Half metallic behavior of Fe_2MnAl and Fe_2MnSi Heusler compounds

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Abstract

Heusler compounds have been very interesting material because of its inherent properties, which make them valuable for spin-dependent materials. In this paper, structural optimization along with electronic properties of Fe_2MnAl and Fe_2MnSi full Heusler compounds have been calculated by using the FP-LAPW method. Both materials found to be half-metallic by showing metallic character within a spin-up and semiconducting character in a spin-down state. Energy and correlation potential have been anticipated by using GGA approximation which gave an idea about the stable ground state. Both materials were stable in the Fm-3m (225) space group.

Keywords: Heusler compounds, Electronic structure, DFT calculation.

1. Introduction

In 1903 Friedrich Heusler was the one who first introduced the concept of Heusler compounds and investigated Cu_2MnAl to be a ferromagnetic material however none of its constituents was magnetic [1, 2]. Since then Heusler compounds have been the hot contenders for the researchers who found their helpful applications in spintronics, magnetoresistive materials, thermoelectric materials, spin value generator and memory devices etc [3-6]. Heusler compounds are generally considered as half-Heusler compounds and full-heusler compounds. Former has an XYZ (1:1:1) composition and latter has X_2YZ (2:1:1) composition [7]. Here X, Y is representing transitions metals whereas Z is from main group [8]. $C1_b$ and $L2_1$ are the structure type for half and full-Heusler compounds respectively. $L2_1$ structure can be stable in two space groups known as Fm-3m (225) which crystallizes in Cu_2MnAl and F-43m (216) which crystallizes in Hg_2CuTi [9].

Heusler compounds contain Co and Mn as their constituents are enormous materials for spintronics devices [10]. Some Fe-Based Heusler compounds (Fe_2MnSi, Fe_2CrSi, Fe_2FeSi, Fe_2NiSi, and Fe_2CoSi) have been studied experimentally as well as theoretically [11-13]. The research for electronic structure of thin films among a number of (111) multi-layers of X_2FeSi (X = Mn, Fe, Co) and Fe_2YSi (Y = Mn, Si) full-Heusler compounds ware carried out by Mori et al. [14]. M. Belkhouane et al. investigated Fe_2MnAl and Fe_2MnSi and found them to be half-metallic [15]. The thought of half-metallicity was initialy presented by de Groot et al. in 1983 [16], which demonstrates a metallic or semiconducting character in either of spin and this special property fascinated interest in spintronics materials [17, 18].

The motivation of the current work is to investigate the electronic structure of Fe_2MnAl in addition to Fe_2MnSi with the help of GGA approximation. The paper is organized in three sections named as computational details, results and discussion and conclusions in a row.

2. Computational Details

The structural optimization of compounds along with the electronic investigations were done by using full-potential linearized augmented plane wave method (FP-LAPW) [19] which depends upon density functional theory (DFT) [20]. It is implemented in WIEN2k code [21]. A generalized gradient approximation (GGA) [22] has examined the minimum energy by considering Cu_2MnAl and Hg_2CuTi structures. To control the energy convergence, the product of least muffin-tin radius and the reciprocal lattice vector was assigned to be 7. The upper limit value of angular momentum was cited as 10 (L_{max} = 10). The energy and charge convergence has been taken into account by considering the common energy and charge difference amid two successive iterations within 0.0001 Ry and 0.001e/a.u.^{3} respectively. 1000 k points are engaged in the integration of Brillouin Zone within the tetrahedral method [23].

3. Results and discussion

3.1 Structural Properties

The minimum energy for Fe_2MnAl and Fe_2MnSi full Heusler compounds have been computed by considering two types of crystal structures in which cubic Heusler compounds generally exist. [24]. First is type is Cu_2MnAl, with Fm-3m (225) SG which label 8c (0.25, 0.25, 0.25), and 4b (0, 0, 0) atomic positions to Fe and Mn respectively, whereas 4a (0.5, 0.5, 0.5) atomic position to Al in Fe_2MnAl and to Si in Fe_2MnSi. While other is Hg_2CuTi with F-43m (216) space group in which Fe atoms have two different positions 4a (0, 0, 0) and 4c (0.25, 0.25, 0.25) while Mn occupy (0.5, 0.5, 0.5) and (0.75, 0.75, 0.75) position occupied by Al or Si in Fe_2MnAl and Fe_2MnSi respectively. To obtain the stable structure for Fe_2MnZ (Z = Al, Si) total energy have been plotted against the reduced volume.

