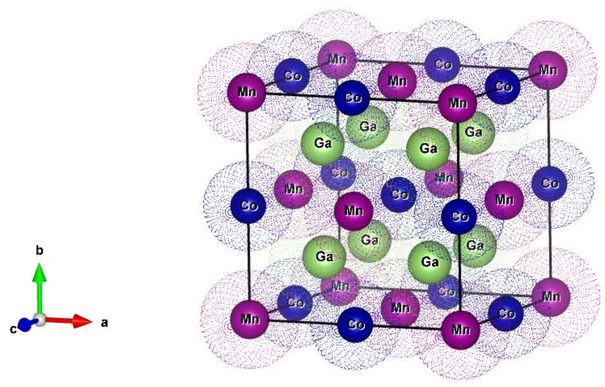
[2] Physics of Materials and Systems Modeling Laboratory (PMSML), Unit Associated at CNRST-URAC: 08, Faculty of Sciences, Moulay Ismail University, Meknes, Morocco

Abstract

First-principles calculations and the mean field approximation were employed to study the structural, electronic and magnetic properties of the full Heusler Ga_2MnCo alloy. The structural analysis unveiled the stability of Ga_2MnCo in a ferromagnetic state. Regarding electronic and magnetic attributes, the calculations demonstrated that Ga_2MnCo exhibits a metallic nature, featuring distinct spin-up and spin-down states. Additionally, the magnetic properties and phase diagrams were computed, and the results were thoroughly examined. The system presents a rich critical behavior, including both first and second-order phase transitions.

Material description

The full Heusler Ga_2CoMn is composed of the magnetic cations Co^{3+} (with spin σ = 3/2) and Mn^{2+} (with spin S = 5/2) and the non magnetic ions Ga^{2+}



The structure of the full Heusler Ga_2CoMn alloy.

Computational method:

The ab-initio calculations are performed using FP-LAPW (fullpotential linearized augmented plane wave), based on the density functional theory (DFT+U). The exchange correlation potential selected is the generalized gradient approximation parameterized by Perdew–Burke–Ernzerhof (PBE-GGA) [1]. Due to the existence of the transition metal (Co and Mn) in the studied compound, the correction by U_{eff} Hubbard parameter is also added. This effective orbital potential U_{eff} is defined as the difference between the Coulomb and the exchange part of the orbital potential (U_{eff} = $U-J$, where U = 3.9 eV for Mn and 3.4 eV for Co also J = 1 (eV)) [2]. U_{eff} parameter value of the iron element is set as 5.8 (eV). The plane wave cutoff is optimized to be $R_{mt} \times K_{max}$ = 7, the K_{max} is the magnitude of the largest wave vector and R_{mt} is the smallest muffintin sphere radius, which are taken as 1.62, 1.88, and 2.22 atomic units (a.u) for Ga, Mn and Co elements, respectively. The self consistent convergence is achieved after 10^{-5} (Ry), we have also use 1000 K-points in the irreducible Brillouin zone.

Model and mean field approximation

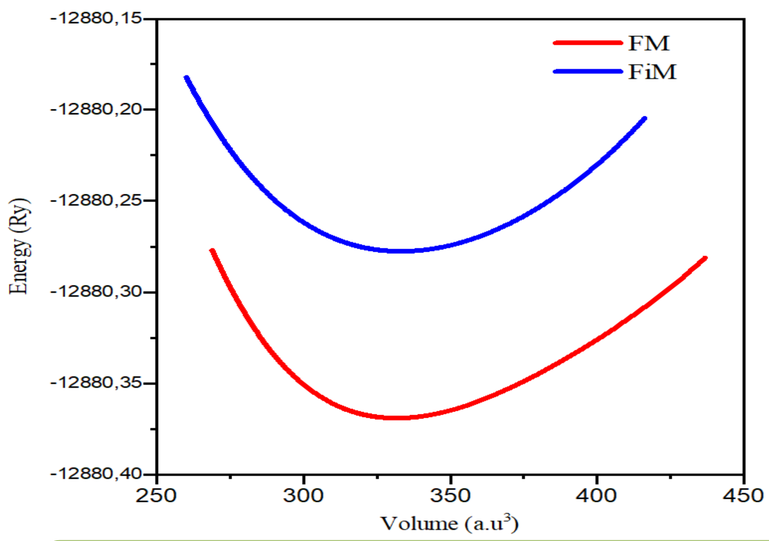
The mean field approximation offers a straightforward theoretical approach that gives a broad overview of system behavior and can also align qualitatively with experimental findings.

$$H = -J_1\sum_{\langle ij\rangle}\sigma_i S_j - J_2\sum_{\langle ij\rangle}S_i S_j - J_3\sum_{\langle ij\rangle}\sigma_i\sigma_j - \Delta_1\sum_{i=1}^{N}\sigma_i^2 - \Delta_2\sum_{j=1}^{N}S_j^2 - h\left(\sum_{i=1}^{N}\sigma_i + \sum_{i=1}^{N}S_i\right)$$

