

Investigation of magneto-electronic and optical properties of rare earth Ag and Co co-doped CdS

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CdS is a potential candidate for material in optoelectronic applications. The magnetic, electronic and optical properties of Ag- doped and Co -codoped CdS were calculated using full potential linear augmented plane wave (FP-LAPW) based on popular density – functional theory (DFT). The band gap and density of states for Ag -doped and Co-codoped CdS have been determined by using Tran Blaha modified Becke-Johnson (TB-mBJ) potential. The optical and electronic properties of Ag-doped and Co-codoped CdS such as absorption coefficient, energy loss function, reflectivity, refractive index, electrical conductivity and extinction coefficient are presented. The results indicate that the magnetic and electro-optical properties are improved by this doping.

(Received February 20, 2022; Accepted November 2, 2022)

Keywords: magneto-electronic, optical properties, rare earth doping

1. Introduction

For their fascinating and potentially valuable structural, physical, and chemical features, nanostructured materials are of both basic and technological interest.

Nanoscale photonic and electronic devices, such as direct-current Nano-generators, light emitting diodes, polarisation sensitive photodetectors, and optically and electrically powered laser, rely heavily on semiconductor nanostructures [1–5].

Nanowires, nanobelts, nanocombs, nanosprings, nanorings, nanotubes, and nanodots are some of the morphologies of semiconductor nanostructures that have been described [6]. Because of its band gap energy (2.52 eV) in the visible range and its nonlinear features, CdS has piqued interest in optoelectronic applications as an II-VI semiconductor compound [7]. In thin-film solar cell systems, CdS has been widely used as an n-type window material. Naturally, there has been a lot of research on both bulk and nanostructured CdS. various methods have been used to create CdS nanostructures, such as nanowires, nanotubes, and nanobelts. 8–11 CdS nanostructures have been studied for their lasing and electronic transport features [10–13].

CdS core-sheath nanowires and tube-wire nanojunctions have not been reported to our knowledge. The thermal evaporation of CdS powder was used to create 1-D CdS nanostructures, nanotubes, core-sheath nanowires, and tube-wire nanojunctions in this letter. With a lower threshold voltage, these CdS nanostructures showed higher emission efficiency.

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<https://doi.org/10.15251/DJNB.2022.174.1263>

The CdS powder was deposited in the centre of a quartz tube to create the 1-D CdS nanostructures. The silicon (100) wafer was placed 10 cm away from the CdS powder downstream, with one face polished and sputtered with a coating of gold (7 nm). In a protective helium (99.999 percent purity) flow at a velocity of 100 sccm, the powder was heated to 900 °C as rapidly as feasible.

This paper proposes a new way to treat and examine the electronic, magnetic, and optical properties of Ag and Co codoped CdS nanostructure using the full-potential linearized augmented plane wave method (FP-LAPW), within the GGA-PBE and GGA+U approaches, to get an idea of the properties of this compound in various fields.

2. Computational details

Structural, electronic, magnetic, and optical properties calculations of Ag and Co codoped CdS nanostructure compound were done using full potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT) as provided by Wien2k package [14]. The exchange-correlation potential was treated by both approximations, the generalized-gradient approximation (GGA) in the scheme of Perdew–Burke–Ernzerh (PBE) [15] and the Hubbard method with PBE functional (GGA+U) are adopted. A super lattice of $(2 \times 2 \times 2)$ k-points in the full Brillouin zone has been employed for the primitive cell (containing Co atom) for the spin-polarization calculations in the antiferromagnetic phase (AFM). The cut-off energy is taken equal to -6 Ry and the energy convergence criterion was set to 10^{-5} . In the interstitial region, plane wave functions are restricted to $R_{mt} * K_{max} = 7.0$, where R_{mt} indicates the smallest atomic sphere radius and K_{max} is the maximum value of the largest K vector in the plane wave expansion. Moreover, to avoid overlap, we have chosen the muffin-tin radii values as follows: 2.0 for the atoms: Ag, Co, Cd and S respectively.

3.1. Density of states

In solid state physics and condensed matter physics the density of states (DOS) of a system determines the number of states that are to be occupied by the system at every level of energy. The density of state is described as existence in the number of states of system whom energies lie down in the range. To clearly understand the nature of the bands in CdS, doped with silver (Ag) and codoped with cobalt (Co), we have calculated the total density of state (TDOS) and projected density of states (PDOS). First of all we discuss the total density of state (TDOS).

