BIBECHANA
Vol. 22, No. 1, April 2025, 80-84

ISSN 2091-0762 (Print), 2382-5340 (Online)
Journal homepage: http://nepjol.info/index.php/BIBECHANA
Publisher: Dept. of Phys., Mahendra Morang A. M. Campus (Tribhuvan University)Biratnagar

(Short Communication)

Exploring the electronic and magnetic properties of half-heusler alloy CoMnSb: implications for spintronics

Binay Limbu, Prem Sagar Dahal

[1] *Central Campus of Technology, Tribhuvan University, Dharan, 56700, Nepal*
*Corresponding author. Email: binay.805511@cdp.tu.edu.np(BL)
prem.dahal@cct.tu.edu.np(PD)

Abstract

Heusler alloys have caught a lot of attention because they can be really useful in modern technology. In this study, we investigated the electronic and magnetic properties of CoMnSb by employing advanced computational methods rooted in Density functional theory and plane-wave pseudo potential approach. Our investigation uncovers that CoMnSb is a half-metallic ferromagnet with a half-metallic gap of 0 eV at the equilibrium lattice constant. The total spin magnetic moments have been computed 3μB per unit cell which is in good agreement with the slater pauling rule $M_t = Z_t - 18$ for Half Heusler alloy. The hybridization of the eg and t2g orbitals of the Co, Mn, and P-orbitals of the Sb are primarily responsible for the band gap. This indicates that these alloys hold great potential as functional materials for spintronics.

Keywords
Half-heusler, Density of states, Half-metallic, bandstructure, spintronic devices, DFT.

Article information
Manuscript Received: April 4, 2024; Accepted: January 18, 2025
DOI https://doi.org/10.3126/bibechana.v22i1.64520
This work is licensed under the Creative Commons CC BY-NC License. https://creativecommons.org/licenses/by-nc/4.0/

1 Introduction

The Half-Heusler alloys composition is represented by the generic formula XYZ where X and Y are transition metal elements and Z is the main group sp element. Half-Heusler [1] structure can be looked at as four-interpenetrating face centre cubic(fcc) lattices and has unique four crystal sites in Wyckoff coordinates. Half-Heusler compounds crystallize in fcc $c1_b$ structure with space group F-43m. In this structure X, Y and Z occupy (0,0,0), (1/4,1/4,1/4) and (3/4,3/4,3/4) sites and (1/2,1/2,1/2) sites are empty. The Half-metallic compounds can also be characterised by their integer value of magnetic moments which is in accordance with the slater-pauling rule $M_t = Z_t - 18$ where M_t is magnetization and Z_t is a total number of valence electron. In this project, we planned to investigate systematically the electronic and magnetic properties of Half-Heusler alloys CoMnSb. In the present time, Heusler compounds having Co and Mn atoms pull large attention because of their

property of strongly ferromagnetic with the high curie temperature. Heusler alloys catch the interest of many one because of possible study within the same family of series of integrating diverse magnetic phenomena like Pauli paramagnetism, helimagnetism, itinerant and localized magnetism or heavy-fermionic behaviour. At Fermi level at low temperture some of oxides(e.g Fe_3O_4 and crO_2) [2], double peroskites (e.g Sr_2FeReO_6) [3] and pyrites (e.g CoS_2) [4] which shows 100% spin-polarization. Mostly Half Heusler [1] are used in the application fields like spin-injection devices,spin-filters [5], tunnel junctions [6] or GMR devices [7]. In most cases, half-metallicity has been lost. It is experimentally found [8] that near surfaces and interfaces half-metallic character is lost. There are also several factors which affect the half-metallic character of Half Heusler alloys [1].

2 Computational details

In this study, we used GGA method imple- mented in the Quantum Espresso software package vaersion 6.7 to investigate electronic and magnetic properties of CoMnSb. In order to optimize the lattice parameter of CoMnSb using the energy minimization method we carried out a convergence test on the kinetic energy-cutoff of the wavefunctions and the number of k-points in Monk-Horst pack grid on the basis of crystal structure and lattice constant of produced CoMNSb determine by experiment. To relax the coordinates we maintain force between atoms less than 10^{-3} Ry/a.u using the optimized lattice parameter of CoMnSb. Taking into account all these computed values, we evaluated the electronic structure employing the plane wave pseudo-potential approach within the Quantum-Espresso distribution of DFT. We use ultra-soft pseudo-potential from the Quantum espresso page for Cobalt, Manganese and antimony. SCF threshold was set to 10^{-8} and energy tolerance was set to 10^{-5}Rydberg Monk-Horst pack grids with dimensions of 8x8x8 were used for the sampling of the brillouin zone. The linear tetrahedral integration approach was used to calculate the density of the states. With the help of the tool XCrySden, crystal structure can be visualized. Graphing and plotting are done with the help of Gnuplot.

