ISSN : 0974 - 7486 Volume 9 Issue 2

Trade Science Inc.

Materials Science

An Indian Journal

Full Paper

MSAIJ, 9(2), 2013 [67-72]

A first principle study of Co_2MnGe a Heusler compound

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Received: 14th June, 2012 ; Accepted: 5th October, 2012

ABSTRACT

We performed the structure optimization followed by the calculation of electronic structure and magnetic properties on Co_2MnGe. The structure optimization was based on generalized gradient approximation (GGA) exchange correlation and linearized augmented plane wave (LAPW) method. The calculation of electronic structure was based on full potential linear augmented plane wave (FP-LAPW) method. We have studied the electronic structure and magnetic properties. The calculated magnetic moment is 5.004 μ_B which is an integral value. The calculated density of states (DOS) and band structures shows the half-metallicity of Co_2MnGe.

KEYWORDS

GGA;
Half-metallicity;
DOS;
Band structure.

INTRODUCTION

NiMnSb a semi-Heusler compound was the first predicted half-metallic ferromagnetism by using first-principle calculation based on density functional theory[1]. After that, half- metallicity attracted much attention[2], because of its prospective applications in spintronics[3]. Recently rapid development of magneto-electronics intensified the research on ferromagnetic materials that are suitable for spin injection into a semiconductor[4]. One of the promising classes of materials is the half-metallic ferrimagnets, i.e., compounds for which only one spin channel presents a gap at the Fermi level, while the other has a metallic character, leading to 100% carrier spin polarization at E_F[5, 6]. Ishida et. al.[7] have also proposed that the full- Heusler alloy compounds of the type Co_2MnZ, where Z stands for Si and Ge, are half- metals. Heusler alloys have been particularly interesting systems because they exhibit much higher ferromagnetic Curie temperature than other half-metallic materials[8]. Among the other properties useful for the applications are the crystal structure and lattice matching compatible with zinc-blende semiconductors used industrially[9, 10]. Jiang et. al.[11] examined the magnetic structure of Mn_2VAl by x-ray diffraction and magnetization measurements. Rai et al.[12, 13] investigated the ground state study of Co_2MnAl and Co_2CrSi using LDA+U and LSDA method respectively and reported the half-metallicity. Rai and Thapa have also investigated the Electronic Structure and Magnetic Properties of X_2YZ (X = Co, Y = Mn, Z = Ge, Sn) type Heusler Compounds by using a first Principle Study and reported HMFs[14]. Rai et al. (2012) also studied the electronic and magnetic properties of Co_2CrAl and Co_2CrGa using both LSDA and LSDA+U and reported the increase in band gap, hybridization of *d-d* orbitals as well as *d-p* orbitals when treated with LSDA+U[15]. Recently, a detailed theo-

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retical study of the magnetism of Mn_2VAl was reported by Weht and Pickett by using GGA[16] for the exchange– correlation potential. The Fermi level was found to lie in the minority spin band.

MOTIVATION

Half-metallic ferromagnetic materials, like Mn_2VZ or Co_2YZ compounds (where Z is the sp elements), are much more desirable in magneto-electronic applications. This is mostly due to the fact that the small value of the total magnetic moment in these systems provides additional advantages. For example, they are less affected by external magnetic fields. In the present paper, we systematically study the electronic and magnetic structure of Co based full Heusler alloys Co_2MnGe to search for new halfmetallic ferromagnetic candidate. Among the systems studied Co_2MnGe are predicted to be nearly half-metallic at theoretical equilibrium lattice constants. In half-metals, the creation of a fully spin-polarized current should be possible that should maximize the efficiency of magnetoelectronic devices[6]. Materials with high spin polarization can be used for tunnel magnetoresistance (TMR) and giant magnetoresistance (GMR)[17]. The Co-based Heusler alloys Co_2YZ (Y: transition metal, Z: *sp* atom) are the most prospective candidates for the application in spintronics. This is due to a high Curie temperature and the simple fabricat ion process such as dc magnetron sputtering in Co_2YZ[18].