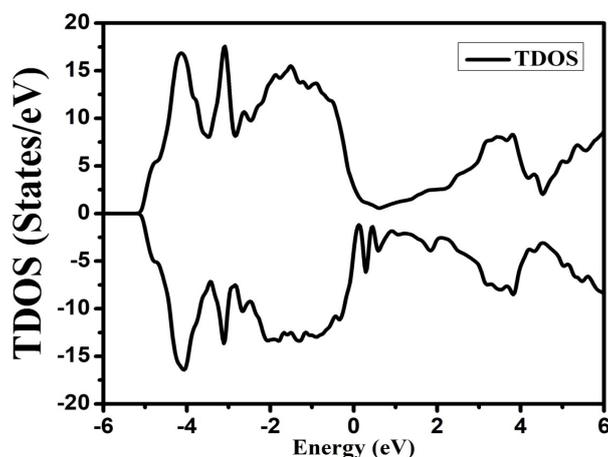


Fig. 1. The graph between total density of states and Energy (eV).

Figure shows that how the total density of state changes with the energy. The figure shows the mirror symmetry of the cadmium for the valance bands. The maximum peak is obtained between -5eV and -3eV. When silver is doped then the mirror symmetry exists. At the Fermi level

mirror symmetry vanishes because when the cobalt is added then there is magnetic moment. And there is no mirror symmetry between 0eV and 2eV. It represents the magnetic properties. So the material is magnetic. It again show mirror symmetry between 2.1eV and 6eV in the conduction band.

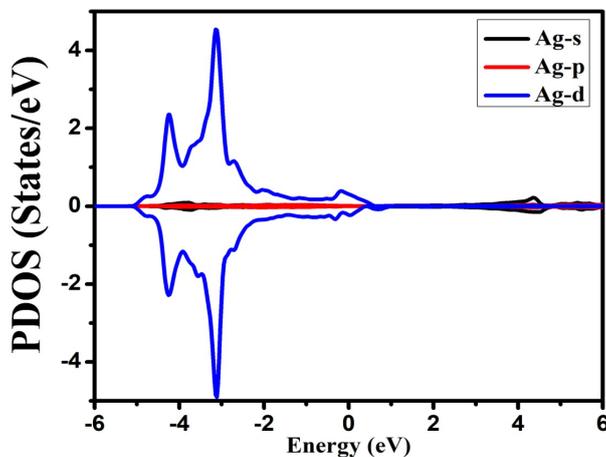


Fig. 2. The graph between the partial density of state of silver and Energy (eV).

Figure 2 shows the mirror symmetry of conduction and valance band. The maximum peak for the valance band is gained by the Ad-d. The highest occurrence of intermediate valance band is between -5eV and -3eV. So there exists greater contribution of Ag-d orbital.

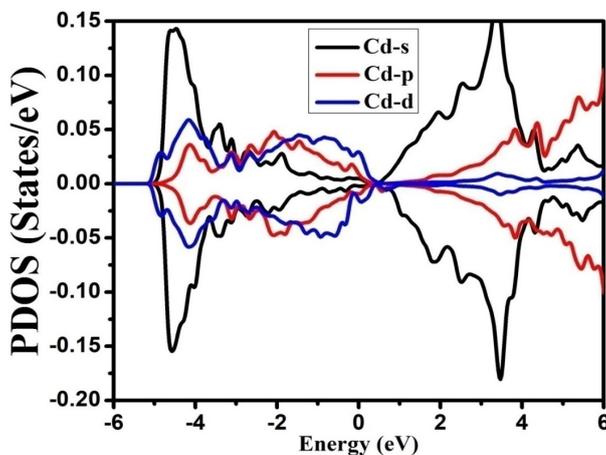


Fig. 3. Graph between the projected density of state of cadmium and Energy (eV).

The graph between the projected density of state of cadmium and energy shows that there is mirror symmetry of valance and conduction band. The maximum peak is attained by the Cd-s. The maximum peak of lower valance band occurs between -5eV and -4eV. The maximum peak in intermediate conduction band is attained between 3eV and 4eV. So we can say that Cd-s orbital has the greater contribution.

