Ab initio study of structural, electronic and optical properties of ternary $CdO_{1-x}Se_x$ alloys using special quasi-random structures

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The structural, electronic, and optical properties of binary CdO, CdSe, and their ternary $CdO_{1-x}Se_x$ alloys ($0 \leq x \leq 1$) in the rock salt and zinc blend phases have been studied by the special quasi-random structure (SQS) method. All the calculations are performed using full-potential linearized augmented plane wave plus local orbital's (FP-LAPW+lo) method within the framework of density function theory (DFT). We use Wu–Cohen (WC) generalized gradient approximation (GGA) to calculate structural parameters, whereas both Wu–Cohen and Engel–Vosko (EV) GGA have been applied to calculate electronic structure of the materials. Our predicted results of lattice constant and bulk modulus show only a slight deviation from Vegard's law for the whole concentrations. The obtained band structure indicates that for the rock-salt phase, the ternary alloys present semi-metallic behavior, while for the zinc blend phase, semiconductor behavior with direct bandgap is observed with decreasing order of x except for CdSe. Finally, by incorporating the basic optical properties, we discuss the dielectric function, refractive index, optical reflectivity, the absorption coefficient, and optical conductivity in terms of incident photon energy up to 14 eV. The calculated results of both binaries are in agreement with existing experimental and theoretical values.

Keywords: density functional theory, structural, electronic, and optical properties

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1. Introduction

The binary compounds of II–VI semiconductors have attracted much consideration due to their stimulating physical properties. The cadmium oxide (CdO) is characterized by wide band gap and high conductivity due to reasonable electron mobility and high carrier concentration.[1] CdO is a favorable transparent conducting oxide that shows metal-like charge transport characteristics with an extremely large carrier mobility and decent optical transparency in the visible region.[2] It is also promising materials for band gap engineering and spintronic applications due to its wide bandgap.[3] These properties make it suitable for application of photodiodes, photovoltaic, phototransistors, transparent electrodes, IR detectors, liquid crystal displays, anti-reflecting coating, solar cells and gas sensors.[4] Cadmium selenide (CdSe) is an II–VI semiconductor which presents a hexagonal andcubic zinc blende phase at atmospheric pressure and generally forms in thin films.[5] For short and medium wavelengths, Cd-based compounds can also be used as an alternative material.[6,7]

The $A_xB_{1-x}C$ types of semiconductors constructed by mixing the elements of AC and BC are scientifically important materials. Their structural, electronic, and optical properties can be incessantly modified by varying the composition x, and thus the range of material properties can be tuned for precise applications.[8] The CdSe crystal developed with the mixing of CdO and additional Se to conquer the formation of Se vacancies was experimentally studied by Chenet,[9] also using first-principles calculation.[10] The variation of band gaps and electronic properties of the ZnCdSe at various concentration of x was studied theoretically.[11] The structural and electronic properties of the low index CdSe and its interface stability were calculated using the well-known first-principles method.[12] To the best of our knowledge, no theoretical and experimental investigations of optical and electronic properties of $CdO_{1-x}Se_x$ ternary alloy have been performed.

In the present theoretical investigation, we calculate structural, electronic, and optical properties of CdOSe by mixing CdO with CdSe at various concentration of $x = 0.0$, 0.25, 0.50, 0.75, and 1.0 in rock salt (RS) and zinc blend (ZB) phase. The lattice constants of the $CdO_{1-x}Se_x$ are calculated by minimizing the total energy with respect to the unit cell volume. Furthermore, we use the calculated lattice constants to research band gaps, electronic properties, and optical properties of the oxides. Accurate full potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method within the framework of density functional theory (DFT) has been used as DFT calculations have time and again provided useful information regarding electronic and optical profile ternary compounds.[13] The obtained results are compared with previous theoretical calculations and available experimental findings.

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2. Calculation method

The structural, electronic, and optical properties of binaries and their ternary alloy $CdO_{1-x}Se_x$ in RS and ZB phase are calculated using a non-relativistic full potential linear augmented plane wave plus local orbital (FP-LAPW+lo) approach in the framework of the density functional theory (DFT) as executed in the WIEN2K package.[14] In order to calculate the structural properties, generalized gradient approximation (GGA) by Wu and Cohen (WC)[15] was used for the exchange correlation potential. For band structure calculations, the WC and Engel–Vosko (EV) GGA schemes[16] were used and it was observed that EVGGA is an improved form of GGA. EVGGA reproduces better exchange potential at the cost of less agreement in the exchange energy, resulting in an enhanced band splitting.

