Ab Initio Study of Co2ZrGe and Co2NbB Full Heusler Compounds

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Abstract : Using the first-principles full-potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method based on density functional theory (DFT), we have investigated the electronic structure and magnetism of some Co2- based full Heusler alloys, namely Co2ZrGe and Co2NbB. The calculations show that these compounds are to be half-metallic ferromagnets (HMFs) with a total magnetic moment of 2.000 µB per formula unit, well consistent with the Slater-Pauling rule. Our calculations show indirect band gaps of 0.58 eV and 0.47 eV in the minority spin channel of density of states (DOS) for Co2ZrGe and Co2NbB, respectively. Analysis of the DOS and magnetic moments indicates that their magnetism is mainly related to the d-d hybridization between the Co and Zr (or Nb) atoms. The half metallicity is found to be robust against volume changes and the two alloys kept a 100% of spin polarization at the Fermi level. In addition, an atom inside molecule AIM formalism and an electron localization function ELF were also adopted to study the bonding properties of these compounds, building a bridge between their electronic and bonding behavior. As they have a good crystallographic compatibility with the lattice of semiconductors used industrially and negative calculated cohesive energies with considerable absolute values these two alloys could be promising magnetic materials in the spintronics field.

Keywords : half-metallic ferromagnets, full Heusler alloys, magnetic properties, electronic properties
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