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Comparative Computational Study of CdSe Cubic And Hexagonal Structures

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Abstract

Structural, electronic and optical properties of 2D CdSe (cadmium selenide) semiconductor cubic and hexagonal structure is determined by the First Principle calculation using PBE and GGA. Obtained the band gap GGA, PBE from Density Of States (DOS), Projected Density Of States (PDOS) and band structure of primitive and crystallized CdSe with both phases. The absorption coefficient, optical conductivity, optical constant, reflectivity, real and imaginary pat of dielectric function and energy loss function is analyzed by optical data using siesta. Optical properties are investigated to find out dielectric constant. Optical properties and excitonic binding energy is determined and are compared to the both structures of CdSe, which shows good relation between them. Existence of direct band gap for both structures is evident from the computational analysis.

Keywords: DFT, SIESTA, Optical Properties.

1. Introduction:

In this study we made a comparative study between computational DFT results data of structural, electronic and optical properties of CdSe Cubic and Hexagonal structures, observing crucial changes in both phases. CdSe-Cubic is stable at the low temperature and above critical temperature it transform to the Hexagonal structure[1]. The experimental energy gap in the Cubic phase is 1.68 eV and in the Hexagonal phase it is 1.74 eV[2]. The structural property are analysed in SIESTA software, DOS, PDOS, electronic band structures are reviles the electronic properties of CdSe and for optical properties we investigate the real and imaginary part of dielectric constant, absorption coefficient and optical conductivity[3-5], the study yields a good understanding of DFT based CdSe-Cubic and Hexagonal structures properties with experimental values[6]. Due to its high absorption coefficient[7], high photosensitivity and technological applications[8-11], as Gamma-rays detectors, solar cell's infrared windows, LEDs, sensors it is considered promising materials and being studied extensively during last few decades.

2. Computational methods:

A computer-quantum mechanical modelling method called DFT is used to determine the electronic and nuclear makeup of many-body systems, including atoms, molecules, and other small-scale objects. This theory states that the properties of a many-electron system can be found using functions [5]. DFT is one of the most popular and practical methods in condensed-matter physics, computational physics, and computational chemistry. First principles total energy calculations have been used to investigate the

structural and electrical properties of cubic and hexagonal CdSe systems [8]. The pseudopotential technique has been used in this code to solve the Kohn Sham (K-S) equations, and the exchange and correlation energies are handled within the GGA in accordance with the PBE parameterization [9]. We performed structural optimization using the cut-off energy and k-points, and by employing reduced lattice constants for both cubic and hexagonal structures, we discovered improved structural parameters [10].

3. Result and discussion:

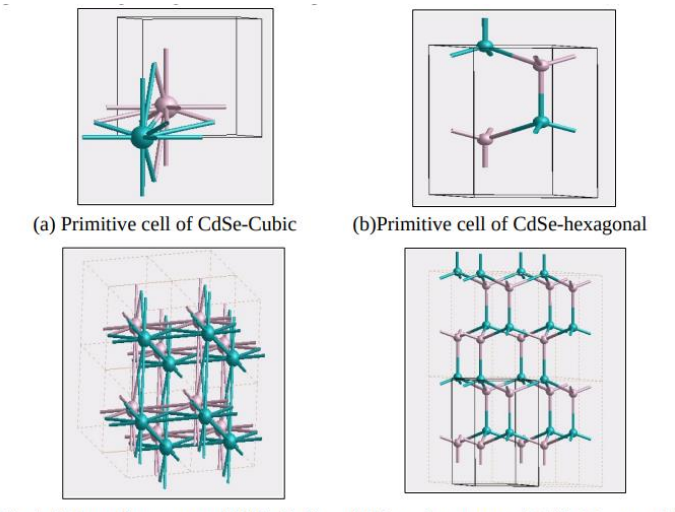
(1) Structural Analysis

To examine the structural properties of CdSe compound in the cubic structure and hexagonal structure, we have started DFT incorporated in the SIESTA package First principles calculation. First, we set the settings, such as the CG steps, lattice constant, mesh-cut-off, and k-point. Table 1 displays a few parameters. Following optimization, molecular structures are created using molecular design software such as Atomistic-Tool-Kit (ATK), GDIS, and Avogadro.

