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DFT Study of Diluted Magnetic Semiconductor $Cd_{1-x}Cr_xS$ at x=3.125%

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Abstract

We investigate the structural, Electronic and Magnetic properties of Cd1-xCrxS diluted Magnetic Semiconductor (x=0.03125) in Zinc Blende (B3) phase. The calculations have been performed using Density functional theory as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms code using local density approximation as exchange-correlation (XC) potential. Calculated electronic band structures and magnetic properties of Cd1-xCrxS are discussed in terms of contribution of Cr 3d5 4s1, Cd 4d10 5s2, S 3s2 3p4 orbital's. Study of band structures shows half-metallic ferromagnetic nature of Cd1-xCrxS. The calculated values of s-d exchange constant Nα and p-d exchange constant Nβ shows the magnetic nature of these compounds.

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Keywords: DMS, CdS, DFT, Mn, Siesta Introduction

1. Introduction

II-VI wide band gap semiconductors represent a large family of compounds having physical properties that are suitable for developing opto electronic devices. They still remain the most netural candidates for red, blue and green lasers and LED's which are widely used for the production of full colour visible optical devices[1,2].Half-metallic

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diluted magnetic semiconductors (DMS) have attracted enormous attention due to their interesting physical properties and possible applications in the spin based devices [3-7].These materials are alloys of semiconductors in which some cations are substituted by transition metal (TM) ions while the crystal field structure of the host material is maintained. Half-metals are considered to be the ideal materials for spintronics.

In 1960, Cr doped II-VI compounds are being used in light emitting diodes, blue lasers and fluorescent displays. These crystals have drawn considerable interest for their possible application in magnetic semiconductors for spintronics, transparent conducting oxides, up and down converters and intermediate band solar cells. [8].The most studied transition metals in DMSs are Mn, Fe and Co. Cr based DMSs present some different and new characteristics which are not present in other DMSs. In the present work we expected half metallic ferromagnetic materials will be obtained by doping CdS semiconductor with 3d transition metal like Cr. CdS is a wide band-gap II-VI semiconductor. These compound are expected to be one of the most vital materials for high-performance opto-electronics devices. Fabrication of these materials is proposed by Saito and Yoshida [9] theoretically, room temperature ferromagnetism in $Zn_{1-x}Cr_xTe$ has been studied experimentally by saito et al. [10]. In this paper, we have performed the first principle calculations to examine the structural, electronic and magnetic properties of $Cd_{1-x}Cr_xS$ in the B3 phase at x= 0.03125.

2. Method of Calculation

The Calculations have been performed using DFT as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms[11] using Local Density Approximation with exchange correlation potential of CA [12]. We consider 2*2*1 standard 32 atoms per super cell of zinc blende phase with cubic symmetry, in which we replace one Cd atom with one Cr atom randomly to simulate 0.03125 concentrations in CdMnS semiconductor. The energy of 80meV is used to define the real space grid and the Brillioun zone is sampled by a 4*4*4 Monk horst-Pack grid. The core electrons are described by norm conserving scalar relativistic pseudo-potentials constructed using Troullier-Martins parameterization [13] including non linear core correction for Transition-metal atoms. Since the super cell contains only one Cr atom and a infinite crystal is constructed by repetition of this super cell, all Cr atoms have the same neighbouring atoms and have same spin. The $Cd_{1-x}Cr_xS$ phases are ferromagnetic and well-ordered. The atomic positions as well as lattice parameters are allowed to relax until forces are smaller than 0.04 eV/Å.

3. Results and Discussion

3.1. Structural Properties

The equilibrium lattice parameters for ferromagnetic state of $Cd_{1-x}Mn_xS$ diluted magnetic semiconductor at x=3.125% calculated by varying the lattice parameter about experimental value. The structural optimization is performed by minimizing the total energy with respect to unit cell volume using Murnaghan's equation of state. The procedure consisted of fitting the values of total energy as functions of the unit cell volume using the Murnaghan's equation [14] given by

$$E(V) - E(V_0) = \frac{B_0 V}{B_0'}\left[\frac{\left(V_0/V\right)^{B_0'}}{B_0'-1}+1\right]-\frac{B_0 V_0}{B_0'-1} \quad (1)$$

$$B_0 = V\frac{\partial^2 E}{\partial V^2} \quad (2)$$

Where B_0 is the bulk modulus given by eq. (2), V_0 is the equilibrium volume, $E(V_0)$ is the energy in equilibrium volume, is the pressure derivative of the bulk modulus .