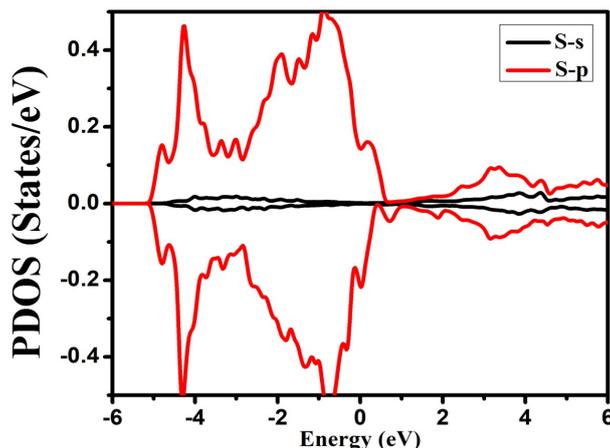


Fig. 4. The graph between the projected density of state of sulphur and Energy (eV).

This graph also shows the mirror symmetry of valence and conduction band. The maximum peaks are attained by the S-p orbital. So S-p has greater contribution shown by this graph. The highest peak in valence band occur between -5eV and 0eV. At almost 0.75eV of energy in conduction band mirror symmetry vanishes for a while but at almost 2eV we again obtain the mirror symmetry. The highest peak in conduction band is attained at almost 3eV.

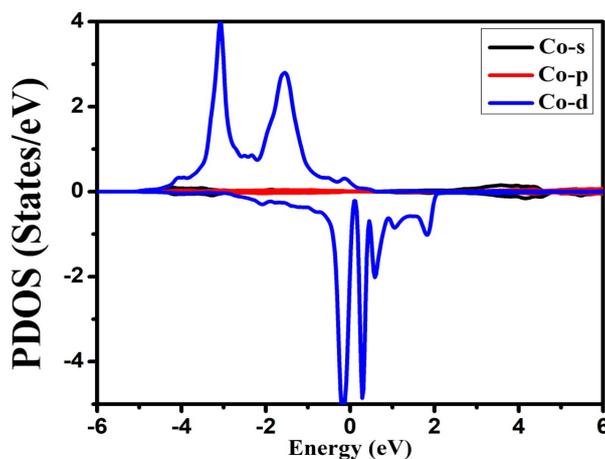


Fig. 5. The graph between the projected density of state of Co and Energy (eV).

This graph shows that there is no mirror symmetry, so there is magnetic moment and the material becomes a magnetic material and shows the magnetic behaviour. Maximum peak in intermediate valence band is obtained between -4eV and -1eV due to the Co-d. And maximum peak for higher valence band is obtained at -0.9 eV and in lower conduction band it is obtained at 0.75eV due to Co-d. So the Co-d has greater contribution.

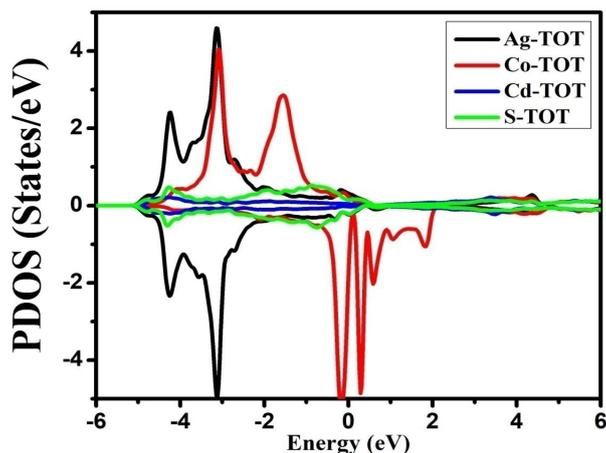


Fig. 6. The graph between the projected densities of state of all material with Energy (eV).

Figure 6 shows that all the materials show mirror symmetry of valance and conduction band except cobalt (Co). The maximum peak of the lower valance band is obtained between -5eV and -3eV by the silver (Ag). So we can say that the silver (Ag) has major contribution. And due to the presence of the cobalt the mirror symmetry of valance band and conduction band vanishes. So then the material has magnetic moment and behaves as a magnetic material. The minimum peak in lower conduction band occurs at almost 0.2eV.

