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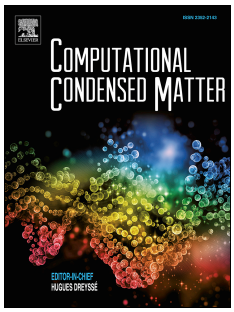

Ab-initio calculations for the electronic and magnetic properties of Cr doped ZnTe

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Ab-initio calculations for the electronic and magnetic properties of Cr doped ZnTe

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Abstract

In this paper, the ab-initio study of the electronic and magnetic properties of ZnTe doped by the transition metal element chromium has been investigated. This work is based on the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method within the local density approximation (LDA). Using the magnetization data, we have calculated the total energy to determine the most stable state in the system and found it to be the ferromagnetic state. On the other hand, we have investigated and plotted the density of states (DOSs) which reveal that the compound exhibits a half metallic character. The spin polarization at Fermi level is estimated and found to be around 100 %, depending on the concentrations [1]of Cr. Furthermore, we have identified the type of mechanism of exchange interactions being double exchange. Moreover, we have estimated the Curie temperature variation T_C which revealed a large value greater than 800 K. In addition, we have studied the effect of the crystal field and the exchange splitting as a function of the concentrations values. Finally, as a comparison study and correction the overestimation of the calculated parameters we have used even more the atomic sphere approximation (ASA).

Keywords: Spintronic; DMS; Cr doped ZnTe; LDA; ASA; Substitution; Half metal;

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