DFT study of optoelectronic spectra of barium cadmium chalcogenides (Ba_2CdX_3 , $\text{X} = \text{S, Se and Te}$)

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DFT analyses of electronic and optical spectra of barium cadmium chalcogenides (Ba_2CdX_3 , $\text{X} = \text{S, Se, Te}$) have been carried out. The study of electronic spectra has been made in terms of band structure and density of states using full potential linear augmented plane wave plus local orbital method. Band structure calculations have been carried out under the approximations PBE-GGA, PBE-Sol, LDA and TB-mBJ. Band structures of these materials show that Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 crystals possess a band gap less than 1 eV, underestimated relative to the experimental/theoretical literature values. Optical spectra of these chalcogenides have been analyzed in terms of real and imaginary parts of dielectric function, reflectivity, refractive index, extinction coefficient, absorption coefficient, optical conductivity and electron energy loss. Optical results show large anisotropy along different directions. These results provide a physical basis of barium cadmium chalcogenides for potential application in optoelectronic devices.

Keywords: *semiconductors; electronic structure; optical properties*

1. Introduction

Recently, a great interest in the narrow/wide bandgap materials has been observed. Narrow bandgap materials are widely used in the area of detectors. Also optoelectronics requires cheap materials which have narrow bandgap. The class of narrow bandgap ternary materials may be a good alternative for other traditional narrow bandgap semiconductors.

Barium cadmium chalcogenides Ba_2CdX_3 ($\text{X} = \text{S, Se, Te}$) show some structural similarities isotypic to Ba_2MnX_3 ($\text{X} = \text{S, Se, Te}$) which are also isotypic to K_2AgI_3 . The Ba_2CdX_3 chalcogenides crystallize in orthorhombic phase with space group Pnma (62) [1]. The structural and configuration studies of Ba_2CdX_3 were carried out by Iglesias et al. [2]. Structural analysis showed that Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 have the lattice parameters, $a = 8.9145 \text{ \AA}$, $b = 4.3356 \text{ \AA}$, $c = 17.2439 \text{ \AA}$ for Ba_2CdS_3 ; $a = 9.2247 \text{ \AA}$,

$b = 4.4823 \text{ \AA}$, $c = 17.8706 \text{ \AA}$ for Ba_2CdSe_3 and $a = 9.8405 \text{ \AA}$, $b = 4.7502 \text{ \AA}$, $c = 19.1008 \text{ \AA}$ for Ba_2CdTe_3 , respectively [2–4]. Ba_2CdS_3 and Ba_2CdSe_3 were formed by heating the mixture of $2\text{BaS}:\text{CdS}$ and $2\text{BaSe}:\text{CdSe}$ in evacuated Vycor ampoules between $1000 \text{ }^\circ\text{C}$ and $1200 \text{ }^\circ\text{C}$ for sulfide and between $700 \text{ }^\circ\text{C}$ and $900 \text{ }^\circ\text{C}$ for selenide [2]. Synthesis and structural properties of Ba_2CdTe_3 were investigated by Wang et al. [1].

Other Ba-based transition metal chalcogenides (viz. Ba_2ZnS_3 , Ba_2ZnSe_3 and Ba_2ZnTe_3) also crystallize in the orthorhombic centrosymmetric space group Pnma [5–7]. Synthesis and luminescent properties of Ba_2ZnS_3 were studied by Lin et al. [5]. Electronic, thermal, optical, and photocatalytic properties of Ba_2ZnSe_3 were studied by Zhou et al. [6] and Reshak et al. [7]. Synthesis and magnetic studies of single crystals of $\text{Ba}_2\text{Fe}_2\text{Se}_3$ were performed by Krzton-Maziopa et al. [8] using X-ray and neutron powder diffraction. They found orthorhombic symmetry and antiferromagnetic ordering below 240 K in $\text{Ba}_2\text{Fe}_2\text{S}_3$. Electronic properties of BaCu_2S_2 were studied

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by Soliman et al. [9]. Structural behavior of some barium transition metal chalcogenides were studied by Andrew in his Ph.D. thesis [10]. To the best of our knowledge, some studies have been made on Ba-based isostructural transition metal chalcogenides but no systemic study has been performed on electronic and optical properties of Ba_2CdX_3 . Thus, barium cadmium chalcogenides have been chosen for the study on their optical and electronic properties.