CRYSTAL STRUCTURE AND COMPUTATIONAL METHODS

Co (red) atoms are at the origin and (1/2, 1/2, 1/2), Mn (yellow) at (1/4, 1/4, 1/4) and Ge (blue) atoms at (3/4, 3/4, 3/4). The cubic *L21* structure consists of four inter-penetrating *fcc* sub-lattices, two of which are equally occupied by Co. The two Co-site *fcc* sub-lattices combine to form a simple cubic sub-lattice as shown in Figure 1.

COMPUTATIONAL METHODS

We performed the structural optimization using parameterization of GGA and linearized augmented plane wave (LAPW) method. The calculation of electronic structure and magnetic properties was performed by using full potential linear augmented plane wave (FPLAPW) method accomplished by using the WIEN2K code[19]. The exchange–correlation potential is chosen in the local spin density approximation (LSDA)[20]. The accuracy is up to 10^{-4} Ry. The self-consistent potentials were calculated on a 20 × 20 × 20 k-mesh in the Brillouin zone, which corresponds to 256 *k* points in the irreducible Brillouin zone. The sets of valence orbitals in the calculations were selected as *3s, 3p, 4s, 4p, 3d* Co atoms, *3s, 3p, 4s, 4p, 3d* for Mn atoms, *3d,4s, 4p* for Ge atoms. All lower states were treated as core states.

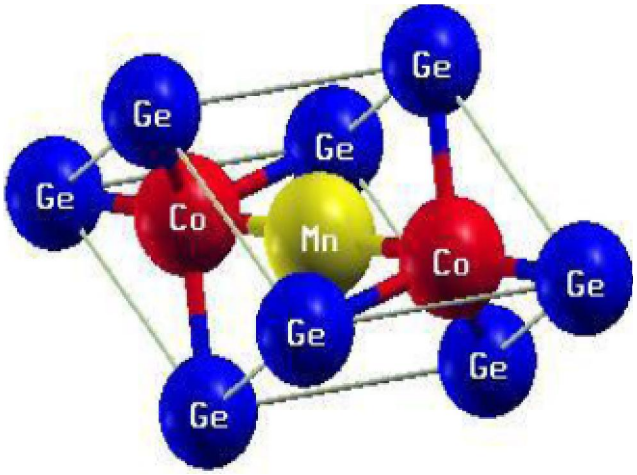

Figure 1 : Unit cell structure of Co_2MnGe Heusler alloy

RESULTS AND DISCUSSIONS

The optimized lattice constant, isothermal bulk moduli, its pressure derivative are calculated by fitting the total energy to the Murnaghan's equation of state[21]. The variation of equilibrium lattice constant and energy

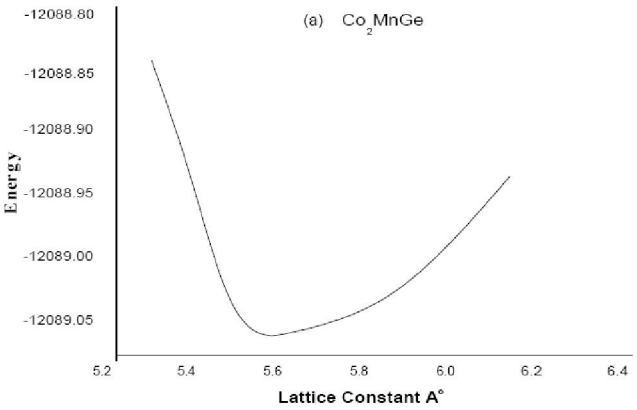

Figure 2 : Plot of energy versus lattice constant: Co_2MnGe

are summerized in Figure 2.

