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Co-author. ***Hakim Baaziz, Hadda Tiouiri, Torkia Ghellab, Zoulikha Charifi.***

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Topic 3: Condensed Matter Physics

First Principales Calculations of the Electronic, Magnetic, and Elastic properties of CoFeVSb Heusler Alloys

I. Bensehil[1,2]✉, H. Baaziz[3,4] , H. Tiouiri[1,4] , T. Ghellab[3,4], Z. Charifi[3,4]

1. Faculty of Technology ,University of M'sila, PO Box 166 , Ichbelia, 28000 M'sila, Algeria

2. Laboratory of Surfaces and Interfaces Studies of Solid Materials,University of Setif 1, Algeria.

3. Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria.

4. Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria.

✉*Corresponding Author Email: ilhem.bensehil@univ-msila.dz*

Abstract

Since Groot's discovery of the first half metallic material, NiMnSb, in 1983, the scientific community has become increasingly interested in the study of Heusler alloys. Due to their unusual and interesting structural characteristics, magnetic properties, and many features, including metallic, insulating, semiconducting, half-metallic, and spin gapless semiconducting, these materials have garnered a lot of attention. These materials are used for spintronics and magnetoelectronics applications such as spin filters, spininjection, magnetic tunnel junctions, giant magnetoresistance, spin transfer torque,memory devices, spin caloritronics, magnetic sensors, and neuromorphic and stochastic computing.

In this work, we have studied the structural, elastic, electronic and magnetic properties of CoFeVSb Heusler compound basing on the density functional theory. The most stable structure has been found to be energetically favorable in face- centered cubic (FCC) structure with space group F43m, in which Co, Fe, V, and Sb atoms are located at 4d, 4c, 4b and 4a Wyckoff positions, respectively. In the stable state, CoFeVSb is ferromagnetic. The determined elastic constants (Cij) show that CoFeVSb is mechanically stable and ductile, and exhibit a notable elastic anisotropy. Electronic calculations indicate that CoFeVSb exhibit half-metallic characteristics with high spin polarisation. For the spin-down, the Fermi level is located between the valence bands 3t1u and the conduction bands 2eu, which leads to a semiconductor behavior with an indirect band gap Γ-X of 0.52 eV. The total magnetic moment of these alloys is found to be equal to 3 μB which follows the Slater Pauling rule, which makes it hopeful in spintronic applications.

Keywords: *Half-metals, quaternary Heusler alloys, Elastic properties, Magnetic moment, Electronic properties*