2. Computational method

Density functional electronic structure calculations for Ba_2CdX_3 , ($X = \text{S, Se, Te}$) were performed in terms of band structure and density-of-state histograms using an accurate full potential linearized augmented plane-wave plus local orbital method (FP-LAPW + lo) with generalized gradient approximations (PBE-GGA) implemented in WIEN2k package [11–13]. The cutoff energy (which defines the separation of valence and core states) was chosen as -6.0 Ry for converging the SCF cycle and $14 \times 29 \times 7$ k points were used to calculate the total and partial density of states. The charge was taken to be 0.0001 EC for convergence criteria. The Fermi energies for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 were found to be 0.126 eV, 0.101 eV and 0.068 eV, respectively.

The optical functions such as dielectric function, reflectivity, refractive index, absorption coefficient, optical conductivity and energy loss function describe the response of materials to the incident photons [14–17]. Optical calculations of Ba_2CdX_3 ($X = \text{S, Se, Te}$) materials have been carried out with self-consistent scheme by solving the Kohn-Sham equation using the FP-LAPW + lo method in the framework of the DFT with the PBE-GGA method [12, 13]. The complex dielectric function has two components which describe the behavior of a material in the applied electromagnetic radiation field, [17, 18] given by:

$$\tilde{\epsilon}(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \quad (1)$$

Here, $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ represent the real and imaginary parts of dielectric function. The real part of dielectric function, $\epsilon_1(\omega)$ is related to dispersion

of incident photons by the material and the imaginary part of the dielectric function, $\epsilon_2(\omega)$ corresponds to the energy absorbed by the materials [19–21]. The total interband contributions to the $\epsilon_2(\omega)$ component are calculated by considering the transition from the occupied to unoccupied states through the transition matrix elements [19–21].

The imaginary part of the dielectric function $\epsilon_2(\omega)$ is expressed as [17, 18]:

$$\epsilon_2(\omega) = \frac{4\pi e^2}{m^2 \omega^2} \sum_{i,j} \langle i|M|j \rangle^2 f_i(1-f_j) \times \delta(E_F - E_i - \omega) d^3k \quad (2)$$

where M is the dipole matrix element, i and j are the initial and final states, respectively, f_i is the Fermi distribution function for the i^{th} state. E_i is the energy of electron in the i^{th} states.

By using the Kramers-Kronig relation [19–21], $\epsilon_1(\omega)$ can be determined from the imaginary part as:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P_0^\infty \int \frac{\omega' \epsilon_2(\omega')}{(\omega^2 - \omega'^2) d\omega'} \quad (3)$$

where P implies the principal value of the integral.

The absorption coefficient $\alpha(\omega)$ and reflectivity $R(\omega)$ in terms of real and imaginary part of complex refractive index describe also the optical behavior, and are expressed as [19–21]:

$$\alpha(\omega) = \sqrt{2\omega} \sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega) - \epsilon_1(\omega)}^{1/2} \quad (4)$$

$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (5)$$

where n and k represent the real and imaginary part of complex refractive index. Refractive index, $n(\omega)$ is expressed as [14, 22]:

$$m(\omega) = \frac{\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} + \epsilon_1(\omega)}{\sqrt{2}}^{1/2} \quad (6)$$

$$k(\omega) = \frac{\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} - \epsilon_1(\omega)}{\sqrt{2}}^{1/2} \quad (7)$$

The electron energy loss (ELOSS), $L(\omega)$ is defined as:

$$L(\omega) = \frac{\epsilon_2(\omega)}{[\epsilon_1^2(\omega) + \epsilon_2^2(\omega)]} \quad (8)$$

3. Results and discussion

3.1. Band structure and density of states

Electronic behavior of Ba_2CdX_3 ($X = \text{S, Se, Te}$) has been analyzed in terms of band structure and total and partial density of states. The band structure along the high symmetry directions W, L, Γ , X and K in the irreducible part of Brillouin zone calculated using PBE-GGA for Ba_2CdX_3 ($X = \text{S, Se, Te}$) are shown in Fig. 1. Different colors in Fig. 1 show the bands lying in different energy range along different symmetry directions W, L, Γ , X and K in the Brillouin zone. These band structure histograms confirm the narrow band gap at the Fermi level.

PBESol functional is intended to provide accurate values of equilibrium structural properties for solids [23, 24]. TB-mBJ potential yields accurate band gaps for semiconductors and insulators and it is less time consuming than the hybrid calculations. This functional is expected to be a significant improvement over PBE, PBESol and LDA functionals for band gap calculations [23–25]. Thus, the band gaps for Ba_2CdX_3 ($X = \text{S, Se, Te}$) were calculated using PBE-Sol, LDA and TB-mBJ exchange correlations and are presented in Table 1. The band gap values displayed in Table 1 for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 show that the band gap values E_g calculated using PBE-GGA, PBE-Sol and LDA are nearly equal but the band gap calculated using TB-mBJ was found to be larger compared to PBE-GGA, PBE-Sol and LDA.