The total and partial DOS plots of Co_2MnGe are shown in Figures (3, 4). From the DOS plots of Co_2MnGe shown in Figure 4 peaks are mostly due to *d* state electrons of Co atoms in the semi-core and the valence region below E_F for both spin channels Figure 4 (a-d). In spin up channel, the DOS intersects E_F showing the metallic nature. In spin up region it is shown in Figures 3(c) and Figure 4 that Mn-*d* electrons mainly contribute in the valence region with sharp peaks at -2.3 eV and -2.7 eV. In spin down channel, peaks are due to *d* states of Co atoms in the valence as well as in the conduction regions. In the conduction region the peaks are observed at 1.0 eV and 2.0 eV, mainly due to *d-eg* and *d-t2g* states of Co and Mn atoms respectively in spin down region shown in Figures 4 (b-d). The *d* electrons of Co atoms are found to be strongly hybridized with Mn-*d* electrons[22]. The partial magnetic moments of Co, Mn and Ge atoms are $0.975\mu_B$, $3.097\mu_B$ and $-0.044\mu_B$ respectively. The effective magnetic moment is $5.004\mu_B$ which is approximately an integer value 5.00 μ_B[23].

TABLE 1 : The calculated lattice constant is compared with the previous results

Compound	Lattice constant a_oÅ		Bulk Modulus (GPa)	Equilibrium Energy (Ry)
	Previous	Our calculation		
Co_2MnGe	5.749[22]	5.678	409.3	-12089.018
	5.737[23]			
	5.743[24]			