In our present work, we have used the special quasi-random structures (SQS), which are particularly designed for small-unit-cell periodic structures that was offered by Zunger *et al*,[17] in order to overcome limitations during the study of various physical properties of disordered solid solutions/random substitutional alloys. SQSs, in which the lattice sites are filled by constituent atoms to reproduce the average correlation functions of the random substitutional alloys, can be completely relaxed within DFT codes to study the effect of local relaxation. First-principles SQSs approach at certain compositions, e.g., $x = 0.25$, 0.50, and 0.75, allows correct prediction of several properties of solid solutions, and has been successfully applied to binary and ternary solid solutions.[18] This approach is effective to reduce the size of the supercell for covering many properties of random alloys. In the FP-LAPW+lo method, the charge density, wave function, and potential are expanded into spherical harmonic functions inside non-overlapping muffin-tin (MT) spheres surrounding the atomic spheres for the wave function, the maximum value of l is $l_{max} = 10$ and for the charge density is Fourier expanded up to $G_{max} = 14$ (Ryd)$^{1/2}$. The convergence parameter $RMTK_{max}$ is equal to 9, which controls the size of the basis sets in these calculations. The RMT for Cd, O, and Se are selected in such a way that the spheres do not overlap. The numbers of integrating points are 72 for binary and 35 for ternary alloy for the Brillion zone integrations in the corresponding irreducible wedge. The optical properties are determined using 3500 k-points for finer k-mesh points are needed to analyze dielectric function. When the total energy convergence is less than 10^{-5} Ry, then the self-consistent calculation is considered to be stable. The orbitals of Cd($4d^{10}$ $5s^2$), O($1s^2$ $2s^2 2p^4$), and Se($3d^{10}$ $4s^2$ $4p^4$) are treated as valence electrons.

3. Results and discussion

3.1. Structural properties

The structural properties of binaries CdO and CdSe compounds and their ternary $CdO_{1-x}Se_x$ alloy with various compositions at $x = 0.0$, 0.25, 0.5, 0.75, and 1.0 are calculated in both RS and ZB phases using SQS approach.[19] The RS and ZB structures are used for binary compounds with space group $Fm3m$ and $F43m$, respectively. The structure is in the simplest form that surroundings of, an eight atoms, simple cubic lattice at the compositions $x = 0.25$ and 0.75 with space group $Pm3m$ for RS and $P43m$ for ZB. The structure acquired at $x = 0.50$ has space group $Pmmm$ and $P222$ in RS and ZB phases, respectively. The atomic positions of binary and their ternary alloys in RS and ZB structures are shown in Figs. 1 and 2. Murnaghan's equation of state (EOS)[20] is used to minimize the total energy for volume optimization. The calculated structural parameters such as the lattice constant 'a' and the bulk modulus B are given in Tables 1 and 2 for RS and ZB, respectively; while variations of the lattice constant and bulk modulus with the concentration of $x$obey Vegard'slaw,[21] as shown in Fig. 3. The calculated lattice constant and bulk modulus depend on the composition. With the increase in composition x, the lattice constant increases, but the bulk modulus decreases, as shown in Figs. 3(a) and 3(b). Our calculated lattice parameters and bulk modulus of $ZnO_{1-x}Se_x$ alloys together with experimental and other theoretical results of both RS and ZB phase are presented in Tables 1 and 2, respectively.

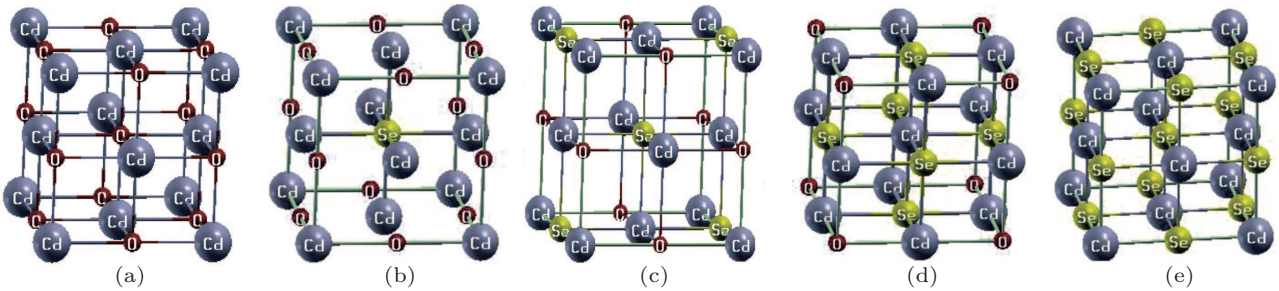


Fig. 1. (color online) Structure of the binary and ternary alloys $CdO_{1-x}Se_x$: (a) 0.0, (b) 0.25, (c) 0.5, (d) 0.75, and (e) 1 in the RS phase.

