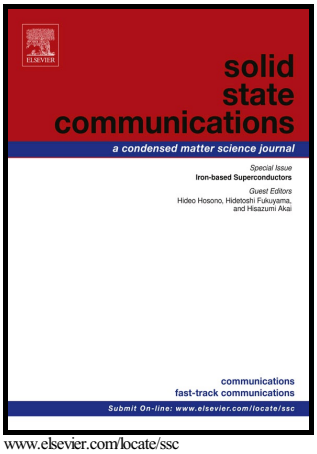
Insight into the origin of magnetism in Iron-doped cadmium sulfide thin films from first principles calculations

Mohammed Benali Kanoun



www.elsevier.com/locate/ssc

PII: S0038-1098(17)30029-7
DOI: http://dx.doi.org/10.1016/j.ssc.2017.01.021
Reference: SSC13131

To appear in: *Solid State Communications*

Received date: 11 August 2016
Revised date: 19 November 2016
Accepted date: 20 January 2017

Cite this article as: Mohammed Benali Kanoun, Insight into the origin o magnetism in Iron-doped cadmium sulfide thin films from first principle calculations, *Solid State Communications* http://dx.doi.org/10.1016/j.ssc.2017.01.021

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

Mohammed Benali Kanoun

College of Science, Department of Physics, Alfaisal University, Riyadh 11533, Saudi Arabia

mkanoun@alfaisal.edu

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