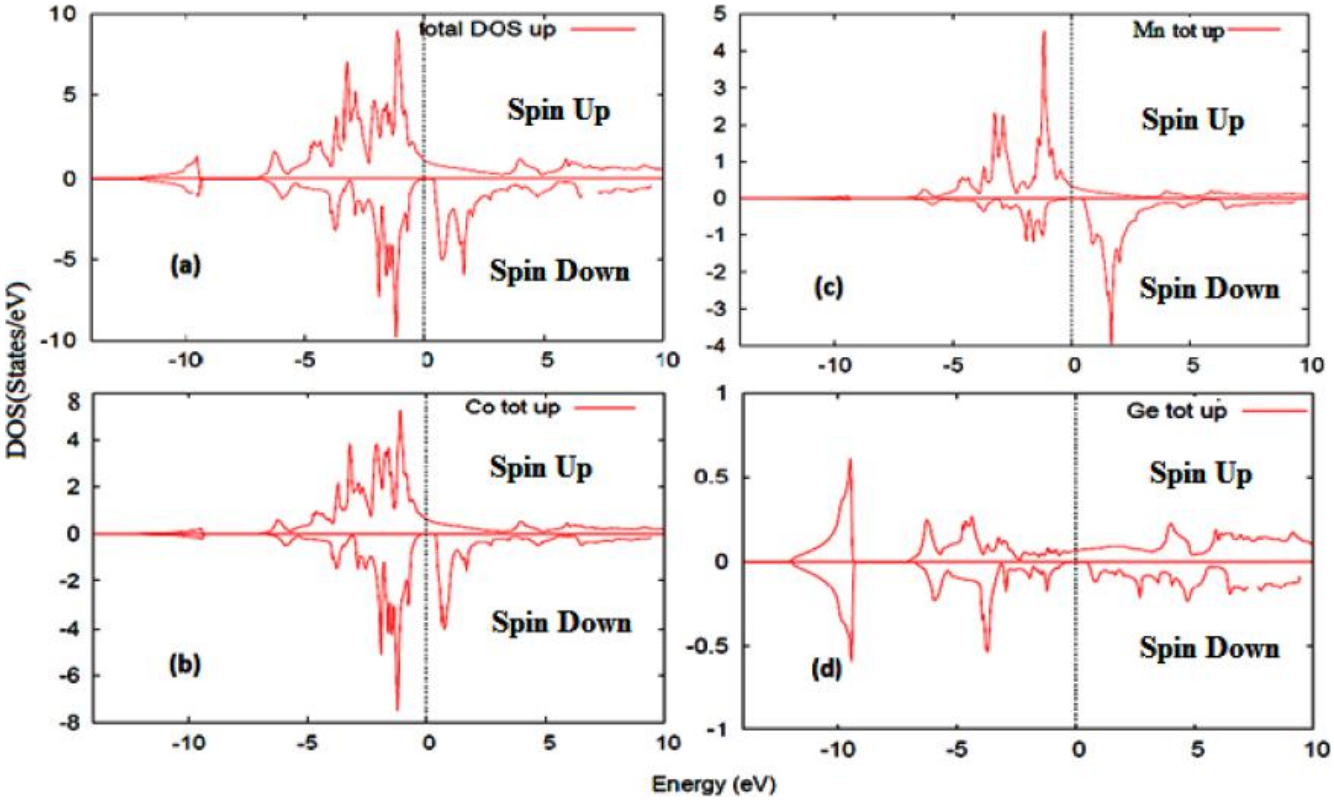

Figure 3 : (a) Total DOS plots of Co_2MnGe; (b) partial DOS plots of Co; (c) partial DOS plots of Mn; (d) partial DOS plots of Ge

Band structures

Figure 5 (a, b) shows the band structure plots of Co_2MnGe in both spin channels. In the valence region of the spin up and down channels, more number of bands were seen which are due to the 3*d* states of Mn atoms. Spin-down channel comprises of thick energy bands in the conduction region above E_F due to *3d* electrons of Mn atoms. The width of energy gap (Eg) is the difference in energies of the highest occupied band at symmetry point Γ in the valence region and the lowest unoccupied band in the conduction region at symmetry point X which is an indirect band gap. With the help of DOS, it is clear that the energy region lower than -3 eV consists mainly of *s* and *p* electrons (not shown) of the Ge atoms in the valence region and the energy region between -3 eV and 2 eV consists mainly of the *d*-electrons of Co and Mn atoms. From Figure 5 (b) it is seen

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that E_F lies almost at the middle of the gap between the valence and the conduction region in spin down channel. The origin of minority gap in Co_2MnGe is explained by Kandpal et. al.[22] as well as by Galanakis and Mavropoulos[25]. Based on the analysis of band structures and DOS calculations it is seen that the 3*d* orbitals of Co atoms from two different sub-lattices, Co1 (0, 0, 0) and Co2 (1/2, 1/2, 1/2) couple and form bonding hybrids. In other words, the gap originates from the strong hybridization between the *d* states of the higher

