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Ab initio study of defects in CdMnTe: Electronic structure and related properties

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Abstract: Band structure, density of states, total energy and magnetic moment are calculated for ideal and defective supercell CdTe and CdMnTe by ab initio method. The optimization of crystal structure and atom relaxation has been carried out. The band gap, local levels in the band gap and magnetic moments are defined for various defective supercell CdTe and CdMnTe in ferromagnetic and antiferromagnetic states. It has been defined that as Mn atoms, the vacancy, interstitial atom and Frenkel pair in the crystal structure form magnetic moment.

Keywords: Semimagnetic Semiconductor, Electron Structure, Defect, Vacancy, Interstitial Atom, Frenkel Pair, Ab Initio, Magnetic Moment, Density of States

1. Introduction

Semimagnetic semiconductors (SMS) are the new class materials, including the properties of both ordinary and magnetic semiconductors. The main qualitative difference between SMS and ordinary semiconductors is the exchange interaction between magnetic ions and band charge carriers, which start to appear only within the external magnetic field [1]. The injection of manganese ions to the crystal lattice of $A^{II}B^{VI}$ compounds and formation of solid solutions $A^{II}MnB^{VI}$ lead to increase of band-gap width. Thus it is possible to manage these materials' photosensitivity by Mn ions concentration in SMS. These features cause strengthening of a number of effects, as well as Faraday effect in these materials [2, 3]. On the other hand, there are unusual changes of electron structure of these materials in magnetic field, which allows managing properties of these materials with magnetic field and temperature.

The energy spectrum and wave functions of electrons for arbitrary wave vector as well as Faraday effect for $Cd_{1-X}Mn_xTe$ thin films were obtained in our previous works [3]. We calculated interband Faraday effect in $Cd_{1-X}Mn_xTe$ in the framework of two band model with taking into account the exchange interaction in a nonquantizing magnetic field.

$Cd_{1-x}Mn_xTe$ SMS are promising materials for γ- and x-ray detectors, solar cells, optic insulator etc. [4]. To obtain high-sensitive and radiation-resistant materials, as well as creation of devices based on them, it is necessary to know the influence of defects on physical properties of $Cd_{1-x}Mn_xTe$. Defects in semiconductors not only influence on electrical and optic properties of these materials, but also display their interesting physical properties.

Ab initio calculations of electron structure and magnetic properties of $Cd_{1-X}Mn_xTe$ were carried out in some works [5-8]. Unlike these works we carried out first principle calculations based on density functional theory (DFT) by using Atomistix ToolKit (ATK) programme for study of defects on structural and magnetic properties of supercell CdTe and $Cd_{1-X}Mn_xTe$. In this work we have theoretically investigated electronic band structure (EBS), density of states (DOS) and magnetic moment (MM) for various ideal and defective supercells CdTe and $Cd_{1-x}Mn_xTe$.

2. Electronic Structure of Ideal and Defective Supercell CdTe

The first-principle calculations of electronic structure of ideal and defective supercells CdTe based on spin- polarized

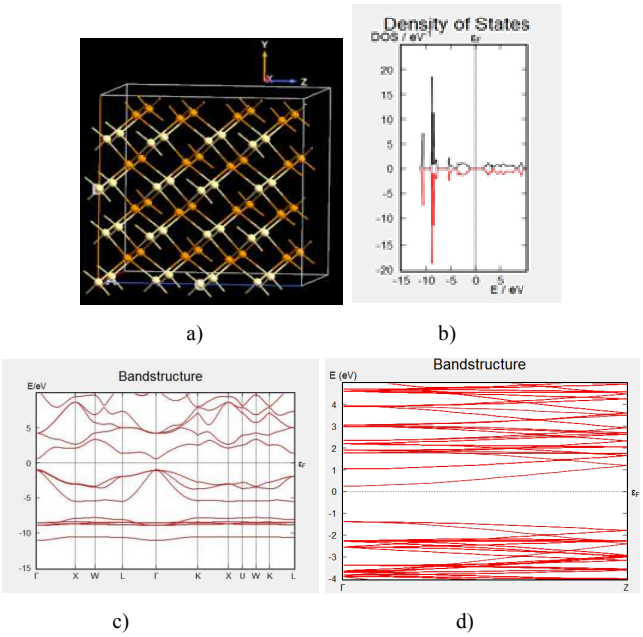
DFT are performed in the local spin density approximation with regard to Hubbard-U correction (LSDA+U) on double zeta double polarized (DZDP) basis set using licensed program software ATK [9].

In this section it was given the results of calculations of EBS, DOS and MM of ideal and defective supercell Cd32Te32.

2.1. Ideal Supercell Cd32Te32

The electronic structures of ideal supercell Cd32Te32 is calculated. It was defined the band gap of ideal supercell Cd32Te32 E_g = 1.64eV, the lower level of conductivity band $E_{c\uparrow}$=0.25 eV and the upper level of valence band $E_{v\downarrow}$=-1.39 eV. The axes indicate to the spin states. The calculated value of the energy gap corresponds to experimentally measured one. In so doing, we have been able to reproduce the experimental value of the energy gap only if Hubbard_U corrections were accounted for. It has been taken the value of Hubbard-U parameter for 5p-states of Te, U_{Te}= 3.7 eV [10]. DOS analysis shows that upper levels of valence band located in the range of [-5; 0] eV, mainly comes from 5p-states of Te atoms, and lower levels of conductivity band - from 5s-states of Cd atoms (Fig.1). The total energy of the ideal supercell Cd32Te32 is E_t=-68285.96eV.

