

Band Structure and optical properties of CDSE compounds calculated using density functional theory (DFT-LDA) and (DFT-GGA)

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ABSTRACT

This work studies the band structure and optical properties of Cadmium selenide (CdSe) are calculated by using density functional theory (DFT) on the implemented in CASTEP cod. By the local density approximation (LDA) and ginneries gradient approximation (GGA) , We have applied plane-wave pseudo potential method to study the band gap energies (E_g), partial density of state (PDOS) , total density of state (TDOS) and optical properties like absorption (α), reflection (R), refraction index (n), dielectric constant (ϵ), conductivity (σ) and extinction coefficient (k) were measured, with band gap energy 0.408 eV (LDA) and 1.105 eV(GGA) are in good agreement with other theoretical calculations as well as available experimental data.

Keywords:

Castep code; DFT (LAD), DFT (GGA), band gap, optical properties

1. Introduction:

Known for their unique electrical and optical devices, chalcogenide semiconductors [1-2]. For optical applications such as solar cells, thermal imaging, infrared power supply, anti-reflection coating, IR emitter, IR detector, tunable laser, wave guide, sensors, rewritable data storage, etc., these are the most crucial materials [3]. They are useful for all-optical switching because they have low-phonon-energy materials, are frequently transparent from the visible to the infrared, and are optically nonlinear. These materials are more adaptable and can change their properties when exposed to a variety of external forces, such as heat, pressure, light, fields, particles, and others. It exhibits a variety of photo-induced phenomena upon illumination by light, including photo crystallization, photodecomposition, photo vaporization, photo polymerization, photo contraction, and

photo expansion. Several parameters have undergone substantial research, including sample volume, absorption edge, refractive index, and bad gap. These materials can be used for solid state batteries because of their intriguing electrical and optical properties. The atomic structure of these materials may be determined by studying their optical and electrical properties, which is crucial for creating new technological applications. In this research, we examine the structural, electrical, and optical characteristics of the semiconductor CdSe chalcogenide. Recently, there has been a lot of interest in the II-VI compound semiconductors from the family of cadmium chalcogenides, both theoretically and experimentally. This is as a result of their unique physical characteristics. Several writers have reported on the cadmium chalcogenides CdX (X = S, Se, and Te) among them [4–13]. The use of these materials in photo-electrochemical

devices is significant. They form in various crystal structures and exhibit varying degrees of covalent, ionic, and metallic bonding (such as zinc-blende and wurtzite). The zinc-blende phase is used in this work. To benefit from them, one must have a solid understanding of the characteristics that are crucial for determining the range of potential applications. Based on the full potential linearized augmented plane wave which is self-consistent from the beginning

2. Method of calculation:

All measurements were performed using the Cambridge serial total energy program (CASTEP) code [14] and were done in accordance with the standard local density approximation (LDA)-CAPZ and generalized gradient approximation (GGA-PBESOL) approach using the non-conserving pseudo potential method and the relativistic treatment Koelling-Hammon [15]. The valence electrons were assumed to be $4d^{10}5s^2$ for Cd and $4s^24p^4$ for Se, for the atoms. Current cell volume (217.89\AA^3) and (231.99\AA^3) are used in this study with tailored energy cut off (480.0 eV) and (450.0 eV) for LDA and GGA, respectively. The grid parameters in the Brillouin region were $6 \times 6 \times 6$ k-points distributed equally. Additionally, the band gap, total density of states, partial density of states, and optical characteristics were computed.

3. Result and discussion:

3.1 Band Structure:

The DFT was taken into account, and the plane wave pseudo potential (PWP) strategy was used to perform the first-principles calculations (FPC) using the CASTEP algorithm. The calculations used DFT as implemented in the CASTEP software included with the Materials Studio package [16]. Due to the applied approach's great efficiency and lack of advanced orbital shape estimates, quick calculations are its

key characteristic. The valence electrons will interact and ensure quick convergence of the ion-electron potential, whereas the inner electrons and nuclei of the ions are thought to make up their cores. Figure (1) shows the band structures calculated for CdSe. The results for the CdSe system's electronic energy structure demonstrate that the band gap is near the high-symmetry point G of the Brillouin zone CdSe band gap (E_g) are lower than experimentally established specifications (0.408 eV) at LDA approximation and (1.105 eV) at GGA approximation. The band structure, total density of states (TDOS) and partial density of states (PDOS) of a substance reflect its electrical properties TDOS stands for density of state (see fig 2). $a = (0, 1/2, 1/2)$, $b = (1/2, 0, 1/2)$, and $c = (1/2, 1/2, 0)$ are the unit-cell vectors of zinc-blende-type structures, where 'a' is the cubic lattice constant. Cd at (0, 0, 0) and Se at (1/4, 1/4, 1/4) are the four CdSe formula units per unit cell. The sites and orbital projected density of states (DOS) for CdSe computed using the LDA and GGA is shown in Figure 2. According to the results of the LDA calculations, VB is made up of four bands, the lowest of which is made up of Se-4s states that have been slightly hybridized by Cd-4d states. Cd-4d bands primarily contribute to the following higher energy band. It has Se-4s and Te-4p bands that are mildly hybridized [23]. The band structure and band gap of CdTe were computed using the localized density approximation (LDA) and generalized gradient approximation (GGA) function in the software CASTEP, as shown in the figures, providing a band gap of roughly 0.408 eV for the CdSe at LDA and (1.105 eV) at GGA approximation, although the experimental band gap is claimed to be 1.7 eV [15]. Because the LDA function constantly underestimates the band gap, this occurs.

