# First-principle Calculations of Electron Band Structure of $Cd_{1-x}Fe_xS$

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***Abstract*—** Cadmium sulfide (CdS) is a significant semiconductor with wide band gap $E_g$ =2.42 eV at the room temperature. CdS has hexagonal lattice structure at the ambient pressure and temperature. The transition metal like iron is employed as a doping material to enhance the spin polarization in CdS compound. Iron (Fe) behave as a good ferromagnetic material (FM). Fe doped CdS band gap can be controlled by variation of Fe concentration. CdS based semimagnetic semiconductors are perspective materials for solar photoconverters, radiation detectors, electronic gadgets like ultra-fast optical switches, spin valves, logic devices and magnetic sensors.

In this work, ab initio calculations were applied to $Cd_{1-x}Fe_xS$ supercells of 64-atom (x=0.0625), 16-atom (x=0.14) and 8-atom (x=0.25). Electronic band structure of semimagnetic semiconductors $Cd_{1-x}Fe_xS$ ($x$= 0.0625, 0.14, 0.25) was calculated by using density functional theory on the Double Zeta Double Polarized basis on Local Spin Density Approximation using Hubbard U potential in Atomistix ToolKit program. We corrected the value of $E_g$ for $Cd_{1-x}Fe_xS$ by applying the Hubbard $U$ potential. It was defined that, band gap of $Cd_{1-x}Fe_xS$ with $x$= 0.0625 is $E_g$ =2.3 eV, with $x$= 0.14 is $E_g$ =2.2eVand with $x$= 0.25 is $E_g$ =2.14eV. As the concentration increases, the value of the band gap decreases, which is due to the interaction of CdS band electrons with d electrons of $Fe^{+2}$ ions.

***Keywords*—**Electronic band structure, ab-initio calculations, semimagnetic semiconductors, band gap.

## I. INTRODUCTION

CdS (band gap 2.43 eV) has a special place among photoconductive, photovoltaic and optoelectronic materials. [1-5]. It should be noted that Mn, Fe, Ni, Co, etc. doping of transition metals in non-magnetic CdS and multifunctionality of this material is of great importance, including in the field of spintronics. [6,7]. At room temperature, CdS-based semiconductors (SMSCs), such as Fe-doped CdS, are considered very good photoluminescent compounds due to their d-states above the valence band as well as inner d-shell transitions [. Initially, our calculations were performed within the framework of Density Functional Theory (DFT) and Local Spin Density Approximation (LSDA) based on Double Zeta Double Polarized (DZDP) in the Atomistix Toolkit (ATK).

In this work, ab-initio calculations of $Cd_{1-x}Fe_xS$ semimagnetic semiconductors (SMSC) using Density Functional Theory (DFT) are investigated. DFT has been used in theoretical studies of magnetic materials [8-12]. It is clear that the band structure of defective $Cd_{1-x}Fe_xS$ is less studied than that of SMSC.

## II. RESULTS

As a result of the calculations, the value of the band gap for CdTe was determined to be Eg =0.5 eV, while the literature shows 2.44 eV [6], but this value difference is related to the DFT theory. We corrected this band gap value for CdTe (fig.1) and $Cd_{1-x}Fe_xS$ (fig.2) by applying a Hubbard U potential. In this study, ab-initio calculations based on DFT with Hubbard U correction to evaluate the crystal structure, Fe impurity formation energy, and electronic structure. This study performed ab initio calculations based on density functional theory with Hubbard U correction to evaluate the crystal structure, Fe impurity formation energy, and

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electronic structure [7].

