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Salim Djaili (s.djaili@ens-lagh.dz)
ENS Laghouat: Ecole Normale Superieure de Laghouat https://orcid.org/0000-0003-3755-2477
Brahim Lagoun
Université Amar Telidji Laghouat: Universite Amar Telidji Laghouat
Taher Smain
Université Amar Telidji Laghouat: Universite Amar Telidji Laghouat
Ali Amour
Université Amar Telidji Laghouat: Universite Amar Telidji Laghouat
Kouider Soleh
Université Amar Telidji Laghouat: Universite Amar Telidji Laghouat
Mohamed Hachi
Université Ziane Achour de Djelfa: Universite Ziane Achour de Djelfa

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Electronic and optical properties of $Cd_xMg_{1-x}O$ alloys, TB-mBJ calculations

S. Djaili[1], **B. Lagoun**[2], T. Smain[2], M A. Amor[2], K. Souleh[2], Hachi[3] .

1- Department of physics, High Teacher's School-Laghouat, 03000, Algeria

2-Laboratory of Physical Chemistry Materials, Faculty of Science, University of Laghouat, 03000, Laghouat, Algeria

3- Laboratoire de chimie organique et de substances naturelles, Université de Djelfa, Algeria.

s.djaili@ens-lagh.dz

Abstract

The magnesium and cadmium oxides (MgO, CdO) are widely used in the optoelectronic technology, for that raison it very interest subject of researches.
In this work, the structural, elastic, electronic and optical properties of rock-salt $Cd_xMg_{1-x}O$ were investigated using both exchange correlations LDA and GGA-WC. The calculations were implemented using Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method in the framework of the Density Functional Theory (DFT). For the electronic and optical properties, the calculations were performed using the Tran-Blaha-modified Beck Johnson potential (TB-mBJ).
The lattice parameter have been reported for different cadmium concentrations x in the rocksalt structure, the calculated lattice parameter to be transmitted quasi-linearly from 4.257 A to 4.43 A for rock-salts MgO and rock-salts CdO respectively, For rs MgO and rs CdO, the obtained results are very acceptable with experimental results existing in the literature. The deviations between our results and experimental data is less than 1%.
The estimated bandgap values to be 7.39eV for rs-MgO (rock salt) and 1.81eV for rs-CdO, the results deviate by less than 5% from experimental results. The energy bandgap (Eg) for x = 0, 0.25, 0.50, 0.75, and x = 1 varied quasi-linearly. Moreover, the optical parameters of $Cd_xMg_{1-x}O$ such as the dielectric function, the reflectivity, the refractive index, and the electron-loss-energy function have also been studied and discussed. Our findings results for rs MgO and rs CdO are also in good agreement with the experimental data, our results prove that the plasma frequency varied non-laniary from 7.33eV for rs MgO to 3.03eV for rs CdO.

Keywords:

Structural properties, electronic properties, optical properties, DFT calculations, TB-mBJ approximation, $Cd_xMg_{1-x}O$ alloys, dielectric function, MgO, CdO.

1. Introduction

The magnesium oxide (MgO) is a transparent dielectric material [1], it's used in technology as an optical window [2][3][4], with a wide direct gap about 7.83eV [5], and 6.5 eV [6]. Furthermore, CdO is a transparent conductor material [7], with an indirect gap about 1.11eV [8], 1.35 eV [9] and 0.84 eV [10]. MgO and CdO are mechanically stables at normal pressure in NaCl structure (B1) [11][12][13].

Actually, the research for new optoelectronic materials, which have a greater flexibility of optical response, is an interest subject. There are a plainly experimental and theoretical studies were performed to study different properties of $Zn_xMg_{1-x}O$ alloys [10][11][12][13][14][15], While the research on the $Cd_xMg_{1-x}O$ a few remain far as we know, whereas it is also equally important oxide of this family.

It is believed that the $Cd_xMg_{1-x}O$ alloys are mechanically stable in the same structure of MgO and CdO oxides in ambient conditions [16][17][18], and those alloys has the flexibility to shifting its properties to new fundamental properties that did not exist in its parent compounds. Furthermore, these alloys can behave the same or must interest in the optoelectronic material technology.

In this paper, the structural, elastic, and their related constants, electronic and optical properties for $Cd_xMg_{1-x}O$ alloys in the rock-salt phase at ambient pressure were investigated.

The calculations were performed using Full Potential Linearized Augmented Plane Wave (FP-LAPW) approach within the Density Functional Theory (DFT), the (TB-mBJ) correction of potential has been used.

The first part will be considered as a method test because the results of rs-MgO, and rs-CdO are precisely known. After that the other concentrations will be studied.

2. Computational details

These calculations were performed using the FP-LAPW method within the DFT theory as implemented in the Wien2 K code [22], we used GGA-WC exchange correlation [16]. In order to more accuracy of the electronic and optical properties, the (TB-mBJ) correction of potential has been included. This approximation has been confirmed to ameliorate effectively the calculations of most properties within the FP-DFT theory, and a more specially, of the electronic and the optical properties [20][18][17].

In order to avoid the calculations convergence affectation, the subsequent values have been optimized. The smallest atomic muffin-tin radius (RMT) are taken to be 2.0, 1.8, 1.6 atomic unit for Cd, Mg, O atoms respectively. The plan wave cut-off energy of $K_{max} \times R_{MT}$ is 7, when K_{max} is the extreme value of the reciprocal lattice vector.