The Cd atoms in bulk configuration (Fig.1a) is indicated by yellow color, Te atoms by red color.



a) b)

c) d)

Fig. 1. *Ideal supercell Cd32Te32 a) Bulk configuration b) DOS c) EBS for CdTe d) EBS for supercell Cd32Te32*

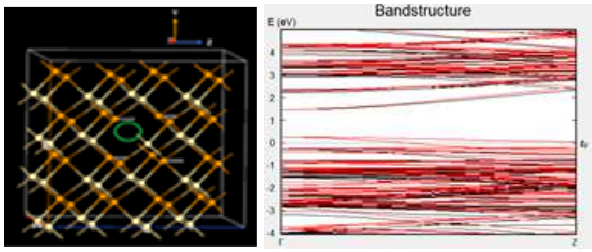
2.2. Defective Supercell Cd32Te32

2.2.1. Vacancy in the Supercell Cd32Te32

The Cd vacancy (V_{Cd}) in supercell Cd32Te32 leads to rupture of Cd bonds with nearest four Te atoms. The main contribution to the MM give these four anionic atoms with 4 dangling bonds totally 4.864μ_B, where μ_B is the Bohr magneton. The MM of all 32 Te atoms is 11.276μ_B, and all 31 Cd atoms is -9.271μ_B. Finally the total MM of all atoms is 2.005μ_B. The total amount of electrons is 564, spins of 283 of them directed upward, 281 downward.

Thus, the main contribution to the MM gives 5p orbitals of Te atoms in the upper of the valence band. The contribution from p_x, p_y, p_z orbitals are the same. Calculations were performed with an accuracy of 0.001 μ_B.

The electronic structure of supercell Cd32Te32 having V_{Cd} is calculated (Fig.2). The band gap is changed from Eg=1.64eV to Eg=1.22eV. It is formed no local level in the band gap. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=1.47eV, $E_{v\uparrow}$=0.25eV. The total energy of the supercell Cd32Te32 with V_{Cd} is E_t=-66730.36eV.



a) b)

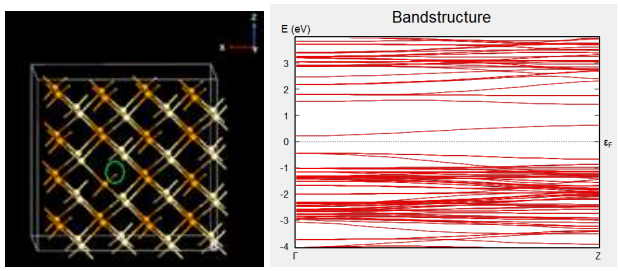
Fig. 2. *Supercell Cd32Te32 with V_{Cd} a) Bulk configuration b) EBS*

The contribution to MM of Cd vacancy (V_{Cd}) in the supercell Cd32Te32 was defined. 4 anion atoms which have 4 broken bonds near the Cd vacancy, acquires MM 4.864μ_B. The MM of all 31 Cd atoms is -9.271μ_B, and all 32 Te atoms is 11.276μ_B. The total MM of all atoms is 2.005μ_B.

The green circle in the Fig.2a indicates to the vacancy site.

The contribution to MM of Te vacancy (V_{Te}) in the supercell Cd32Te32 is insignificant. 4 cation atoms which have 4 broken bonds near the Te vacancy, acquires insignificant value of MM 0.004μ_B. The MM of all 31 Te atoms is 0.004μ_B, and all 32 Cd atoms is 0.011μ_B. The total MM of all atoms is 0.015μ_B.

The band gap is changed from E_g=1.64eV to E_g=1.97eV. It is formed 1 local level in the band gap: $E_{\uparrow}$=0.21eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\uparrow}$=1.53eV, $E_{v\uparrow}$=-0.44eV (Fig.3). The total energy of the supercell Cd32Te32 having V_{Te} is E_t=- 67692.97eV. The total amount of electrons is 568 and spins of 284 of them directed upward, 284 downward.



a) b)

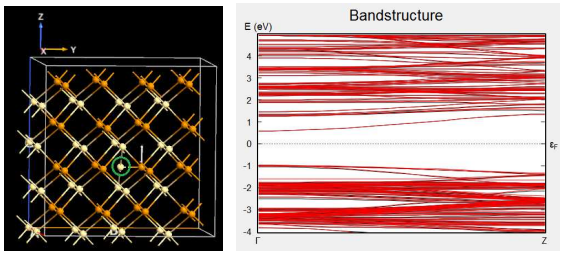
Fig. 3. *Supercell Cd32Te32 with V_{Te} a) Bulk configuration b) EBS*

Thus, V_{Cd} decrease the band gap in the supercell Cd32Te32 but V_{Te} increase it and forms 1local level in the band gap.

2.2.2. Interstitial Atom in the Supercell Cd32Te32

The electronic structure of supercell Cd32Te32 having interstitial Cd atom (I_{Cd}) has been calculated. The band gap doesn't changed. It is formed no local level in the band gap. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\uparrow}=E_{c\downarrow}=0.58$eV, $E_{v\uparrow}=E_{v\downarrow}=-1.05$eV (Fig.4). The total energy of the supercell Cd32Te32 having V_{Cd} is $E_t=-69844.74$eV.

I_{Cd} atom has 3 bonds: 2 bonds with Cd atoms and 1 bond with Te atom. I_{Cd} leads to forming MM. The main contribution to the MM give interstitial Cd atom $0.489\mu_B$, two Cd atoms each of them is $0.399\mu_B$ and Te atom $1.516\mu_B$ having bonds with interstitial Te atom. The MM of all 33 Cd atoms is $-1.469\mu_B$ and all 32 Te atoms is $1.464\ \mu_B$. Finally the total MM of all atoms is $-0.005\mu_B$.