3 Results and discussion

3.1 Electronics properties

The electronic band structure is one of the most used analytical techniques in the determination of a crystal's first-principles electronic structure, particularly within the Kohnsham framework of density functional theory [9]. Electronic properties of solids can be determined and analyzed by using their band structures. It includes the fundamental components for practically all crystal characteristics. When many atoms are brought together, their interaction causes the initial atomic levels to be perturbed because the atoms in a solid are tightly packed. According to Pauli's exclusion principle, which states that no two electrons can occupy the same energy state. The orbitals are completely occupied with electrons [10]. In a solid, the valence electrons group together and compete to occupy the same energy level, creating energy bands. The core electrons, on the other hand, do not change energy levels and continue to be bound to the nuclei. Within each energy band, the outcome is a continuum of energy levels. In semiconductors and insulators, a band gap forms as a result of the periodic potential of the ion cores in the material and how the electrons react to this potential. The energy range between the highest occupied and lowest vacant energy levels is known as the band gap. The material's electronic characteristics are determined by the band gap size, which is dependent on the substance. For instance, conductors have no band gap whereas insulators have a wide band gap. Materials can be categorized as conductors, semiconductors, or insulators. It depends on the width of their energy bands and the relative position of their Fermi level, which is the energy level of the highest occupied state. The Fermi level is located in the conduction band because the valence bands in conductors are broad and overlap. The Fermi level is found in semiconductors and insulators near the top of the valence band or within the band gap. A material's density of states (DOS), or the number of electronic states per unit energy range, may also be used to describe its electronic structure. Density functional simulations were used to examine the electronic structures of the CoMnSb [11] alloys at their equilibrium lattice constants (a=5.82350 a.u). We focus on the DOS in the range of the Fermi level, which is set to zero and varies from -5 to 3eV since the DOS distribution at the Fermi level influences the electronic characteristics. Around the Fermi level, it is clear that there is a significant exchange splitting between the majority-spin and minority-spin states. Particularly, the bands of the minority-spin states for CoMnSb [11] have an indirect energy gap at the Fermi level, but the majority-spin states crossing the Fermi level are partially filled. As a result, CoMnSb shows half-metallic [12] characteristics. The computed spin-polarized band structures for CoMnSb alloy at the equilibrium lattice constant along the high symmetry directions in the first Brillouin zone are represented in Figures 1a and 1b, respectively. We computed the band structure along the Brillouin zone route $\Gamma - X - W - K - \Gamma - L - U - W - L - K$ which

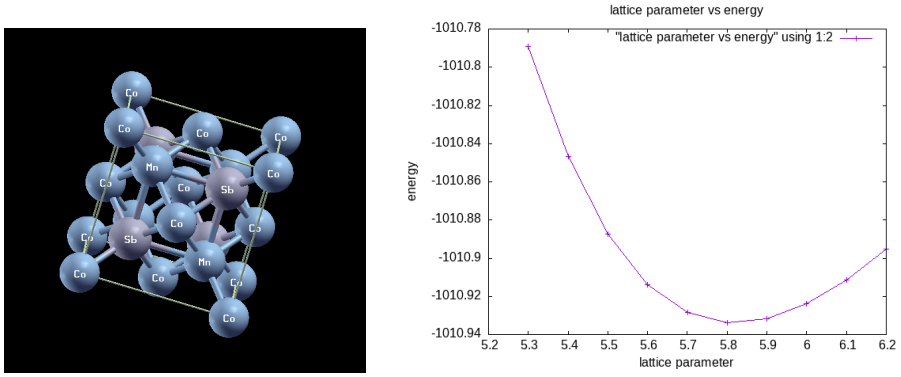

Figure 1: (a)Unit cell and (b) Optimized lattice parameter.