After the convergence study, a grid of 11×11×11 meshes has been used. In order to more accuracy for optical properties the number of special K-points meshes was 21×21×21 k-points.

3. Results and discussions

3.1 Structural properties

The total energy using both GGA-WC approximations was calculated for different compositions x, using the Burch-Murnaghan equation of state the lattice parameter a_0 due to the zero pressure was estimated. The results of a_0 for various concentrations x are summarized in **table 1**. In this table, our results are compared with the other theoretical and experimental data reported in the literature. We note that our theoretical results agree well with other experimental results. The deviation between our finding results for rs-MgO and rs-CdO and experiment results is less than 1%.

The **figure1** shows the variation in lattice parameter a_0 as a function of Cd concentration in the rock-salt structure, the line curve in this figure represent variation in a_0 as a function of x calculated using GGA-WC approximation. The dotted curve line represent the variation in a_0 as a function of x estimated using Vegard's law [33]. We note that exchange of Mg atom with Cd atom leads to the

decrease quasi-laniary of lattice parameter a_0 (The deviation of the calculated lattice parameter is less than 1% from those estimated using Vegard's Law).

3.2 Electronic properties

Using the TB-mBJ approximation, the total and partial density of state partial (TDOS, PDOS), and the band structure along the various representative directions symmetry points in the Brillouin zone of rs-MgO and rs-CdO have been calculated. The results are presented in **figure 2** (rs-MgO), and **figure 2** (rs-CdO). Starting with partial density of state that presented in **figure 2(a)**, it is evident that O(2p) like orbital with a low contribution of the Mg(3p), Mg(3s) like orbitals compose the valence band, and Mg(3p), Mg(3s), O(2s) compose the conduction band, these states are responsible for the strong Mg-O liaison.

In **figure 2(b)**, it is clear that the maximum of the valence band is at point Γ, and the minimum of the conduction band is at the point Γ, which gives us a wide-direct-gap semiconductor (Γ-Γ) for rs-MgO. From these results, the direct gap of rs-MgO at zero pressure is 7.39eV, which is close to 7.83 eV [45], 7.1eV [46] obtained by experimental data. It represents a good accuracy in comparing with previously found theoretical results 5.35 [47], 5.05 [8] obtained by other approximations. These results confirm that the TB-mBJ is a good method for study the electronic properties.

Figure 3 shows the calculated TDOS, PDOS, and band structures of rs-CdO at zero pressure. the partial density of state are presented in **figure 3(a)**, this figure proves that the Cd(3d), and O(2p) like orbitals with a low contribution of Cd(3s) like orbital form the valence band, and the Cd(3p), Cd(3s), O(2p) form the conduction band. The calculated band structure is shown in figure 3(b), which clearly present that the maximum of the valence band is at point L, and the minimum of the conduction band is at the point Γ. Which prove that the fundamental gap nature of rs-CdO is indirect between the L and the Γ states. The calculated fundamental indirect gap is Eg=1.81eV is in good agreement of the experimental values 1.11 eV[9], 1.35 eV[10][48], 0.84 eV[8]. These founding was of more accuracy then theoretical results -0.5 eV[7][49], -0.66 eV[50][51], -0.667eV[11]. The direct gap is about of 1.81 eV, which also a good result compared with experimental results 2.28 eV [8], 2,40 eV [48], It is also a more accuracy then the results obtained by other methods 0.66 eV [50], 0.7 eV [7]. Therefore, we estimate that the results obtained using the TB-mBJ approximation are good for the $Cd_xMg_{1-x}O$ alloys

Figure 4 presents the calculated partial density of states of rs-$Cd_xMg_{1-x}O$ alloys at zero pressure, it shows that the O(2p) like orbitals with a low contribution of the Mg(3p), Cd(3s) form the valence band, and Cd(3s), Cd(3p), O(2p), Mg(2p) states form the conduction band. In this figure, we shows also the calculated band structure of rs-$Cd_xMg_{1-x}O$. It proves that the rs-$Cd_xMg_{1-x}O$ is an indirect band gap semiconductor between the L and the M states for x = 0.25, 0.50 and 0.75. It is clear that the nature of the gap is changed from direct (rs-MgO) to indirect (x=0.25, 0.50, 0.75, 1). A qualitatively like tendency has been reported for $Mg_xZn_{1-x}O$ semiconductors [18][52].

The variation in the calculated direct and indirect energy band gap as a function of Cd content are displayed in **Figure 5**. Four curves are showed in this figure; the black curves show the variation in direct and indirect band gap E_g versus x, and the red curves obtained by fitting those to a second order polynomial equation. From this Figure, it is clear that the substitution of Mg with Cd leads to the decrease of E_g. The behavior appears to be quasi-linear. The bowing parameter of the energy

band-gaps has been determined from a polynomial fitting of the energy band-gaps E_g curve according to the equation:

$$E_g^{Cd_xMg_{1-x}O} = x.E_g^{CdO} + (1-x)E_g^{MgO} - b.x.(1-x)$$

From this fitting, the direct band gap energy of rs-$Cd_xMg_{1-x}O$ can be estimated by the equation:

$$E_g^{Cd_xMg_{1-x}O} = 7.40\text{-}6.95.x\text{+}2.58.x^2$$

The indirect band gap of rs-$Cd_xMg_{1-x}O$ ($x\neq 0$) can be estimated by the equation:

$$E_g^{Cd_xMg_{1-x}O} = 4.81\text{-}4.98.x\text{+}2.0.x^2$$

3.4 Optical properties

The Kramers-Kronig model was tested to obtain the corresponding real and imaginary parts of the complex dielectric function $\varepsilon = \varepsilon_1 + i\,\varepsilon_2$, which is defined to describe the optical response of the alloy system at all phonon energies E=hω. The study of this response drives us to describe the optical properties [24]. The imaginary part ε_2 is calculated from the probabilities of electronic transitions between valence bands and conducting band (Inter-band transition), depending on the following equation [25]:

$$\varepsilon_2 = \frac{Ve^2}{2\pi \mathrm{h} m^2\omega^2}\int d^3k \sum_{n,n'} \left\langle kn\left|P\right|kn'\right\rangle^2 \times f\,(kn)\left(1-f\,(kn')\right)\delta\left(kn-kn'-\mathrm{h}\omega\right) \quad \text{.....(5)}$$

Where V is the volume of the cell, e and m are the charge and the mass of the electron, hω the energy of the incident photon, f(kn) is the Fermi-Dirac distribution, P is the angular momentum operator and kn is the wave function. By using the Kramers-Kronig relation, we can calculate the real part[26]:

$$\varepsilon_1 = 1 + \frac{2}{\pi}\int_0^{\infty} \frac{\varepsilon_2.\omega'.d\,\omega'}{\omega'^2-\omega^2} \quad \text{.....(6)}$$

It is possible to describe the absorption and refraction by a single term called the complex refractive index with real(n) and imaginary (k) parts, which called (refractive index (n), and extinction coefficient (k)) [27]. Those constants usually described by:

$$n = \sqrt{\frac{|\varepsilon| + \varepsilon_1}{2}},\ k = \sqrt{\frac{|\varepsilon| - \varepsilon_1}{2}} \quad \text{.....(7)}$$

The following relations can give the reflectivity and the energy loss:

$$R = \left|\frac{\sqrt{\varepsilon_1}-1}{\sqrt{\varepsilon_1}+1}\right|^2,\ L = -\frac{\varepsilon_2}{\left(\varepsilon_1^2+\varepsilon_2^2\right)} \quad \text{.....(8)}$$

Using TB-mBJ approximation, the imaginary ε_2 part of the dielectric functions calculated in different energy photon for rs-MgO, and rs-CdO. While, using the Kramers–Kronig expression one can estimate the real ε_1 part of the dielectric functions from ε_2, whilst, the reflectivity, loss function, and refraction can be computed using the expressions (7), (8). In addition, In **figure 6**; the results concerning the real and imaginary parts, reflectivity, loss function, and refraction a function of photon e for rs-MgO.

In **figure 6(a)**, the real part ε_1 spectrum analysis of the dielectric function present a few peaks, the first peak is located at about 7.33eV. This value essentially due to the electronic transitions between

valence band and conduction band, this value is close to the band gap energy. Thereafter, the real part ε_1 shows a minimum value at around a photon frequency of 20.4eV. Afterwards it exhibits a set of negative values at energy area [20.5eV, 21.9eV], so at this area the rs-MgO have a metallic behavior. At height energies, it tends towards zero so at this area the rs-MgO have a dielectric behavior.

The curve of the reflectivity presented in **figure 6(b)** indicates that, at low energies the reflectivity peak are generally not affected by the elevation of the photon energy, above 7.33 eV the peak of reflectivity is present a small increasing as the photon energy becomes higher. The reflectivity peaks are set to be 13.33%, 19.02%, 20.9%, and 20.9% for the photon energies 11.33 eV, 14.02 eV, 17.64 eV, and 19.33eV, respectively, and gets a maximum reflectivity (33%) for the photon energy 21eV. According to our results, the static dielectric constant which defined as the real part of the dielectric function at zero energy ($\varepsilon(0) = \varepsilon_{1\ (\omega=0)}$) is about 2.45, this value is close to the experimental and theoretical results 2.94 [53][54][55], 3.20 [56], 3.12 [57]. Furthermore, the imaginary parts of dielectric function as a function of photon energy curve is shown in **figure 6(a).** It's clear that the fundamental optical absorption for rs-MgO is limited to photon energies below 21eV This curve shows that a pronounced peak (E) near to the absorption edge [58]for photon energy of about 7.33eV, that are correspond a direct transition between the valence band and the conduction band at the Γ point. It results from a Wannier-Mott-like excitonic state [59]. Upward of the absorption edge in the spectrum, we can discuss four main peaks originates mainly from transitions between VB and CB at 11.49 eV, 13.94 eV, 10.28 eV, 13.75 eV. Those energetic positions are a good agreement with that of experiment measured [1][55].

In **figure 6(c)**, the results for the electron-energy-loss function for rs-MgO as a function of photon energy was shown. The fundamental peak is existing in the photon energy area [22.5eV, 30eV], the large peak report the fine structure of this material. The refractive index spectra as a function of the photon energy is presented in **figure 6(d),** the evident peaks are resulted from the excitonic transitions. The static refractive index n(0) is 1.5 for rs-MgO.

The real ε_1 and imaginary ε_2 parts of the dielectric functions, reflectivity, loss function, and refraction also calculated for rs-CdO. It is plotted a function of photon energy in **figure 7**. The **figure 7(a)** presents the real part of dielectric function as a function of photon energy, it shows a few of peaks for ε_1, the first peak essentially due to the electronic transitions between valence band and conduction band, it is located at around 3.27eV, this value is close to the band gap energy. Thereafter, the real part ε_1 shows negative values at energy area [15.27, 15.75eV], so Rs-CdO have a metallic behavior at this zone of energy. Above this zone, ε_1 toward to zeros, so it have a dielectric behavior above 15.75eV. The curve of ε_2 shows that the pronounced peak (E) near to the absorption edge for photon energy of about 3.78eV. We can discuss three main peaks 8.11 eV, 10.29 eV, and 13.72eV, those energetic positions are in good agreement with the experimentally measured ones [61].