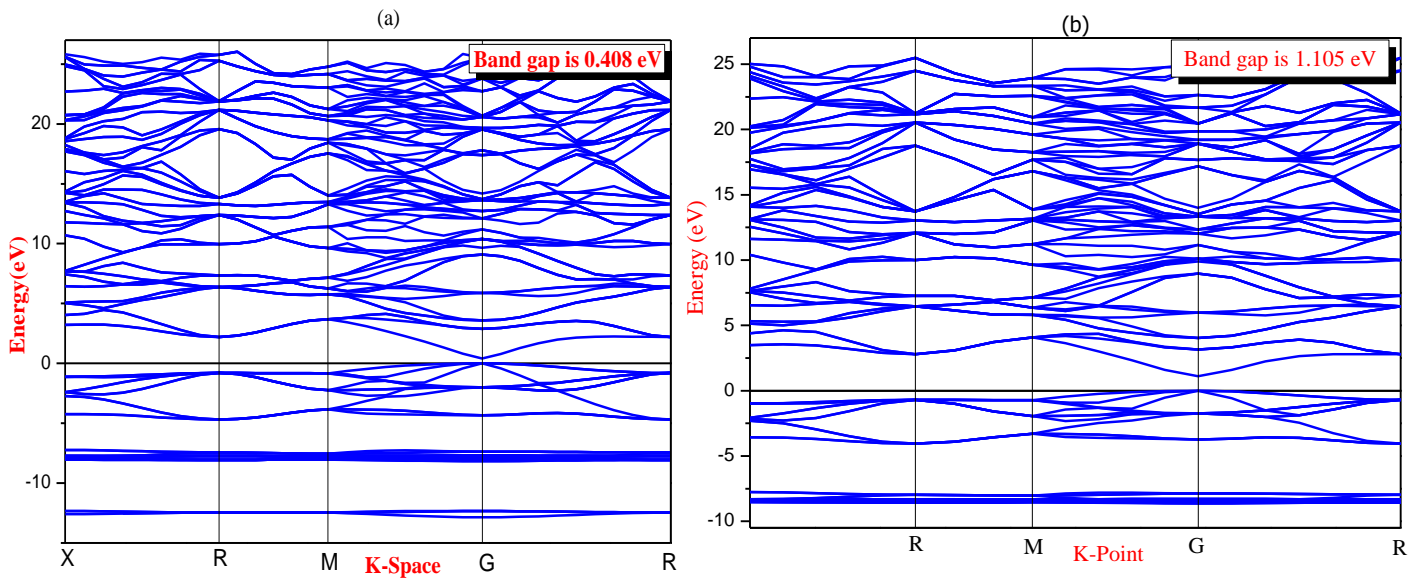


Fig. 1: Band gap structure of CdSe applying (a)LDA, (b)GGA approximation.

