World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Spin-Polarized Structural, Electronic, and Magnetic Properties of Co and Mn-Doped CdTe in Zinc-Blende Phase

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Abstract : Structural, electronic, and magnetic properties of Co and Mn-doped CdTe have been studied by employing the full potential linear augmented plane waves (FP-LAPW) method within the spin-polarized density functional theory (DFT). The electronic exchange-correlation energy is described by generalized gradient approximation (GGA) as exchange–correlation (XC) potential. We have calculated the lattice parameters, bulk modulii and the first pressure derivatives of the bulk modulii, spin-polarized band structures, and total and local densities of states. The value of calculated magnetic moment per Co and Mn impurity atoms is found to be 2.21 μB for CdCoTe and 3.20 μB for CdMnTe. The calculated densities of states presented in this study identify the half-metallic of Co and Mn-doped CdTe.

Keywords : electronic structure, density functional theory, band structures, half-metallic, magnetic moment
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020