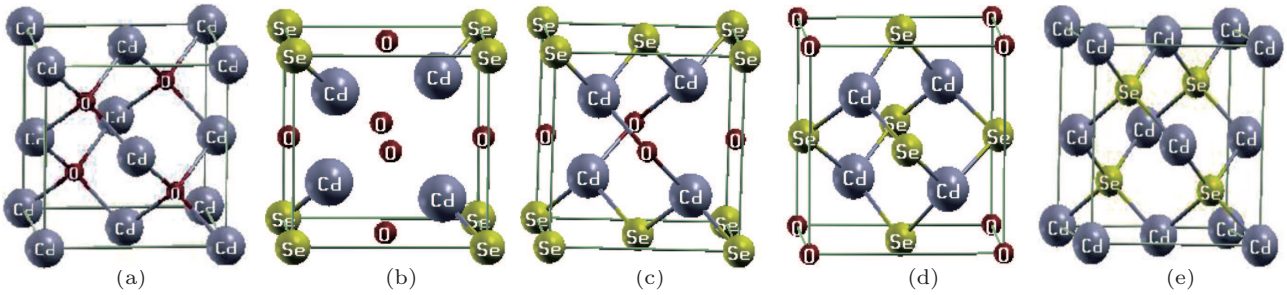


Fig. 2. (color online) Structure of the binary and ternary alloys $CdO_{1-x}Se_x$: (a) 0.0, (b) 0.25, (c) 0.5, (d) 0.75, and (e) 1 in the ZB phase.

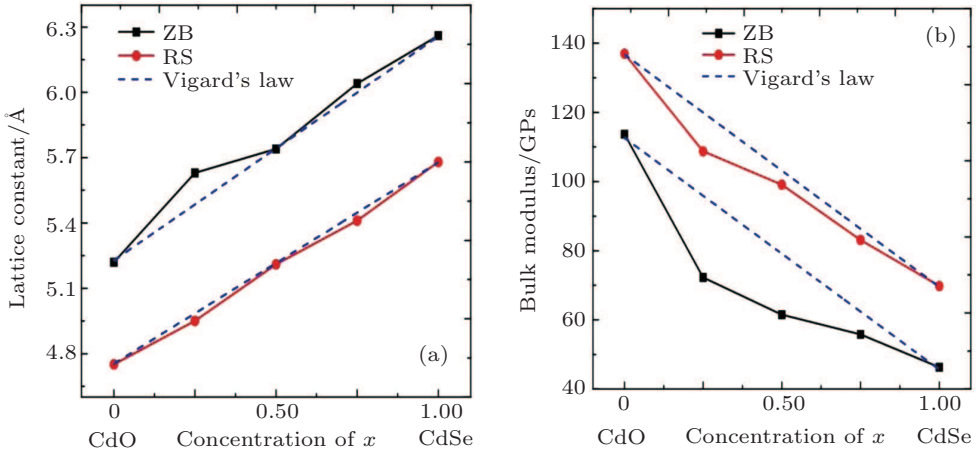


Fig. 3. (color online) Variation of the calculated lattice parameters and bulk modulus with x for $CdO_{1-x}Se_x$alloys.

Table 1. Calculated lattice parameters and bulk modulus of $CdO_{1-x}Se_x$ alloys together with experimental and other theoretical results in the RS phase.

x	a/Å			B/GPa		
	This work	Expt.	Other Cal.	This work	Expt.	Other Cal.
0.00	4.69	4.7[a], 4.69[b]	4.7[c], 4.76[d]	139.2	148[b]	123.6[c],133.2[d]
0.25	4.97	–	–	109.8	–	–
0.50	5.22	–	–	99.08	–	–
0.75	5.43	–	–	84.9	–	–
1.0	5.61	5.61[e]	5.717[f]	73.78	86.7[e]	64.3[f]

[a]Ref. [22], [b]Ref. [23], [c]Ref. [24], [d]Ref. [25], [e]Ref. [26], [f]Ref. [27].

Table 2. Calculated lattice parameters and bulk modulus of $CdO_{1-x}Se_x$ alloys compared with experimental and other theoretical results in ZB phase.

x	a/Å			B/GPa		
	This work	Expt.	Other Cal.	This work	Expt.	Other Cal.
0.00	5.2	–	5.14[a], 5.15[b]	113.5	–	93.9[a],83[b]
0.25	5.6	–	–	71.4	–	–
0.50	5.72	–	–	61.54	–	–
0.75	6.02	–	–	52.83	–	–
1.00	6.16	6.05[c]	6.09[d], 6.17[e]	47.83	53[c]	55.91[d]

[a]Ref. [28], [b]Ref. [29], [c]Ref. [30], [d]Ref. [31], [e]Ref. [32].

3.2. Electronic band structures and density of states

The band structures of the materials in semiconductor play an important role in manufacturing the electronic and optoelectronic devices. The band structures have been calculated using WC and EV GGA schemes. Even the EV-GGA was used only for the energy band gaps calculations and not used for the optimization of the lattice constant. The calculated band structure has indirect band gaps for binary compounds in RS phase and direct band gaps in ZB phase. The band structure has semi-metallic behavior for ternary alloys in the RS phase (see Fig. 4) and direct band gap in the ZB phase (see Fig. 5) at the Γ point within a range of $0 \leq x \leq 1$. The band gap decreases

with increasing concentration of Se. It has been observed that the calculated band gap values with the EV-GGA scheme have better band splitting and agree well with the experimental values. The direct-band-gap semiconductor nature is observed at the Γ-symmetry point in the ZB phase and their calculated values are given in Table 3.