S. N	Compound Name	Mesh-Cut-off (Ry)	Lattice constant	Fermi Energy (eV)	Cell Volume
1.	CdSe_Cubic	250	1.0	-4.681	59.9952
2.	CdSe_Hexagonal	250	1.0	-4.696	119.89

Table-1: Input Parameter of CdSe Cubic and CdSe Hexagonal structure.

The calculated ground state lattice parameter in Cubic phase is 6.21 Å, while in the Hexagonal phase it is found that a = b = 4.39 Å and c = 7.71 Å, it is also observed that there is a little difference in the Fermi level of both structures CdSe-Cubic (-4.681 eV) and CdSe-Hexagonal (-4.696 eV). The calculated bond length between Cd and Se atoms is 2.69 Å in both phase.



(a) Primitive cell of CdSe-Cubic (b)Primitive cell of CdSe-hexagonal

Fig-1:(a)Crystal structure of CdSe Cubic (b)Crystal structure of CdSe Hexagonal

The CdSe crystal structure and unit cell of the cubic and hexagonal models are shown in Figures 1(a) and (b). The pink and blue balls in the picture represent selenide and cadmium atoms, respectively. The most symmetric CdSe structure is stable, according to other papers. Here, we were able to get both phases' symmetric structures. Tables 2(a) and (b) display the bond lengths and bond angles between the atoms.

S. No.	Compound Name	Bond Name	Bond Length
1	CdSe_Cubic	Cd1-Se2	2.69Å
2	CdSe_Hexa	Cd1-Se4	2.69Å
3	CdSe_Hexa	Se3-Cd2	2.69Å
4	CdSe_Hexa	Se4-Cd2	2.69Å

Table-2(a): Bond Lenght for CdSe Cubic and CdSe Hexagonal structure

S. No.	Compound Name	Angle Name	Bond Angle
1	CdSe_Cubic	Cd1-Se2	180˚
2	CdSe_Hexa	Cd1-Se4-Cd2	109.36˚
3	CdSe_Hexa	Se3-Cd2-Se4	109.36

Table-2(b): Bond Angle for CdSe Cubic and CdSe Hexagonal structure

The bond length between the CD and Se atoms in table 1 is marginally longer than the experimental value; this is consistent with the general pattern that GGA typically overestimates the lattice parameters. For both cubic and hexagonal compounds, our GGA results correspond well with other computed values and experimental evidence.[7]

(2) Electronic Property Analysis:

Investigation of optical properties of CdSe for optoelectronic applications, real and imaginary dielectric function are calculated by equation

ε(ω) = ε 1 (ω) + iε2 (ω).

Frequency dependent imaginary dielectric function ε2(ω) is given by:

$$\varepsilon_2(\omega) = \frac{8}{2\pi\omega^2}\sum_{nn\prime}\int_{BZ}|P_{nn'}(k)|^2\frac{dS_k}{\nabla\omega_{nn'}(k)}$$

Where ∫ is an integration over the entire Brillouin zone,

∑ ′ is the sum over all initial valence $B\mathbf{Z}$ nn band and final conduction band states,

| ′ ( )| 2 is the dipole matrix element between final and P nn k initial states, is energy surface with constant value, ω nn ′

(k) is the energy difference between dS k two states.

The real part of dielectric function ε 1 (ω) can be extracted from imaginary part using Kramer Kroning relation.

