AB INITIO CALCULATIONS OF ELECTRONIC BAND STRUCTURE OF CdMnS SEMIMAGNETIC SEMICONDUCTORS

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I. INTRODUCTION

CdS is an attractive semiconductor in the photoconductive, photovoltaic, optoelectronic materials. Doping of transition metals in nonmagnetic CdS is very important to make this material multifunctional. Room temperature CdS based semimagnetic semiconductors (SMSC), such as Mn doped CdS is a very good photo-luminance compound due to d states at the top of the valence band and intra-d shell transitions. [1].

This work devoted to theoretical investigations of $Cd_{1-x}Mn_xS$ SMSC. The Mn-CdS sheet with 16 atom supercell is analyzed by Kumar et al. [2]. The electronic band structure of wurtzite CdS calculated by Rantala et al. using two different self-consistent ab initio LDA methods [3]. Nabi [4] investigated electronic and magnetic properties of Mn doped CdS in wurtzite phase, using ab-initio calculations based on LDA, GGA and LDA + U exchange and correlation functionals. Ahmed et al. [1] investigated electronic band structure of $Cd_{1-x}Mn_xS$ (x = 6.25 %) using spin-polarized density functional theory (DFT) within the framework of Generalized Gradient Approximation (GGA), its extension via on-site Hubbard U interactions (GGA + U) and a model for exchange and correlation potential Tran modified Becke-Johnson (TB-mBJ).

The purpose of this work was to calculate the electronic band structure of ideal and defective $Cd_{1-x}Mn_xS$ SMS in both antiferromagnetic (AFM) and ferromagnetic (FM) phases.

II. METHODS AND RESULTS

Ab initio calculations are performed in the Atomistix Toolkit (ATK) program within the Density Functional Theory (DFT) and Local Spin Density Approximation (LSDA) on Double Zeta Double Polarized (DZDP) basis. We have used Hubbard U potential U_{Mn} = 3.59 eV for 3d states for Mn atoms [5, 6]. Supercells of 8 and 64 atoms were constructed. After the construction of $Cd_{1-x}Mn_xS$ (x = 0; 6.25 %; 25%) supercells, atom relaxation and optimization of the crystal structure were carried out. Electron band structure, density of states were calculated, total energy have been defined in AFM and FM phases (fig.1).

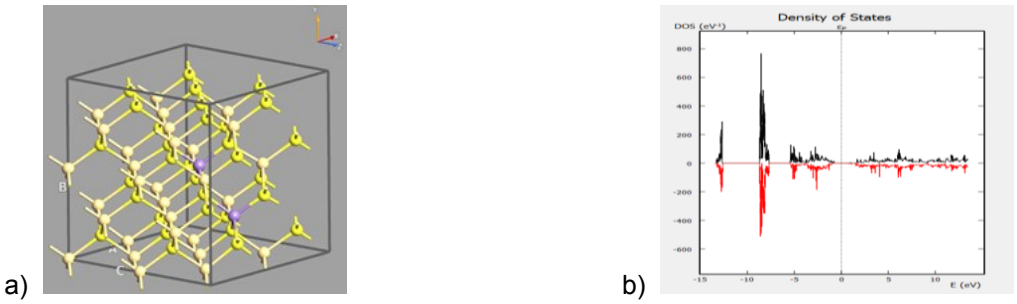

Figure 1. $Cd_{30}Mn_2S_{32}$ supercell a) bulk configuration b) density of states

Our calculations show that the band gap increases with the increases in Mn ion concentration. Obtained theoretical results correspond to experimental investigations carried out by Selma M.H [7]. It has been established that Cd or S vacancy in the crystal structure leads to the change of band gap, deep levels appear in the band gap, Fermi level shifts towards the valence or conduction band (fig.2).

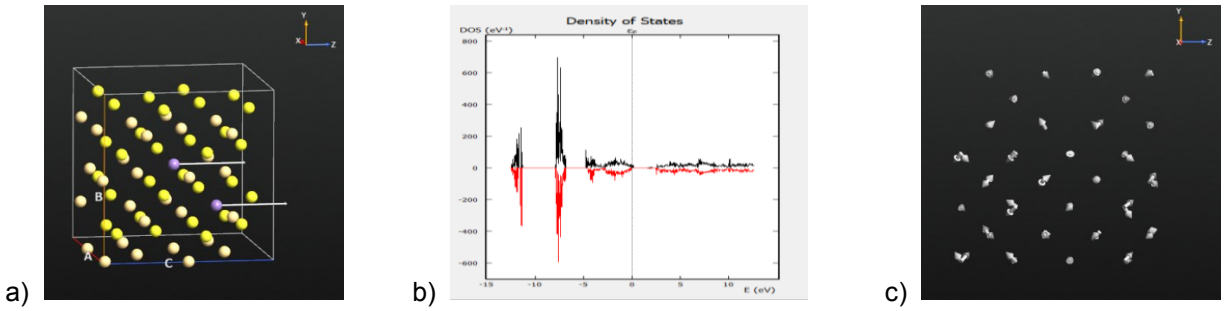

Figure 2. Cd vacancy in $Cd_{30}Mn_2S_{32}$ supercell a) bulk configuration b) density of states c) forces

III. CONCLUSIONS

It was defined that band gap of $Cd_{1-x}Mn_xS$ SMSC increases with the increases in Mn ion concentration. It has been established that defects as Cd or S vacancy in the crystal structure leads to the change of band gap, formation of deep levels in the band gap, shifting of Fermi level towards the valence or conduction band.

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