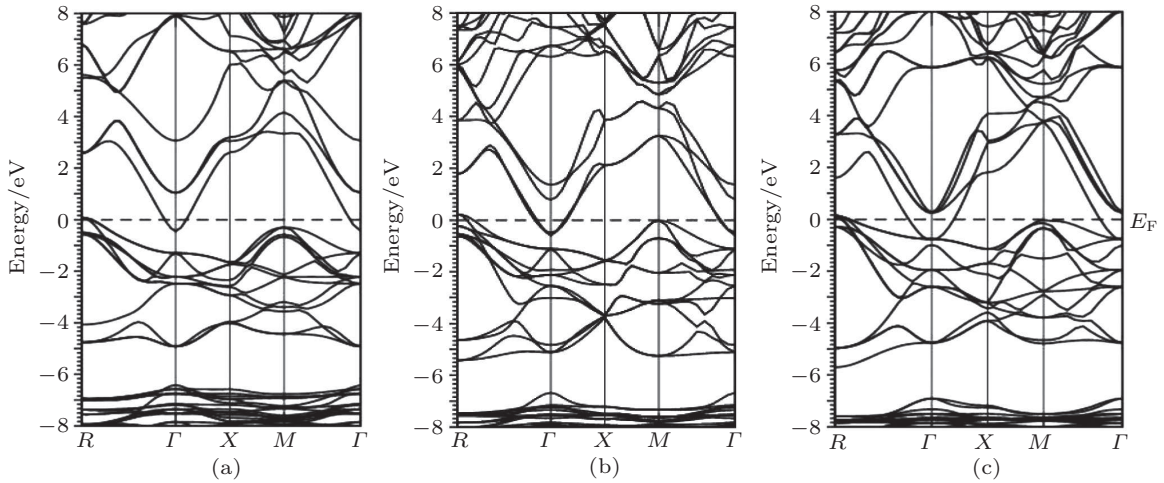


Fig. 4. Band structures of (a) $CdO_{0.75}Se_{0.25}$, (b) $CdO_{0.50}Se_{0.50}$, and (c) $CdO_{0.25}Se_{0.75}$ using WC-GGA in RS Phase.

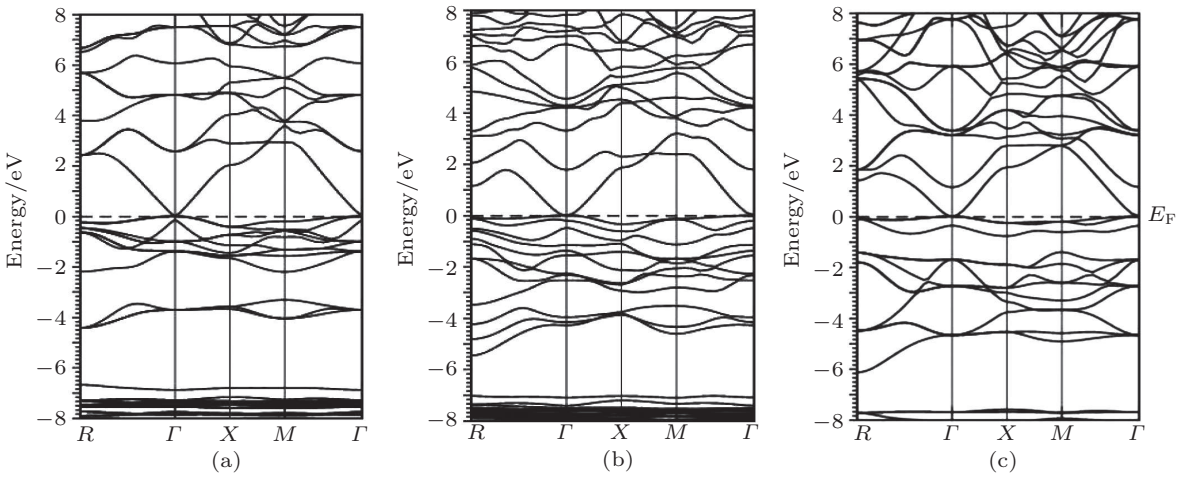


Fig. 5. Band structures of (a) $CdO_{0.75}Se_{0.25}$, (b) $CdO_{0.50}Se_{0.50}$, and (c) $CdO_{0.25}Se_{0.75}$ using WC-GGA in ZB Phase.

Table 3. Calculated band gaps for $CdO_{1-x}S_x$ at Γ–Γ symmetry points in ZB phase.

x	Band gap energy/eV			
	GGA	EVGGA	Expt.	Other work
0.00	0.09	0.42	2.26[a)]	0.01[b)]
0.25	0.14	0.45		
0.50	0.02	0.15		
0.75	0.04	0.23		
1.00	0.46	1.351.9[c)]		0.47[d)],0.4[e)]

[a)]Ref. [33], [b)]Ref. [34], [c)]Ref. [35], [d)]Ref. [36], [e)]Ref. [37].