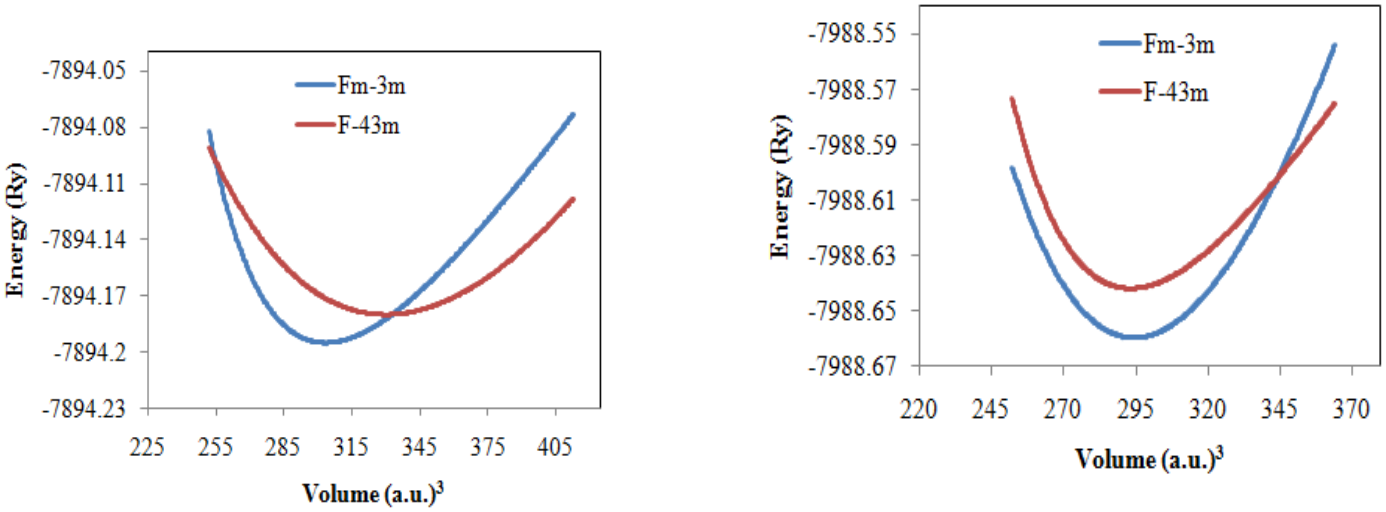


Fig.1: Energy versus volume curve for Fe_2MnAl and Fe_2MnSi within GGA.

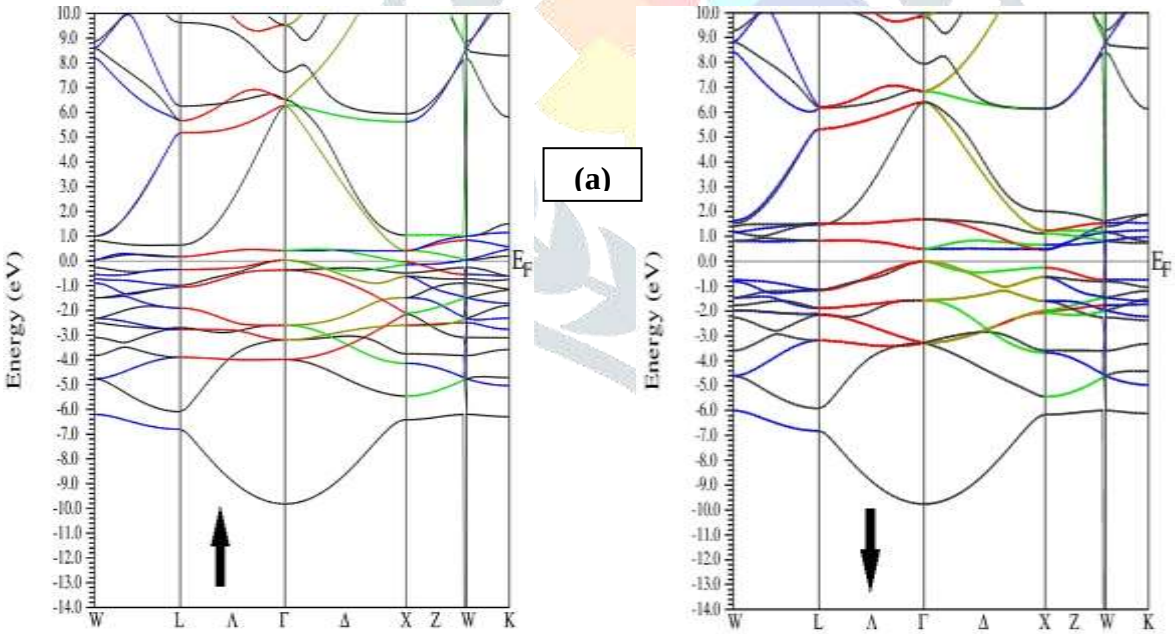
The E-V curve in Fig. 1 depicts the Cu_2MnAl as a more stable phase in contrast to Hg_2CuTi for both the compounds seeing that it got the minimum energy. Fitting of total energies to the Murnaghan's equation of state [25] specified the equilibrium structure parameters and are specified in Table 1, compared with the existing theoretical and experimental result.

