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Understanding Optical Attributes of Wet Chemically Synthesized Quantum Dots

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Abstract: - This paper investigates the optical properties of wet chemically synthesised cadmium selenide (CdSe) quantum dots (QDs). Because of its distinct optical and electrical properties, quantum dots exhibit an increase in band gap energy (Eg) which can be further used as a suitable material for solar cell application. The size quantization effect in CdSe particles is also responsible for blue shifts observed in the adsorption and fluorescence spectra. Swanepoel method is used to evaluate refractive index of the given material and after analysing the graph it has been observed that as wavelength increases, refractive index of the prepared material decreases. The interaction between electrons and photons with regard to the photon energy is shown by the imaginary(εi) and real parts(εr) of dielectric constants. Optical conductivity (σ_opt) using the absorption coefficient was also calculated.

Keywords: Quantum dots, optical conductivity, dielectric constant, refractive index, finite difference time domain.

I. INTRODUCTION

Due to their distinctive optical and electrical characteristics, zero-dimensional semiconductor nanoparticles have gained a huge amount of attention in the last decade and are applied in numerous biological applications [1, 2]. The nanoparticles are typically referred to as quantum dots (QDs) when their size is lower than its initial Bohr radius and quantum confinement characteristics like an increase in the band gap (E_g) and blue shifts in the fluorescence and adsorption spectra appear [2-6]. To alter the special optical and electrical properties while maintaining the chemical composition of the material, number of atoms in a QDs can be changed. Many studies have focused on the optical initiation of synthesised II-VI semiconductors [7-10]. By tuning the size of these QDs, the E_g can be tuned over most of the visible spectrum. By reducing the diameter of the dot from 20 to 2 nm in the case of CdSe, the E_g can be changed from a deep red (1.7 eV) to a green (2.4 eV) [7-9]. Quantum dots shows enhanced properties like reduced particle size for electrical and optical devices like light emitting diodes and solar cells because they may be used as a variable to adjust the required features of the system [7, 8,11]. For CdSe both dark red hexagonal and cubic crystal forms are possible. At 300 K, the E_g of CdSe is 1.74 eV for n-type Semiconductor. Cd is 58.74% and Se is 41.26% of the molecular weight of CdSe, which is 191.37g/mol [13,12]. Although CdSe in large scale form is not particularly attractive, CdSe nanoparticles are one of the most fascinating semiconductors and lots of recent studies have prioritised their properties and uses. The development of controlled synthesis of CdSe nanoparticles is a current research focus [12]. The CdSe QDs' synthesis is very important as it directly affects the optical functionality of the coated CdSe QDs. CdSe QDs with optical features suitable for biological applications and research can currently be prepared by two synthetic techniques: organic-phase and aqueous-phase [6]. Since aqueous synthesis is more reagent-effective, less hazardous, and more feasible, it increases the water consistency and biological adaptability. While, organic-phase synthesised QDs are not soluble in aqueous solutions and does not go with the biological system [6,14]. As a result, a lot of work has been devoted to the synthesis of II-VI semiconductor QDs such as CdS, ZnS, CdSe and CdTe in aqueous solutions [6,15-18]. Shah et al. [19] created PVA-capped CdSe NPs using a straightforward chemical process. They then examined the effects of precursor concentration, ageing duration, and reaction temperature on the size and optical characteristics of the as-synthesised CdSe NPs. By adopting colloidal chemistry techniques, Mansur et al. reported the synthesis and characterisation of CdSe nanoparticles via an aqueous approach at room temperature, employing acid-functionalized PVA as capping ligands [20]. The reduced size of nanoparticles enables the control of optical properties which further enhances solar cell performance.

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II. Synthesis

After nine hours of refluxing 96mM sodium sulphite (Na_2SO_3) with 24mM selenium (Se) in deionized water at 90°C, sodium selenosulfate was produced (Na_2SeSO_3). Se stock solution was kept in the dark since light makes it unstable. Following reflux, the ultimate mixture was filtered using a Whatman filter paper and kept at (60 ± 5) ∘ C in the dark to avoid decomposition due to its instability at normal temperature.
Deionized water was mixed with 40mM of cadmium acetate (Cd ($CH_3C00)_2$) and 20ml of Se stock solution for 15 minutes at 30°C to create CdSe aqueous solution. 5 minutes later, 0.025ml of 2-mercaptoethanol was added. After 10-15 minutes of continuous stirring, an aqueous solution of CdSe was produced. The particle size of CdSe nanoparticle was found to be 100nm which is confirmed by X-ray diffraction spectra [21].

