

Ab-Initio Calculations of Structural, Electronic, and Optical Properties of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$

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Abstract—We have reported ab-initio calculations of the electronic, structural and linear optical properties of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ compounds. Ab-initio calculations are performed in the framework of full potential linearized-augmented plane-wave plus local orbitals (FP-LAPW+ l_0) method based on the density functional theory (DFT) within the generalized gradient approximation (GGA). Murnaghan's equation of state (EOS) is used for volume optimization by minimizing the total energy with respect to the unit cell. The linear optical properties such as dielectric function, reflectivity, and refractive index are obtained. In the plots of the imaginary part of the complex dielectric function, the absorption threshold shifts toward higher energy with the increase in Mn contents.

Index Terms—Ab initio calculations, density-functional theory, equations of state, optical properties, dielectric function.

I. INTRODUCTION

A great deal of attention has been attributed to the study of diluted magnetic semiconductor due of their potential applications in a wide spectrum of optoelectronic devices, photovoltaic solar cells, laser screen materials and various luminescence devices, etc. [1]. $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ is one of them, especially important due to variation of its electronic and optical properties by changing the Cd:Mn doping. In this paper we have reported the ab-initio calculations for the investigation of electronic, structural, and optical properties of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ alloys using full potential linearized-augmented plane-wave plus local orbitals (FP-LAPW+ l_0) method based on the density functional theory (DFT) within the generalized gradient approximation (GGA) [2].

II. COMPUTATIONAL DETAILS

FP-LAPW+ l_0 method as implemented in the Wien2k code [3] with GGA parameterized by Perdew, Burke and Ernzerhof (PBE) [4] is employed to deal with the exchange and correlation effects. The equilibrium structural parameters are carried out by optimizing total energy with respect to the unit cell volume using Murnaghan's equation of state [5]. The calculations were done with $R_{MT}k_{max} = 7$, to achieve energy eigen value convergence. R_{MT} is the smallest radius of the muffin-tin (MT) spheres and k_{max} is the maximum value of the wave vector. The wave function has been expanded inside the atomic spheres with the maximum value of the

angular momentum l_{max} as 10. The irreducible Brillouin zone (BZ) has been decomposed into a matrix of $10 \times 10 \times 10$ Monkhorst–Pack k -points [6]. The iteration procedure is continued with total energy and charge convergence to 0.0001Ry and 0.001e, respectively [7], [8].

III. RESULTS AND DISCUSSIONS

The $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ has a cubic symmetry with space group F-43M. The total energy is optimized with respect to the unit-cell volume by fitting Murnaghan's equation of state [5]:

$$E_T(V) = \left[\frac{B_0 V (V_0/V)^{B_0'}}{B_0' - 1} + 1 \right] + E_0 - \frac{V_0 B_0}{B_0' - 1} \quad (1)$$

For $x = 0, 0.25, 0.5, 0.75, 1$, Table I shows the energy minimization occurring for $a_0 = 6.617, 6.548, 6.487, 6.422$ and 6.371 \AA , which agree well with the experimental values [9]–[11].

TABLE I: EQUILIBRIUM LATTICE CONSTANT a_0 (Å), BULK MODULUS B_0 (GPa) AND ITS PRESSURE DERIVATIVE B_0' OF $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$

x	a_0 (Å)		B_0 (GPa)		B_0'	
	Present	Others	Present	Others	Present	Others
0.0	6.617	6.56 [9]	37.02	–	3.58	–
0.25	6.548	6.481[11]	34.92	44.50[11]	4.54	6.40[11]
0.5	6.487	6.354[10]	35.61	47.10[10]	4.64	4.58[10]
0.75	6.422	6.32 [8]	37.78	49.94[8]	4.99	7.46[8]
1.0	6.371	6.26 [9]	36.12	–	3.58	–