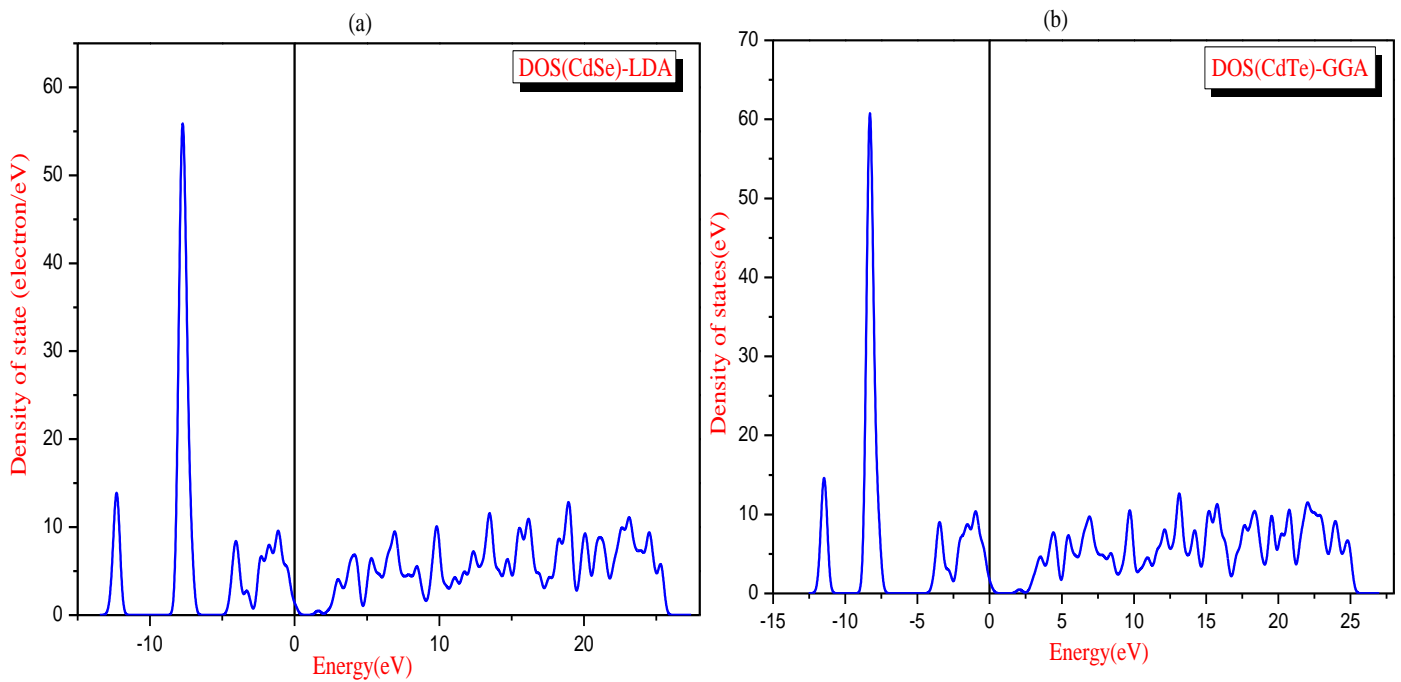


Fig. 2: The total density of states of compounds binary CdSe using the LDA and GGA approaches.

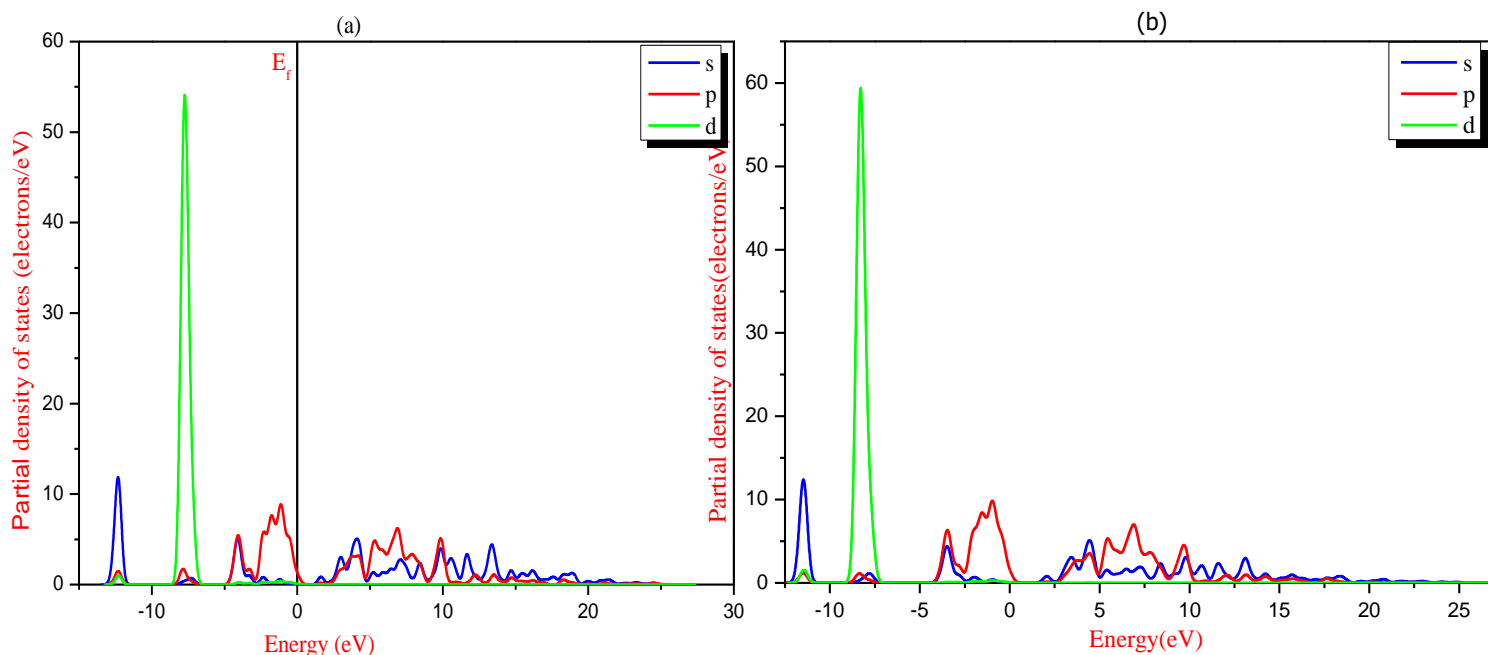


Fig. 3: The partial density of states of compounds binary CdSe using the LDA and GGA approaches.

