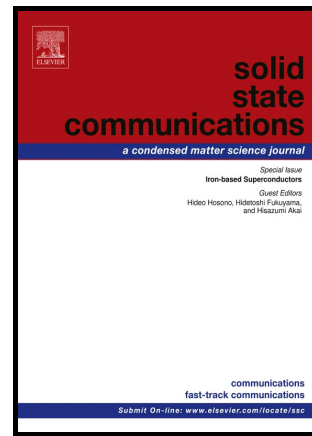


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Insight into the origin of magnetism in Iron-doped cadmium sulfide thin films from first principles calculations

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Abstract

We report a theoretical study of electronic structures and magnetic properties of Fe-doped CdS (10-10) thin films using first principle calculations within the density functional theory. It is shown that Fe atoms occupying Cd sites prefer to reside on the surface and couple antiferromagnetically. However, our results show the existence of competition between ferromagnetic and antiferromagnetic coupling because of the smaller total energy difference. Moreover, our density of states show the existence of a simultaneous hybridization between the Fe d and S p states near the Fermi level.

Key words: Thin films, magnetism, spintronic, ab initio

The development of new spintronic materials with high Curie temperatures remains priority of many scientists [1, 2]. As a particular magnetic material, dilute magnetic semiconductors (DMSs) have received a much attention due to combine of magnetic and semiconductor properties, hence high potential for spintronic materials [3-7]. Moreover, the importance of ferromagnetic semiconductors has increased due to their potential as spin-polarized carrier sources and the relative ease of their integration into spintronic devices [8, 9]. Nowadays, experimental and theoretical studies have been achieved to show ferromagnetic properties into the host semiconductor (e.g., GaAs, ZnTe, CdS) materials doped with transition metal impurities (e.g., V, Cr, Mn, Fe, Co or Ni). Following the prediction of Dietl *et al.* [10] based on the Zener mean-field model that the transition metals doped wide band gap semiconductors should result in a Curie temperature exceeding room temperature. Recently, the

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