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Structural, Electronic and Magnetic Properties of Co and Mn Doped CDTE

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Abstract : The structural, electronic, and magnetic properties of transition metal Co and Mn doped zinc-blende semiconductor CdTe were calculated using the density functional theory (DFT) with both generalized gradient approximation (GGA). We have analyzed the structural parameters, charge and spin densities, total and partial densities of states. We find that the Co and Mn doped zinc blende CdTe show half-metallic behavior with a total magnetic moment of 6.0 and 10.0 μB, respectively.The results obtained, make the Co and Mn doped CdTe a promising candidate for application in spintronics.

Keywords : first-principles, half-metallic, diluted magnetic semiconductor, magnetic moment
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