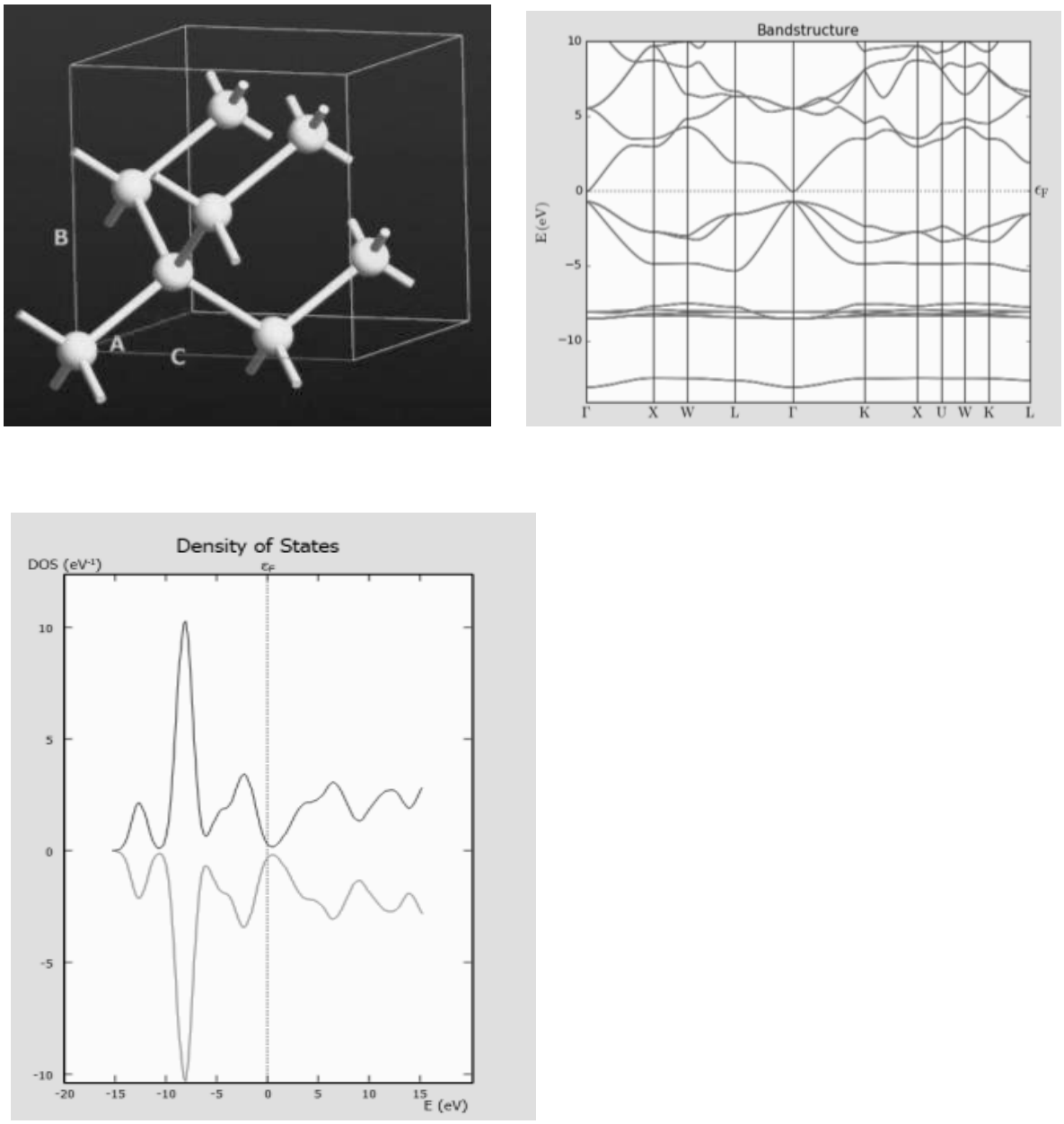


Fig.1. Supercells of CdS of 8 atoms for FM phase a) bulk configuration b) electronic band structure **c**) density of states

We should also note that the calculated band gap Eg value of $Cd_{1-x}Fe_xS$ SMSC for x = 0.14, x = 0.25 and x= 0.0625 was found to be Eg = 2.20 eV, Eg = 2.14 eV and Eg = 2.3 eV, respectively. It is clear that the Eg value decreases with increasing Fe concentration, which is attributed to the interaction of CdS band electrons with d electrons of Fe+2 ions (Table1.)

The theoretical results obtained by us are consistent with the experimental data on $Cd_{1-x}Fe_xS$ with different Fe concentrations prepared by the electrodeposition technique [6]. In our previous works, we calculated the electronic band structure, DOS and specific band gap, total energy, and magnetic moments of some SMSC by the ab-initio method.