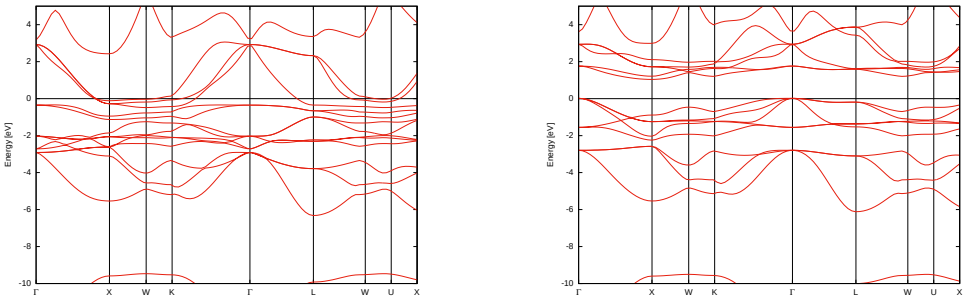

Figure 2: Band structure plots of CoMnSb (a) Spin-up and (b) Spin-down.

is shown in Figure 1. We learn that CoMnSb's electronic structures exhibit the typical half-metallic characteristics, the majority-spin band structures are metallic, but the minority-spin band structures are semiconducting with a band gap of 1 eV. This finding is in good accordance with findings from earlier studies [11]. The augmented spherical waves investigation was used by Kübler [13] to conduct a theoretical study of CoMnSb [14]. He discovered a DOS that was exactly like ours in terms of its size gap and the Fermi level, which was situated at the left edge of the spin-minority gap. The bottom of the minority-spin conduction bands is placed at 1.3 eV, whereas the top of the minority-spin valence bands is at 0 eV [14]. The half-metallic gap for CoMnSb [14] is 0 eV, which is decided minimum of Ec and Ev. Ec is the energy level of the bottom minority-spin conduction band in relation to the Fermi level, and Ev is the absolute value of the top minority-spin valence band energy in relation to the Fermi energy. The DOS nature perfectly matches the band's results. The hybridization of the eg and t2g orbitals of the Co, Mn, and P-orbitals of the Sb are primarily responsible for the band gap. The delocalized electrons may be responsible for Co and Mn's eg and t2g orbitals contribution.

3.2 Magnetic properties

The spin and orbital angular momentum of electrons in their electronic shells give rise to the magnetic properties of atoms or ions. The total spin of the atom or ion is determined by the combination of the spin and angular momentum vectors of the electrons. This behaviour is regulated by the laws of quantum mechanics. It is clear from Hund's rule states are energetically favoured. Three quantum numbers total spin S, orbital angular momentum L, and total angular momentum J can be used to describe the state of an atom or ion. According to the Pauli exclusion principle and Hund's rule, the electronic shells of atoms are filled up. The valence orbitals of the atoms hybridize with those of neighbouring atoms when they are brought together to form a solid, creating bonding and anti-bonding states. These states are able to have electrons added to them in ways that are energetically advantageous, leading to varied magnetic behaviour in solids. Some substances contain spontaneous magnetic moments, which means they have a magnetic moment even in the absence of an external magnetic field. The presence of such spontaneous moments shows that electronic spins and magnetic moments are arranged in a predictable way. The magnetic materials ferromagnets, anti-ferromagnets, and ferrimagnets all result from distinct configurations of

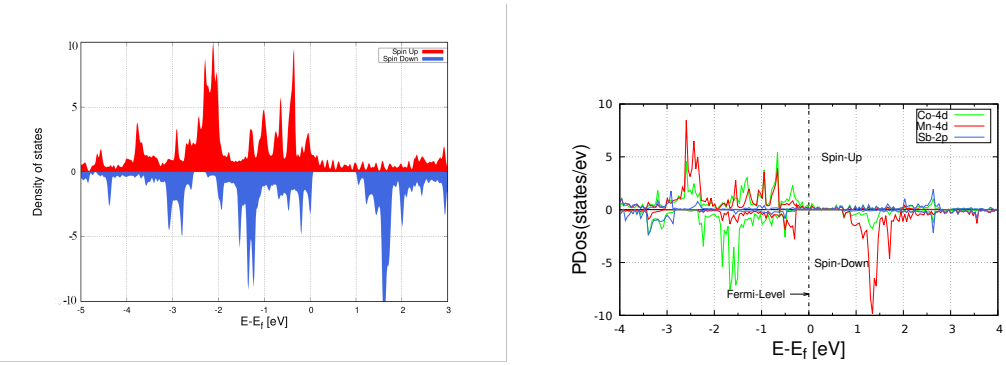

Figure 3: Total and Partial density of state plots of CoMnSb (a) DOS and (b) Pdos.