Hence well-defined structural properties are sufficient for further study of electronic and optical properties. The equilibrium lattice constants are used to calculate the density of states (DOS) and electronic band structures for $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ (shown in Fig. 1 and Fig. 2). The zero of the energy scale is set at the Fermi level (E_F). The energy band structures are calculated along the directions containing high symmetry points of the first Brillouin zone, namely $\text{W} \rightarrow \text{L} \rightarrow \Gamma \rightarrow \text{X} \rightarrow \text{W} \rightarrow \text{K}$. Each member of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ demonstrates the existence of the valence band maximum and conduction band minimum at the same symmetry point. This confirms the direct energy gap between the top of the valence band and the bottom of conduction band at Γ point. These plots provide a qualitative explanation of the atomic and orbital origins of the different band states.

From the DOS plots we observe that near the Fermi level, the upper part of the valence band possesses Mn-3d and Te-5p characteristics.

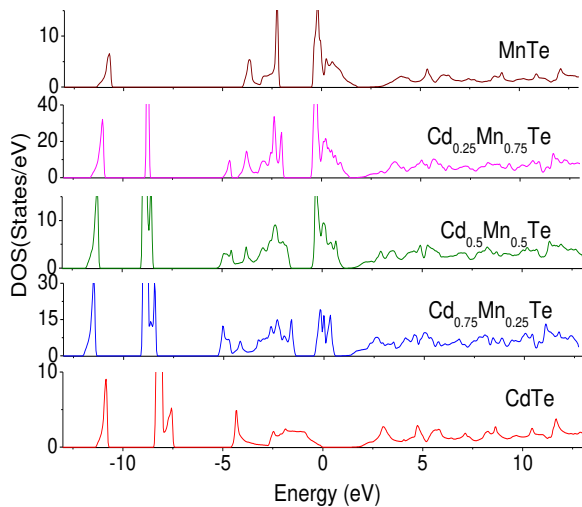


Fig. 1. Electron density of states for $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$.

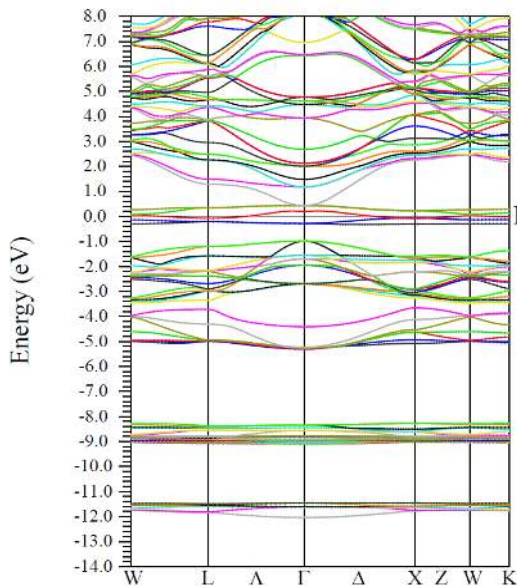


Fig. 2. Electronic band structure for $\text{Cd}_{0.75}\text{Mn}_{0.25}\text{Te}$.

The first structure in the total DOS is small and centered at around -11.19 eV, -11.28 eV, -11.58 eV and -11.87 eV for $x=1.0, 0.75, 0.5$ and 0.25 respectively. This structure arises from the Te s states and it corresponds to the lowest lying band with the dispersion in the region around the Γ point in the Brillouin zone. The next structure appears at -8.20 eV, -8.18 eV, -8.11 eV and -8.01 eV for $x=0.75, 0.5, 0.25$ and 0.0 respectively. It is an attribute of Cd d states with some p states of the Te atoms and occupies largest number of states with flat bands clustered between -9.0 eV and -8.2 eV. Less dispersion of these bands results in sharp peaks. There is a wide spread in DOS in the energy range of -5.0 eV and zero energy for these compounds. The peaks in this energy interval arise from the Te p states partially mixed with Cd s states and they contribute to the upper Valence Band. Above the Fermi level, the feature in the DOS originate mainly from the s and p states of Cd partially mixed with little of Te d states. Band width of valence band as determined from the width of the peaks in DOS dispersion below Fermi level