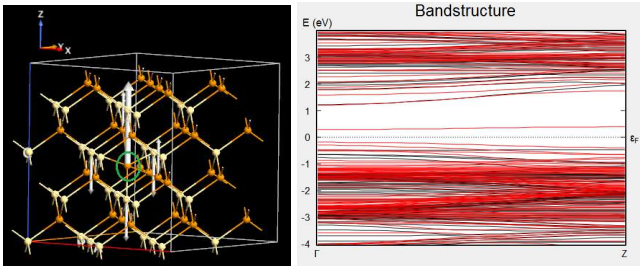


a) b)

Fig. 4. *Supercell Cd32Te32 with I_{Cd} a) Bulk configuration b) EBS*

The electronic structure of supercell Cd32Te32 having interstitial Te atom I_{Te} has been calculated. The band gap doesn't changed. It is formed 1 local level in the band gap: $E_{\uparrow}=0.29$eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\uparrow}=1.2$eV, $E_{v\uparrow}=-0.44$eV (Fig.5). The total energy of the supercell Cd32Te32 with V_{Cd} is $E_t=-68890.2$eV.

I_{Te} atom has 5 bonds: 2 bonds with Te atoms and 3 bonds with Cd atoms. I_{Te} leads to forming large MM. The main contribution to the MM give interstitial Te atom $5.467\mu_B$, two Te atoms each of them $2.521\mu_B$ and 3 Cd atoms each of them $2.9\mu_B$ having bonds with interstitial Te atom. The MM of all 32 Cd atoms is $-15.264\mu_B$ and all 33 Te atoms is $19.891\ \mu_B$. Total MM of all atoms is $4.627\ \mu_B$.



a) b)

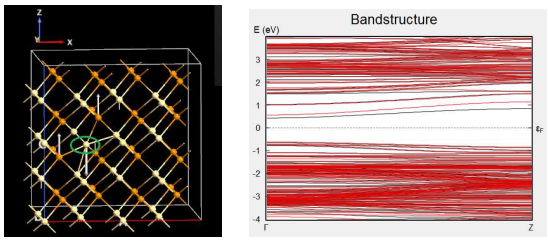
Fig. 5. *Supercell Cd32Te32 with I_{Te} a) Bulk configuration b) EBS*

Thus, I_{Cd} and I_{Te} atoms in the supercell Cd32Te32 don't change the band gap. It is formed large MM and 1local level in the band gap in the supercell Cd32Te32 having I_{Te}.

2.2.3. Frenkel Pair in the Supercell Cd32Te32

The displaced Cd atom has 5 bonds with neighboring 2 Cd atoms and 3 Te atoms in the case of Frenkel pair F_{Cd} in the supercell Cd32Te32. F_{Cd} in the supercell Cd32Te32 leads to forming 2 local levels in the band gap: $E_{\uparrow}=0.57$eV, $E_{\downarrow}=0.43$eV. The band gap doesn't changed. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow\uparrow}=1.0$eV, $E_{v\downarrow\uparrow}=-0.64$eV (Fig.6). The total energy of the supercell having F_{Te} is $E_t=-68283.4$eV.

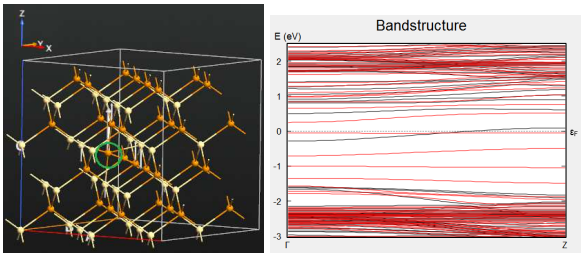
Frenkel pair F_{Cd} leads to forming MM. The main contribution to MM give interstitial Cd atom $-2.36\mu_B$, two Te atoms each of them $1.768\mu_B$ and 2 Cd atoms each of them $0.751\mu_B$ having bonds with interstitial Cd atom and neighboring Te atom $0.7451\mu_B$. The MM of all 32 Cd atoms is $-4.351\mu_B$ and all 32 Te atoms is $4.35\ \mu_B$. Totally MM's of all atoms compensate each other.



a) b)

Fig.6. *Supercell Cd32Te32 with F_{Cd} a) Bulk configuration b) EBS*

In the case of Frenkel pair F_{Te} in the supercell Cd32Te32 the displaced Te atom has 5 bonds with neighboring 2 Te atoms and 3 Cd atoms. F_{Te} in the supercell Cd32Te32 leads to forming 4 local levels in the band gap: $E_{\uparrow}=-0.05$eV, $E_{\downarrow}=-0.3$eV, $E_{\uparrow}=-0.7$eV, $E_{\uparrow}=-1.0$eV. The band gap doesn't changed. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\uparrow}=0.25$eV, $E_{v\downarrow\uparrow}=-1.35$eV (Fig.7). The total energy of the supercell Cd32Te32 having F_{Te} is $E_t=-68286.9$eV.



a) b)

Fig. 7. *Supercell Cd32Te32 with F_{Te} a) Bulk configuration b) EBS*

Frenkel pair F_{Te} leads to forming MM. The main contribution to MM give interstitial Te atom $3.112\mu_B$, two Te atoms each of them is $1.53\mu_B$ and 3 Cd atoms each of them is $0.751\mu_B$ having bonds with interstitial Cd atom and neighboring Te atom $1.694\mu_B$. The MM's of all 32 Cd atoms

is -5.35μ_B and all 32 Te atoms is 6.133 μ_B. Finally the total MM of all atoms is 0.783μ_B .

F_{Cd} and F_{Te} atoms in the supercell Cd32Te32 don't change the band gap. F_{Cd} forms 2 local levels and F_{Te} forms 4 local levels in the band gap in the supercell Cd32Te32. It is formed MM in the supercell Cd32Te32 having F_{Cd} or F_{Te} atom.

3. Electronic Structure of Defective Supercell $Cd_{1-x}Mn_xTe$

The calculations are performed in ATK program within the spin-polarized DFT and LSDA+U on DZDP basis. We have used U_{Mn} = 3.59 eV for 3d states for Mn atoms and U_{Te} = 3.7 eV for 5p states of Te atoms [10, 11]. It has been given the results of calculations of EBS, DOS and MM of defective supercell Cd30Mn2Te32 in both ferromagnetic and antiferromagnetic states.