III. Results And Discussion

3.1 Refractive Index

The refractive index (*n*) of a material can be calculated using transmission spectra and the commonly recognised Swanepoel method is used [22].

$$n = \sqrt{H^2 + \sqrt{H^2 - S^2}}$$

Where $H = \frac{4S^2}{(S^2+1)T^2} - \frac{S^2+1}{2}$, *T* stands for the material's transmission and *S* is the air's refractive index. *n* decreases as wavelength increases which may be contributed to the material's normal dispersion behaviour. Various real-world applications including real-time holography, phase conjugators and optical correlators are being studied that require materials with higher nonlinearity and quick response times. The nonlinearity of materials is studied using a variety of theoretical models. The Boling relation is one of the most used techniques for calculating nonlinear refractive index (n_2) [23, 24].

$$n_2 = 391\,\frac{n_d-1}{(v_d)_{5/4}} \quad (1)$$

where v_d is abbe number and given by

$$v_d = \frac{n_d-1}{n_f-n_c} \quad (2)$$

In Eq. (1) n_d, n_f and n_c represent the linear refractive index at wavelengths of 587.5 nm, 486.1 nm and 656.3 nm respectively. The nonlinear refractive index (n_2) values for CdSe quantum dot are 1.74×10^{-11} (e.s.u.).

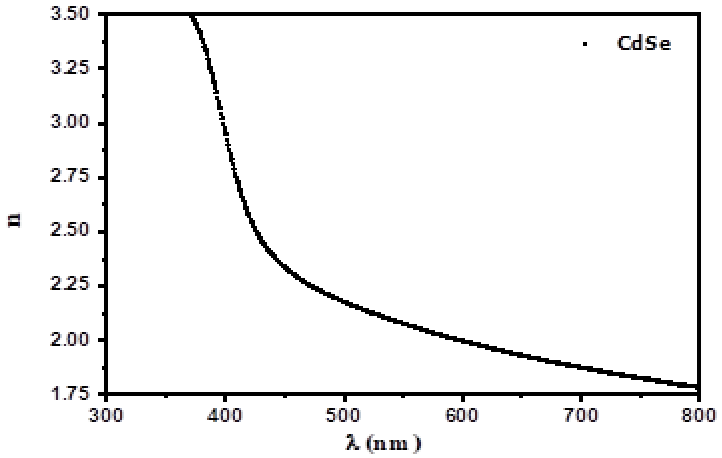

Fig. 1. Plot of Refractive index with respect to wavelength for CdSe quantum dot

Fig.1 depicts the relationship between the CdSe quantum dots refractive index (*n*) and wavelength (λ). To design optical components, modelling, and optical coatings, it is crucial to understand the material's refractive index [25,26 which will provide time-dependent solutions across an extensive time span through a single simulation.

IV. Dielectric Constant

Two methods have been used to calculate the dielectric constant. The first approach makes use of the photon incident dispersion relation. According to the Moss [26,31] model, only very little free carriers are actually involved in dispersion. It means that the refractive index value that lies below the absorption edge can be used. The complex dielectric constant is defined as the sum of the real (ε_r) and imaginary (ε_i) components of the dielectric constant and it is represented as $\varepsilon(\omega)=\varepsilon_r+\varepsilon_i$ where ε_r and ε_i are defined as $\varepsilon_r = n^2 - k^2$ and $\varepsilon_i=2nk$ respectively. The interaction between electrons and photons with regard to the photon energy is shown by the real (ε_r) and imaginary parts (ε_i). The dispersion and rate of dissipative propagation of electromagnetic waves in a medium are related in ε_r and ε_i. The variation of ε_r and ε_i in relation to photon energy is depicted in Fig.s 5 and 6. The graph illustrates how ε_r and ε_i's values grow as photon energy increases for the CdSe quantum dot [26].