The curve of the reflectivity for rs-CdO is displayed in **figure 7(b),** The reflectivity peaks are set to be 18.25%, 15.42%, 12.25%, and 20.10% for the photon energies 8.32eV, 10.45eV, 12.75eV, and 13.86eV, respectively, and gets a maximum reflectivity (23.35%) for the photon energy 15.75eV. We note that the reflectivity for rs-CdO. From our results, the static dielectric constant for rs-CdO is about 3.78, this value is close to the experimental results 3.8 [54], our obtained results are better than the results obtained by other methods 6.07 [49], 7.19 [60], 4.0 [7]. In **figure 7(c)** the results for the electron-energy-loss function for rs-CdO are shown, we discuss two large fundamental peaks correspond to resonance frequency at about 17, and 22.5 eV.

We note that our results for rs-MgO and rs-CdO are in good agreement with experiment data, those good results support us to following study for leftover values of x. The real ε_1 and imaginary ε_2 parts for leftover Cd concentrations of rs-$Cd_xMg_{1-x}O$ (x=0.25, 0.50, 0.75) have been studied using TB-mBJ approximation, the real and imaginary parts versus the photon energies are displayed in **figure 8((a)** and **(b))** for different values of x, we note that the change of the cadmium concentration has a strong influence on the dielectric function. The curve of real part ε_1 **(figure 8(a))** presents that the estimated static dielectric constant $\varepsilon_1(0)$ are about 2.62, 2.98, and 3.30 for the cadmium concentrations x= 0.25, 0.50, and 0.75 respectively, When proceeding x=0.25 to 0.5 to 0.75 the all the critical point shows a shift towards lower photon energies. This shift can be results to the change of the energy band gaps.

Figure 9((a) and **(b))** illustrates the reflectivity and loss function spectra for rs-$Cd_xMg_{1-x}O$. We note that all the peaks of $R(\omega)$ shifts to lower photon energy when x increases from 0.25 to 0.5 to 0.75, and the values of reflectivity decreases when the x increases. Almost the same observation for the main peaks of L(ω) in **figure 11(b).**

4. Conclusion

In this paper, the structural parameters of the $Cd_xMg_{1-x}O$ alloys in the rock-salt structure were investigated, the calculations were performed within the DFT approach, and we used the LAPW-FP method with GGA exchange correlations. The equilibrium lattice parameters for all cadmium concentration x were reported, besides, using GGA-TB-mBJ method we have studied the band structure, total and partial density of states, the dielectric function, the electron-energy-loss function, and the reflectivity of $Cd_xMg_{1-x}O$ in the rock-salt phase at zero pressure.

All calculated parameters for MgO (x=0) and CdO (x=1) were found to be in good reasonably with the experimental data available in literature, unfortunately, there are no experimental data available for other cadmium composition (0.25, 0.50, 0.75). Our results predict that $Cd_xMg_{1-x}O$ alloys for different x are stable in rock-salt phase, we can estimate also tha rs- $Cd_xMg_{1-x}O$ ternary alloys showed the lowest reflection and highest absorption in a large energy zone. Our results may offer a good prediction as a reference for future studies.

5. References

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Figures

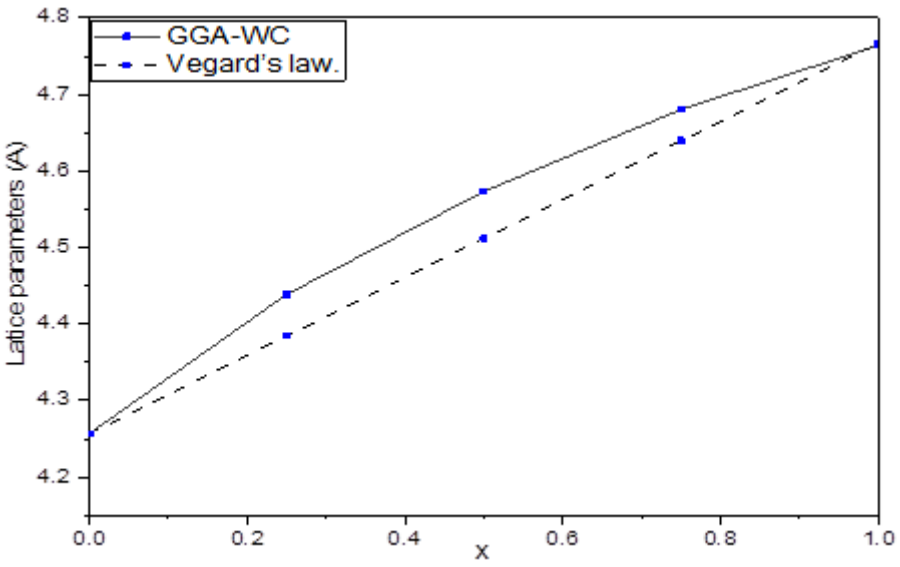


Figure 1

Lattice parameters a_0 a function of cadmium composition x for rock-salt $Cd_xMg_{1-x}O$ calculated using, GGA-WC methos