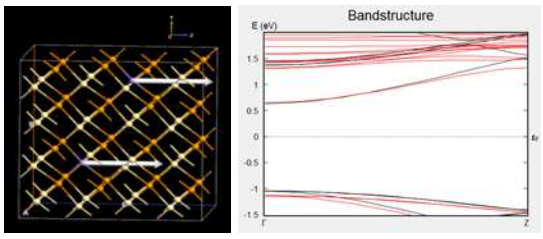
3.1. Supercell Cd30Mn2Te32

MM of *s*upercells Cd3MnTe4 and Cd15Mn2Te16 was calculated by ab initio method in the work [13].

We have investigated *s*upercell Cd30Mn2Te32 and have obtained that DOS of *s*upercell Cd30Mn2Te32 consist of three parts in the valence band: 1) the upper part of the valence band is mainly formed from p-states of Te atoms with some contribution of Cd s-states at bottom of the upper part 2) the middle part is formed from d-state of Mn atoms and from s-states of Cd atoms, which are below the valence band maximum on 7eV 3) the main peak at 10 eV below of the valence band maximum is formed mainly from s- states of Te atoms,.

The bottom of the conductivity band is formed from s states of Cd atoms and p states of Te atoms. The peak of 2 eV above the conductivity band minimum is formed mainly from d states of Mn atoms [12].

The calculated band gap in ferromagnetic supercell Cd30Mn2Te32 is Eg=1.73eV, the lower level of conductivity band is $E_{c\uparrow}$=0.632eV and the upper level of valence band is $E_{v\uparrow}$=-1.05eV (Fig.8). The total energy of the supercell Cd30Mn2Te32 in ferromagnetic supercell Cd30Mn2Te32 is E_t=-66403.14eV.



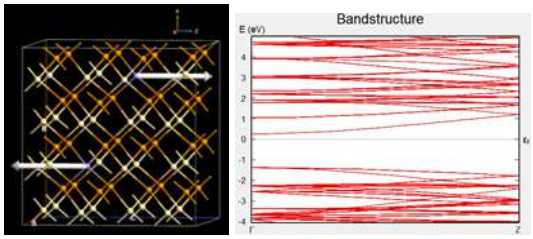
a) b)

Fig. 8. *Supercell Cd30Mn2Te32 in ferromagnetic state a) Bulk configuration b) EBS*

For the ferromagnetic *s*upercell Cd30Mn2Te32 the main contribution to the MM give 3d-orbitals of two Mn atoms, the total MM of them is 10,30μ_B. The MM of all 30 Cd atoms is -0.311μ_B and all 32 Te atoms is 0.406 μ_B, they are practically compensate each other.

The calculated band gap of supercell Cd30Mn2Te32 in antiferromagnetic state is E_g=1.73eV, the lower level of conductivity band is $E_{c\uparrow}$=0.31eV and the upper level of valence band is $E_{v\downarrow}$=-1.42eV (Fig.9). The total energy of supercell Cd30Mn2Te32 in antiferromagnetic state is E_t=-66403.1eV.

For the *s*upercell Cd30Mn2Te32 in antiferromagnetic state the main contribution to the MM give two Mn atoms, each of them leads to formation of MM 5.113μ_B. The MM of all 30 Cd atoms -0.02 μ_B, and all 32 Te atoms 0.024 μ_B. The total MM's of all atoms practically compensate each other. The total amount of electrons is 556 and spins of 278 of them directed upward, 278 downward.



a) b)

Fig. 9. *Supercell Cd30Mn2Te32 in antiferromagnetic state a) Bulk configuration b) EBS*

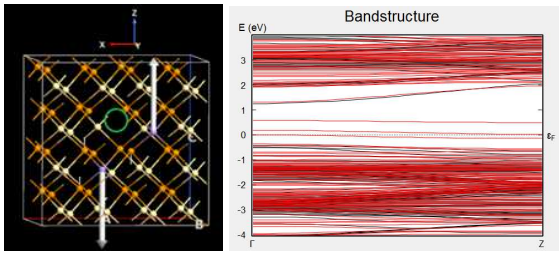
Thus, impurity of two Mn atoms into the supercell Cd30Mn2Te32 leads to forming large MM. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the antiferromagnetic state is more stable.

3.2. Defective Supercell Cd30Mn2Te32

3.2.1. Vacancy in the Supercell Cd30Mn2Te32

V_{Cd} in the supercell Cd30Mn2Te32 in antiferromagnetic state forms insignificant value of MM. The main contribution to MM give two Mn atoms, each of them leads to formation of MM 5.321μ_B. The MM which is acquired by four broken Te atoms with dangling bonds near the Cd atom is 0.319μ_B. The MM of all 29 Cd atoms is -0.119μ_B and all 32 Te atoms is 0.186μ_B. Finally the total MM of all atoms is -0.008μ_B .

The band gap doesn't changed Eg=1.73eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=1.25eV, $E_{v\downarrow\uparrow}$=-0.5eV. It is formed 3 local levels in the band gap $E_{\uparrow}$=0.eV, $E_{\uparrow}$=0.2eV, $E_{\uparrow}$=0.6eV (Fig.10).



a) b)

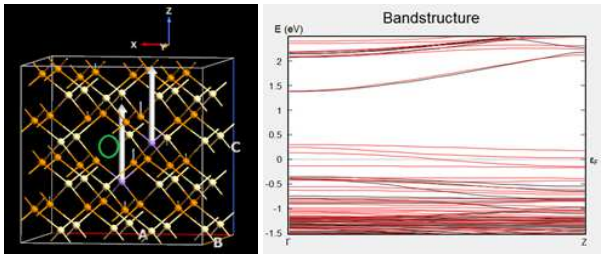
Fig. 10. *Supercell Cd30Mn2Te32 with V_{Cd} in antiferromagnetic state a) Bulk configuration b) EBS*

The total energy of supercell Cd30Mn2Te32 having V_{Cd} in antiferromagnetic state is E_t=-64848.24eV.

