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AB-INITIO STUDY OF STRUCTURAL, OPTOELECTRONIC AND MAGNETIC PROPERTIES OF CO2MNSI HEUSLER ALLOYS

M Matougui[1], B Bouadjemi[1], M Houari[1], S Haid[1], T Lantri[1] and S Bentata[1,2]

[1]Laboratory of Technology and of Solids Properties-University of Abdelhamid Ibn Badis, Algeria
[2]University of Mascara, Algeria

We performed first-principle calculations to investigate the structural, optoelectronic, and magnetic properties of Co2MnSi Heusler alloys using density functional theory based on full- potential linearized augmented plane wave (FP-LAPW) method. We employed three approaches LSDA, LSDA+U and Hybrid on-site exact exchange, where the Hubbard correction U is calculated by constraint LDA for Co and Mn. Our results showed the half- metallicity character with integral magnetic moment of 5μB, which agrees with the Slater- Pauling rule. Our findings suggest that these materials are potential candidates for manufacturing Spintronic devices and Nanotechnology.

matouguimohamed@hotmail.com