4. Optical properties

4.1. Dielectric function

It is widely required to describe the optical and electronic properties and constant dispersion and scattering of the CdS, in the sense to recognize their optoelectronic applications. For this some important optical constant dispersions are noticed to energy 0 to 14eV of incident photon is discussed in this report. The significant part of the calculated optical possessions is calculating complex dielectric constant $\epsilon(\omega)$. Epsilon is constitute complex dielectric constant is explained as ability of substances to transport external magnetic field. $\epsilon(\omega)$ has well-built dependence on frequency. $\epsilon(\omega)$ is a calculated electron band structure function.

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$$

i-e, complex dielectric constant is an amalgamation of its real $\epsilon_1(\omega)$ and imaginary parts $\epsilon_2(\omega)$. Momentum matrix elements allow $\epsilon_1(\omega)$ [81]. Where as using Kramer Kroning relation real components of complex dielectric function may be computed [82]. $\epsilon(\omega)$ take part as the essential role to discover further parameters e.g. absorption coefficients, optic reflectivity $R(\omega)$ and refractive index $n(\omega)$ etc.

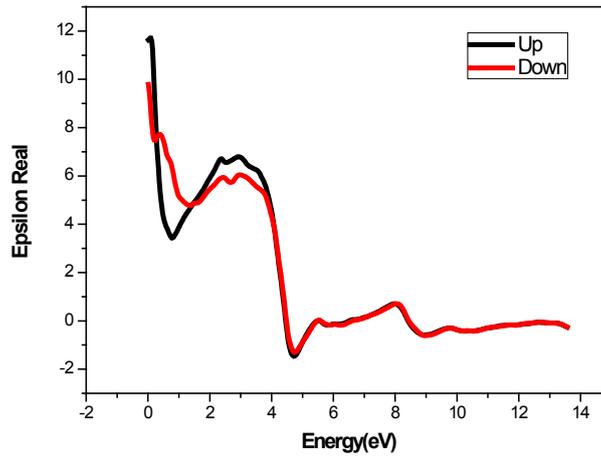


Fig. 7. (a). Real part of dielectric function for Ag and Co codoped CdS nanostructure.

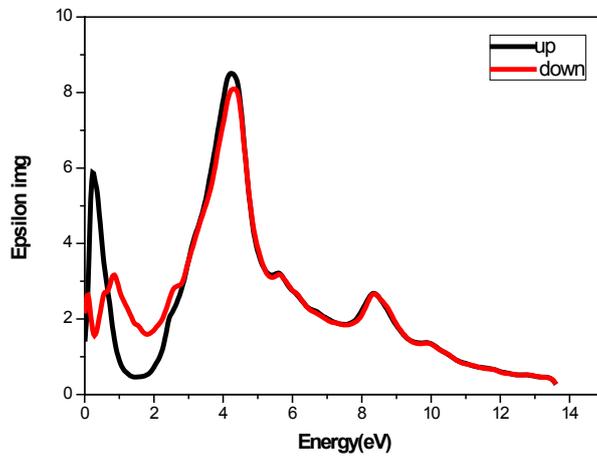


Fig. 7. (b): Figure 1(a): Imaginary part of dielectric function for Ag and Co codoped CdS nanostructure.

Figure 7 (a) and (b) are the graphs between energy and epsilon real and imaginary parts respectively. The graph (a) shows that the dielectric function has its maximum value at <1eV, for up state at almost 1eV and has minimum peak at <5eV. The graph (b) shows that the threshold energy for the CdS is about 4eV for up and down polarizations. For both electron transitions occurring from symmetry / balance point of valance band and conduction band are the principal source of threshold. For CdS the main peaks are caused by the transition of the states of electrons. These measured and computed optical and electronic possessions in this content of study represent that the CdS under study can be used in optical devices as they are required. The optical properties such as absorption coefficient $I(\omega)$, reflectivity $R(\omega)$, refractive index $n(\omega)$ and energy loss function $L(\omega)$ are calculated from the imaginary part and the real part of the dielectric function using the following equations. [83-86]

$$I(\omega) = \frac{\omega}{c} \sqrt{2(\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} - \epsilon_1(\omega))} \quad (i)$$

$$R(\omega) = \left| \frac{\sqrt{\epsilon(\omega)} - 1}{\sqrt{\epsilon(\omega)} + 1} \right|^2 \quad (ii)$$

$$n(\omega) = \sqrt{\frac{\epsilon_1^2(\omega) + \epsilon_2^2(\omega) + \epsilon_1(\omega)}{2}} \quad (\text{iii})$$

$$K(\omega) = \sqrt{\frac{\epsilon_1^2(\omega) + \epsilon_2^2(\omega) - \epsilon_1(\omega)}{2}} \quad (\text{iv})$$

$$L(\omega) = \frac{\epsilon_2(\omega)}{\epsilon_2(\omega) + \epsilon_1(\omega)} \quad (\text{v})$$

