# Ab-initio calculations of Co-based diluted magnetic semiconductors $Cd_{1-x}$ $Co_x$ X (X=S, Se, Te)


## Abstract

Ab-initio calculations are performed to investigate the structural, electronic and magnetic properties of spin-polarized diluted magnetic semiconductors composed of II-VI compounds $Cd_{1-x}$ $Co_x$ X (X=S, Se, Te) at x=0.25. From the calculated results of band structure and density of states, the half-metallic character and stability of ferromagnetic state for $Cd_{1-x}$ $Co_x$ S, $Cd_{1-x}$ $Co_x$ Se and $Cd_{1-x}$ $Co_x$ Te alloys are determined. It is found that the tetrahedral crystal field gives rise to triple degeneracy $t_{2g}$ and double degeneracy $e_g$ . Furthermore, we predict the values of spin-exchange splitting energies $\Delta_x$ (d) and $\Delta_x$ (p-d) and exchange constants $N_0$ α and $N_0$ β produced by the Co 3d states. Calculated total magnetic moments and the robustness of half-metallicity of $Cd_{1-x}$ $Co_x$ X (X=S, Se, Te) with respect to the variation in lattice parameters are also discussed. We also extend our calculations to x=0.50, 0.75 for S compounds in order to observe the change due to increase in Co.



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## Author Keywords

Ab-initio calculations; Density functional theory; Dilute magnetic semiconductors; Electronic and magnetic properties