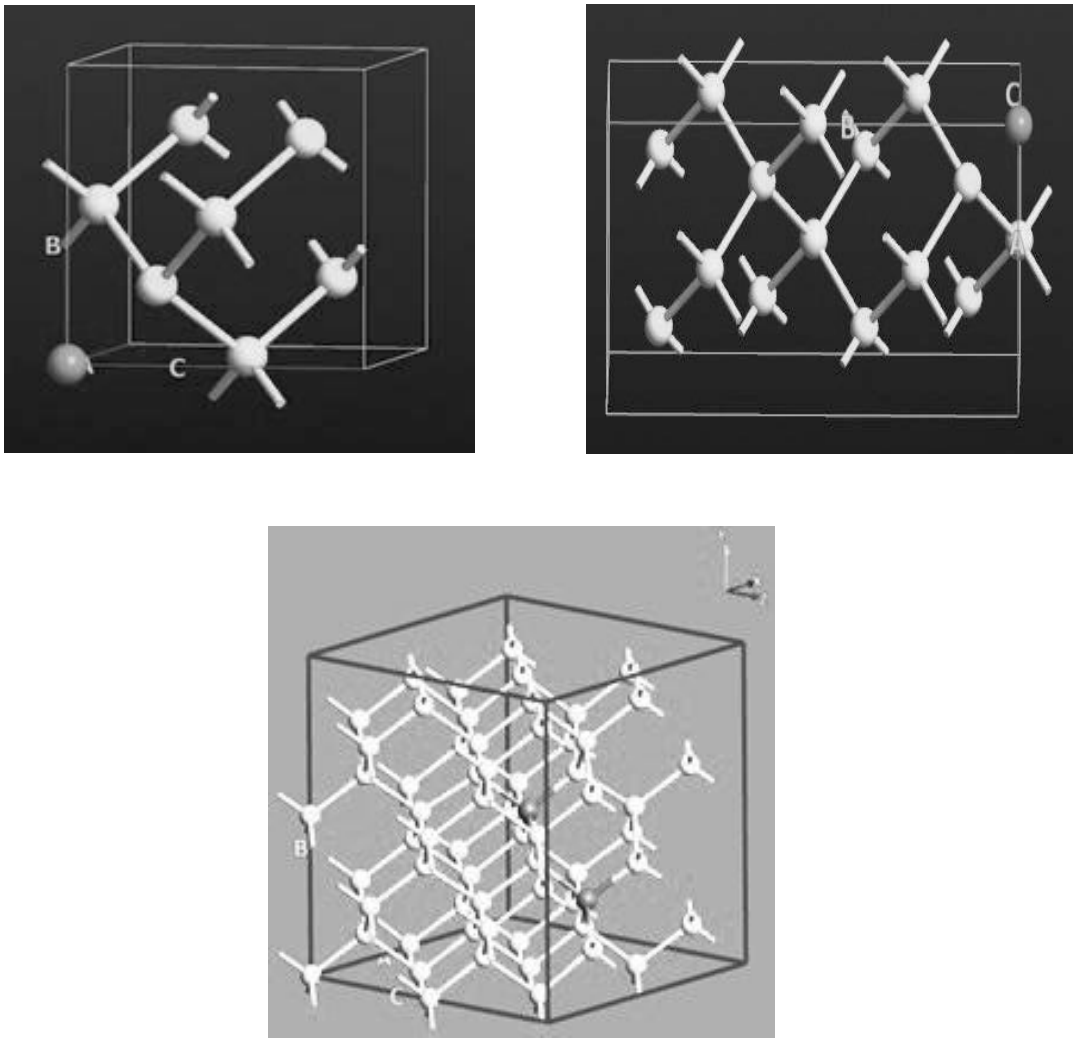


Fig.2. Bulk configuration of $Cd_{1-x}Fe_xS$ in FM phase a) $x = 0.25$, b) $x = 0.14$, c) x=0.0625

Table1.
The band gap data for $Cd_{1-x}Fe_xS$

| № | *x* | *Eg* (300 K), eV |
|---|---|---|
| 1 | 0 | 2.44 |
| 2 | 0.14 | 2.20 |
| 3 | 0.25 | 2.14 |
| 4 | 0.0625 | 2.3 |

In $Cd_{1-x}Mn_xTe$ and $Cd_{1-x}Fe_xTe$ SMSC, it was determined that the band gap value increases as the concentration of Mn, Fe in transition metals increases, but in $Cd_{1-x}Mn_xSe$ and $Cd_{1-x}Fe_xS$ SMSC, the band gap value decreases when the concentration of Mn, Fe in transition metals increases.

## III. Conclusion

In the presented work, the electronic behavior and optical properties of the Fe-doped CdS compound at different concentrations were studied using the DFT method. Ab initio

calculations were applied to 64-atom (x=0.0625), 16-atom (x=0.14) and 8-atom (x=0.25) $Cd_{1-x}Fe_xS$ supercells. Electronic band structure, density of states, band gap were calculated by ab initio method by applying Density Functional Theory. It was determined that the value of the band gap decreases as the concentration increases, and it was determined that the CdS band electrons are related to the interaction of $Fe^{+2}$ ions with d electrons.

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