4.2. Absorption coefficient

Absorption is a condition in which something takes in another substance. Transition depends upon the band gap. In metals it starts from zero energy because of the overlapping of conduction band and valance band. The energy where transition takes place is known as threshold energy or critical energy. Mostly absorption takes place in ultraviolet region but we want the absorption in visible region. So the imaginary part is absorption. And the real part shows the scattering which depends upon the band gap of the substance. Band gap is inversely proportion to the graph transition.

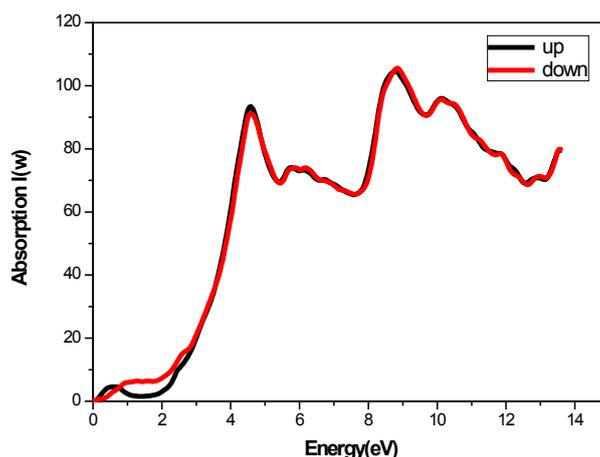


Fig. 8. Absorption coefficient for Ag and Co codoped CdS nanostructure

Figure 8 shows the average absorption coefficient $I(\omega)$ for the CdS. The most active and dynamic absorption region of the CdS is almost 4eV and 10 eV. From the calculated result the sharp edge of absorption coefficient subsist near 3eV for CdS. Semiconductor substances that exist with large band gap retain the possession of having precise edge in spectrum of absorption coefficient. The maximum absorption domains occur just near 5-8 eV and 10-13 eV for the CdS. CdS may be used as potential prospects for their implementations in optoelectronic gadgets working in the range of ultraviolet frequency.

4.3. Energy loss function

When energy is transferred from one state to another or travel from one position to another, or from one system to another then the energy loss occur. So we aware that when energy is transformed to a distinct set up, some of the input energy is converted into a extremely disarranged state of energy like heat.

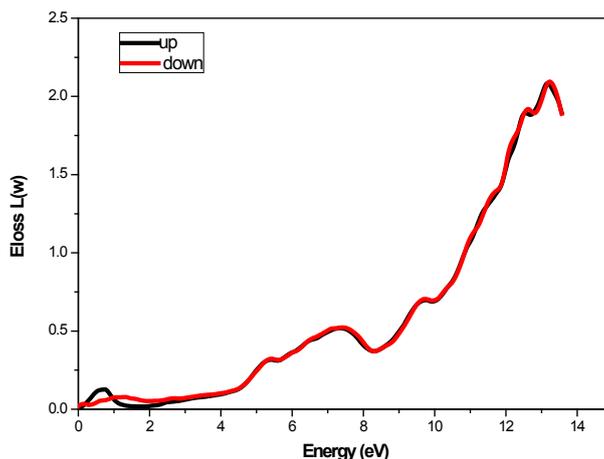


Fig. 9. Energy loss function of Ag and Co codoped CdS nanostructure.

This is the graph between the Eloss $L(\omega)$ and energy (eV) of the CdS. There are two lines for up and down, black and red respectively. The energy loss is maximum when energy is zero. As the energy increases the energy loss decreases. In the beginning the graph for up and down is slightly different from each other but at the energy of 2 eV the graphs is same for both the up and down and energy loss is decreasing gradually. As the energy is increasing the energy loss is reduced. The least value of the energy loss is obtained at the 13 eV of energy. Then the energy loss is again increasing.