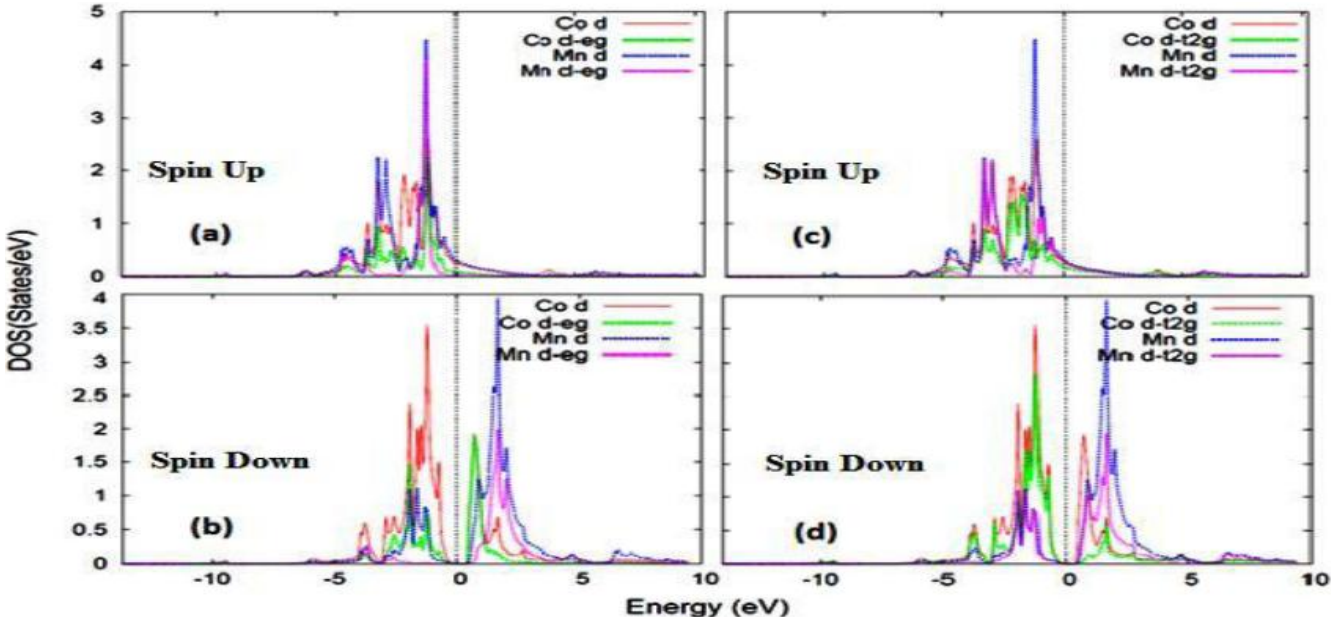

Figure 4 : DOS plots of Co_2MnGe, (a) Co (d, deg) and Mn (d, deg) states in spin-up; (b) Co (d, deg) and Mn (d, deg) states in spin-down; (c) Co (d, dt2g) and Mn (d, dt2g) states in spin-up; (d) Co (d, dt2g) and Mn (d, dt2g) states in spin-down