V_{Cd} in the supercell Cd30Mn2Te32 in ferromagnetic state forms large MM due to the two Mn atoms, each of them leads to formation of MM 5,065μ_B, and 4 broken Te atoms with dangling bonds near the Cd atom. The MM of all 29 Cd atoms is 6.309 μ_B and all 32 Te atoms is -4.463 μ_B. Finally the total MM of all atoms is 11.997μ_B .

The band gap doesn't changed Eg=1.73eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=1.377eV, $E_{v\downarrow}$=-0.35eV. It is formed 3 local levels in the band gap $E_{\uparrow}$=0.3eV, $E_{\uparrow}$=0.13eV, $E_{\uparrow}$=-0.132eV (Fig.11). The total energy of the supercell Cd30Mn2Te32 in ferromagnetic state with V_{Cd} is E_t=-64847.4eV.

Thus, in the supercell Cd30Mn2Te32 having V_{Cd} it is formed 3 local levels in the band gap. It is formed MM due to the Mn atoms and Te and Cd vacancies. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the ferromagnetic state is more stable.

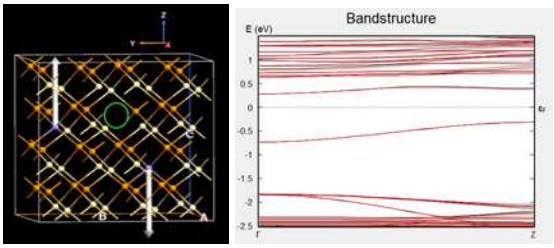


a) b)

Fig. 11. *Supercell Cd30Mn2Te32 with V_{Cd} in ferromagnetic state a) Bulk configuration b) EBS*

V_{Te} in the supercell Cd30Mn2Te32 in antiferromagnetic state doesn't form large MM. The main contribution to MM give two Mn atoms, each of them leads to formation of MM 5.108μ_B. The MM of all 30 Cd atoms is -0.024μ_B and all 31 Te atoms is 0.011 μ_B. Finally the total MM of all atoms is -0.011μ_B .

The band gap is changed from Eg=1.73eV to Eg=2.1eV. It is formed 1 local level in the band gap: $E_{\uparrow}$=-0.731. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=0.283eV, $E_{v\downarrow}$=-1.83eV. The total energy of the supercell Cd30Mn2Te32 in antiferromagnetic state having V_{Te} is E_t=-65817.21eV (Fig.12).

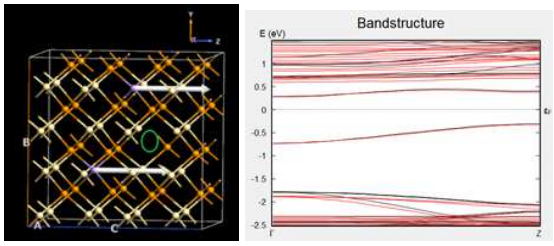


a) b)

Fig. 12. *Supercell Cd30Mn2Te32 with V_{Te} in antiferromagnetic state a) Bulk configuration b) EBS*

V_{Te} in the supercell Cd30Mn2Te32 in ferromagnetic state doesn't form large MM. The main contribution to MM ferromagnetic supercell Cd30Mn2Te32 give two Mn atoms each of them is 5.095μ_B. The MM of all 30 Cd atoms is -0.248 μ_B and all 31 Te atoms is 0.06 μ_B. The total MM of all atoms is 10.002μ_B .

The band gap is changed from Eg=1.73eV to Eg=2.08eV It is formed 1 local level in the band gap below the Fermi level $E_{\uparrow\downarrow}$=-0.73eV. The top of valence band and the bottom of conductivity band are displaced to the energy levels $E_{c\downarrow}$=0.3eV, $E_{v\downarrow}$=-1.78eV (Fig.13). The total energy of the supercell Cd30Mn2Te32 in ferromagnetic state having V_{Te} is E_t=-65817.15eV.



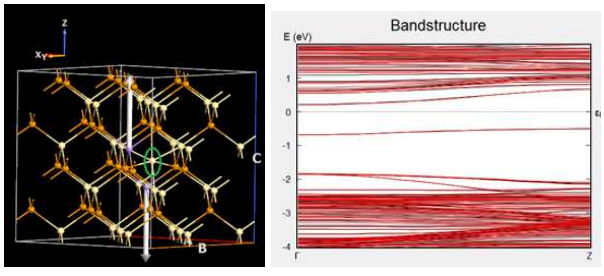
a) b)

Fig. 13. *Supercell Cd30Mn2Te32 with V_{Te} in ferromagnetic state a) Bulk configuration b) EBS*

Thus, in the supercell Cd30Mn2Te32 having V_{Te} it is formed 1 local level in the band gap and band gap is increased. Contribution of V_{Te} to MM ts insignificant. The main contribution to MM gives two Mn atoms. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the ferromagnetic state is more stable.

3.2.2. Interstitial Atom in the Supercell Cd30Mn2Te32

Interstitial Cd (I_{Cd}) *atom in the supercell Cd30Mn2Te32 in antiferromagnetic state leads to formation of 1* local level in the band gap: $E_{\uparrow\downarrow}$=-0.68 eV. The band gap is changed from Eg=1.73eV to Eg=2.03eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=0.2eV, $E_{v\downarrow}$=-1.83eV (Fig.14). The total energy of the supercell Cd30Mn2Te32 in antiferromagnetic state having I_{Cd} is E_t=-67953.46eV.



a) b)

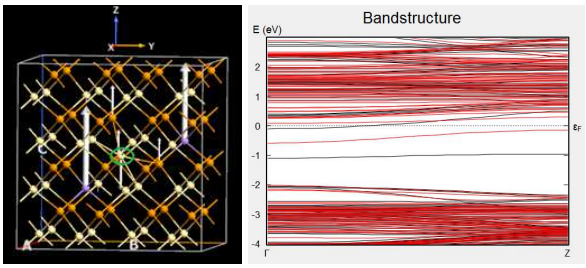
Fig. 14. *Supercell Cd30Mn2Te32 with I_{Cd} in antiferromagnetic state a) Bulk configuration b) EBS*

Main contribution to the MM give two Mn atoms, each of them is 5,114μ_B. The contribution of I_{Cd} to MM insignificant.