4.2 Optical properties

Optical properties of CdSe in the reststrahlen region have been studied by several authors [11-15]. The Figures below shows the, absorption coefficient (α), refractive index (n), conductivity (σ), extinction coefficient (k), reflectivity (R), response functions (ϵ_1) and (ϵ_2) and derived using the LDA and GGA approximations for CdSe. The outcomes are contrasted with published experimental CdSe data [15]. The locations of all the peaks in the spectrum distribution of the optical spectra computed using DFT is pushed toward lower energy when compared to ones that have been empirically measured. A strict shift toward higher energies was made in order to correct the DFT's underestimation of the band gaps. The locations of every peak in the resulting optical spectra are largely similar with those discovered experimentally. Understanding a solid's electrical characteristics is aided by studying its optical characteristics, and optical conductivity of direct band gap It has been established that semiconductor binary compounds are optically active materials, and that these compounds' associated characteristics, such as their frequency-dependent dielectric function, The optical characteristics in this paper include In comparison to experimental data, the amplitude of the peaks corresponding to the basic absorption gap is overestimated. To ascertain the CdSe's optoelectronic uses, it is important to investigate its optical properties. For this, necessary optical properties are required. The complicated dielectric constant calculation, which assesses how an external electromagnetic field affects a system's linear response, makes up the majority of computed optical properties. Since the $\epsilon(\omega)$ depends on the estimated electronic band structure, we use the mBJ functional to evaluate the optical properties. The real and imaginary components of the function are indicated by $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$, respectively, in the definition of the complex dielectric function: $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ [28]. When $\epsilon(\omega)$ is known, additional important optical properties, such as the refractive index $n(\omega)$, extinction coefficient $k(\omega)$, optical reflectivity $R(\omega)$, optical conductivity, and absorption coefficient, can be estimated. This threshold is mostly caused by the transfer of electrons from the VB X to the CB G symmetry point for both molecules. Fig 8 (a,b) displays the real and imaging portion of the dielectric function The electronic component of the static dielectric constant, or zero frequency limit $\epsilon_1(0)$, is the most significant quantity in the spectra. It's computed values for CdSe-LDA and CdSe-GGA are 7.97 and 7.89, respectively. The refractive index $n(\omega)$ and extinction

coefficient $k(\omega)$ of CdSe-LDA and CdSe-GGA are shown in Figs. 5 and 7, respectively. The refractive index $n(\omega)$ value spectrum covers a wide energy range up to 35 eV. Similarities between the characters of $n(\omega)$ and $\epsilon_1(\omega)$ It is evident from Fig 5(a, b) that $n(\omega)$ rises with energy to reach a peak at values of 3.2 eV for CdSe-LDA and 3.1 eV for CdSe-GGA, respectively. The UV is shown by this behaviour of peak in the transparency zone, which goes to minimal level 12.6 eV and 10.17 eV, respectively. The computed values for the static refractive index $n(0)$ of CdSe-LDA and CdSe-GGA are 3.02 eV and 2.6eV, respectively Similar to how the band gap changes, this index does as well. Fig. 7(a, b) also demonstrates that local extinction coefficient $k(\omega)$ peaks connect to the static section of $\epsilon_1(0)$. Overall consistency of the $n(\omega)$ and $k(\omega)$ peak behaviour of both compounds is found, and it is in good agreement with previously published work on the subject. Our computed values of zero frequency reflectivity for CdSe-LDA and CdSe-GGA are 0.25 eV and 0.20 eV, respectively. Based on Fig. 9(a, b). It should be noticed that while switching from CdSe-LDA to CdSe-GGA, the value of zero frequency reflectivity $R(0)$ increases similarly to $\epsilon_1(\omega)$. Figure 4(a,b) displays the absorption coefficients $\alpha(\omega)$ for the perovskites CdSe-LDA and CdSe-GGA. The strong absorption zones of the tested materials are justified. When compared to Fig. 8(a,b), it can be seen that these distinct boundaries in the absorption coefficients are a characteristic of broad band gap semiconductor components, which only allow photons with energy suitable for stimulating an electron from the occupied levels of the valence band to the unoccupied levels in the conduction band to be detected into the material. Both of the perovskites' occurrence of high absorption areas between 13 and 15 eV may point to them as prospective candidates for use in UV frequency range optoelectronic devices. According to the measured optical conductivity (Fig. 6(a, b)), the optical conductivity of CdSe-LDA and CdSe-GGA respond to the applied energy at 0.72 eV and 1.24 eV, respectively.