Fig. 2 shows total density of states (TDOS) for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 , whereas Fig. 3 shows total density of states (TDOS) along with partial density of states (PDOS) spectra for Ba_2CdS_3 . Fig. 3a depicts that there are mainly two peaks below the Fermi level at around -8.0 eV and -4.0 eV. The peak at around -8.0 eV is mainly due to Cd-d orbitals with small contribution of S-p orbitals. The small peak at around -4.0 eV is mainly caused by hybridization of Cd-s and S-p orbitals. Some DOS also exist above the Fermi level at around 2.0 eV. These are empty states available for the conduction. These orbitals are mainly contributed by local Ba-d orbitals. The PDOS

Fig. 1. Electron dispersion curves for Ba_2CdS_3 ; (b) Ba_2CdSe_3 ; (c) Ba_2CdTe_3 along high symmetry directions in the Brillouin zone.

for Ba_2CdSe_3 and Ba_2CdTe_3 have not been shown (only TDOS Ba_2CdSe_3 and Ba_2CdTe_3 are shown in Fig. 2b and Fig. 2c) because almost all features of TDOS and PDOS for Ba_2CdSe_3 and Ba_2CdTe_3 have been found to be similar to Ba_2CdS_3 .

3.2. Optical properties

3.2.1. Dielectric function

Optical properties of barium cadmium chalcogenides have been illustrated in Fig. 4 to Fig. 7. The dispersion spectra of real part of dielectric

Table 1. Calculated and experimental values of band gap, E_g [eV] for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 using PBE-GGA, PBE-Sol, LDA and TB-mBJ exchange correlation.

	Ba_2CdS_3	Ba_2CdSe_3	Ba_2CdTe_3
PBE-GGA	0.088	0.154	0.441
PBE-Sol	0.048	0.118	0.387
LDA	0.069	0.122	0.423
TB-mBJ	0.187	0.296	0.638
Theoretical [26–29]	2.140, 1.735	1.610, 1.575	1.402
E_f	0.126	0.101	0.068

Fig. 2. Calculated total density of (a) Ba_2CdS_3 ; (b) Ba_2CdSe_3 ; (c) Ba_2CdTe_3 .

Fig. 3. Calculated total and partial density of states for (a) Ba_2CdS_3 -total; (b) Ba-total; (c) Cd-total; (d) S-total; (e) Gd-d orbital; (f) Gd-f; (g) Cd-d; (h) S-s, p orbital.

function, $\epsilon_1(\omega)$ have been illustrated in Fig. 4. It is seen that $\epsilon_1(\omega)$ extends in the energy range of ~ 0.1 eV to 14.0 eV for all three compounds Ba_2CdTe_3 , Ba_2CdSe_3 and Ba_2CdS_3 . It is clear from these figures that a major difference between $\epsilon_1^{xx}(\omega)$, $\epsilon_1^{yy}(\omega)$ and $\epsilon_1^{zz}(\omega)$ occurs in the energy

range from 0 eV to 10 eV and after this range there is no major difference among its values. Thus, there is a large anisotropy in the energy range of 0 eV to 10 eV, whereas beyond it, the anisotropy becomes small. The anisotropy is found to be larger along