The electronic density of state (DOS) for $CdO_{1-x}Se_x$ alloys ($x = 0$, 0.25, 0.50, 0.75, and 1.0) in RS and ZB phases give surplus insight of various states of the conduction and valence bands. The calculation of total density of states (TDOS) and partial density of states (PDOS) for $CdO_{1-x}Se_x$alloys can be useful in identifying the character of the band states at given composition x. The total and partial DOS along with the Cd(d, s), O(p, s), and Se(s, p) for $CdO_{1-x}Se_x$ at various concentration of $x = 0.0$, 0.25, 0.5, 0.75, and 1.0 are shown in Figs. 6(a) and 6(b). The region from the Fermi level to -4 eV is due to O 2p and the region from -5.8 eV to -7 eV is due to Cd 4d electrons in both RS and ZB phases for CdO binary compounds. In case of CdSe, the region from the Fermi level to -4.5 eV is originated from Se 4p and the energy range from -7.4 eV to -8.3 eV ensues due to Cd 4d in both phases (see Fig. 6). The total and partial DOS of the ternary alloys have been shown in Fig. 6(a) for RS and Fig. 6(b) for ZB. The conduction band consists of Se 3p and Cd 5s states in ternary alloys. With the increase in the concentration of Se, the peak of oxygen shifts towards the Fermi level in the ZB phase. The lower region

of the valence band is completely occupied by Cd 4d and Se 3p states and the region just below the Fermi level in valence band is occupied by O 2p and 2s states, while the lower part of the conduction band is dominated by Se 3p and Cd 5s states for ternary alloy $CdO_{1-x}Se_x$ ($x = 0.25$, 0.50, and 0.75) in both RS and ZB phases.