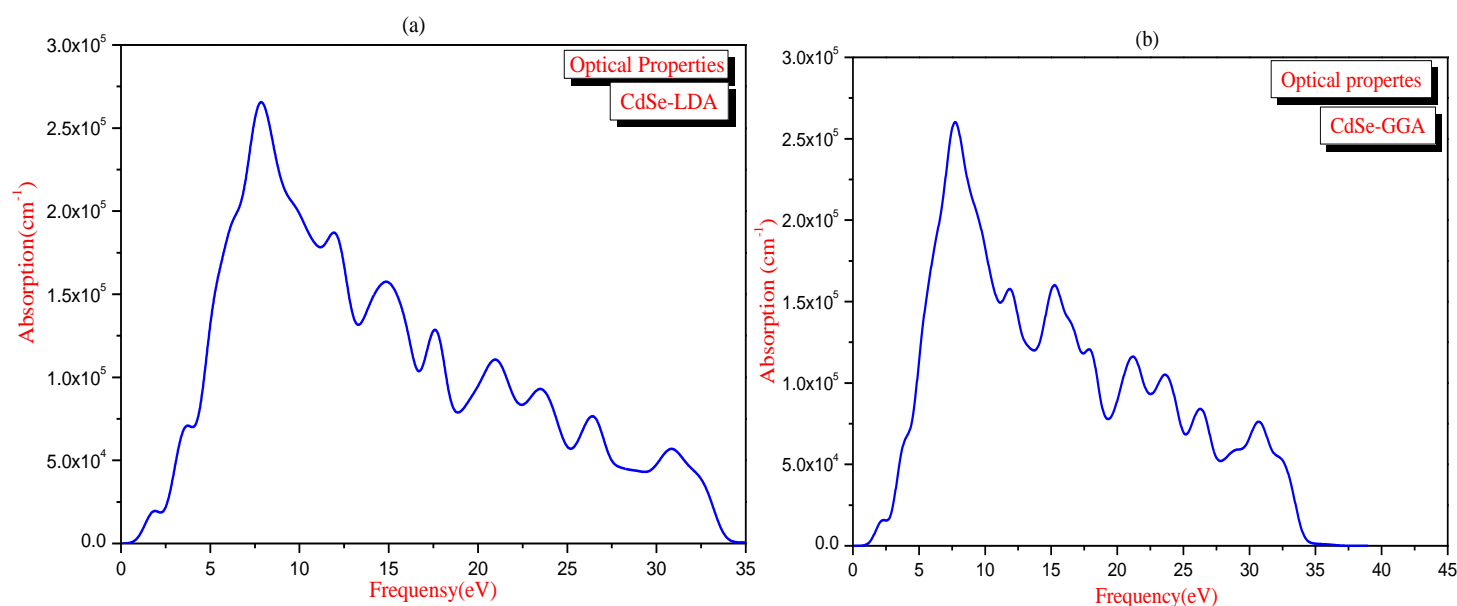


Fig. 4(a, b): The absorption coefficients compound binary CdSe using the LDA and GGA approaches.