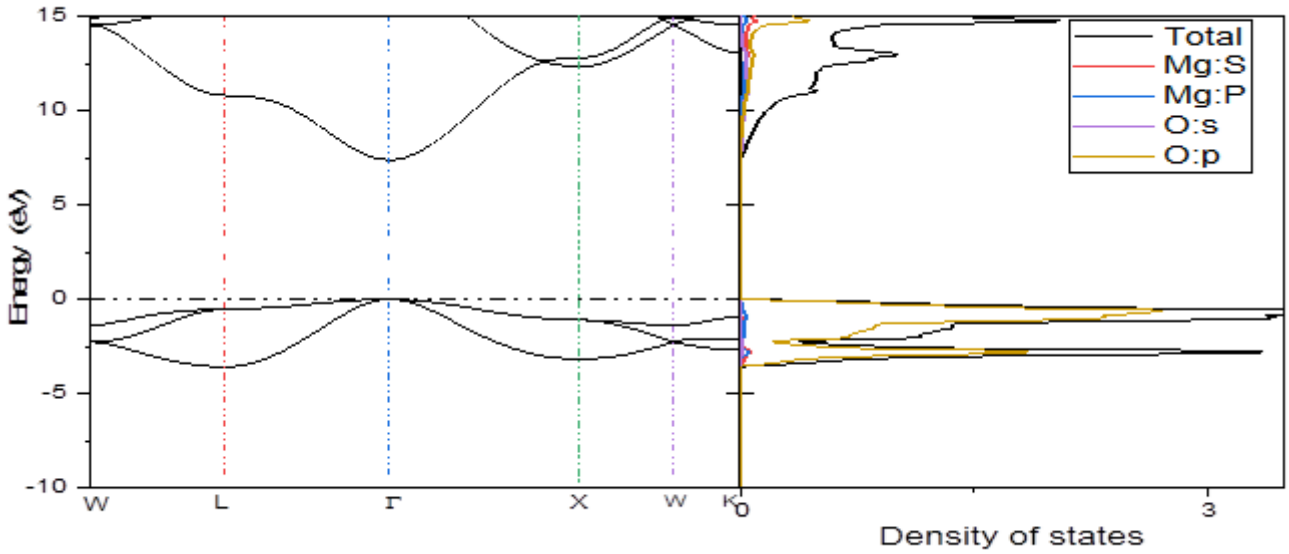


Figure 2

Band structure and density of states of rs-MgO

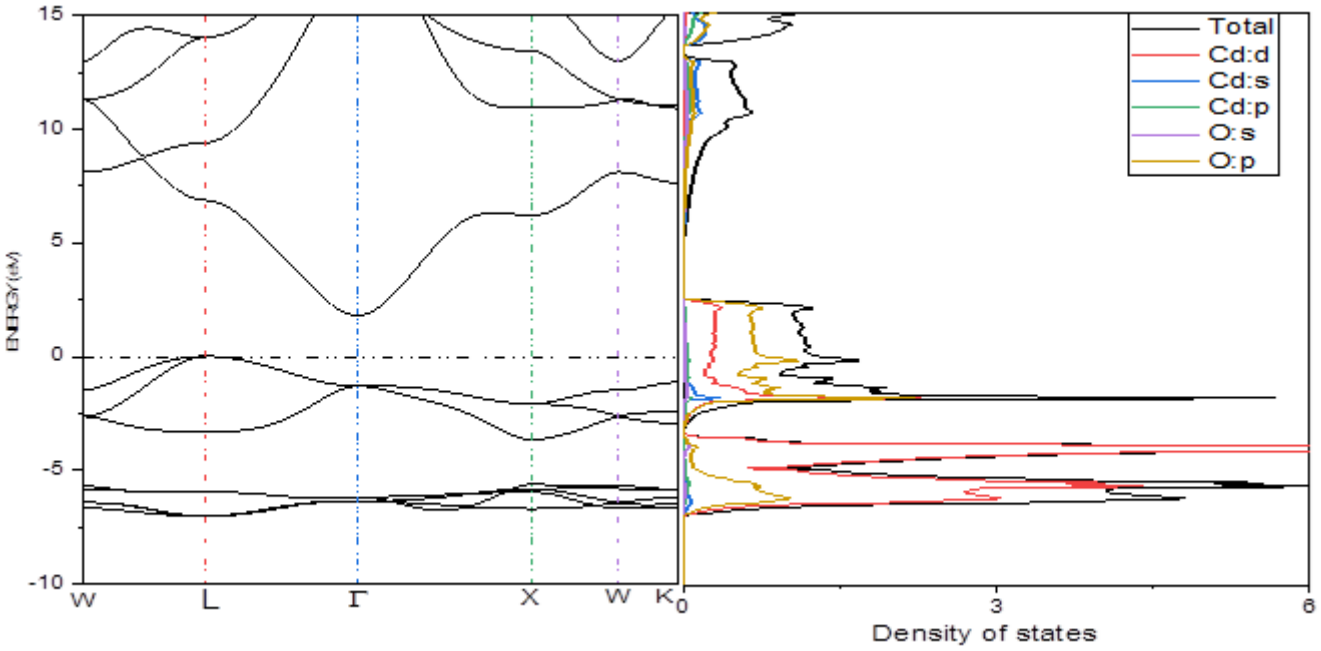
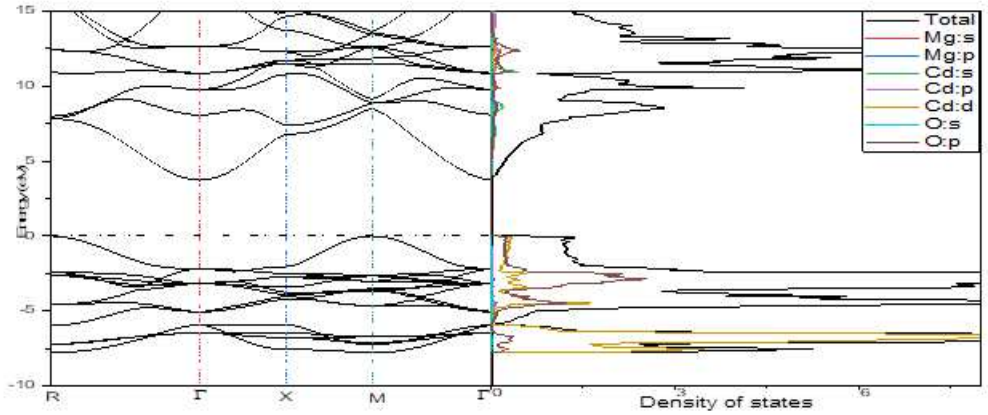
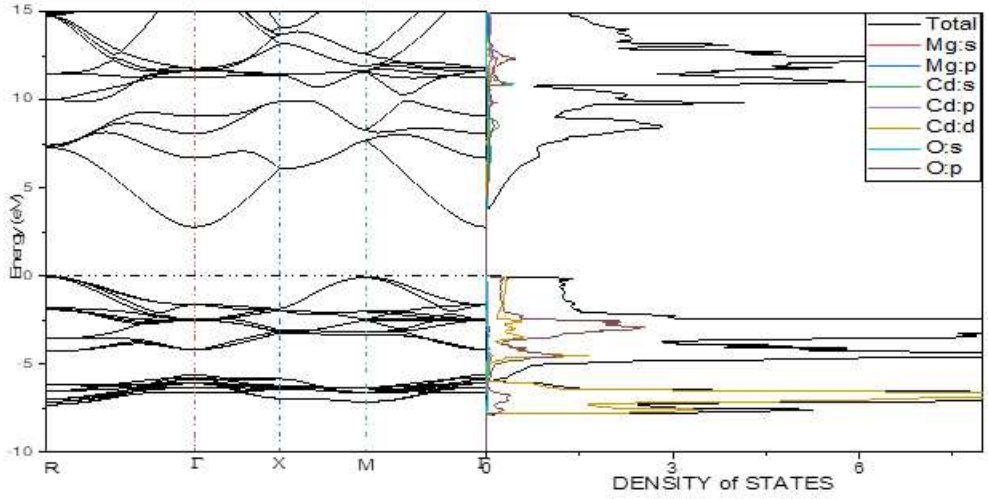