For a given material system, the complex dielectric constant is,

$$\varepsilon^* = \varepsilon_r - j\varepsilon_i \quad (3)$$

Here, ε_r denotes energy that has been stored, while ε_i denotes energy that has been lost due to the applied electric field. Because four different types of polarisations are involved, namely space charge, dipole, electronic and ionic, ε_r and ε_i are of the utmost importance in the ionic conduction process [23,32]. The dielectric constant is measured using the relationship: $\varepsilon_r=\frac{C_p d}{\epsilon_0 A}$ for the measured value of parallel capacitance C_p.

where the film's area is A, its thickness is d, and its permittivity to free space is ε_o. It is obvious that at low frequencies, the dielectric constant is larger. This further supports the non-Debye behaviour by demonstrating that electrode polarisation and space charge polarisation have both occurred [33-34].

Dielectric losses ε_i denotes energy loss brought on by polarisation and ionic conduction. ε_i displays a constant value as the frequency increases. This particular behaviour of ε_i with respect to temperature and frequency correlates to the moment of charge carriers [35-39] and dielectric relaxation of the material [23]. Ionic and electronic polarisation dominate the space charge polarisation as frequency rises. At this point, ε_r is said to be intrinsically responsive because it does not change while the frequency varies [40].

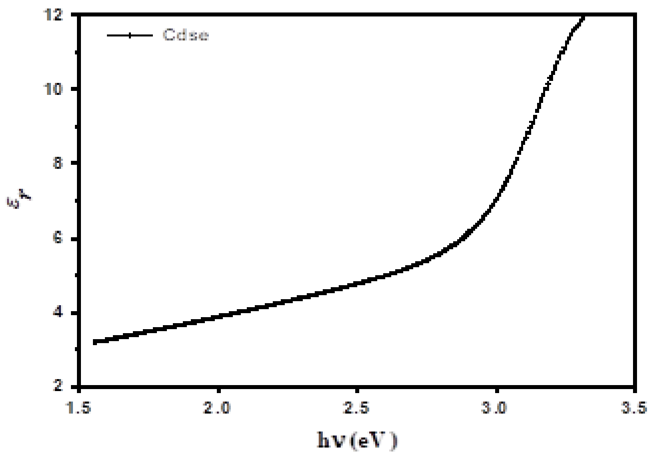

Fig. 5. Plot of Real part of dielectric constant for a CdSe quantum dot

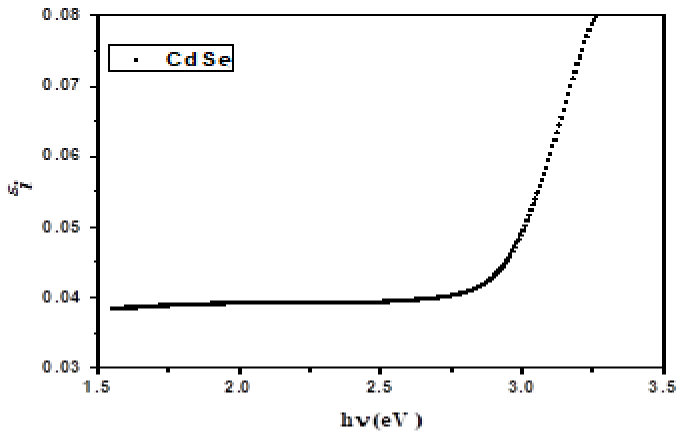

Fig. 6. Plot of Imaginary part of Dielectric constant for a CdSe quantum dot

V. Extinction Coefficient

The behaviour of the material during light propagation with respect to wavelength is described as the extinction coefficient *k*. It displays how the absorption changes as electromagnetic waves go through the substance. More specifically, *k* which is computed using the relation $K=\frac{\alpha\lambda}{4\Pi}$, affects the loss of light during propagation. Fig. 7 shows how *k* behaves in relation to λ for the CdSe quantum dot [26]. A change in the *k* value indicates that photons and electrons are interacting. The grain boundaries of nanocrystalline materials absorb more light. A change in the behaviour of *k* with CdSe has also been found by Sharma et al [41] and other authors [42].

