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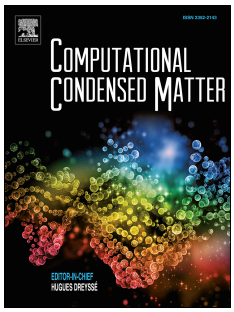

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Calculated magnetic properties of co-doped CdTe(V, P): first-principles calculations

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Abstract

In order to shed light on the magnetic properties of the host compound CdTe co-doped with the vanadium and the phosphorus elements. This work aims to contribute to the research for development and innovation to find new materials used in spintronic devices. For this purpose, we apply the first-principles calculations. We have investigated and discussed the half-metallic ferromagnetic behavior and the polarization as function of the concentrations of the diamagnetic compound phosphorus. The Korringa–Kohn–Rostoker (KKR) method is combined with the coherent potential approximation, within the local density approximation. Moreover, analyzing the calculated density of states, the mechanism of the exchange coupling interaction has been investigated. Furthermore, the stability of the system is studied by calculating the total energies. Besides, we have estimated and compared the evolution of the Curie temperature in connection with the room temperature. The theoretical Curie temperature is estimated by using the mean field approximation. Finally, as a function of the concentrations of phosphorus we have shown how the crystal field and the exchange splittings vary.

Keywords: DMS; Semiconductors II-VI; CdVTe; Diamagnetic; Half metal; Double exchange;

1 Introduction

A major asset has been involved in the field of condensed matter research since the appearing, in the last century, the ferromagnetism in semiconductors initially nonmagnetic. This change of state is due to the substitution doping by the transition metals or the rare earths [1], the ions bearing a magnetic moment or densities of charges [5]. These compounds are known by the diluted magnetic semiconductor (DMS) and are several. The fact of associating the usual properties of a semiconductor with magnetic properties remains the most obvious way to carry out a polarization and the injection of a polarized current into a semiconductor because this solution, DMS / semiconductor is free from the fundamental problem of conductivity mismatch that exists between a metal junction ferromagnetic / semiconductor [6]. The host materials constituting the DMSs, depend on a combination set within the periodic table, III–V, II–VI, IV–VI and IV. The properties of these compounds differ according to their structures crystalline and to the doping elements. The polarization of a charge current would be carried out via an exchange coupling existing between the electrons of the 3d levels of the dopants with the electrons responsible for the charge flow, that is to say those coming from the valence band. The hope is to obtain a ferromagnetic coupling for interesting magnetic properties. The Curie temperature of these materials

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