Figure 3

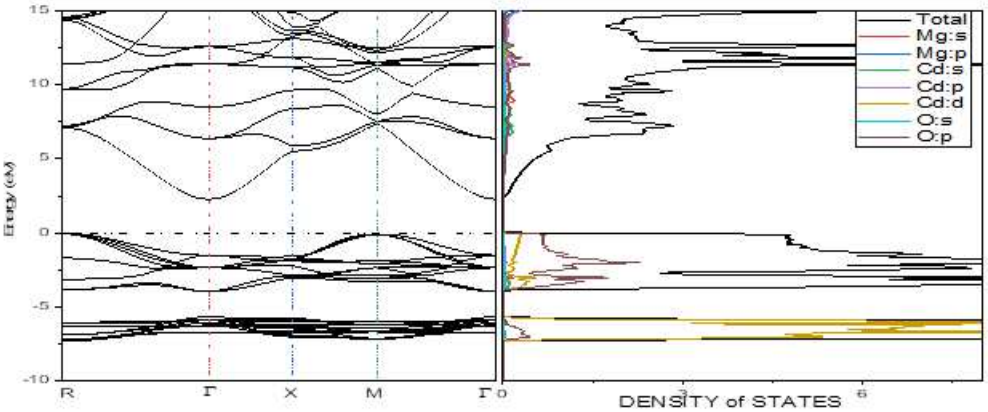
Band structure, total and partial density of states of rs CdO



x=0.25 (a)



x=0.50 (b)



x=0.75 (c)

Figure 4

Band structure and density of states of rs-$Cd_xMg_{1-x}O$ (x=0.25, x=0.50, x=0.75).

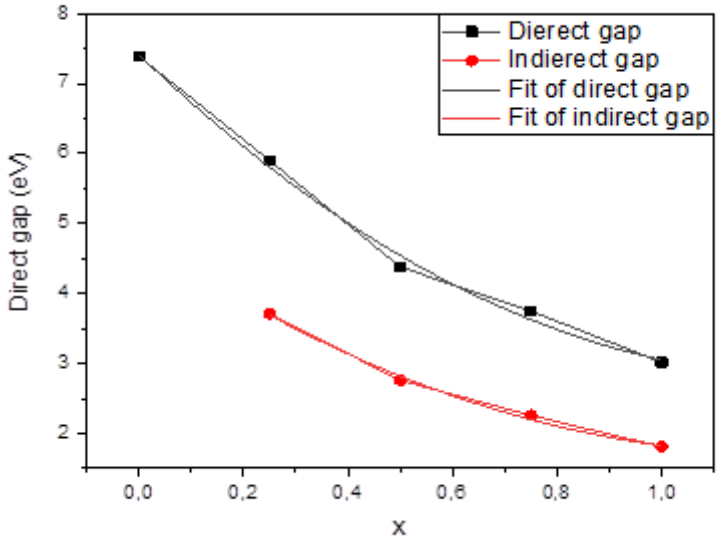


Figure 5

Variation of direct and indirect ban gap energy E_g as a function of x for rs-$Cd_xMg_{1-x}O$.