The MM of all 31 Cd atoms is -0.023 μ_B and all 32, Te atoms is 0.079 μ_B. The total MM of all atoms is 0.006μ_B .

I_{Cd} atom in the supercell Cd30Mn2Te32 in ferromagnetic state forms 1 local levels in the band gap: E↓=-1.1eV. The band gap doesn't changed from. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{v\uparrow}$=-2.31eV, $E_{c\uparrow}$=-0.58eV (Fig.15). The total energy of the supercell Cd30Mn2Te32 in ferromagnetic state having I_{Cd} is E_t=-67953.26eV.

I_{Cd} atom has 6 bonds: 3 bonds with Te atoms and 3 bonds with Cd atoms. The main contribution to the MM give two Mn atoms each of them is 5.153μ_B, interstitial Cd atom -2.143μ_B and 3 Te atoms having bonds with interstitial Cd atom, each of them 2.049μ_B. The MM of all 31 Cd atoms is -4.709 μ_B and all 32 Te atoms is 4.689 μ_B. The total MM of all atoms is 10.005μ_B .

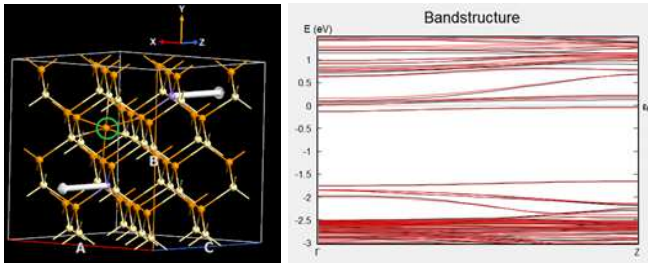


a) b)

Fig. 15 *Supercell Cd30Mn2Te32 with I_{Cd} in ferromagnetic state a) Bulk configuration b) EBS*

Thus, in the supercell Cd30Mn2Te32 having I_{Cd} it is formed 1 local level in the band gap. Band gap is increased in antiferromagnetic state and doesn't changed in ferromagnetic state. The contribution of I_{Cd} atom to MM in antiferromagnetic state ts insignificant. The main contribution to MM give two Mn atoms and I_{Cd} atom in ferromagnetic state. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the ferromagnetic state is more stable.

I_{Te} in the supercell Cd30Mn2Te32 in antiferromagnetic state it is formed no local level in the band gap. The band gap doesn't changed. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\uparrow}$=-0.1eV, $E_{v\downarrow}$=-1.6eV. The total energy of the supercell Cd30Mn2Te32 in antiferromagnetic state having I_{Te} is E_t=-66981.54eV (Fig 16).



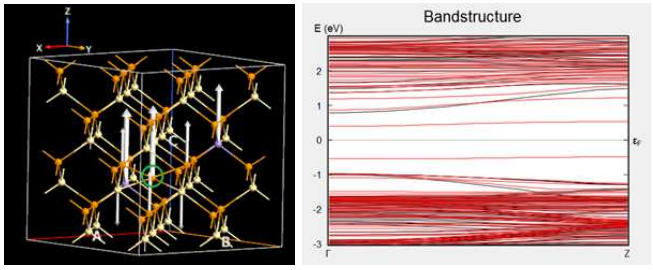
a) b)

Fig. 16. *Supercell Cd30Mn2Te32 with I_{Te} in antiferromagnetic state a) Bulk configuration b) EBS*

Main contribution to the MM give two Mn atoms each of them is 5.64 μ_B. I_{Te} doesn't lead to formig large MM. The MM of all 30 Cd atoms is 0.107 μ_B and all 33 Te atoms is -0.491 μ_B. The total MM of all atoms is -0.006μ_B .

I_{Te} in the supercell Cd30Mn2Te32 in ferromagnetic state leads to forming 2 local levels in the band gap: E↑=0.4eV, E↑=-0.54eV. The band gap doesn't changed Eg=1.73eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=0.783eV, $E_{v\downarrow}$=-0.955eV (Fig 17). The total energy of the supercell Cd30Mn2Te32 in ferromagnetic state with I_{Te} is E_t=-66997.02eV.

To move Te atom from its position to the interstitial one it is have to break 4 bonds with Cd atoms. After the displacement the interstitial Te atom has 6 bonds - 3 bonds with Te atoms and 3 bonds with Cd atoms. Contribution to MM give these 6 atoms, each Cd atom -2.443μ_B and each Te atom 2.823μ_B, interstitial Te atom itself 4.632μ_B and two Mn atoms each of them 4.806μ_B. The MM of all 30 Cd atoms is -9.16 μ_B and all 33 Te atoms is 13.52 μ_B. The total MM of all atoms is 12.994μ_B .



a) b)

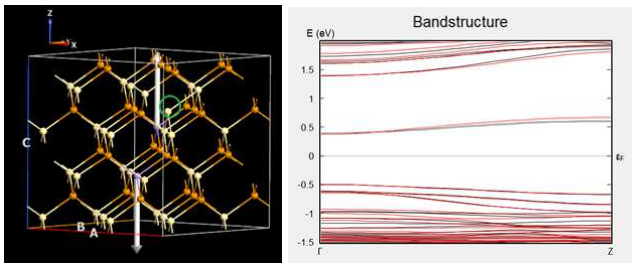
Fig. 17. *Supercell Cd30Mn2Te31 with I_{Te} in ferromagnetic state a) Bulk configuration b) EBS*

Thus, in the supercell Cd30Mn2Te32 having I_{Te} it is formed no local level in the band gap in antiferromagnetic state and 2 local levels in ferromagnetic state. Contribution of I_{Te} atom to MM in antiferromagnetic state is insignificant. The main contribution to MM give two Mn atoms and I_{Te} atom in ferromagnetic state. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the antiferromagnetic state is more stable.

