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AB INITIO CALCULATIONS OF DEFECTS IN $Cd_{1-x}Mn_xTe(Se)$ SEMIMAGNETIC SEMICONDUCTORS

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Abstract: Ab initio calculations were used to define electronic band structure and density of states of ideal and defective $Cd_{1-x}Mn_xTe(Se)$ (x=0.13). Total energy, magnetic moment, number of valence electrons for the ideal and defective supercells were determined. The calculated band gap for $Cd_{1-x}Mn_xTe$ was E_g =1.69 eV and for $Cd_{1-x}Mn_xSe$ E_g =1.66 eV. Vacancy leads to an increase in the band gap, change in the total energy, formation of local levels in the band gap, and magnetic moments near the defects.

Keywords: Semimagnetic semiconductor, defect, ab initio, band structure, density of states, band gap.

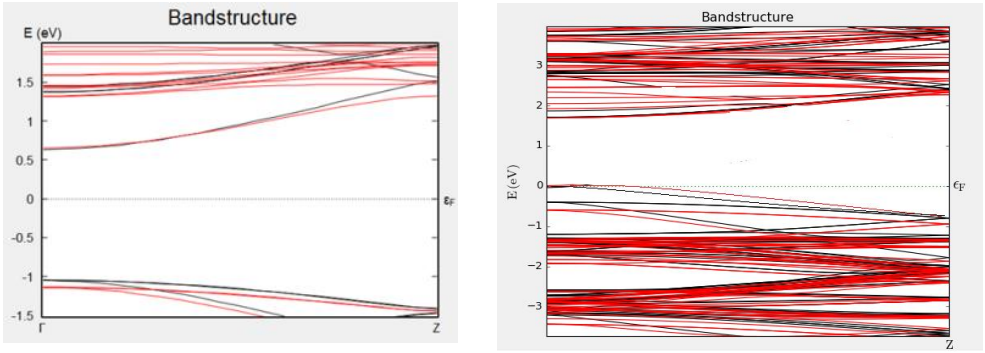
1. Introduction

Semimagnetic semiconductors (SMS) $Cd_{1-x}Mn_xTe(Se)$ are considered a good material for microelectronics, optoelectronics, and spintronics. Several instruments, including solar cells, radiation detectors, IR detectors, photodetectors, optical isolators, etc. were created based on of these semiconductors [3,4,7,12,13,15]. Obtain of radiation-resistant and radiation-sensitive materials with stable electrical and optical characteristics is one of the actual issues of modern physics. It should be noted that there are some works [1,2,5,6,14] devoted to the study of the processes of radiation defect formation (RDF) in bulk crystals. However, there are no unique models for the formation, mechanism, and evolution of RDF in SMS, their epitaxial films and structures based on them.

In our previous works, we have calculated electronic band structure (EBS), the density of states (DOS) by ab-initio method and defined band gap, total energy, magnetic moments of the ideal and defective $Cd_{1-x}Mn_xTe(Se)$ semimagnetic semiconductors for some supercells [8-11]. In the present paper, it has been studied defect states of $Cd_{1-x}Mn_xTe(Se)$ for x = 0.13 concentration of Mn atoms.

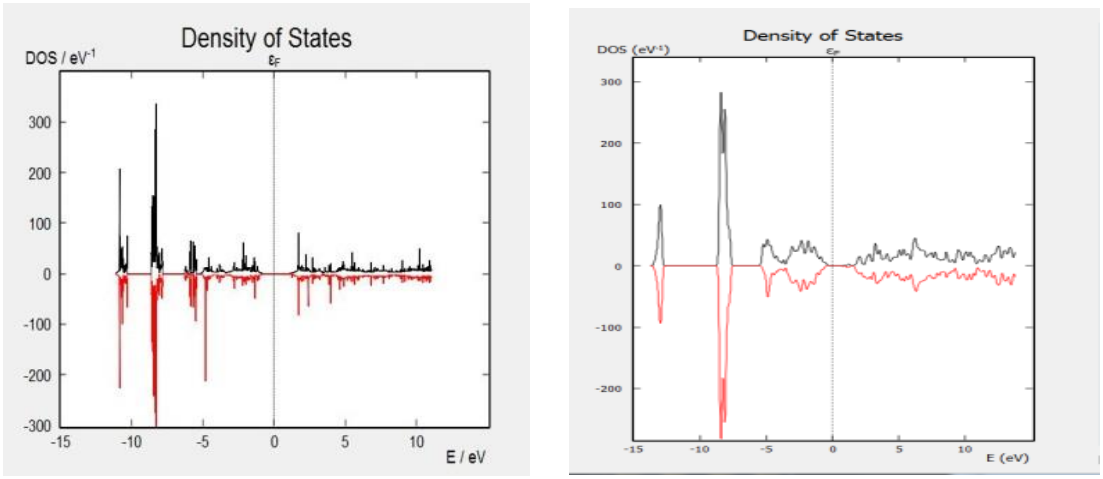
2. Ab initio calculations of electronic band structure for $Cd_{1-x}Mn_xTe(Se)$

The purpose of this work was to calculate the electronic band structure of ideal and defective $Cd_{1-x}Mn_xTe(Se)$ SMS of x = 0.13. 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 [4, 15]. After the construction of supercells $Cd_{1-x}Mn_xTe(Se)$ (x=0.13), atom relaxation and optimization of the crystal structure were carried out. Supercells of 32 (x = 0.13) atoms are considered. EBS, DOS was calculated and total energy, magnetic moment, number of valence electrons for the of ideal and defective supercells $Cd_{1-x}Mn_xTe(Se)$ (x = 0.13) have been defined in both antiferromagnetic (AFM) and ferromagnetic (FM) phases (fig.1, fig.2). The calculated band gap for $Cd_{1-x}Mn_xTe$, x=0.13 was E_g =1.69 eV, for $Cd_{1-x}Mn_xSe$, x=0.13 was E_g =1.66 eV.