4.4. Reflectivity

Reflectivity is one of the optical properties of the material, which determines how much light is reflected from the material in relation to an amount of light incident on the material. The phenomenon of reflection occurs always on the surface of the material, for light diffusing (translucent) materials also in the volume of material.

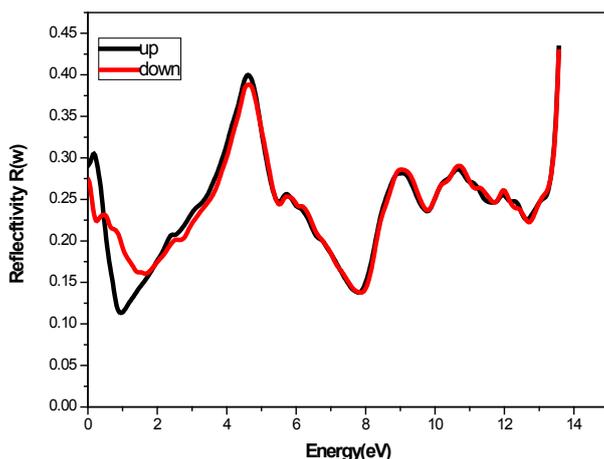


Fig. 10. Reflectivity for Ag and Co codoped CdS nanostructure.

We need a shielding material. So this shielding material, we get from the reflectivity. Figure 10 shows the values of average reflectivity at zero frequency. Computed in the current instance have values of 0.27 and 0.29 for the CdS. It is important that the value of average reflectivity at zero frequency $R(0)$ decreases while going from CdS. Attractively maximum reflectivity take place when energy is zero. Substances are metals if they have negative value of energy. Matallicity of a compound can be directly identified of that calculated and the value of

average $R(\omega)$ is maximum when the value of $\epsilon(\omega)$ is negative. This reflectivity is inversely proportion to the Eloss. This behaviour of peak of peak within the transparency area represents the ultraviolet region. The minimum is attained at the energy of 13.8eV. There is inverse relation between the values of band gap and static average refractive index $n(\omega)$ for the CdS, computed values are 0.25 and 0.375 respectively.

3.5. Refractive Index

In optics, the refractive index of a material can be described as the dimensionless number that determines how rapid light travels through the material. It is described as:

$$n = c/v$$

where c is the speed of light in vacuum and v is the phase velocity of light in medium.

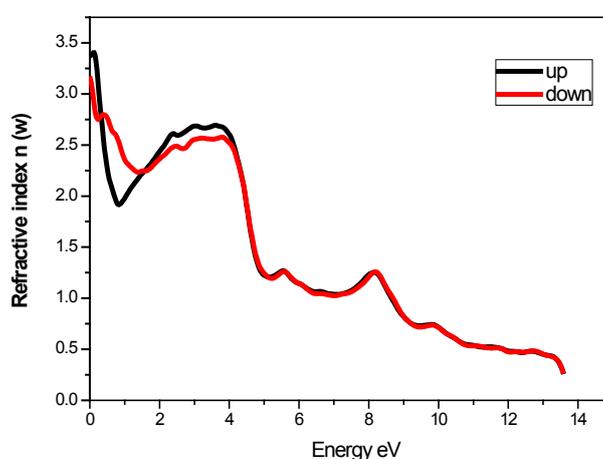


Fig. 11. Refractive index for Ag and Co codoped CdS nanostructure.

Figure 11 shows that the values of average refractive index $n(\omega)$ increase and decrease gradually with increasing energy. The first peak is attained when energy is $< 1\text{eV}$ for up and down states. The second peak value is attained at the energy $< 5\text{eV}$ for both the states of the CdS material.

4.6. Optical conductivity

How much distinct material conducts electricity, can be calculated as the ratio of the current density in the material to the electric field that give rise to the flow of current. The rate, at which heat passes through a distinct material, can be expressed as the quantity of heat that flows per unit time through a unit area with a temperature gradient of one degree per unit distance.