y-direction compared to x- and z-directions. In addition, Fig. 4 depicts that $\epsilon_1(\omega) < 0$, in the energy range of ~ 6.0 eV to 10.0 eV for Ba_2CdS_3 ; 5.0 eV to 10.0 eV for Ba_2CdSe_3 and 3.0 eV to 8.0 eV for Ba_2CdTe_3 . $\epsilon_1(\omega)$ is negative in two energy ranges: from 0 eV to 2.0 eV and 3.0 eV to 10 eV for all the compounds. In energy range 0.0 eV to 2.0 eV the width and negative value of $\epsilon_1(\omega)$ on y-axis for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 changes in the order $\text{Ba}_2\text{CdS}_3 > \text{Ba}_2\text{CdSe}_3 > \text{Ba}_2\text{CdTe}_3$ for $\epsilon_1(0)^{yy}$, which implies that forbidden region and loss increases in the order $\text{Ba}_2\text{CdTe}_3 \rightarrow \text{Ba}_2\text{CdSe}_3 \rightarrow \text{Ba}_2\text{CdS}_3$ along y-direction. Moreover, in the energy range of 3.0 eV to 8.0 eV, $\epsilon_1(\omega) < 0$ in larger degree for x- and y-directions compared to z-direction, whereas in Ba_2CdTe_3 , $\epsilon_1(\omega) < 0$ in higher degree in x- and z-directions compared to y-direction. The energy range in which the real part of dielectric function $\epsilon_1(\omega) < 0$, indicates the forbidden region for the propagation of electromagnetic wave [30]. It means, Ba_2CdS_3 and Ba_2CdSe_3 have larger forbidden region in x- and y-directions compared to z-direction whereas Ba_2CdTe_3 has larger forbidden region in x- and z-directions compared to y-direction. Again, the static constant values of $\epsilon_1^{xx}(0)$, $\epsilon_1^{yy}(0)$ and $\epsilon_1^{zz}(0)$ (dielectric constant at zero frequency limit) are 6.30, 25.80 and 5.90 for Ba_2CdS_3 ; 6.0, 15.0 and 5.0 for Ba_2CdSe_3 ; and 14.0, 16.60 and 7.40 for Ba_2CdTe_3 . Smaller values of energy gap produce larger $\epsilon_1(0)$, which can be explained by the Penn model [31]. According to Penn model, $\epsilon_1(0)$ depends on the band gap of material and is related to refractive index in accordance to the relation $n(0) = \sqrt{\epsilon_1(0)}$ [30]. The values of $n(0)$ and $\epsilon_1(0)$ have been shown in Table 2. It is clear from Table 2 that the values of $n(0)$ and $\epsilon_1(0)$ satisfy the relation $n(0) = \sqrt{\epsilon_1(0)}$, which in turn justify the bandgap values of these compounds.

The variation of imaginary parts of dielectric constant, $\epsilon_2(\omega)$ along x-, y- and z-directions – ($\epsilon_2^{xx}(\omega)$, $\epsilon_2^{yy}(\omega)$ and $\epsilon_2^{zz}(\omega)$), as a function of photon energy have been illustrated in Fig. 4d, Fig. 4e and Fig. 4f for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 , respectively.

Fig. 4d, Fig. 4e and Fig. 4f show that for $\epsilon_2(\omega)$, the threshold energy (called first critical

Table 2. Values of refractive index for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 calculated using PBE-GGA.

	Ba_2CdS_3	Ba_2CdSe_3	Ba_2CdTe_3
$n(0)^{xx}$	2.51	2.45	3.74
$n(0)^{yy}$	5.07	3.87	4.08
$n(0)^{zz}$	2.47	2.23	2.72
$\epsilon_1(0)^{xx}$	6.30	6.0	14.0
$\epsilon_1(0)^{yy}$	25.80	15.0	16.60
$\epsilon_1(0)^{zz}$	5.90	5.00	7.40
$R(0)^{xx}$	0.18	0.17	0.34
$R(0)^{yy}$	0.46	0.35	0.37
$R(0)^{zz}$	0.17	0.15	0.22

Fig. 4. Real parts of dielectric function along x-, y- and z-directions for (a) Ba_2CdS_3 ; (b) Ba_2CdSe_3 ; (c) Ba_2CdTe_3 ; imaginary parts of dielectric function along x-, y- and z-directions for (d) Ba_2CdS_3 ; (e) Ba_2CdSe_3 ; (f) Ba_2CdTe_3 .

point) of the dielectric function occurs at 0.088 eV for Ba_2CdS_3 and 0.154 eV for Ba_2CdSe_3 and 0.441 eV for Ba_2CdTe_3 compounds which is equal to the bandgap (shown in the band structures and Table 1). It is also known as fundamental