electronic spins and magnetic moments. By counting the number of unpaired electrons and multiplying the result by Bohr's magneton, one may get the total magnetic moment of a substance. 21 valence electrons in the CoMnSb half-Heusler alloy contribute to magnetism. Four of the 21 valence electrons will initially occupy the Co and Mn 4s states since these states are lower in energy than the 4p levels. Seven of them are in majority-spin states for Co and Mn, while the other ten are in minority-spin states for Co and Mn. According to Hunds Rules, a 3d orbital has space for 10 electrons, hence the 3d orbital of majority-spin states are not entirely filled. The majority spin has a three-hole band, and the total magnetic moment for a spin should be 3μB per formula unit. Table 1 contains the computed total spin magnetic moments. It is clear that these are integral values, which for CoMnSb equals 3μB. The total spin magnetic moments are known to be $M_t = Z_t - 18$ for half-metallic, where M_t is the total magnetic moment per unit cell and Z_t is the total number of valence electrons. These total spin magnetic moments are required to follow the Slater-Pauling rule [15]. In half-metals [12], the Fermi energy is often confined in the minority-spin gap, which makes the spin magnetic moment integral and the number of occupied minority-spin states an integer. They have 21 valence electrons in the CoMnSb. According to the Slater-Pauling rule [15], CoMnSb's total spin magnetic moment is 3μB, which is consistent with the findings of our first principles. The computed magnetic moments have been found to be in accordance with previous CoMnSb [14] theoretical studies. As can be observed, various atoms contribute differently to the magnetic characteristics due to differences in their spin magnetic moments. The CoMnSb alloy's Mn atom has the highest spin magnetic moments, while Sb contributes very little to the alloy's overall spin moment. These quantitative findings show that Mn atoms, which are present in the compounds in a high spin state, account for the majority of the total spin magnetic moments. The magnetic moments of Co and Sb in the half-Heusler alloy CoMnSb [14] have a negative sign. The induced magnetic polarization of the Co and Sb atoms is antiparallel to that of the Mn atoms, as seen by the negative sign in their local magnetic moments. It also demonstrates the existence of ferromagnetic coupling in CoMnSb [11].

Table 1: Calculated total magnetic moment (M^T) for CoMnSb.

Magnetic moments in (μ_B)	GGA
Co	-0.0879
Mn	3.1275
Sb	-0.0605

4 Conclusion

With the help of DFT, GGA, and Quantum ESPRESSO code, this paper has effectively analyzed the electronic and magnetic characteristics of CoMnSb. First, we created the optimized unit cell of the FCC structure of CoMnSb [11]. The kinetic energy (cut-off energy) with a k-point grid of 9x9x9, is discovered to be 90 Ry during optimization. The estimated lattice parameter was then determined to be 5.82350 a.u, which is only 0.4% deviated from the experimental data but still extremely close to them. As a result, the lattice parameter of CoMnSb [11] computed with the GGA approach agrees well with experimental data. The GGA technique in the QE package is then used to investigate the band structure and density of states. This demonstrates that the plane-wave pseudopotential approach may be employed with the quantum ESPRESSO code to do first-principles calculations to analyze more complicated electronic and other systems. Between the majority-spin and minority-spin bands of the Co 3d and Mn 3d states, there is a significant exchange splitting. CoMnSb is a half-metallic ferromagnet with a half-metallic gap of 0 eV at an equilibrium lattice constant. The total spin magnetic

moments that have been computed is 3μB per unit cell, which is in good agreement with the Slater-Pauling law [15]. It is discovered that the observed results agree with previous experimental and theoretical results.

Acknowledgments

We are grateful to Roshan Basnet of South Carolina, Ashim Bhujel of University of Marryland, and Rickky Rai of Tribhuvan University for providing us value pieces of advice throughout our work.

References

[1] C Felser and A Hirohata. Properties, growth, applications, 2016.