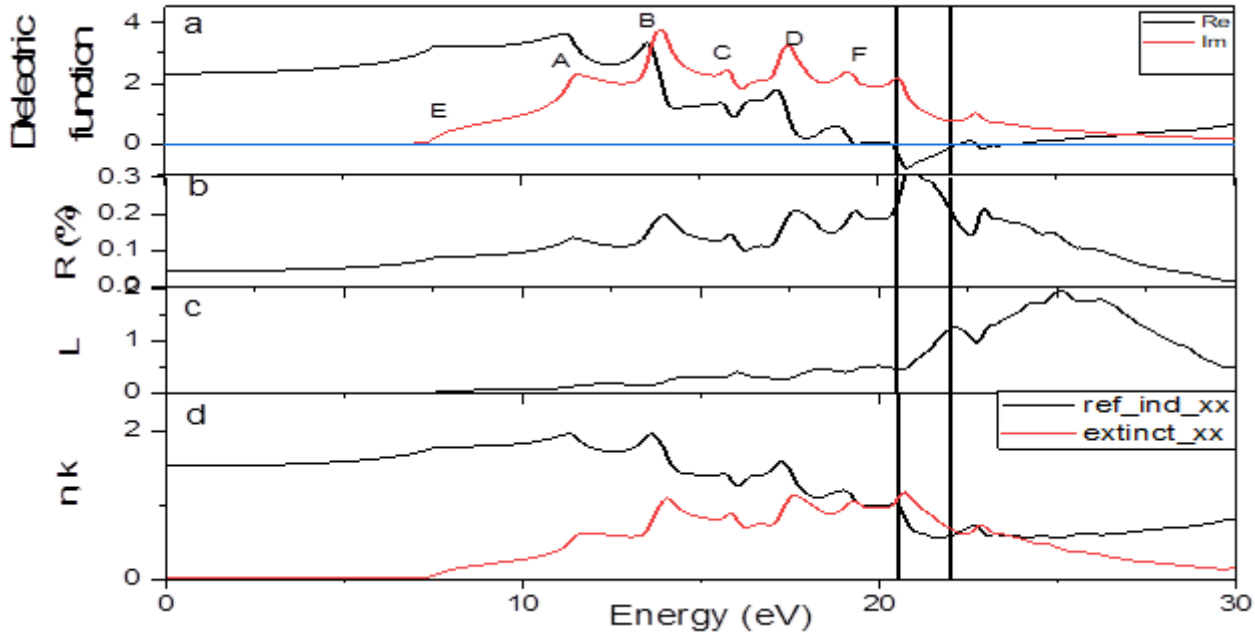


Figure 6

real and imaginary parts of dielectric function, reflectivity, loss function, and refraction for (a) rs-MgO displayed a function of photon energy.

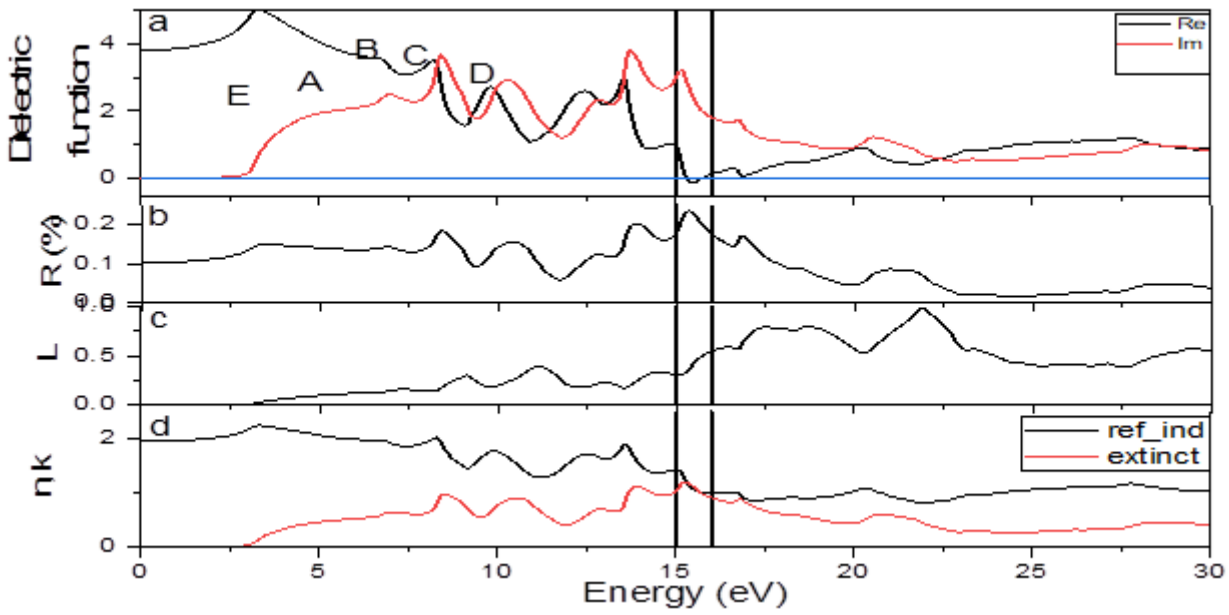


Figure 7

Rreal and imaginary parts of dielectric function, reflectivity, loss function, and refraction for rs- CdO displayed a function of photon energy.