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

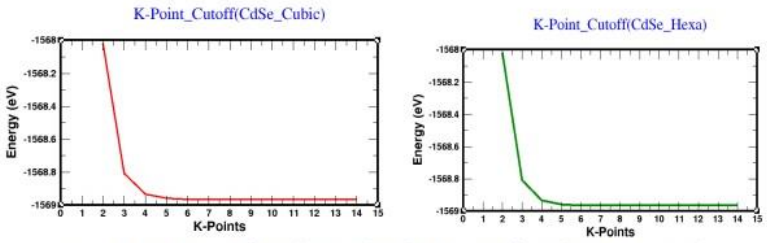


Fig.2: (a) K-point for CdSe_Cubic, (b) K-point for CdSe_Hexagonal

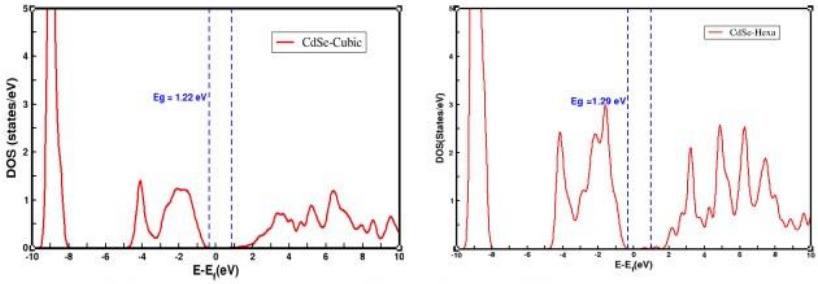


Fig-3: Density of States (a) CdSe_Cubic, (b) CdSe_Hexagonal

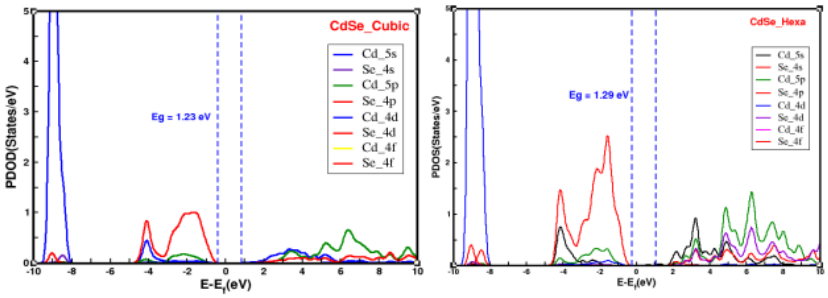


Fig-4: Projected Density of States (a) CdSe_Cubic, (b) CdSe_Hexagonal

The calculating density of states for the CdSe cubic and hexagonal phases is shown in Figures 3 (a) and (b), while the projected density of states is shown in Figures 4 (a) and (b). The hexagonal structure has intense energy levels in both the valence and conduction bands, while the cubic structure's DOS shows a very intense region in the conduction band.

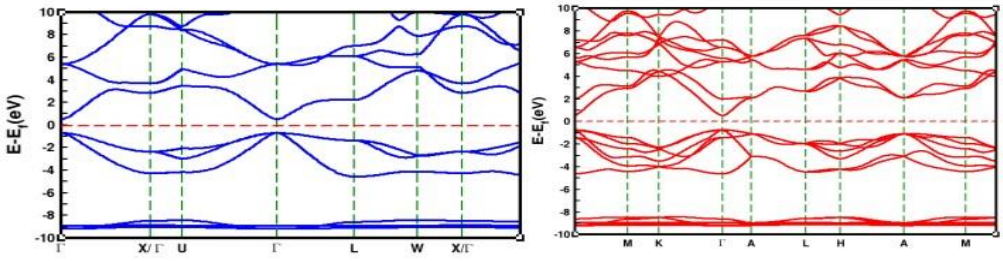


Fig-5: Electronic band structure of (a) CdSe_Cubic, (b) CdSe_Hexagonal

The band structures of CdSe in various cubic and hexagonal structures are depicted in Figure 5: (a) and (b), respectively. This research was conducted using approximations. For the cubic and hexagonal configurations, it is demonstrated that the band gap is a straight bang gap in the Γ point. Consequently, the gap values in the cubic and hexagonal structures, 1.22 eV and 1.29
eV, respectively, are lover than the observed band gap value. Because excited states are not
taken into account in the normal DFT, the band gap is typically underestimated by GGA, resulting in 1.68 eV in cubic and 1.74 eV in hexagonal.

(3) Optical Property Analysis:

The variation of the absorption in the region of ultraviolet and visible light of Hexagonal does not present a large difference with the cubic structure.