absorption edge that is dominated by direct optical transition between valance band maxima and the conduction band minima. The main structure of $\epsilon_2^{xx}(\omega)$, $\epsilon_2^{yy}(\omega)$ and $\epsilon_2^{zz}(\omega)$ extends between threshold energy to 14.0 eV. The spectra of $\epsilon_2^{xx}(\omega)$, $\epsilon_2^{yy}(\omega)$ and $\epsilon_2^{zz}(\omega)$ for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 show one prominent sharp peak for $\epsilon_2^{yy}(\omega)$ at ≈ 1.0 eV which is shifted from lower to higher energy ranges of $0.5 \text{ eV} \rightarrow 0.6 \text{ eV} \rightarrow 0.7 \text{ eV}$; sharp peak of $\epsilon_2^{zz}(\omega)$ at ≈ 4.0 eV shifts from higher to lower energy range of $4.20 \text{ eV} \rightarrow 3.9 \text{ eV} \rightarrow 3.7 \text{ eV}$ and $\epsilon_2^{xx}(\omega)$ is shifted from lower to higher energy ranges by replacing S by Se or Te. This is due to the increase in bandgap and change in band energy dispersion [7]. One can see that the spectral structure of $\epsilon_2^{xx}(\omega)$, $\epsilon_2^{yy}(\omega)$ and $\epsilon_2^{zz}(\omega)$ for all the compounds have nearly the same pattern but large variation in the spectra of $\epsilon_2^{xx}(\omega)$, $\epsilon_2^{yy}(\omega)$ and $\epsilon_2^{zz}(\omega)$ of each compound indicate considerable anisotropy.

3.2.2. Reflectivity

Fig. 5 shows the reflection spectra for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 . The reflectivity x-, y- and z-components: $R(\omega)^{xx}$, $R(\omega)^{yy}$ and $R(\omega)^{zz}$, are significantly enhanced in comparison to zero frequency (static part of reflectivity) components. From the reflectivity spectra, we observe the large anisotropic behavior in low energy range (< 2 eV) and it becomes less anisotropic in higher frequency range. Moreover, anisotropy is larger in $R(\omega)^{yy}$ compared to $R(\omega)^{xx}$ and $R(\omega)^{zz}$ for Ba_2CdS_3 , Ba_2CdSe_3 in low energy range, whereas it becomes higher for $R(\omega)^{xx}$ and $R(\omega)^{zz}$ components in mid frequency range. In case of Ba_2CdTe_3 , the reflectivity is larger in x-direction in low frequency range and becomes higher in y- and z-direction compared to x-direction in mid energy range. The calculated values of reflection coefficient along x-, y- and z-axis are displayed in Table 2 from which we found the reflection values along x-, y- and z-axis which are 18 %, 46 % and 17 % for Ba_2CdS_3 ; 17 %, 35 % and 15 % for Ba_2CdSe_3 and 34 %, 37 % and 22 % for Ba_2CdTe_3 at 0 eV. These static values show that reflection is maximum along y-axis and minimum along z-axis.

Fig. 5. Reflectivity along x-, y- and z-directions for (a) Ba_2CdS_3 ; (b) Ba_2CdSe_3 ; (c) Ba_2CdTe_3 . Absorption coefficient along x-, y- and z-directions for (d) Ba_2CdS_3 ; (e) Ba_2CdSe_3 ; (f) Ba_2CdTe_3 .

3.2.3. Absorption coefficient

The spectrum of absorption coefficient, $\alpha(\omega)$ illustrates the relationship between the incident photons energies and their absorption by a material. Absorption coefficient as a function of photon energy has been calculated from dielectric constants (ϵ_1 and ϵ_2) and is shown in Fig. 5 for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 .

It is worth noting that the most intense part of the calculated radiations lies in the energy range between 0.0 eV and 6.0 eV. Absorption coefficient reveals the manner by which the compound absorbs the incident radiation. Absorption spectra and electronic spectra enable basic understanding of scintillating characteristics of materials. The imaginary part of dielectric constants is directly connected with the absorption spectra [32]. It is clear from the absorption spectra that the optical gap is very small ~ 0.08 eV for Ba_2CdS_3 , 0.15 for Ba_2CdSe_3 and 0.44 eV for Ba_2CdTe_3 . This is the region below which materials behave like a transparent medium. For all the three compounds, absorption spectra

are observed in the energy range ~ 0.1 eV to 14 eV for Ba_2CdS_3 and Ba_2CdSe_3 , and 0.4 eV to 14 eV for Ba_2CdTe_3 , i.e. they fall in the visible and near UV region which can be used in the study of spectra of radiation energy emitted by sun (solar emission) and the spectra of energy emitted by the stars (stellar emission) and in CCD video detectors. The higher values of absorption coefficients are observed in the energy range of 2 eV to 10 eV which indicates the promising application of all the compounds in fabrication of solar cells.