3.2.3. Frenkel Pair in the Supercell Cd30Mn2Te32

Frenkel pair F_{Cd} in the supercell Cd30Mn2Te32 in antiferromagnetic state leads to forming of 1 local level in the band gap: $E_{\downarrow\uparrow}$=0.38eV. The band gap is changed from E_g=1.73eV to E_g=1.9eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\downarrow}$=1.4eV, $E_{v\downarrow}$=-0.5eV (Fig.18). The total energy of the supercell Cd30Mn2Te32 in antiferromagnetic state having I_{Te} is E_t=-66400.55eV.

The displaced Cd atom has 3 bonds with neighboring Cd atoms. Frenkel pair F_{Cd} in the supercell Cd30Mn2Te32 in antiferromagnetic state leads to forming MM. The main contribution to MM give two Mn atoms each of them is 5,241 μ_B. The MM of all 30 Cd atoms is 0.221μ_B and all 32 Te atoms is -0.707 μ_B. The total MM of all atoms is -0.619μ_B.

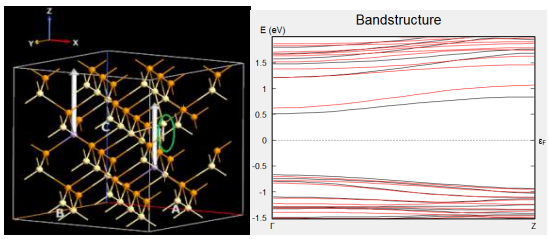


a) b)

Fig. 18. *Supercell Cd30Mn2Te31 with F_{Cd} in antiferromagnetic state a) Bulk configuration b) EBS*

Displacement of Cd atom in the supercell Cd30Mn2Te32 in ferromagnetic state leads to forming F_{Cd}. Cd atom breaks 4 bonds with Te atoms displaces to the interstitial and forms 4 new bonds with 2 Cd atoms and 2 Te atoms. F_{Cd} in the supercell Cd30Mn2Te32 in ferromagnetic state leads to forming of 2 local levels in the band gap: $E_{\downarrow}$=0.51eV, $E_{\uparrow}$=0.62eV. The band gap is changed from Eg=1.73eV to Eg=1.89eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{v\downarrow\uparrow}$=-0.67eV, $E_{c\downarrow\uparrow}$=1.215eV (Fig.19). The total energy of the supercell Cd30Mn2Te32 in antiferromagnetic state having I_{Te} is E_t=-66400.88eV.

Frenkel pair F_{Cd} in ferromagnetic state leads to forming MM. The main contribution to MM give two Mn atoms, each of them 5.081μ_B , interstitial Cd atom with MM of 1.372μ_B and two Te atoms with MM of 1.91μ_B and 0.3964μ_B. The MM of all 30 Cd atoms is -2.663 μ_B and all 32 Te atoms is 2.623 μ_B. The total MM of all atoms is 10.002μ_B .



a) b)

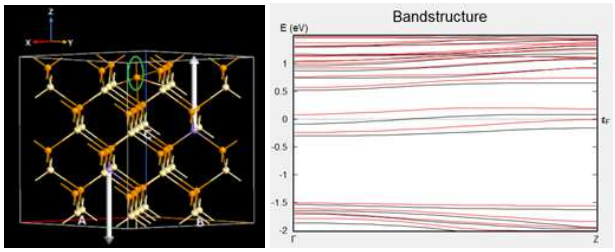
Fig. 19. *Supercell Cd30Mn2Te31 with F_{Cd} in ferromagnetic state a) Bulk configuration b) EBS*

Thus, in the supercell Cd30Mn2Te32 having F_{Cd} it is formed 1 local level in the band gap in antiferromagnetic state and 2 local levels in ferromagnetic state. The band gap is increased. Contribution of F_{Cd} atom to MM is insignificant. The main contributionto MM give two Mn atoms. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the antiferromagnetic state is more stable.

Displacement of Te atom leads to formation of F_{Te} in the supercell Cd30Mn2Te32. Te atom brakes 4 bonds with Cd atoms displace to the interstitial position and forms 4 new bonds with 2 Cd atoms and 2 Te atoms.

Frenkel pair F_{Te} in the supercell Cd30Mn2Te32 in antiferromagnetic state leads to formation of 4 local levels in the band gap: $E_{\uparrow}$=0,8 $E_{\downarrow}$=-0.1eV, $E_{\uparrow}$=-0.25eV, $E_{\downarrow}$=-0.3eV. The band gap is changed from Eg=1.73eV to Eg=2.0 eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{v\downarrow\uparrow}$=-1.5eV, $E_{c\downarrow\uparrow}$=0.5eV (Fig.20). The total energy of the supercell Cd30Mn2Te32 in antiferromagnetic state with F_{Te} is E_t=-66398.475eV.

F_{Te} forms insignificant MM. The main contribution to MM gives two Mn atoms each of them 5,241μ_B. The MM of all 30 Cd atoms is -0.221 μ_B and all 32 Te atoms is 0.707 μ_B. The total MM of all atoms is 1.022μ_B .