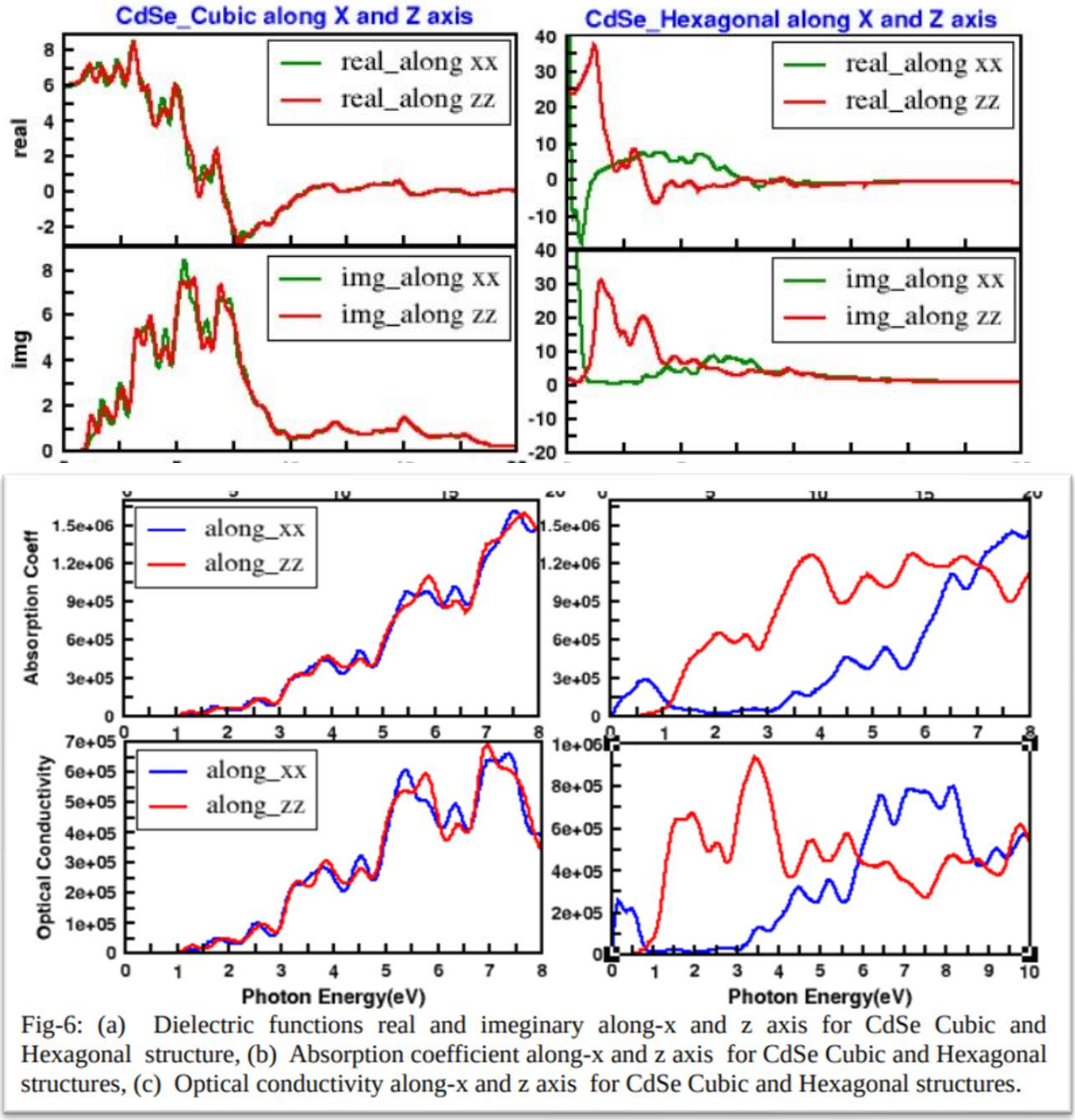


Fig-6: (a) Dielectric functions real and imeginary along-x and z axis for CdSe Cubic and Hexagonal structure, (b) Absorption coefficient along-x and z axis for CdSe Cubic and Hexagonal structures, (c) Optical conductivity along-x and z axis for CdSe Cubic and Hexagonal structures.

In order to calculate significant optical functions, the frequency-dependent imaginary and real dielectric functions are both examined.[] Figure 6(b), which displays the fluctuation in absorbance as a function of wavelength for the CdSe compound in both forms, demonstrates that the hexagonal structure is not fully isotopic whereas the cubic structure is. The radiation's hv propagation along the x and z directions stays constant in the CdSe-Cubic system, but there is a notable absorption in the UV spectrum. CdSe has a low absorption in the visible light spectrum between 450 and 650 nm, which is significantly lower than the ultraviolet. Because CdSe is hexagonal, radiation propagates differently in the xx and zz directions.

4. Conclusions:

The DFT study of the structural, electronic, and optical properties of CdSe cubic and hexagonal have been reported in present findings, have reflected the compositional dependent changes in lattice constants and band gaps. Calculated values of the band gap of CdSe for both cubic and hexagonal structures found smaller then experimental values which is reflective of fact that GGA underestimate band gap. The obtained results with LDA approach are found to be an enhancement to experimental values.

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