Table 1: The Calculated values for lattice constant (a_0), Volume (V), Bulk modulus (B_0) and Energy (E_0) at equilibrium.

Compound	Space Group	a_0 (Å)	V (a.u.^{3})	B (GPa)	E_0 (Ry)
Fe_2MnAl	Fm-3m	5.645	303.5344	205.2280	-7894.195306
	F-43m	5.805	330.1525	109.5636	-7894.180252
Fe_2MnSi	Fm-3m	5.589	294.6519	245.4900	-7988.659637
	F-43m	5.581	293.4339	210.8287	-7988.641849

3.2 Electronic Properties

To obtain the Electronic properties in density function theory spin dependent band structure and density of states have been plotted by using the optimized lattice parameter given in the Table 1. The band structure for both the compounds in Fm-3m (225) and F-43m (216) space group are represented in Fig. 2, 3.



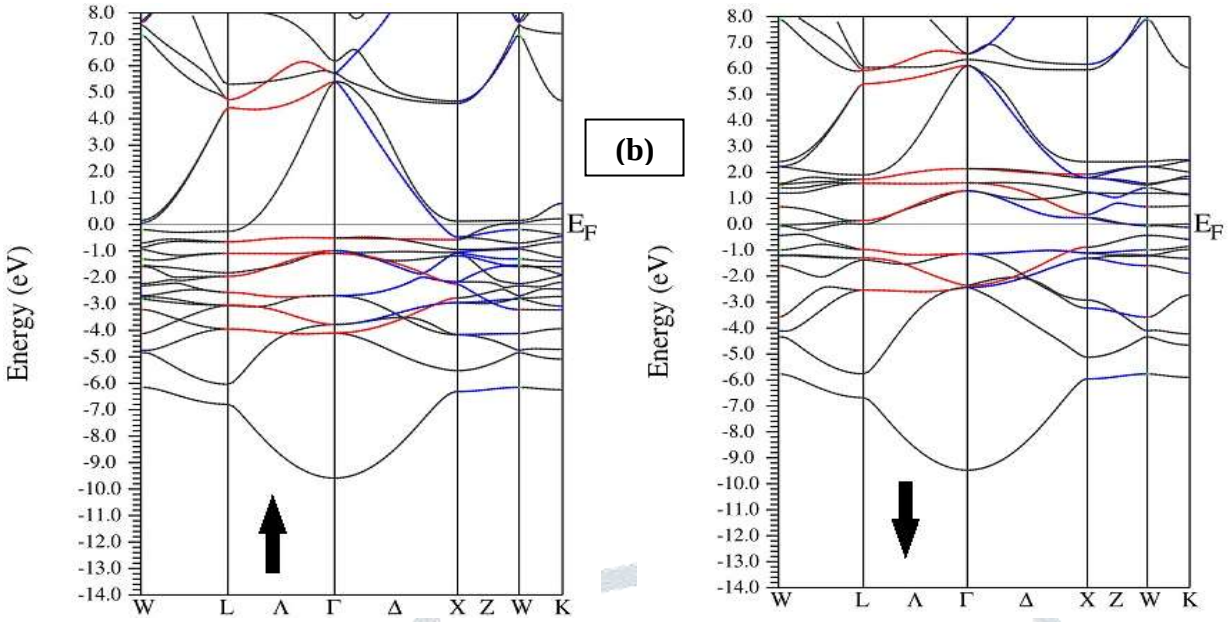
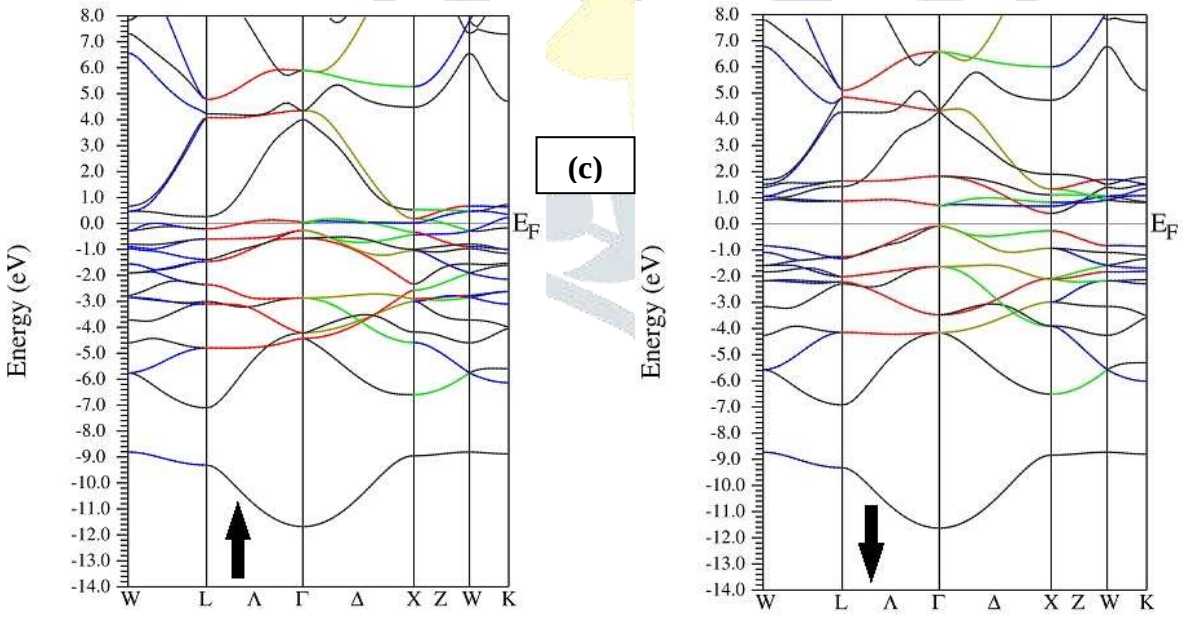


Fig. 2: The Band structure for Fe_2MnAl in (a) Fm-3m (b) F-43m

These figures are clearly representing the half-metallic behavior in Fm-3m space group and metallic behavior in F-43m space group for both the compounds. In spin-up electronic bands are crossing the Fermi level which has set at 0 eV, whereas in spin-down bands have gap of 0.48 eV in Fe_2MnAl and 0.494 eV in Fe_2MnSi for Cu_2MnAl structure. In Hg_2CuTi structure, it is found that bands are crossing the Fermi level and consequently representing the metallic nature for both the compounds.