equal to 12.42 eV, 12.13 eV, 12.17 eV for $x=0.75, 0.5, 0.25$, respectively. The results showing valence band width minimum for $\text{Cd}_{0.75}\text{Mn}_{0.25}\text{Te}$, clearly indicate that the wave function for $\text{Cd}_{0.75}\text{Mn}_{0.25}\text{Te}$ is more localized than that for others. This is in consistence with the fact that when the atomic number of the anion increases, a material becomes non-polar covalent with valence band states being more localized. The dielectric function $\epsilon(\omega)$ can describe the interaction of photons with electrons in the form of linear response of the system to electromagnetic radiation [12]. Dielectric function comprises of the imaginary part $\epsilon_2(\omega)$ and the real part $\epsilon_1(\omega)$. The momentum matrix elements between the occupied and unoccupied wave functions within the selection rules play the main role for the determination of $\epsilon_2(\omega)$. The expression for ϵ_2 is given by

$$\epsilon_2(\omega) = \frac{Ve^2}{2\pi\hbar m^2 \omega^2} \int d^3k \left| \langle kn | p | kn' \rangle \right|^2 f(kn) \times [1 - f(kn')] (E_{kn} - E_{kn'} - \hbar\omega) \quad (2)$$

where $\hbar\omega$ is the energy of the incident photon, p is the momentum operator, $|kn\rangle$ is the eigenfunction with eigenvalue E_{kn} and $f(kn)$ is the Fermi distribution function.

The real part $\epsilon_1(\omega)$ of the dielectric function follows the Kramer-Kronig relations and can be expressed in terms of $\epsilon_2(\omega)$ as follows

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\epsilon_2(\omega') \omega' d\omega'}{\omega'^2 - \omega^2} \quad (3)$$

The variation of the dielectric functions, $\epsilon_2(\omega)$ and $\epsilon_1(\omega)$ of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ as function of photon energy is displayed in Fig. 3 and Fig. 4 respectively, in the range of 0–14 eV.

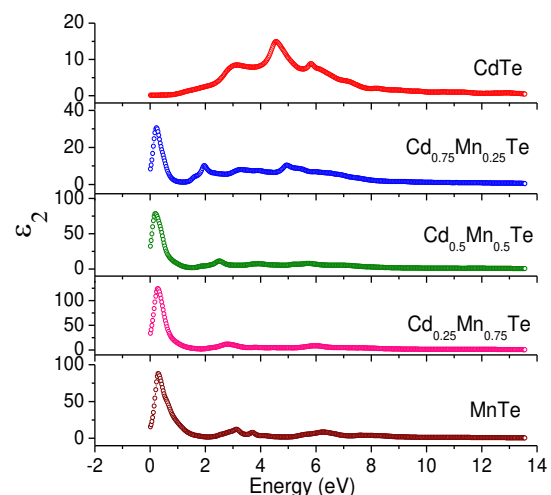


Fig. 3. The variation of the dielectric functions, ϵ_2 of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ as function of photon energy.

It is observed that the imaginary part of the complex dielectric function, the absorption threshold shifts toward higher energy with the increase in Mn contents. With the knowledge of the imaginary part $\epsilon_2(\omega)$ and the real part $\epsilon_1(\omega)$ of the dielectric function, one can calculate different optical properties. The following equations are used for the

calculation of refractive index n and reflectivity R [13]–[15]:

$$n(\omega) = \frac{1}{\sqrt{2}} \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) + \varepsilon_1} \quad (4)$$

$$R(\omega) = \left| \frac{\sqrt{\varepsilon(\omega)} - 1}{\sqrt{\varepsilon(\omega)} + 1} \right|^2 \quad (5)$$