[2] RJ Soulen Jr, JM Byers, MS Osofsky, B Nadgorny, T Ambrose, SF Cheng, Pr R Broussard, CT Tanaka, J Nowak, JS Moodera, et al. Measuring the spin polarization of a metal with a superconducting point contact. *science*, 282(5386):85–88, 1998. DOI: https://doi.org/10.1126/science.282.5386.85.

[3] H Kato, T Okuda, Y Okimoto, Y Tomioka, K Oikawa, T Kamiyama, and Y Tokura. Structural and electronic properties of the ordered double perovskites a 2 m reo 6 (a= sr, ca; m= mg, sc, cr, mn, fe, co, ni, zn). *Physical Review B*, 69(18):184412, 2004. DOI: https://doi.org/10.1103/PhysRevB.69.184412.

[4] Tatsuya Shishidou, AJ Freeman, and Ryoji Asahi. Effect of gga on the half-metallicity of the itinerant ferromagnet cos 2. *Physical Review B*, 64(18):180401, 2001. DOI: https://doi.org/10.1103/PhysRevB.64.180401.

[5] KA Kilian and RH Victora. Electronic structure of ni 2 mnin for use in spin injection. *Journal of Applied Physics*, 87(9):7064–7066, 2000. DOI: https://doi.org/10.1063/1.372932.

[6] Clifford T Tanaka, Janusz Nowak, and Jagadeesh S Moodera. Spin-polarized tunneling in a half-metallic ferromagnet. *Journal of applied physics*, 86(11):6239–6242, 1999. DOI: https://doi.org/10.1063/1.371678.

[7] Ch Hordequin, JP Nozieres, and J Pierre. Half metallic nimnsb-based spin-valve structures. *Journal of magnetism and magnetic materials*, 183(1-2):225–231, 1998. DOI: https://doi.org/10.1016/S0304-8853(97)01072-X.

[8] Silvia Picozzi, Alessandra Continenza, and Arthur J Freeman. Role of structural defects on the half-metallic character of heusler alloys and their junctions with ge and gaas. In *Half-metallic Alloys*, pages 41–66. 2005. DOI: https://doi.org/10.1103/PhysRevB.69.094423.

[9] Manoj K Harbola and Arup Banerjee. Many-electron problem in terms of the density: From thomas–fermi to modern density-functional theory. *Journal of Theoretical and Computational Chemistry*, 2(02):301–322, 2003. DOI: https://doi.org/10.1016/S0304-8853(97)01072-X.

[10] Rajendra A sharma Amrit, SB Thapa. Study of structural and electronic properties of chromium and molybdenum(unpublished master's thesis. *Tribhuvan university,Nepal*, 2020.

[11] HM Huang, SJ Luo, and KL Yao. First-principles investigation of the electronic structure and magnetism of heusler alloys comnsb and co2mnsb. *Physica B: Condensed Matter*, 406(8):1368–1373, 2011. DOI: https://doi.org/10.1016/j.physb.2011.01.031.

[12] MP Ghimire, TP Sinha, RK Thapa, et al. First principles study of the electronic and magnetic properties of semi-heusler alloys nixsb (x= ti, v, cr and mn). *Journal of alloys and compounds*, 509(41):9742–9752, 2011. DOI: https://doi.org/10.1016/j.jallcom.2011.08.017.

[13] Vadim Ksenofontov, Gennadiy Melnyk, Marek Wojcik, Sabine Wurmehl, Kristian Kroth, Sergey Reiman, Peter Blaha, and Claudia Felser. Structure and properties of comnsb in the context of half-metallic ferromagnetism. *Physical Review B*, 74(13):134426, 2006. DOI: https://doi.org/10.1103/PhysRevB.74.134426.

[14] Rajendra Dahal and Gopi Chandra Kaphle. Structural, electronic and magnetic properties of xyz type half-heusler alloys. *Journal of Nepal Physical Society*, 5(1):97–102, 2019. DOI: https://doi.org/10.3126/jnphyssoc.v5i1.26938.

[15] I Galanakis, PH Dederichs, and N Papanikolaou. Slater-pauling behavior and origin of the half-metallicity of the full-heusler alloys. *Physical Review B*, 66(17):174429, 2002. DOI: https://doi.org/10.1103/PhysRevB.66.174429.