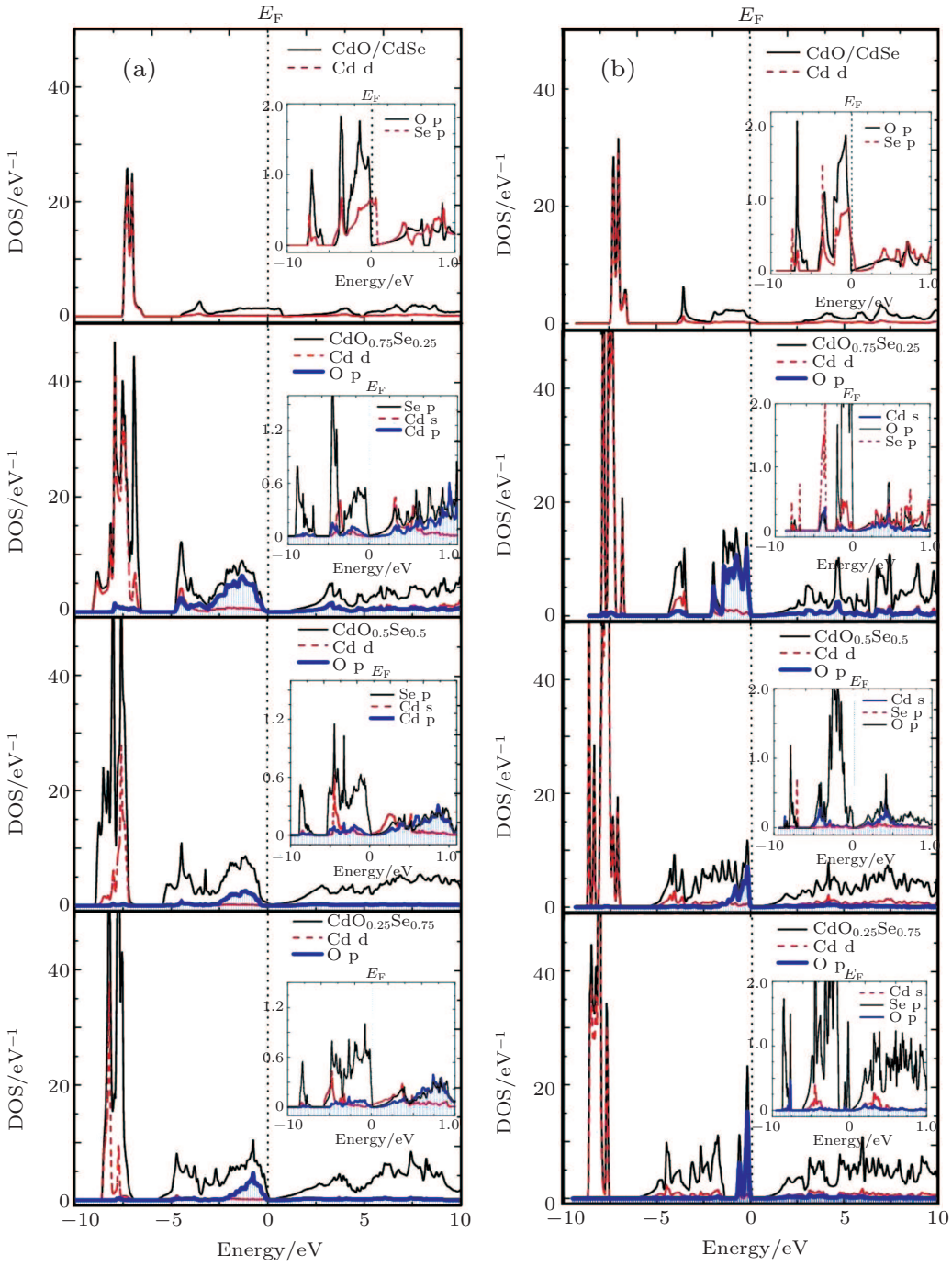


Fig. 6. (color online) Total density of states (TDOS) of $CdO_{1-x}Se_x$ alloys at $x = 0.25$, 0.50, and 0.75 in (a) RS and (b) ZB phase.

3.3. Optical properties

The electronic structure of solids gives rise to two types of band contributions, namely, inter-band and intra-band transitions. The intra-band transitions exist only in metals and semimetals, while inter-band transitions occur in semiconductors. Therefore, only direct and indirect inter-band transitions are considered in semiconductors, disregarding intra-band transitions. The direct inter-band transitions are related with the dielectric function and the indirect part is negligible due to its trivial involvement in dielectric function.[38] The optical properties of $CdO_{1-x}Se_x$ depend on dielectric function $\varepsilon(\omega)$, which relates to the interaction of photons with electrons.[39] The $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary components of the dielectric function and it can be found by addition of all possible occupied to the unoccupied states of transitions and

that is Ambrosch-Draxl and Sofo.[40] The real part $\varepsilon_1(\omega)$ of dielectric function is obtained from $\varepsilon_2(\omega)$ using the Kramers–Kronig transformation.

The real part of the dielectric function shown in Fig. 7(a) exemplifies the dispersion of the incident photons by the material. The ε_1 helps us to find important physical quantity such as static dielectric constant $\varepsilon_1(0)$. The $\varepsilon_1(0)$ is the low energy boundary of the real part of the dielectric function and it gives the dielectric response of a material to a static electric field. The value of $\varepsilon_1(\omega)$ is positive up to 10.9 eV and after 11.1 eV it becomes negative for CdO. For CdSe, the value of $\varepsilon_1(\omega)$ is positive up to 6.7 eV, abruptly decreases after this point, and then becomes negative. Similarly, the values of $\varepsilon_1(\omega)$ for $CdO_{0.75}Se_{0.25}$, $CdO_{0.5}Se_{0.5}$, and $CdO_{0.25}Se_{0.75}$ are positive up to 8.3 eV, 7.4 eV, and 6.9 eV, respectively, as shown in Fig. 7(a). This indicates that as the concentration of Se increases, the value of $\varepsilon_1(\omega)$ tends to be negative. When the $\varepsilon_1(\omega)$ is positive, the photons transmit through alloys. For negative values of $\varepsilon_1(\omega)$, the electromagnetic wave is damped. The calculated $\varepsilon_2(\omega)$ for CdO has a solid absorption region from 7.8 eV to 12.4 eV, whereas CdSe has strong absorption region and the highest peak from 4.9 eV to 5.7 eV. These patterns are also repeated in the ternary alloys when $\varepsilon_2(\omega)$ goes from the maximum to the minimum in these energy ranges, as shown in Fig. 7(b). The study of $\varepsilon_2(\omega)$ curve explains that the first critical points (threshold energy) of the dielectric function take place at 0.9, 0.32, 0.98, 0.67, and 0.12 eV for the CdO, $CdO_{0.75}Se_{0.25}$, $CdO_{0.5}Se_{0.5}$, $CdO_{0.25}Se_{0.75}$, and CdSe, respectively.