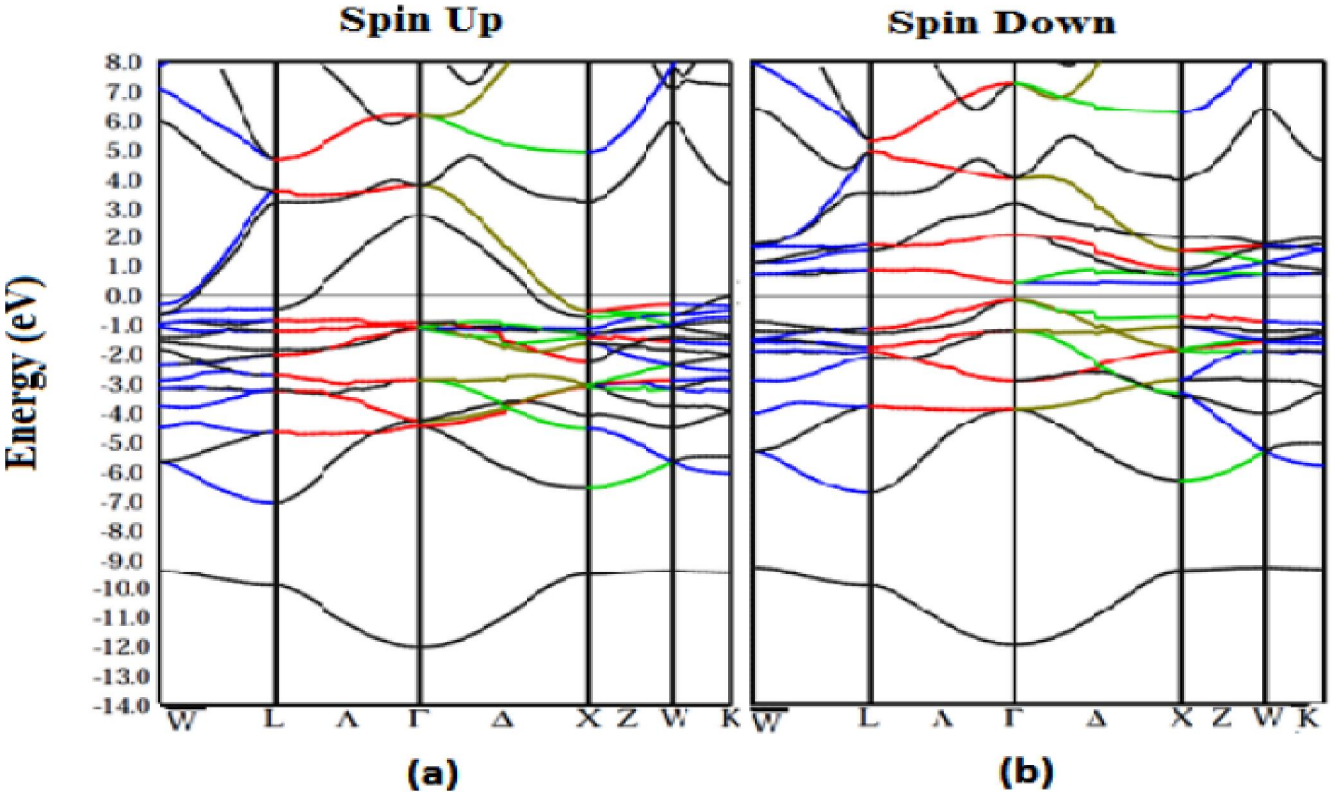

Figure 5 : (a) Energy bands of Co_2MnGe; (b) Energy bands of Co_2MnGe for spin down

valent and the lower valent transition metal atoms. As a result the interaction of Mn with the Z-*p* states splits the Mn-*3d* states into a low lying triplet of t_{2g} states and a higher lying doublet of eg states. The splitting is partly due to the different electrostatic repulsion, which is strongest for the eg states which is directly point at the Z atoms. In the majority band the Mn-*3d* states are shifted to lower energies and form a common *3d* band with X (Co) *3d* states, while in the minority band the Mn-*3d* states are shifted to higher energies and are unoccupied, so that a band gat at E_F is formed, separating the occupied *d* bonding states from the unoccupied *d* antibonding states. Thus X_2YZ is a half-metal with gap at E_F in minority band and a metallic DOS at the Fermi level in majority band. This explains half metallicity in Co_2MnGe. Less number of bands were found in the conduction region of the spin-up channel indicating the absence of DOS contributions. For Co_2MnGe an indirect energy gap obtained between symmetry point Γ and X is 0.60 eV which almost equals 0.581 eV reported by Kandpal et. al.[22].

TABLE 2: The calculated magnetic moment is compared with the previous results

Compound	Magnetic Moment μ_B		Energy gap Eg (eV)	
	Previous	Our calculation	Previous	Our calculation
Co2MnGe	5.00[24]	5.004	0.581[22]	0.600
	5.00[22]			

CONCLUSIONS

We have studied the possibility of appearance of half-metallicity in the case of the full Heusler compounds Co_2MnGe where Ge is a sp atom belonging to the IVB column of the periodic table. We found that in Co_2MnGe the ferromagnetic is stable at the equilibrium lattice constant. Although all compounds are not half-metallic at their equilibrium lattice constant. Thus these compounds follow the Slater–Pauling behaviour and the 'rule of 24'[25]. The lighter the transition elements and the smaller the number of valence electrons, the wider is the gaps and the more stable is the half-metallicity. We have calculated the DOS, magnetic moments and band structures of Co_2MnGe using FP-LAPW method using LSDA+U approximation. The results were in support of the HMF nature for Co_2MnGe. The existence of energy gap in the DOS for spin down region is an indication of being a potential HMF. This is also evident from the energy band Figure 5b. The calculated magnetic moment for Co_2MnGe is 5.004 μ_B which is almost an integral value. The observed results are in qualitative agreement with the integral value, supporting the HMF nature of Co_2MnGe.

ACKNOWLEDGMENTS

DPR acknowledges DST Inspire research fellowship and RKT a research grant from DAE (BRNS), Mumbai.

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