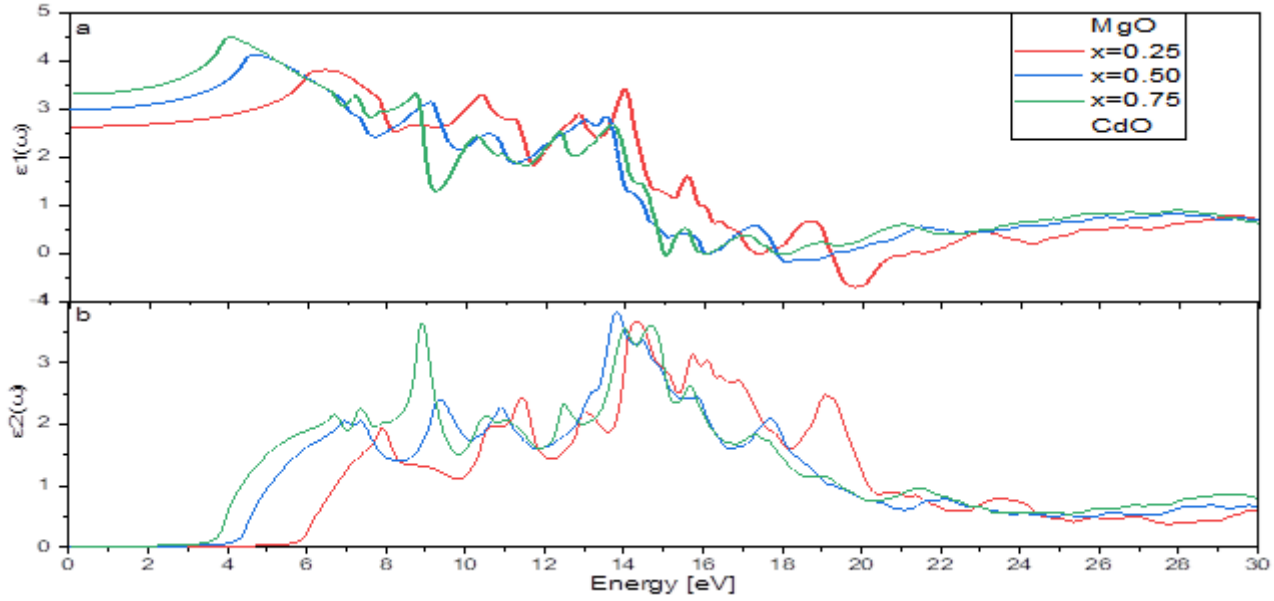


Figure 8

Real and imaginary parts of dielectric function for $Cd_xMg_{1-x}O$ for different values of x displayed a function of photon energy.

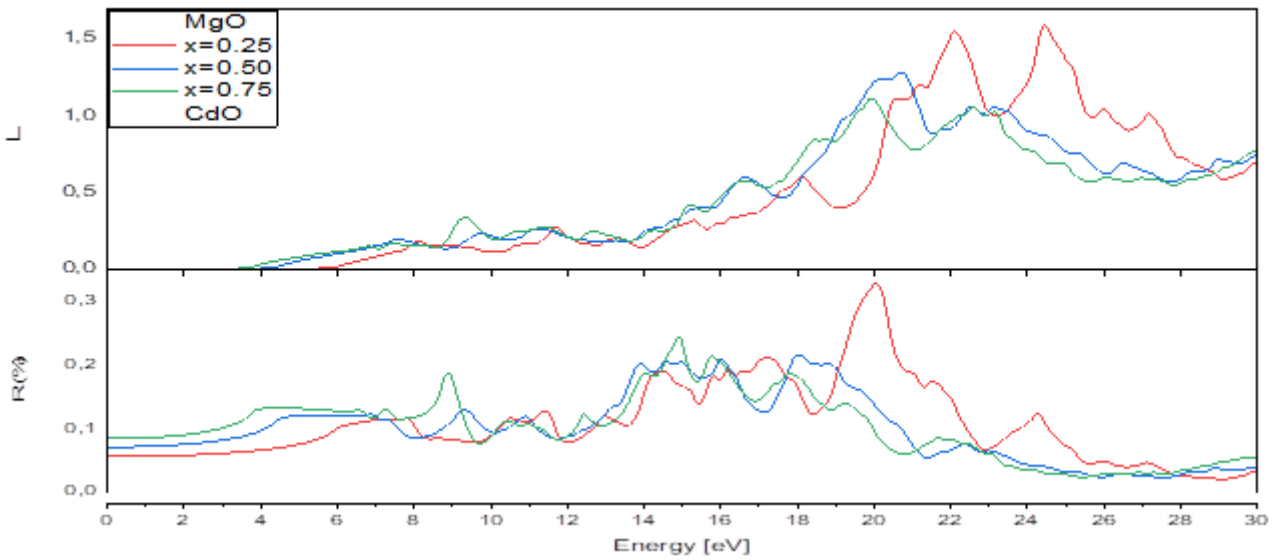


Figure 9

Reflectivity and loss function spectra for rs-$Cd_xMg_{1-x}O$ (x = 0, 0.25, 0.50, 0.75and 1).