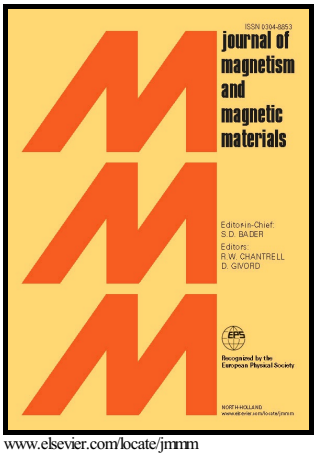

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Abstract

In this study, we investigated the structural, electronic and magnetic properties of $Cd_{0.9375}TM_{0.0625}S$ (TM = Ni, Co and Fe) compounds in zinc blende (B3) ferromagnetic phase using all-electron full-potential linear muffin tin orbital (FP-LMTO) calculations within the frame work of the density functional theory and the generalized gradient approximation. The analysis of electronic structures shows that $Cd_{0.9375}Ni_{0.0625}S$, $Cd_{0.9375}Co_{0.0625}S$ and $Cd_{0.9375}Fe_{0.0625}S$ compounds are half-metallic ferromagnets with 100% spin polarization at the Fermi level. This half-metallic behavior is confirmed by the total calculated magnetic moment per Ni, Co and Fe substituted transition metal (TM) atom, which is found to be 2 μ_B, 3 μ_B and 4 μ_B for $Cd_{0.9375}TM_{0.0625}S$ (TM = Ni, Co and Fe) compounds, respectively. Furthermore, we found that the TM-3d states are responsible for generating spin-polarization and magnetic moment in these compounds and we establish that the p-d hybridization reduces the local magnetic moment of TM atoms from its free space charge value and produces small local magnetic moments on nonmagnetic Cd and S host sites. Also, we predicted exchange splitting energy Δ_x(pd) and exchange constants $N_0\alpha$ and $N_0\beta$. The calculated values validate the ferromagnetic nature of these compounds.

Key words

Ab-initio calculations, Diluted magnetic semiconductor, Half-metallic ferromagnetism, Electronic structure, Magnetic properties.