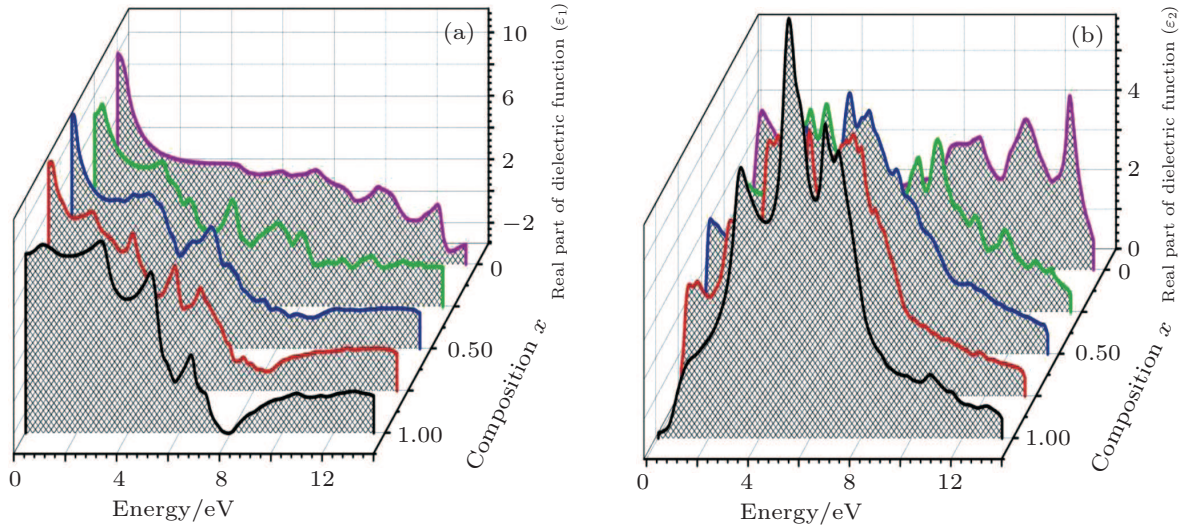


Fig. 7. (color online) Calculated (a) $\varepsilon_1(\omega)$ and (b) $\varepsilon_2(\omega)$ spectra for the binary and ternary alloys $CdO_{1-x}Se_x$.

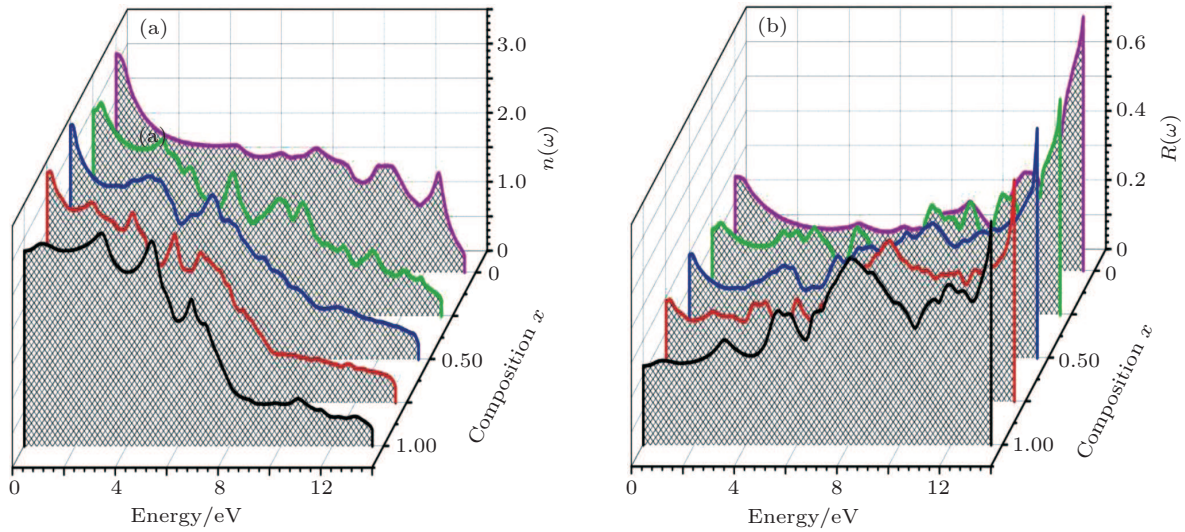


Fig. 8. (color online) Complex refractive index for $CdO_{1-x}Se_x$ alloys corresponding to different x for (a) $n(\omega)$ and (b) $R(\omega)$.

The real and imaginary parts of the dielectric function offer the information that one can calculate the refractive index $n(\omega)$ and reflectivity $R(\omega)$ using the following equation:

$$n(\omega) = \left[\frac{\varepsilon_1}{2} + \frac{\varepsilon_1^2(\omega) - \varepsilon_2^2(\omega)}{2}\right]^{1/2}.$$

The spectra of dielectric, refractive index, reflectivity, absorption, and optical conductivity (ω) are taken for a radiation up to 14 eV for binary compounds and their ternary alloys. The considered values of the static refractive indices $n(0)$ from the static optical dielectric constant at various compositions of x have been assessed using the relation $n(0) = \varepsilon^{1/2}(0)$. This is an expectable behavior of $\varepsilon(0)$ with respect to x, which is similar to that of $n(0)$. It can be seen from Fig. 8(a) that the refractive index of the material is inverse behavior with the band gap as the band gap of CdSe is maximum but refractive index is minimum similarly behavior for rest of composition x. The reflectivity $R(\omega)$ for the binary and their ternary alloys CdO, $CdO_{0.75}Se_{0.25}$, $CdO_{0.5}Se_{0.5}$, $CdO_{0.25}Se_{0.75}$, and CdSe are shown in Fig. 8(b). The reflection is directly related to refraction and the maximal reflectivity occurs in the region from 7.6 eV to 9.8 eV.[41] The calculated values of dielectric function, refractive index, and refraction are consistent with the values of binary compounds,[37,42] which are given in Table 4.