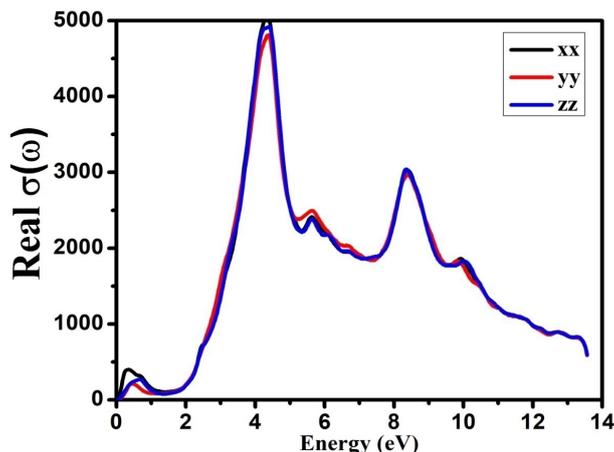


Fig. 12. Graph b/w the electrical conductivity $\sigma(\omega)$ and energy (eV).

Figure 12 is the graph between the optical conductivity $\sigma(\omega)$ and energy (eV). This graph shows that the electrical conductivity is zero when energy is zero and increases gradually with the increase in energy. At almost 4eV the electrical conductivity gains its maximum peak then it starts to decrease with increase in energy. At almost 7eV it again starts increasing with increasing energy. At 8eV of energy the second maximum peak is gained, and then optical conductivity decrease slowly with increasing energy.

4.7. Extinction coefficient

The expression molar extinction coefficient (ϵ) is an estimate of how strongly a chemical species or material absorbs light at a specific wavelength. It is intrinsic property of chemical species which is dependent upon their chemical composition and structure. The extinction coefficient is the absorbance divided by the concentration and the path length, in accordance with Beer's law.

$$\epsilon = \frac{\text{absorbance}}{\text{concentration} \cdot \text{path length}}$$

The units of extinction coefficient are usually $M^{-1}cm^{-1}$ but for proteins it is frequently extra convenient to use $(\frac{mg}{ml})^{-1}cm^{-1}$.

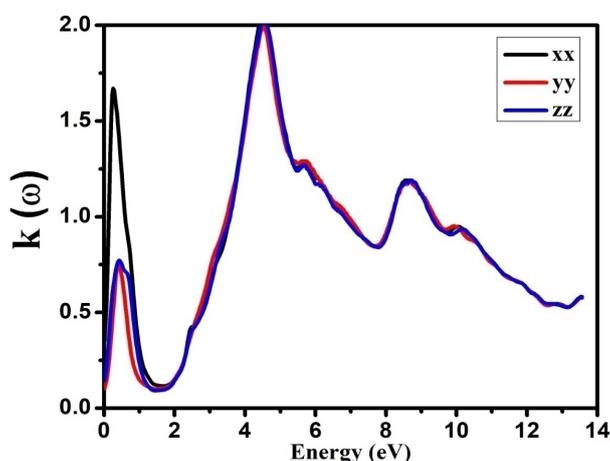


Fig. 13. Graph b/w extinction coefficient $k(\omega)$ and energy (eV).

Figure 13 shows a graph between the extinction coefficient $k(\omega)$ and the energy (eV). The graph shows that the first maximum peak is attained when energy is almost $< 1\text{eV}$ and 2nd maximum peak is observed when the energy is $> 4\text{eV}$. This graph plotted shows that the extinction coefficient magnitude increases rapidly for energies higher than 4eV for (E||X), (E||Y) and (E||Z) directions respectively.

5. Conclusion

Magneto-electronic and optical properties of transition metal Ag doped and Co co-doped CdS nanostructure has been calculated for magneto-electronic and optical applications. The calculations are performed using the density functional theory (DFT) with in the full potential linearized augmented plane waves (FP-LAPW) method. The electronic and optical properties calculations are calculated which is implemented in Wien2k package. The band gap obtained is 2eV. This value is close to the experimental value. The complex dielectric function, absorption, energy loss function, reflectivity, refractive index, electrical conductivity and extinction coefficient were calculated and discussed. Ag dopes and Co co-dopes effects the properties of the CdS. Finally our results show that the Ag and Co have potential to improve the optical and magneto-electronic performance of CdS. These measured and computed optical and electronic possessions in this content of study represent that the CdS under study can be used in optical devices as they are required.

Acknowledgment

The authors H. Elhosiny Ali extend their appreciation to the Research Center for Advanced Materials Science (RCAMS), King Khalid University, Saudi Arabia, for funding this work under grant number RCAMS/KKU/012-22.

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