Abstract

Investigation of the structural, electronic and magnetic properties of full-Heusler Co_2VIn as well as half-Heusler CoVIn Cobalt based Heusler compounds using density functional theory (DFT) leads to the general conclusion that Co_2VIn and CoVIn are half-metallic materials with a gap at the Fermi level in the minority states and majority states respectively. A Hubbard-like Coulomb correlation term *U* has been included in the DFT (DFT+*U*) for the computation of the electronic and magnetic properties of the compounds. The structural properties have been calculated for the paramagnetic and ferromagnetic phases, and both Co_2VIn and CoVIn are found to be stable in the ferromagnetic phase. The calculated magnetic moments are 2 μB2 μB and 0.9 μB0.9 μB per formula unit for Co_2VIn and CoVIn respectively.