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Half-Metallic Ferromagnetism in CdCoTe and CdMnTe: Ab-Initio Study

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Abstract : Using the first-principles method, we investigate the structural, electronic, and magnetic properties of the diluted magnetic semiconductors CdCoTe and CdMnTe in the zinc blende phase with 12.5% of Cr. The calculations are performed by a developed full potential augmented plane wave (FP-L/APW) method within the spin density functional theory (DFT). As exchange–correlation potential, we used the new generalized gradient approximation GGA. Structural properties are determined from the total energy calculations and we found that these compounds are stable in the ferromagnetic phase. We discuss the electronic structures, total and partial densities of states and local moments. Finally, CdCoTe and CdMnTe in the zinc-blend phase show the half-metallic ferromagnetic nature and are expected to be potential materials for spintronic devices.

Keywords : DFT, GGA, band structures, half-metallic, spintronics
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