Abstract

First principles calculations are reported on perpendicular magnetic anisotropy (PMA) in nearly fully compensated ferrimagnetic Heusler compound $Mn_{0.75}Co_{1.25}VIn$. The structural, electronic and magnetic properties of $Mn_{2-x}Co_xVIn$ Heusler compounds (x = 0.0, 0.25, 0.50, 0.75, 1.0, 1.25, and 1.75) have been investigated using Density Functional theory (DFT) as implemented in the Vienna *ab initio* simulation package (VASP). The Perdew Burke Ernzerhof parametrization of the generalized gradient approximation (GGA) was used to treat the exchange and correlation in the system. The crystal structure of the compounds with x = 0.75, 1.00 and 1.25 are found to be tetragonally distorted. While the former exhibits inplane magnetocrystalline anisotropy (IMA) energy of 0.035 meV, the latter two exhibit perpendicular magnetocrystalline anisotropy (PMA) energy of 11.700 meV and 96.800 meV respectively. Additionally, the magnetic moments for x = 0.75 and 1.25 are found to be ∼0.5 μ_B/f.u. while for x = 1.00, it is found to be ∼0 μ_B/f.u., in agreement with the Slater Pauling rule for half metallic systems. Through Co replacement of Mn in Mn_2VIn which is not half metallic at the optimized volume, a composition whose crystal structure is tetragonally distorted is found, which is not only a highly spin polarized nearly fully compensated ferrimagnet but also exhibits PMA.