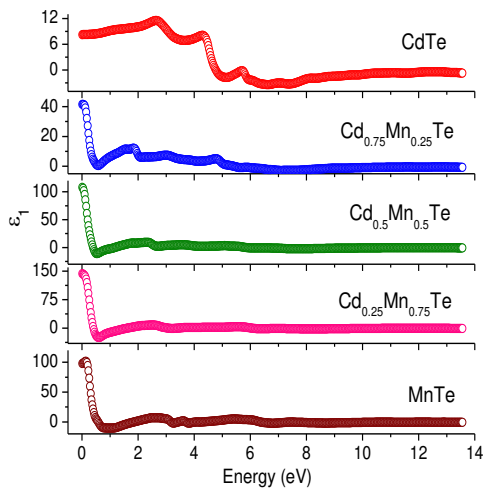


Fig. 4. The variation of the dielectric functions, ε_1 of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ as function of photon energy.

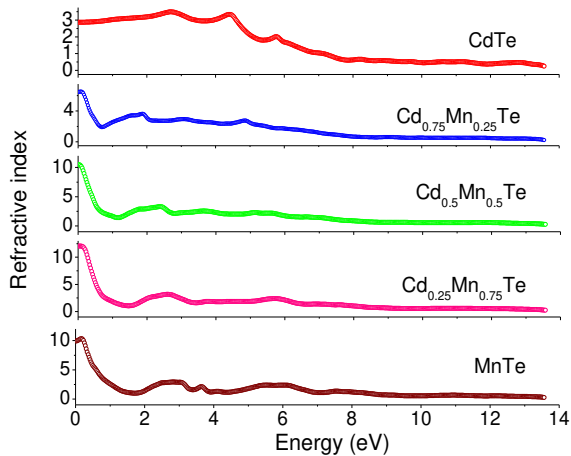


Fig. 5. The variation of the refractive index, (n) of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ as function of photon energy.

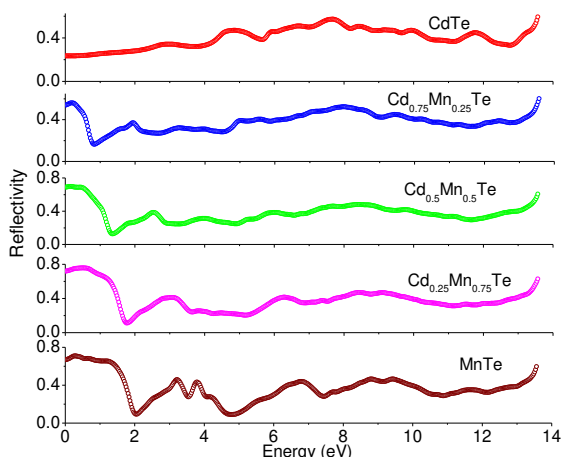


Fig. 6. The variation of the reflectivity (R) of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ as function of photon energy.

The calculated optical parameters, viz., refractive index $n(\omega)$ and reflectivity $R(\omega)$ are shown in Fig. 5 and Fig. 6 respectively. It is clear from the reflectivity spectrum that CdTe possesses more transmitting nature than Mn doped compounds.

IV. CONCLUSION

The structural, electronic, and optical properties of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ have been studied with FP-LAPW + l_0 method in the framework of density functional theory. The quantities such as band structure, dielectric constants, and refractive index were obtained. The generalized gradient approximation (GGA) was considered for the exchange and correlation effects calculations. The band structure of all compounds confirms the direct energy gap between the top of the valence band and the bottom of conduction band at Γ point. In the linear optical response, the absorption threshold shifts toward higher energy with the increase in Mn contents.

ACKNOWLEDGMENT

We acknowledge the support in part by the Department of Science and Technology through computing resources provided by the High Performance Computing Facility at the Inter University Accelerator Centre, New Delhi. The author (BKS) is thankful to Galgotias University for its support.

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