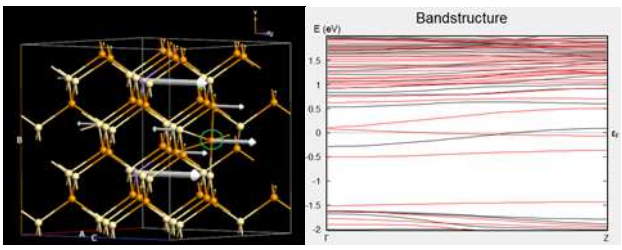


a) b)

Fig. 20. *Supercell Cd30Mn2Te31 with F_{Te} in antiferromagneticstate a) Bulk configuration b) EBS*

Frenkel pair F_{Te} in the supercell Cd30Mn2Te32 in ferromagnetic state leads to formation of 3 local levels in the band gap: $E_{\uparrow}$=0.1, $E_{\downarrow}$=-0.3eV, $E_{\uparrow}$=-0.5eV. The band gap is changed from Eg=1.73eV to Eg=2.0eV. The top of valence band and the bottom of conductivity band are shifted towards the energy levels $E_{c\uparrow}$=0.5eV, $E_{v\uparrow}$=-1.5eV. The total energy of the supercell Cd30Mn2Te32 in ferromagnetic state having I_{Te} is E_t=-66405.26eV.

Frenkel pair F_{Te} in the supercell Cd30Mn2Te32 in ferromagnetic state leads to forming MM. The main contribution to MM give two Mn atoms each of them have MM 5.113 μ_B and 4 broken bonds of Cd atoms with Te atom -1.717 μ_B, -2.175 μ_B, -1.667μ_B, -0.919 μ_B, and 3 Te atoms 2.445 μ_B, 2.42 3 μ_B, 3.495 μ_B. The MM of all 30 Cd atoms is -9.279 μ_B and all 32 Te atoms is 9.9 μ_B. The total MM of all atoms is 10.821μ_B .



a) b)

Fig. 21. *Supercell Cd30Mn2Te31 with F_{Te} in ferromagnetic state a) Bulk configuration b) EBS*

Thus, in the supercell Cd30Mn2Te32 having F_{Te} it is formed 4 local levels in the band gap in antiferromagnetic state and 3 local levels in ferromagnetic state. The band gap is increased. Contribution of F_{Te} atom to MM in the supercell Cd30Mn2Te32 in antiferromagnetic state is insignificant. The main contribution to MM give two Mn atoms and F_{Te} in ferromagnetic state. Comparison of total energies for

ferromagnetic and antiferromagnetic states shows that the antiferromagnetic state is more stable.

4. Conclusion

It was calculated band structure, density of states and magnetic momentum for ideal and defective supercell CdTe and CdMnTe by ab initio method. The band gap, local levels in the band gap and magnetic momentum are defined for various defects in ferromagnetic and antiferromagnetic states. It has been defined, that as Mn atoms, the vacancy, interstitial atom and Frenkel pair in the crystal structure form magnetic moment.

It has been defined that V_{Cd} decrease the band gap in the supercell Cd32Te32 but V_{Te} increase it and forms 1local level in the band gap.

I_{Cd} and I_{Te} atoms in the supercell Cd32Te32 don't change the band gap. It is formed large MM and 1local level in the band gap in the supercell Cd32Te32 having I_{Te}.

F_{Cd} and F_{Te} atoms in the supercell Cd32Te32 don't change the band gap. F_{Cd} forms 2 local levels and F_{Te} forms 4 local levels in the band gap in the supercell Cd32Te32. It is formed MM in the supercell Cd32Te32 having F_{Cd} or F_{Te} atom.

Impurity of two Mn atoms into the supercell Cd30Mn2Te32 leads to forming large MM. The antiferromagnetic phase is more stable in the supercell Cd30Mn2Te32.

In the supercell Cd30Mn2Te32 having V_{Cd} it is formed 3 local levels in the band gap. It is formed MM due to the Mn atoms, Te and Cd vacancies. The antiferromagnetic state in the supercell Cd30Mn2Te32 having V_{Cd} is more stable.

In the supercell Cd30Mn2Te32 having V_{Te} it is formed 1 local level in the band gap and band gap is increased. The contribution of V_{Te} to MM tsinsignificant. The main contribution to MM give two Mn atoms. The ferromagnetic state is more stable in the supercell Cd30Mn2Te32 having V_{Te}.

In the supercell Cd30Mn2Te32 having I_{Cd} it is formed 1 local level in the band gap. The band gap is increased in antiferromagnetic state and doesn't changed in ferromagnetic state. The contribution of I_{Cd} atom to MM in antiferromagnetic state ts insignificant. The main contribution to MM give two Mn atoms and I_{Cd} atom in ferromagnetic state. Comparison of total energies for ferromagnetic and antiferromagnetic states shows that the ferromagnetic state is more stable.

In the supercell Cd30Mn2Te32 having I_{Te} it is formed no local level in the band gap in antiferromagnetic state and 2 local levels in ferromagnetic state. The contribution of I_{Te} atom to MM in the supercell Cd30Mn2Te32 in antiferromagnetic state having I_{Te} is insignificant. The main contribution to MM give two Mn atoms and I_{Te} atom in ferromagnetic state. The antiferromagnetic state is more stable.

In the supercell Cd30Mn2Te32 having F_{Cd} it is formed 1 local level in the band gap in antiferromagnetic state and 2 local levels in ferromagnetic state. The band gap is increased. Contribution of F_{Cd} atom to MM is insignificant. The main contribution to MM give two Mn atoms.. The antiferromagnetic state is more stable *in the supercell Cd30Mn2Te32* having F_{Cd}.

In the supercell Cd30Mn2Te32 having F_{Te} it is formed 4 local levels in the band gap in antiferromagnetic state and 3 local levels in ferromagnetic state. The band gap is increased. Contribution of F_{Te} atom to MM in the supercell Cd30Mn2Te32 in antiferromagnetic state having F_{Te} is insignificant. The main contribution to MM give two Mn atoms and F_{Te} in erromagnetic state. The antiferromagnetic state is more stable *the supercell Cd30Mn2Te32* having F_{Te}.

Acknowledgment

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