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Structural and Electronic Properties of Cd0.75V0.25S Alloy

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Abstract : The first principles calculations based on the density functional theory (DFT) by using the full-potential linearized augmented plane wave (FP-LAPW) method within the generalized gradient approximation (GGA) in order to investigate the structural and electronic properties of Cd1-xVxS alloy at x = 0.25 in zincblende structure. For the structural properties, we have calculated the equilibrium lattice parameters, such as lattice constant, bulk modulus and first pressure derivatives of the bulk modulus. From the electronic structure, we obtain that Cd0.75V0.25S alloy is nearly half-metallic. The analysis of the density of states (DOS) curves allow to evaluate the spin-exchange splitting energies Δx(d) and Δx(pd) that are generated by V-3d states, where the effective potential for spin-down case is attractive than for spin-up case. Calculations of the exchange constants N0α (valence band) and N0β (conduction band) are served to describe the magnetic behavior of the compounds.

Keywords : first-principles calculations, structural properties, electronic properties
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