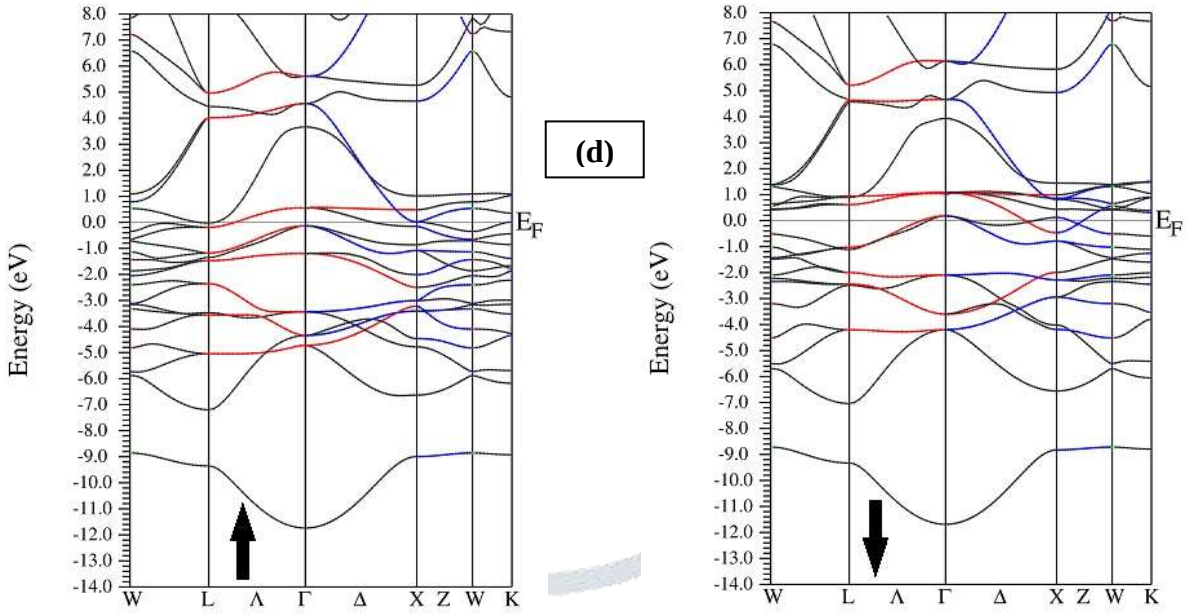


Fig. 3: Band structure of Fe_2MnSi in (c) Fm-3m and (d) F-43m.

The band structure results are also verified by the density of states (DOS) result as can be seen in Fig. 4, 5. It is also understandable from Fig. 6 that the contribution to the DOS at fermi level is mainly because of Fe-d and Mn-d which make these compounds metallic in spin-up. In spin-down case Mn-d move inside the conduction band and on the other hand Fe-d shift towards the valence band due to which compounds show semiconducting behavior in the same.