The system model described by the Hamiltonian will be analyzed using the mean field approximation, which is formulated as a variational method based on the Gibbs-Bogoliubov inequality [3]

Results

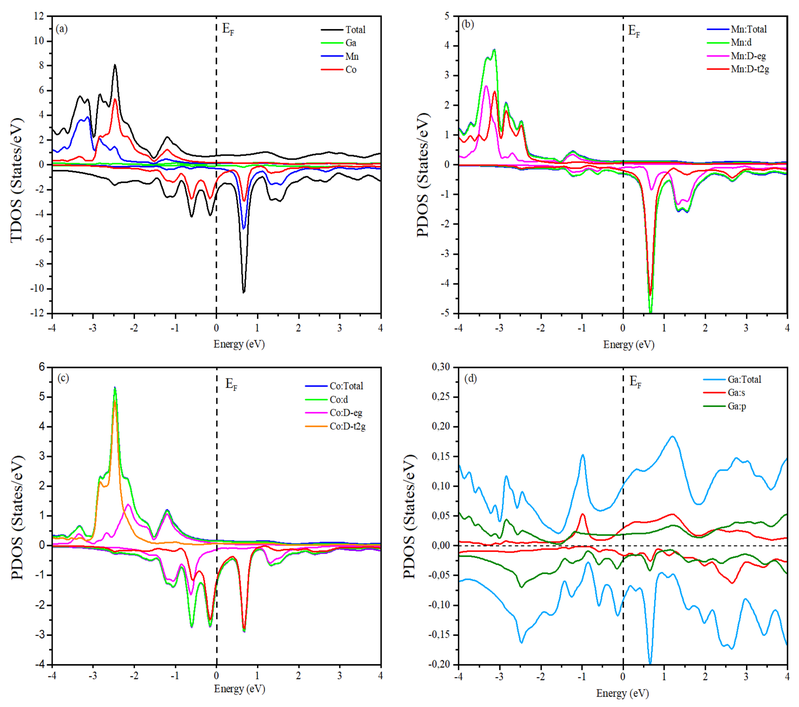
1- Structural properties



Energy versus volume curve of the full Heusler Ga_2MnCo alloy

Table 1: Calculated magnetic moment of the full Heusler Ga2MnCo alloy using GGA, GGA+U and GGA+SOC approximations.

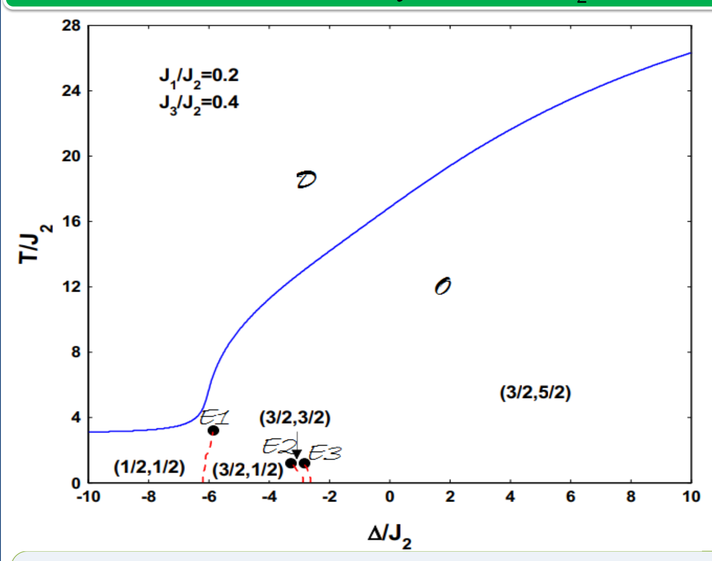
	GGA	GGA+U	GGA+SOC
μ_{Ga}	-0.02	-0.02	-0.02
μ_{Mn}	3.36	4.00	3.37
μ_{Co}	0.98	2.02	1.00
μ_{Total}	4.45	6.11	4.47



Total and partial density of states of the full Heusler Ga_2MnCo alloy with GGA+U

The band structures of the full Heusler Ga2MnCo alloy with GGA+U

2- Effect of the crystal field Δ/J_2



Phase diagram in the (Δ/J_2, T/J_2) plane for fixed values of J_1/J_2 = 0.2 and J_3/J_2 = 0.4

Conclusion

In summary, by using the first-principles calculations and the mean field approximation, we investigated the structural, electronic, and magnetic properties of the full Heusler Ga_2MnCo alloy. we have found that, the full Heusler Ga_2MnCo alloy presents a metallic behavior given to the electronic density of state and the band structure analysis. It is also found that the total magnetic moment are attributed to the Cobalt and Manganese cations with the spins 3/2 and 5/2, respectively. In addition, Concerning the mean field approximation, we have studied the magnetic properties of our Heusler alloy. It is shown that the system presents a first and second order transition when $\Delta_1 = \Delta_2 = \Delta$

References

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