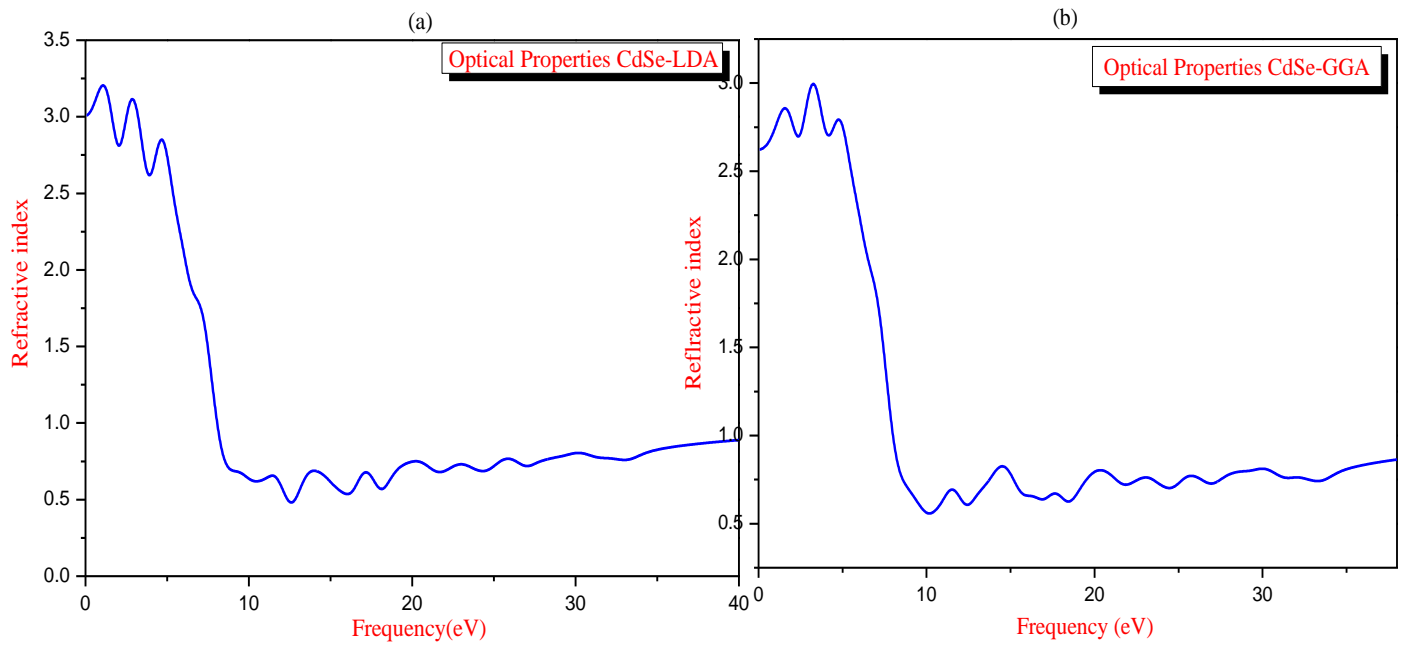


Fig. 5: The Refractive index compounds binary CdSe using the LDA and GGA approaches.

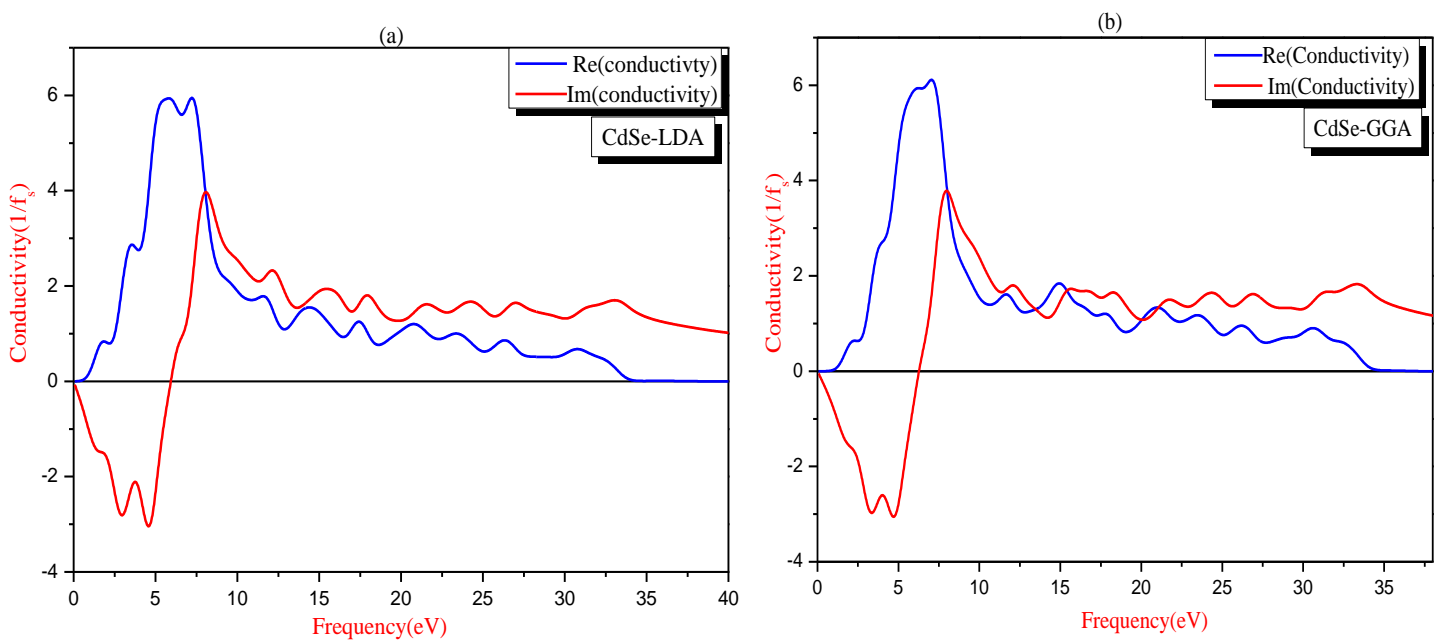


Fig.6: show the conductivity with real and imaginary part of conductivity. The real part is only positive value while the imaginary part is starting from negative part and going to positive part.