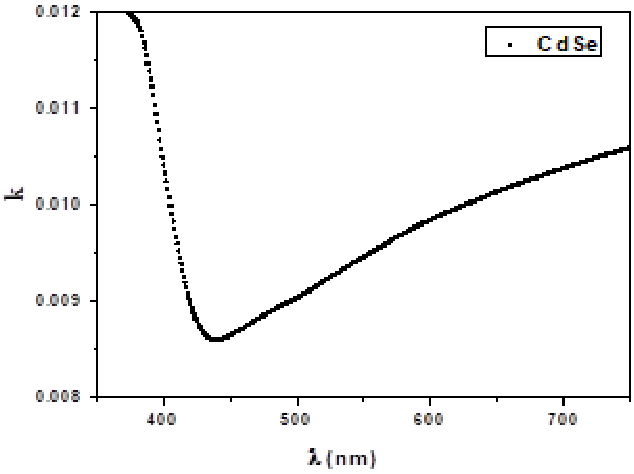

Fig. 7. Plot of Extinction Coefficient of CdSe quantum dot

VI. Optical Conductivity

The most effective way to study optical response is optical conductivity. The optical conductivity (σ_{opt}) can be obtained using the absorption coefficient by the following equation [43]:

$$\sigma_{opt} = \frac{\alpha n c}{4\pi} \quad (4)$$

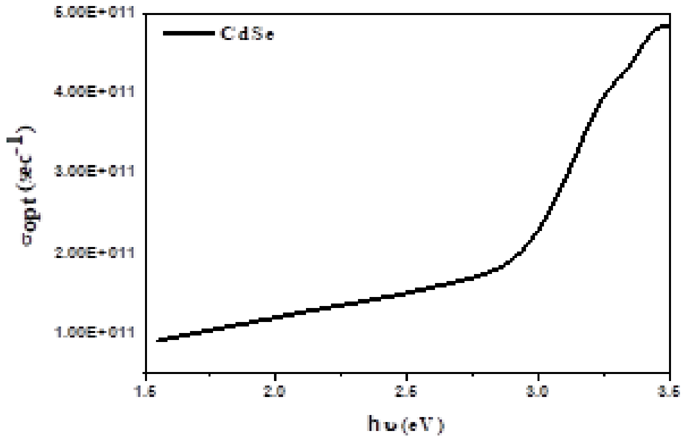

Fig. 8. Variation of optical conductivity with photon energy of CdSe Quantum dot

Above eq. provides the optical conductivity, which is directly dependent on the material's refractive index. Fig. 8 illustrates how the presence of nanoparticles causes conductivity to rise. This is due to the photon energy that helps to excite the electrons. The value of optical conductivity of CdSe quantum dot from Fig. 8 is calculated as 5 x 1011 Sec-1. M. Sharma et. al. [41] investigation of CdSe nanorods submerged in a polyvinyl alcohol matrix reveals a similar effect [26].

VII. Conclusions

CdSe QDs can be synthesized using organic-phase and aqueous-phase techniques, with aqueous-phase being more reagent-effective and less hazardous. The synthesis of CdSe QDs has been studied for their optical properties, which can enhance solar cell performance. The refractive index (n) of CdSe quantum dots is crucial for designing optical components, modeling, and optical coatings. The absorption spectra reveal distinct characteristics in their optical responses, with the absorption peak of CdSe of 15 nm diameter occurring around 688 nm. The dielectric constant, a measure of the material's resistance to electromagnetic waves, is a crucial factor in the performance of quantum dot solar cells. It is calculated using the photon incident dispersion relation and the complex dielectric constant, which is the sum of the real and imaginary components of the dielectric constant. The extinction coefficient, which describes the material's behavior during light propagation, shows how absorption changes as electromagnetic waves pass through the substance. The optical conductivity, which is directly dependent on the material's refractive index, is another important factor to consider. The presence of nanoparticles in CdSe quantum dots leads to a rise in conductivity due to photon energy excitation. Simulated absorption spectra reveal distinct characteristics in their optical responses, with the absorption peak of CdSe nanoparticles occurring around 688 nm.

VIII. Conflicts Of Interest

There are no conflicts to declare.

IX. Funding Declaration

There is no funding agency for the present work.

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