a) b)

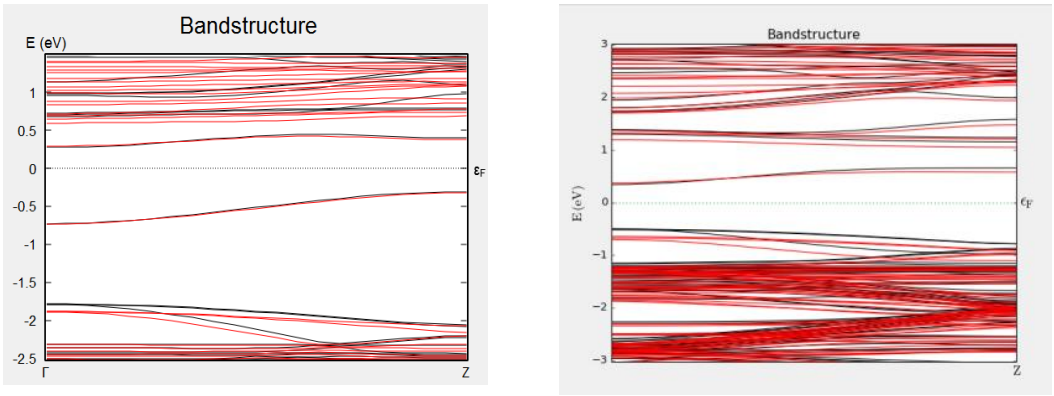
Fig.1 Electronic band structure for FM phase for x = 0.13 a) $Cd_{1-x}Mn_xTe$ b) $Cd_{1-x}Mn_xSe$



a) b)

Fig.2 Density of states for FM phase for x = 0.13 a) $Cd_{1-x}Mn_xTe$ b) $Cd_{1-x}Mn_xSe$

Ab initio calculations of EBS have been carried out for defective supercells $Cd_{1-x}Mn_xTe(Se)$, $x = 0.13$. Vacancy type defect was considered. It has been established that vacancy leads to the following changes: the band gap changes, deep levels appear in the band gap, Fermi level shifts towards the valence or conduction band, magnetic moments appear near the defects, the transition occurs from FM to AFM phase and vice versa (fig.3).



a) b)

Fig.3 Electronic band structure of supercells a) $Cd_{1-x}Mn_xTe$ (x=0.13), Te vacancy b) $Cd_{1-x}Mn_xSe$ (x=0.13), Se vacancy

3. Conclusion

It has been calculated the electronic band structure, density of states, band gap, total energy of the ideal and defective $Cd_{1-x}Mn_xTe(Se)$ (x=0.13) by the ab-initio method using the Functional Density Theory. It has been established that, with the change of Mn concentration, the band gap changes too. The calculated band gap for $Cd_{1-x}Mn_xTe$, x=0.13 was E_g =1.69 eV, for $Cd_{1-x}Mn_xSe$, x=0.13 was E_g =1.66 eV. Vacancy type defects lead to an increase in the band gap, change in the total energy, formation of local levels in the band gap and magnetic moments near the defects.

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РАСЧЕТЫ ИЗ ПЕРВЫХ ПРИНЦИПОВ ДЕФЕКТОВ В ПОЛУМАГНИТНЫХ ПОЛУПРОВОДНИКАХ $Cd_{1-x}Mn_xTe(Se)$

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Резюме: Из первых принципов были рассчитаны электронная зонная структура и плотность состояний идеального и дефектного $Cd_{1-x}Mn_xTe(Se)$ (x=0,13). Определены полная энергия, магнитный момент, количество валентных электронов для идеальной и дефектной суперячеек. Рассчитанная ширина запрещенной зоны для $Cd_{1-x}Mn_xTe$ составляла E_g=1,69 эВ, а для $Cd_{1-x}Mn_xSe$ E_g=1,66 эВ. Определено, что вакансия приводит к увеличению ширины запрещенной зоны, изменению полной энергии, образованию локальных уровней в запрещенной зоне и магнитных моментов вблизи дефектов.

Ключевые слова: Полумагнитный полупроводник, дефект, из первых принципов, зонная структура, плотность состояний, запрещенная зона.

$Cd_{1-x}Mn_xTe(Se)$ YARIMMAQNİT YARIMKEÇİRİCİLƏRİNDƏ DEFEKTLƏRİN TƏMƏL PRİNSİPLƏRDƏN HESABLANMASI

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Xülasə: Təməl prinsiplərdən ideal və defektli $Cd_{1-x}Mn_xTe(Se)$ (x=0.13) yarımmaqnit yarımkeçiricilərinin elektron zona quruluşu və hal sıxlığı hesablanmışdır. İdeal və defektli super özəklər üçün tam enerji, maqnit moment, valent elektronların sayı müəyyən edilmişdir. Qadağan olunmuş zonanın eni $Cd_{1-x}Mn_xTe$ üçün E_g=1.69 eV, $Cd_{1-x}Mn_xSe$ üçün E_g=1.66 eV təşkil etmişdir. Müəyyən edilmişdir ki, vakansiya tipli defekt qadağan olunmuş zonanın eninin artmasına, ümumi enerjinin dəyişməsinə, qadağan olunmuş zonada lokal səviyyələrin əmələ gəlməsinə və defektlərin ətrafında maqnit momentlərinin yaranmasına səbəb olur.

Açar sözlər: Yarımaqnit yarımkeçirici, defekt, təməl prinsip, elektron zona quruluşu, hal sıxlığı, qadağan olunmuş zonanın eni.