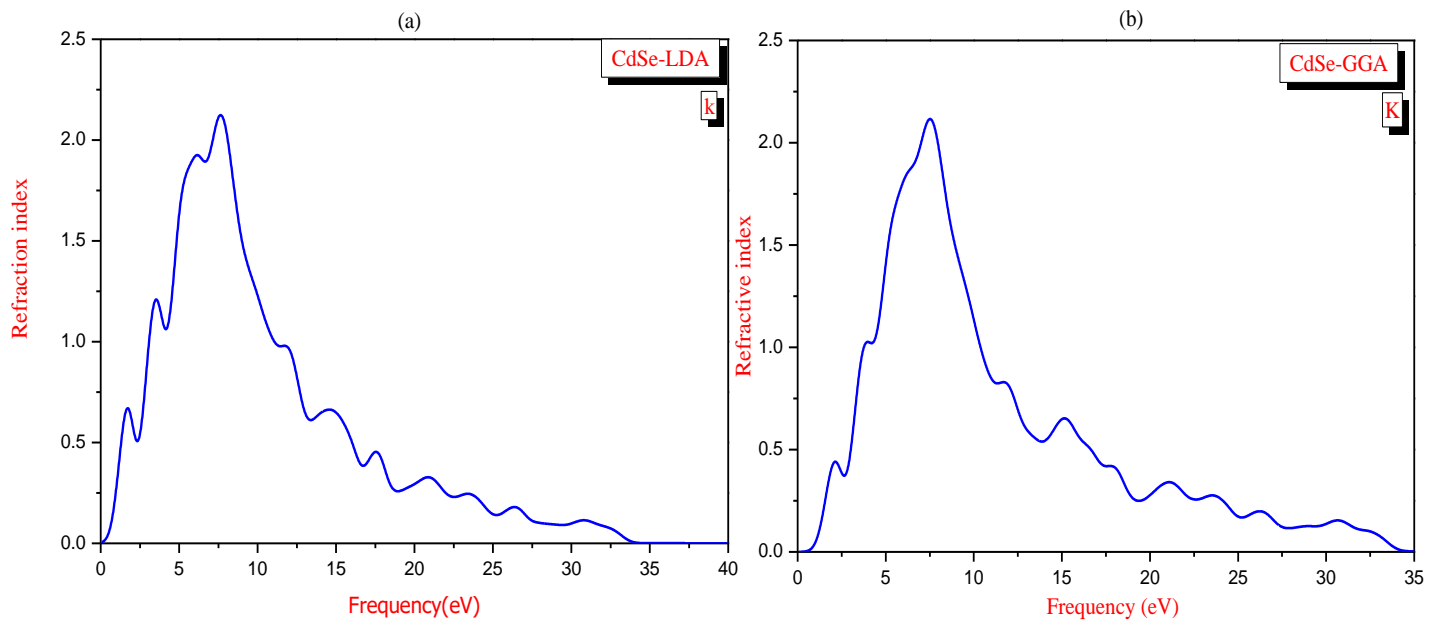


Fig.7: The refractive index compounds binary CdSe using the LDA and GGA approaches.

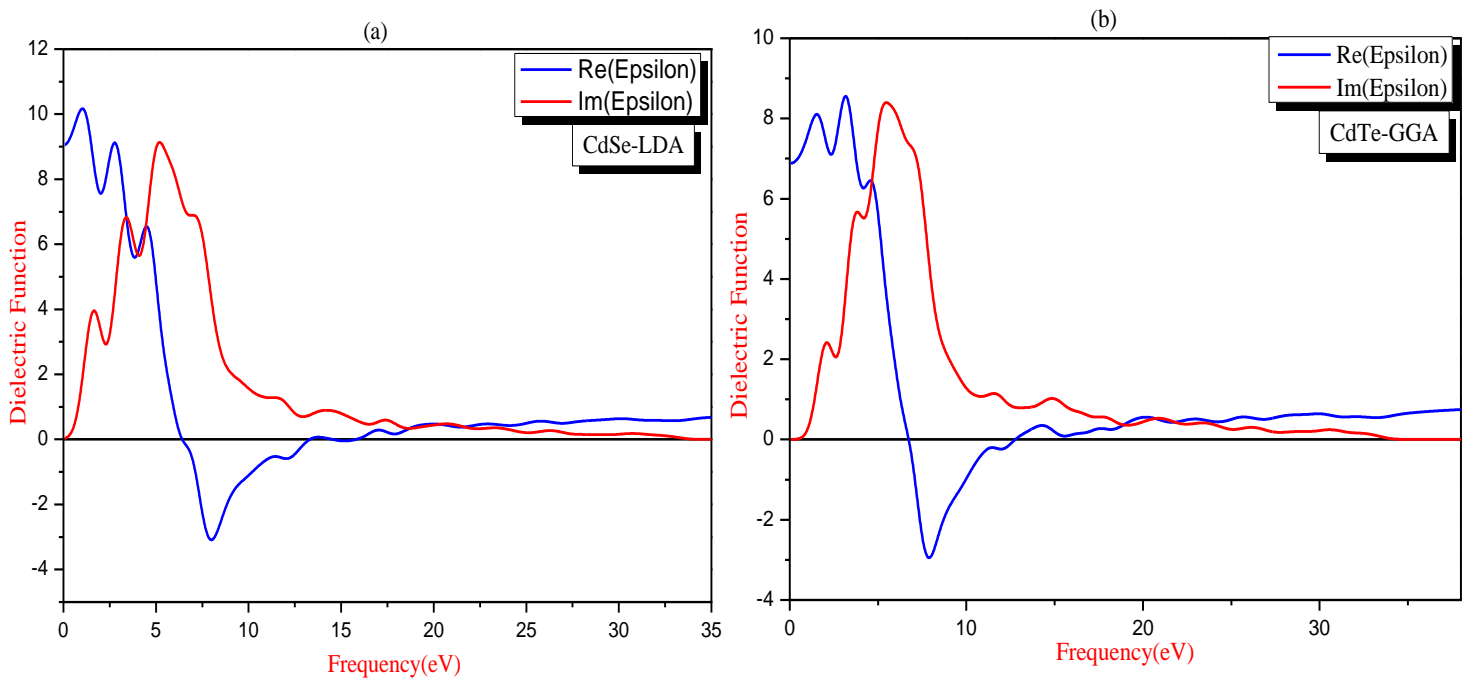


Fig 8: show the real and imaginary part of dielectric function where the peak of real part is 2.4 and the image is 10.8 for compounds binary CdSe using the LDA and GGA approaches.

