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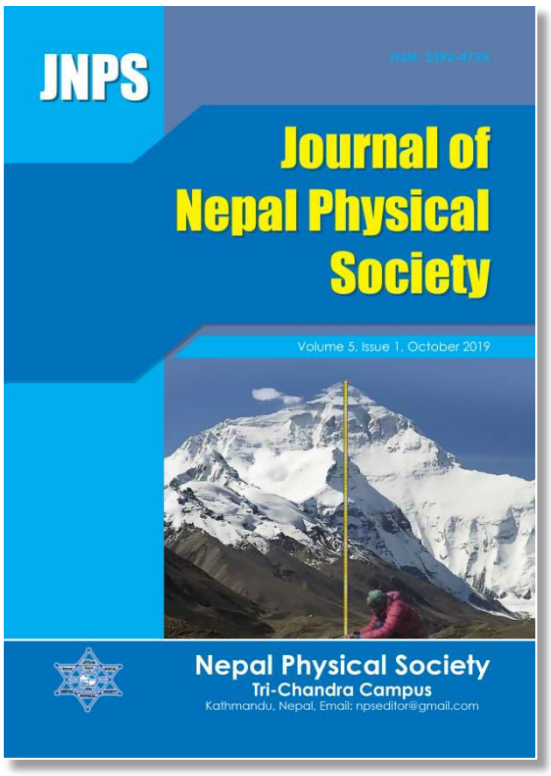
Journal of Nepal Physical Society

Volume 5, Issue 1, October 2019

ISSN: 2392-473X



JNPS, **5** (1), 97-102 (2019)

Published by:

Nepal Physical Society

P.O. Box: 2934

Tri-Chandra Campus

Kathmandu, Nepal

Email: npseditor@gmail.com

JNPS 5 (1), 97-102 (2019)
ISSN: 2392-473X

Research Article

STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF XYZ TYPE HALF-HEUSLER ALLOYS

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ABSTRACT

The spintronic devices have played an important role in modern technological era . Heusler alloys have attracted lot of interest in spintronic applications due to their half-metallic properties predicted by band structure calculations. We investigate the electronic, magnetic and structural properties of half-Heusler alloys FeMnGe and CoMnSb using first principles based density functional theory (DFT) implemented on Tight Binding Linear Muffin-Tin Orbital within Atomic Sphere Approximation (TB-LMTO-ASA) code. The calculation reveal that CoMnSb and FeMnGe are half-metallic Ferro-magnet in nature of with magnetic moment 1.00 μB and 2.99 μB per formula unit at equilibrium lattice parameter respectively. The magnetic moment mainly originates from the strong spin polarization of d electrons of X atom and partial contribution of p electrons of Y atom. The half metallic gap of FeMnGe and CoMnSb is found to be 0.38 eV and 0.95 eV respectively. This shows that these alloys are very promising spintronic functional materials.

Keywords: TB-LMTO-ASA, half-Heusler Alloy, half-Metallicity, DOS, Spintronic applications

INTRODUCTION

The spintronic devices have played an important role in modern technological era. It is also very important for fundamental aspect of Physics. Half-metallic (HM) materials are those one which one of the spin bands out of two, is semiconducting with a gap at the Fermi level, but another spin band is metallic, leading to 100% spin polarization at the Fermi level, have attracted more and more attention because of their promising applications in spintronic devices. First de Groot et al. [1] predicted the half metallic property in half-Heusler alloy of NiMnSb and PtMnSb, since then much attention has been paid to half-Heusler alloys [2]. The term Heusler alloy is named after a German mining engineer and chemist Friedrich Heusler in 1903 [3, 4]. Surface reconstruction has been an active area of research in field of semiconductors. The basic thing of the electronic devices is to inject the spin polarized electrical current into semiconductors [5]. In Ferromagnet the spin population is not balance at Fermi level. Hence ferromagnetic materials with full spin polarization at Fermi level will be the most applicable for spin injecting. This phenomenon can be applicable in half metallic Ferromagnet. Half-Heusler composition of XYZ, where X and Y are transition metal elements, Z is a main group element. In recent year, Heusler compounds containing Co and Mn atoms have attracted particular attention as they are strongly ferromagnetic with high Curie temperature [6]. The half-Heusler alloy is trust worthy materials to be applied as spin injector in the rapidly developing field of spin electronics (spintronic) [7]. The rapidly developing field of electronics technology is owing to the discoveries of GMR and TMR which opened the line of research in spintronic [8, 9]. In half metallic Ferro magnet (HMFs) the majority of the spin band is metallic and the minority of the spin band is superconducting with an energy gap at the Fermi level. DOS of half metals compared with metals and semiconductors is shown in Fig. (1).

From figure 1 above it is lucid that there is no band gap in the Fermi region for metals but in case of semiconductors there is gap. Half metals have no band gap in spin up channel at the Fermi level but has considerable band gap in the spin down channel. This shows that spin up electrons of Fermi level shows metallic nature while spin down electrons Fermi level shows non-metallic nature. Combining these two parts we can conclude that system is half metallic. Thus Heusler alloy are