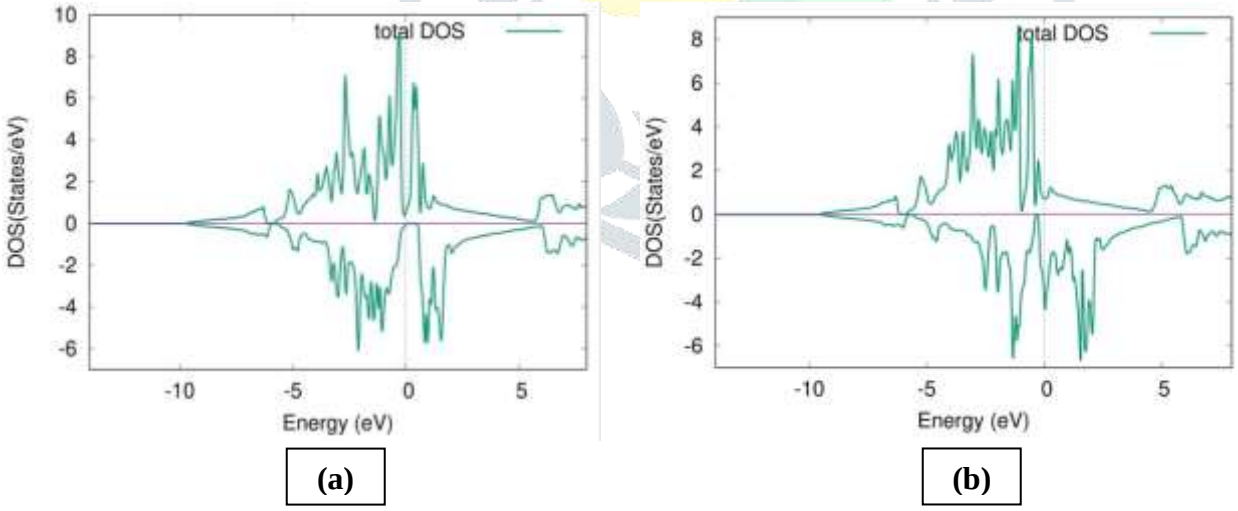


Fig. 4: Spin dependent total density of states for Fe_2MnAl (a) Fm-3m (b) F-43m

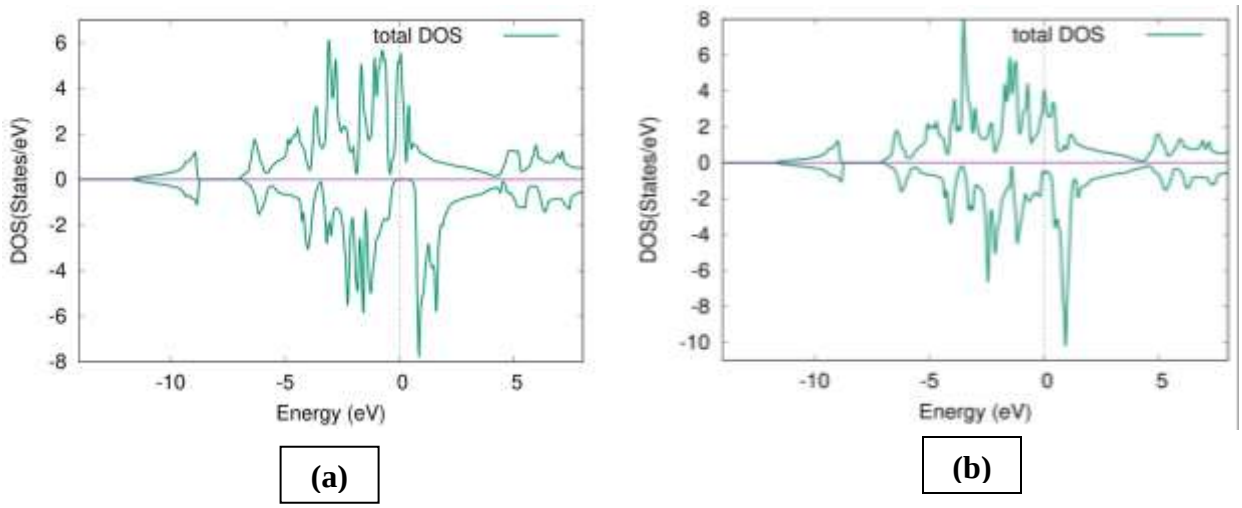


Fig. 5: Spin dependent total density of states for Fe_2MnSi (a) Fm-3m (b) F-43m

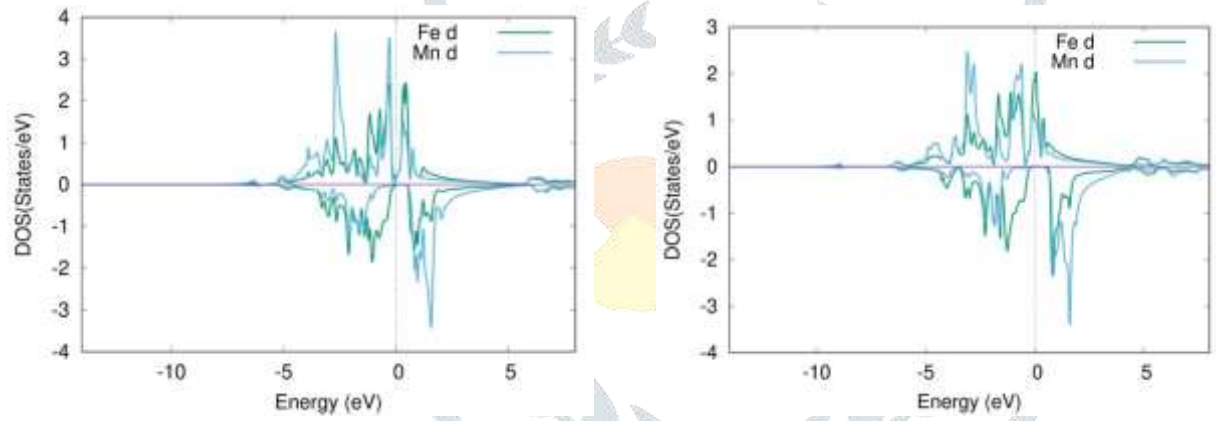


Fig. 6: Spin dependent partial density of states (a) Fe_2MnAl (b) Fe_2MnSi

4. Conclusion

Two Heusler compounds Fe_2MnAl and Fe_2MnSi have been studied within GGA under WIEN2k code. Their stable structures were given by the structural optimization. The results showed that at ambient conditions both materials are stable in Cu_2MnAl structure as compare to second structure type. Electronic properties from band structure and density of states were calculated. From where, it is concluded that both materials have half-metallic character in Cu_2MnAl structure and metallic within Hg_2CuTi type structure.

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