Table 4. Calculated optical parameters for $CdO_{1-x}Se_x$ at different Se concentrations.

x	$\varepsilon_1(0)$	$n(0)$	$R(0)$	$\varepsilon_2\sigma$	σ
0.00	9.2	3.1	0.27	0.92	1.69
0.25	8.3	2.9	0.24	0.32	0.63
0.50	6.9	3.4	0.29	0.97	1.71
0.75	6.8	3.3	0.28	0.68	1.23
1.00	5.9	2.8	0.22	0.14	0.24

We also calculate the absorption coefficient $\alpha(\omega)$ and optical conductivity $\sigma(\omega)$ for $CdO_{1-x}Se_x$ alloys for $x = 0.0$, 0.25, 0.50, 0.75, and 1.0, as shown in Figs. 9(a) and 9(b), respectively. A relative analysis of band structure with $\alpha(\omega)$ indicates that the incident radiation may be absorbed in these materials. In the calculation of $\alpha(\omega)$, absorbance peak for CdO and CdSe occurs at 12.3 eV and 7.6 eV, respectively (see Fig. 9(a)). As the concentration of Se is increased, the peak shifts toward lower energies. Since the optical conductivity $\sigma(\omega)$ is related to $\varepsilon_2(0)$, the conductivity behavior seems to follow the pattern of $\varepsilon_2(0)$.

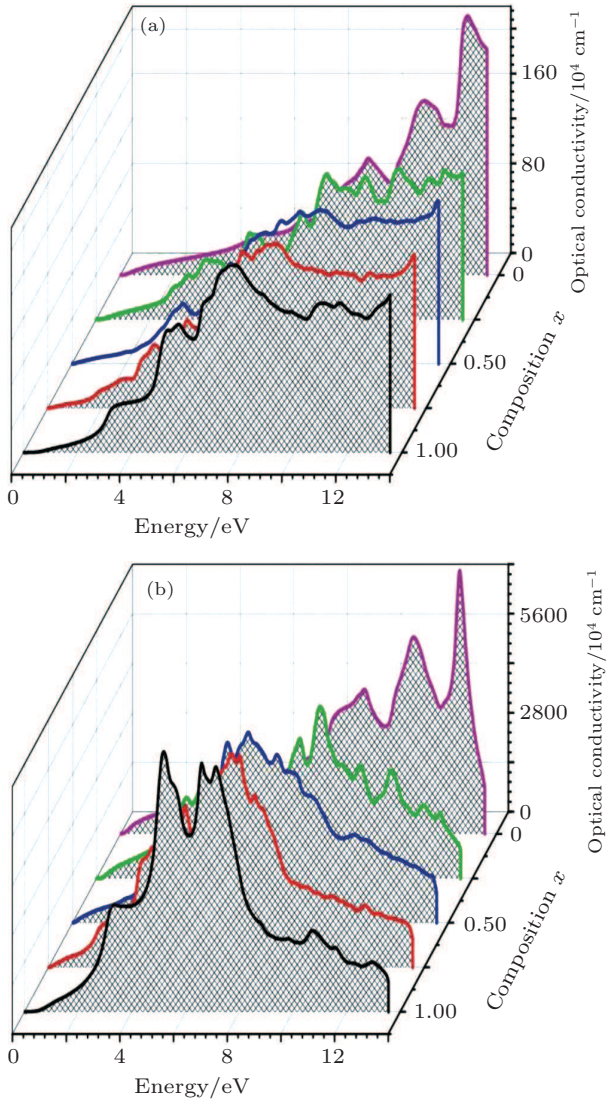


Fig. 9. (color online) (a) Absorption coefficient $\alpha(\omega)$ and (b) optical conductivity $\sigma(\omega)$ for $CdO_{1-x}Se_x$ with different concentrations.

4. Conclusions

In this work, we present first-principles calculations within the framework of density functional theory for the analysis of fundamental properties like electronic band structures, density of states, and optical measurements in RS and ZB phases. These fundamental properties of the ternary $CdO_{1-x}Se_x$ alloys ($x = 0.25$, 0.5, 0.75) are studied in both phases by using the special quasi-random structures (SQS) approach of Zunger to consider the effect of randomness of the alloys in first few shells around the considered site. It is found that our calculated lattice constants of the binary compounds are in good agreement with the experimental values, whereas the composition-dependent structural parameters of the ternary alloys seem to deviate slightly from Vegard's law. To calculate electronic band structures, a technique EV GGA has also been used for comparison and the results are in good agreement with experimental results. The achieved structural properties are in reasonable agreement with other theoretical

and experimental results for the binary compounds and support for the first time used ternary alloys. In the ZB phase, the behavior of band structures show that $CdO_{1-x}Se_x$ alloys in each composition have direct band gaps decreasing with concentration of Se. DOS and PDOS have been studied in terms of dissimilar orbitals of the basic atoms. Finally, the optical properties are calculated using WC GGA in the ZB phase and good agreement with available data is found. Our results predict the improvement of optical functionality for the $CdO_{1-x}Se_x$ alloys with increasing concentration of Se, which may support an assessable theoretical expectation for such properties.

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