3.2.4. Refractive index

Refractive index plays a key role in the optoelectronics. Fig. 6a to Fig. 6c and Fig. 6d to Fig. 6f show the dispersion spectra for refractive index, $n(\omega)$ and extinction coefficient, $k(\omega)$, respectively. The complex refractive index describes the refraction as well as absorption of the material. The real part, $n(\omega)$ describes the bending nature of light beam when the light beam penetrates into the material whereas $k(\omega)$ represents the energy loss of light in the optical medium. Since the compounds have orthorhombic phase, so three tensor components – $n(\omega)^{xx}$, $n(\omega)^{yy}$, $n(\omega)^{zz}$ and $k(\omega)^{xx}$, $k(\omega)^{yy}$, $k(\omega)$ are required to describe the optical properties defining the linear properties of the studied materials. The values of $n(\omega)^{xx}$, $n(\omega)^{yy}$, and $n(\omega)^{zz}$ are enhanced beyond the zero frequency limit reaching their maximum values and then they start to decrease and around the unity, few oscillations are observed.

The extinction coefficient, $k(\omega)$ reveals the shortest absorption edge as the extinction coefficient $k(\omega)$ closely follows the $\epsilon_2(\omega)$ (Fig. 4d to Fig. 4f and Fig. 6d to Fig. 6f).

3.2.5. Optical conductivity

Optical conductivity, σ illustrates the conduction of free charge carriers over a defined range of photon energies. There is a change in optical conduction caused by illumination. Fig. 7 shows the optical conductivity of the studied compounds. One can observe from Fig. 7 that optical conduction starts at energy ~ 0.08 eV for Ba_2CdS_3 , 0.15 eV for Ba_2CdSe_3 and 0.44 eV for Ba_2CdTe_3 along all three axes. We notice that on increasing photon

Fig. 6. Refractive index along x-, y- and z-directions for (a) Ba_2CdS_3 ; (b) Ba_2CdSe_3 ; (c) Ba_2CdTe_3 ; extinction coefficient along x-, y- and z-directions for (d) Ba_2CdS_3 ; (e) Ba_2CdSe_3 ; (f) Ba_2CdTe_3 .

energy, the optical conduction rises up and reaches its highest value. Though the plots of σ_{xx} , σ_{yy} and σ_{zz} have many peaks but in each case, at least two sharp high peaks exist. The high sharp peaks are observed at 1.7 eV and 5.2 eV for σ_{xx} ; at 0.7 eV and 6.0 eV for σ_{yy} and 1.8 eV and 4.0 eV for σ_{zz} for Ba_2CdS_3 and Ba_2CdSe_3 , whereas these peaks are observed at 0.6 eV and 5.0 eV for σ_x , 0.7 eV and 4.0 eV for σ_{yy} and 1.0 eV and 3.8 eV for σ_{zz} for Ba_2CdTe_3 . These sharp peaks show that conduction achieves there large energy values. Moreover, the highest peak values of optical conduction at about 5.5 eV of σ_{xx} 6.0 eV of σ_{yy} and 4.0 eV of σ_{zz} shift towards lower energy values as cation S is replaced by Se or Te. This corresponds to the results obtained for ϵ_2 (Fig. 4d to Fig. 4f). The optical conduction curves consist of several other peaks representing plasma excitations which are caused by electrons transition from the valance to conduction band.

3.2.6. Electron energy loss

The electron energy loss, $L(\omega)$ represents the motion of the fast electron across the medium that loses an energy per unit length. Fig. 7 shows the energy loss as a function of photon energy for Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 . The peaks in energy loss represent the combined nature of plasma resonance and the related plasma frequency above which matter behaves like a dielectric and below which it reveals metallic character. A sharp peak existing at about 1.0 eV along y-direction, indicates larger loss at 1.0 eV in y-direction.

Fig. 7. Optical conductivity along x-, y- and z-directions for (a) Ba_2CdS_3 ; (b) Ba_2CdSe_3 ; (c) Ba_2CdTe_3 ; energy loss along x-, y- and z-directions for (d) Ba_2CdS_3 ; (e) Ba_2CdSe_3 ; (f) Ba_2CdTe_3 .

Some other peaks also exist in energy ranges of 7.0 eV to 12.0 eV. There are high peaks at 11.2 eV, 10.7 eV and 10.2 eV along x-, y- and z-directions for Ba_2CdS_3 ; at 10.80 eV along x- and y- directions and at 10.0 eV along z-direction for Ba_2CdSe_3 and at 9.0 eV for y- and z-directions and at 10.0 eV along x-direction for Ba_2CdTe_3 . Furthermore, the peaks for Ba_2CdS_3 and Ba_2CdSe_3 indicate

that energy loss in x-direction is higher than in y- and z-directions while the peaks for Ba_2CdTe_3 indicate that the loss in x-direction is smaller than in y- and z-directions.

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Received 2018-05-29

Accepted 2019-04-23