First-principles study of spin-polarized electronic band structures in ferromagnetic Zn_{1-x} TM_x S (TM = Fe, Co and Ni)

Abstract

We report a first-principles study of structural, electronic and magnetic properties of crystalline alloys Zn_{1-x} TM_x S (TM = Fe, Co and Ni) at x = 0.25. Structural properties are computed from the total ground state energy convergence and it is found that the cohesive energies of Zn_{1-x} TM_x S are greater than that of zincblende ZnS. We also study the spin-polarized electronic band structures, total and partial density of states and the effect of TM 3d states. Our results exhibit that $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ are half-metallic ferromagnetic with a magnetic moment of $4\mu_B$, $3\mu_B$ and $2\mu_B$, respectively. Furthermore, we calculate the TM 3d spin-exchange-splitting energies Δ_x (d), Δ_x (x-d), exchange constants N_0 α and N_0 β, crystal field splitting ($\Delta E_{cryst} \equiv E_{t2\,g} - E_{eg}$), and find that p-d hybridization reduces the local magnetic moment of TM from its free space charge value. Moreover, robustness of Zn_{1-x} TM_x S with respect to the variation of lattice constants is also discussed.