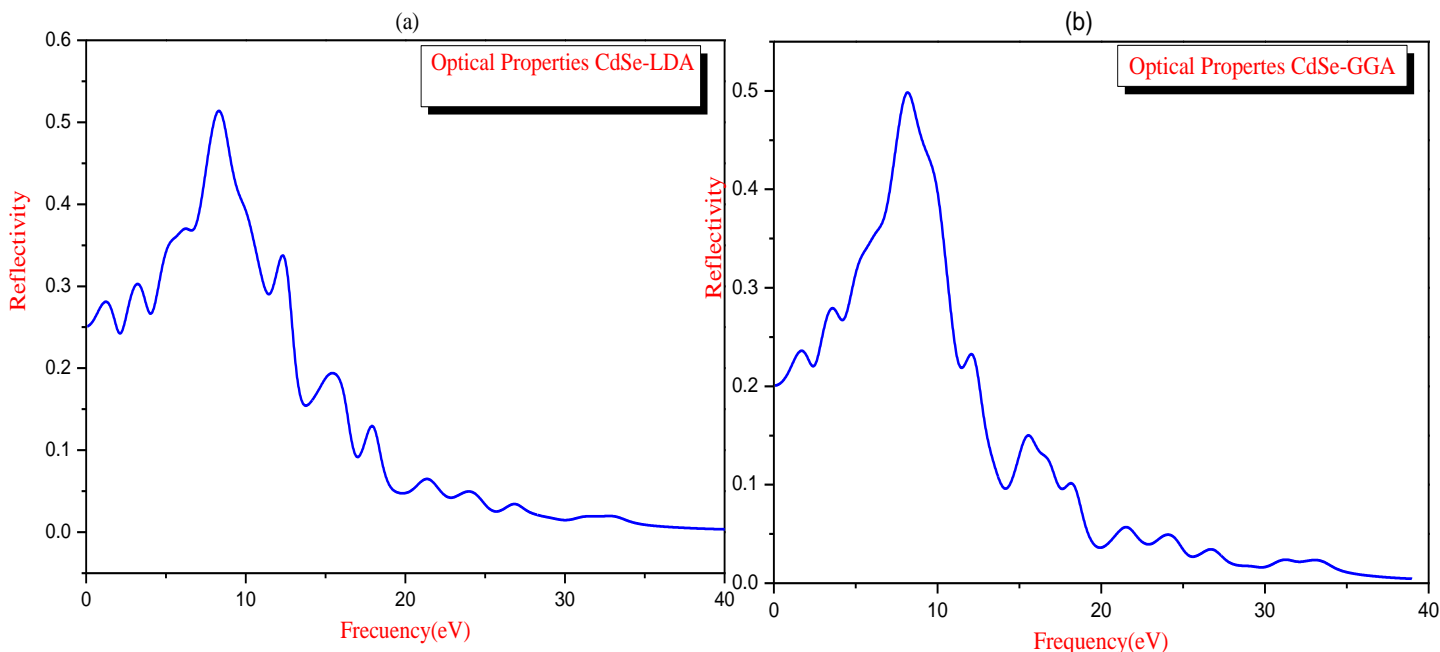


Fig. 9: The reflectivity compounds binary CdTe using the LDA and GGA approaches.

Conclusion

This work studies the band structure and optical properties of Cadmium selenide (CdSe) are calculated by using density functional theory (DFT) on the implemented in CASTEP code. By the local density approximation (LDA) and generalized gradient approximation (GGA), we have applied plane-wave pseudo potential method to study the band gap energies (E_g), total density of state (TDOS), partial density of state (PDOS), and optical properties like absorption (α), reflection (R), refraction index (n), dielectric constant (ϵ), conductivity (σ) and extinction coefficient (k) were measured). $a = (0, 1/2, 1/2)$, $b = (1/2, 0, 1/2)$, and $c = (1/2, 1/2, 0)$ are the unit-cell vectors of zinc-blende-type structures, where 'a' is the cubic lattice constant. Cd at $(0, 0, 0)$ and Se at $(1/4, 1/4, 1/4)$ are the four CdSe formula units per unit cell. With band gap energy (0.408 eV) and (1.105 eV) for LDA and GGA respectively, they are in good agreement with other theoretical calculations as well as available experimental data although the experimental band gap is claimed to be 1.7 eV.

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