First principles study of structural, electronic and magnetic properties of $Mg_{1-x}Mn_xTe$ alloys

Abstract

Density functional FP-LAPW + lo calculations have been performed to study the structural, electronic and magnetic properties of $Mg_{1-x}Mn_xTe$ for compositional parameter x = 0.25, 0.50, 0.75 and 1. Our calculations reveal the occurrence of ferromagnetism in these compounds in which the transition-metal atom is ordered in a periodical way thereby interacting directly with the host atoms. Results extracted from electronic band structure and density of states (DOS) of these alloys show the existence of direct energy band gap for both majority- and minority-spin cases, while the total energy calculations confirm the stability of ferromagnetic state as compared to anti-ferromagnetic state. The total magnetic moment for $Mg_{1-x}Mn_xTe$ for each composition is found to be approximately 5 μ_B, which indicates that the addition of Mn content does not affect the hole carrier concentration of the perfect MgTe compound. Moreover, the s-d exchange constant ($N_0\alpha$) and p-d exchange constant ($N_0\beta$) are also calculated which are in accordance with a typical magneto-optical experiment. The estimated spin-exchange splitting energies originated by Mn 3d states energies, i.e. Δ_X(s-d) and Δ_X(p-d), show that the effective potential for minority-spin is more attractive than that of the majority-spin. Also, the p-d hybridization is found to cause the reduction of local magnetic moment of Mn and produce small local magnetic moments on the nonmagnetic Mg and Te sites.