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Half-metallic ferromagnetism in Co doped CdS diluted magnetic semiconductor[1)]

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In the present study, magnetic properties of Co doped CdS has been investigated by first principle calculations using GGA + U approximation. The study reveals the ferromagnetic ordering of Co doped CdS at lower concentrations of Co, whereas, at higher concentrations, the antiferromagnetic interactions dominate. The observed ferromagnetic nature in the present study is not due to the presence of any secondary phases as confirmed by the purity of phase revealed in XRD spectra [1]. The magnetic dipoles located on the surface of the nanoparticles having higher surface-to-volume ratio play a crucial role in the formation of the ferromagnetic state. At lower concentrations of Co, a large number of magnetic dipoles are located at the surface of the nanoparticles which tends neighboring dipoles align in the same direction. Subsequently, a prominent ferromagnetic nature is observed for the nanoparticles [2, 3].

The electronic structures reveal the half metallic character with spin up state being semiconducting and spin down state being metallic signifying 100 % spin polarization [4]. The corresponding density of states of the Co doped CdS system shows reasonable $p-d$ hybridization at Fermi level between d states of Co ions and p states of S ions, which implies half metallic ferromagnetism of CdS induced by Co. The estimated defect formation energy of Co doped CdS was found to be −1.10 eV, indicating that the dopant is easily incorporated into the host lattice. The smaller value of formation energy promises superior stability and indicates that Co doped CdS can be easily fabricated experimentally [5].

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