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DFT based study of structural and magnetic properties of full-Heusler compounds

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Abstract

Recent developments in the field of magneto-electronics and spintronics have motivated the research on ferromagnetic materials such as Heusler compounds. Full-Heusler compounds of type X_2YZ (X= Co, Y= Mn, Z= Si/Ge) are interesting as they exhibit higher Curie temperature than other half-metallic materials. Small value of total magnetic moment for such systems gives them additional advantage. In the present paper, we have used pseudo potential plane wave method based on density functional theory (DFT) and studied various properties of Co_2MnSi Heusler compound. Density of states (DOS) and band structure calculations show half-metallicity for such alloy. The magnetic moment comes out to be 5.09 Bohr magneton/cell. The observed results are in qualitative agreement with other theoretical and experimental predictions.

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*Keywords:*density functional theory; huesler alloys; electronic properties ; magnetic properties

Introduction

Heusler compounds have been a subject of intensive study since the discovery by F. Heusler [1]. Ferromagnetic thin films of these compounds are very relevant for spintronic application [2]. Various theoretical calculations [3, 4, 5, 6,7] have been done on their electronic, mechanical, elastic and other properties. Recent experimental observation [8] of half-metallicity in Co_2MnSi by ultraviolet-photoemission spectroscopy has further motivated research on these

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compounds. It has been observed that 100% spin polarization take place in Co_2MnSi at Fermi-energy [8]. But there is lack of study on magnetic properties of these compounds. In the present work, we use pseudo potential plane wave method based on density functional theory (DFT) to study various properties of Co_2MnSi and Co_2MnGe type Heusler compounds. Density of states (DOS) and band structure calculations show half-metallicity for such alloys. The calculated magnetic moment is about 5.09 Bohr magneton/cell. The observed results are in qualitative agreement with other theoretical and experimental predictions.

Theoretical and computational approach

Co_2MnSi is face centered cubic (FCC) structure with primitive translation vectors **a**= a(0,1/2,1/2), **b**= a(1/2,0,1/2) and **c**= a(0,1/2,1/2) where a is lattice parameter. The structure symmetry of Co_2MnSi is O_h^5, the corresponding space group is Fm-3m. There are four atoms in primitive unit cell. The four sites can be specified in the irreducible unit cell as, Co : a(0,0,0) and a(1/2,1/2,1/2) , Mn : a(1/4,1/4,1/4), Si : a (3/4,3/4,3/4). This compound is half-metallic in nature because majority spin-band is metallic and minority-spin band is semiconducting. The present electronic calculations are performed using density functional theory (DFT) with the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) [9] using plane wave pseudo potential method as implemented in Quantum Espresso package 5.1.1 [10]. Norm-conserving pseudo potential based on the Troullier–Martins scheme were utilised to model core electrons. The cutoff for the kinetic energy was set to 50 Ry for the plane-wave expansion of the electronic wave functions. The marzari-vanderbilt smearing size was fixed at 0.003 Ry. The starting magnetization was fixed at 0.3 for each atom. The Brillouin zone integration was performed over a Monkhorst–Pack [11] 4 × 4 × 4 meshes. The lattice constant of Co_2MnSi was optimized until the total energy converged to at least 10^{-8} Ry. A denser k-mesh of 24 × 24 × 24 was used for calculations of density of states.

Results and Discussions

Our calculated lattice constant is 5.6541 Å (Table 1) which is in good agreement with theoretical data reported by Amari etal [2] and experimental data reported by Webster [12]. Also, the calculated Fermi-energy is 14.6536 eV

Table 1. Calculated lattice constant

Properties	Calculated (this work)	Previous theoretical and experimental work
Lattice constant (Å)	5.6541	5.642[2],5.6357[12],5.665[5]

In figure 1, density of states for Co_2MnSi is shown as function of energy. It is clear from the figure that for up spin electrons (red color), there is no band-gap around Fermi-energy while for down spin electrons (green color), there is small band-gap around Fermi-energy. Thus, up-spin electrons are behaving as metal while down-spin electrons are behaving as semi-conductor. Therefore, the compound Co_2MnSi is half-metallic.

In figure 2, band-structure for spin-up is shown. Fermi-level is shown with horizontal dotted line. The high symmetry lines are X, L, W, r. It is clear from figure that there is no forbidden gap between valence and conduction bands. The general features of band structure are similar to band structure reported by Rai et al [5]. Corresponding band-structure for down-spin is shown in figure 3. It is clear from the figure that there is small band gap between valence and conduction bands.

In figure 4, magnetic moment is shown as a function of lattice constant. It can be clearly seen from figure that lattice expansion favours magnetism. The magnetic moment at optimized lattice constant comes out to be 5.09 Bohr magneton/cell. This value is in good agreement with experimental results [13,14].