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**Research Article** 

# A theoretical study of optical properties of CdS quantum dots and evaluation of optical band gap of CdS nanoparticles, particle size and temperature dependent intensity of PL-spectra as a function of photon energy

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Abstract: Using the theoretical formalism of N. Soltani etal [Chalcogenide Lett. 9, 321(2012)], N. Q. S. Sabir [Int. J. Nanosci. Nanotechnol. 8, 111 (2012)], P. Ghosh et al.. [arXiv:1606.06711v][cond-mat.mtrl-Sci] 21 June 2016 and Silan Baturang [J. BAUN Inst. Sci. Technol. 19, 264 (2017)], we have theoretically studied CdS nanoparticle and CdS QDs. We have evaluated energy band gap and particle size of fcc and hcp structure nanoparticle. Our theoretically obtained results show that particle size increases with increase of the irradiation times whereas energy band gap decreases with increase of irradiation times. The particle size obtained for hcp structure is large compared to fcc structure. We have evaluated time dependent PLintensity as a function of photon energy for different temperature and Full width at half maximum (FWHM) broadening as a function of temperature. Our evaluated results show that temperature dependent PL-intensity increase, attain maximum value and then decrease as a function of photon energy for each temperature. However the maximum value of peak enhances as one increase the temperature. Our results of FWHM broadening as a function of temperature increase with temperature. The results show that the large no of relaxation processes are involved in this broadening.

The dominant contribution comes from exciton-phonon coupling and ionized impurity scattering. Our theoretically evaluated results are in good agreement with those of the other theoretical workers. The entire evaluation in this paper is based on time independent Schrodinger equation with Density Functional method (DST), Brus equation and empirically established Varshni relation. These studies will be quite helpful in order to understand the different relaxations processes involved in light emission from CdS nanoparticle and CdS QDs. These are very important for future applications in photonic and optoelectronic devices.

**Keywords:** Direct band semiconductor, Hexagonal close packed (hcp) structure, Face centered cubic (fcc) structure, Quantum size Effect, Band gap widening, Electrochemical potential, Photocatalytic activities, Density Functional theory (DST), Brus equation for particle size determination, Semiemperical Varshni relation, Full width at half maximum (FWHM) broadening, Relaxation process, Exciton-phonon coupling, Ionized impurity scattering, TDPL (temperature dependent photoluminescence) spectra, Ultrasonic spray pyrolysis method.

### INTRODUCTION

Quantum dots are semiconductors whose electronic characteristics are closely related to the size and shape of the individual crystal. Generally the smaller the size of the crystal the larger will be the band gap. This causes large difference between the highest valence band and the lowest conduction band. Therefore, one needs more energy to excite the dot, when the dots return to the resting state more energy is released. CdS is our II-IV semiconductor consisting of Cadmium from group II and Sulphur from group IV of the periodic table of element. Due to Cadmium Sulphur it exhibit intrinsic n-type of conductivity. This is because of the sulphur vacancies and the depth of the acceptor level. CdS in bulk has hexagonal Wurtizite type structure with melting point<sup>1</sup> 1600°C. It is well known direct band semiconductor. CdS bulk has band  $gap^2 E_g = 2.42 \text{ eV}$  (515nm) at room temperature and pressure. In recent years the progress of new synthesis methods<sup>3-5</sup> have been developed which demonstrate that the quantum size effects of nanoscale CdS. This has attracted considerable attention due to its unique optoelectronic, photochemical and photocatalytic properties of the dot. This is quite different from their bulk counterpart. CdS quantum dots exhibit unique size-tunable optical and electronic properties. These properties are band gap widening, change of electrochemical potential of band edge and enhancement of photo-catalytic active with decreasing crystalline size<sup>6-9</sup>. These properties are due to large number of sulphur atoms and three dimensional confinement electrons<sup>10,11</sup>.

The increase of the band gap upon a decrease of particle size is one of the characteristics which are observed by optical spectroscopy. Upon a decrease of the particle radius, the onset of the absorption shifts towards the higher energy. In order to compute band gap of quantum dot theoretically, one calculates the optical absorption energy of the electronic transitions between the valence and conduction bands of quantum dots. The transition takes place when the incident photon strikes the quantum dots and the valence band electrons of Cd atoms absorb these photons and go to excited higher energy level of conduction band of sulphur atoms. Since the band gap energy of quantum dots is dependent on particle size and lattice structure therefore to understand the transition between the electronic states, one uses an approach based on density functional theory (DST)<sup>12</sup> to simulate the electronic transitions. This is one of the methods of calculating band gap of quantum dots. Several theoretical approaches<sup>13-17</sup> have been proposed to compute the electronic states of quantum dots.

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In this paper using the theoretical formalism of N. Soltani etal<sup>18</sup>, N. Q. S. Sabir<sup>19</sup>, P.Ghosh *et al.*.<sup>20</sup> and S. Baturay<sup>21</sup>, we have studied experimental and theoretical works of CdS QDs of fcc and hcp structure synthesized from Sulphur source of Sodium Sulphate and thiocetamide respectively via microwave – hydrothermal method, chemical precipitation method,  $\gamma$ -irradiation technique and ultrasonic spray pyrolysis method respectively. The QDs were characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM), UV-Visible spectroscopy respectively. We have valuated Absorbance (A) as a function of wavelength (nm) for both type of CdS nanoparticle synthesized using Sodium Sulphide and thioacetamide as Sulphur source for different irradiation time.

In both the case Absorbance decreases with wavelength for each irradiation time. We have also evaluated  $[d(\ln \alpha h\nu)/d(h\nu)]$  as a function of  $h\nu$  for both types of synthesized CdS nanoparticle for different irradiation time. Our evaluated results show that  $[d(\ln \alpha h\nu)/d(h\nu)]$  increase attains maximum value and then decrease for each value of irradiation time. From these results, one calculates the particle size and band gap energy of CdS nanoparticle. Our theoretical results indicate that particle size increase with irradiation time whereas band gap energy decrease with irradiation time. We have also evaluated temperature dependent intensity of PL-spectra as a function of photon energy at different temperatures. Our theoretically evaluated results show that PL-intensity increases with photon energy attain maximum value and then decrease with each temperature. However the peak values enhance as one increase the temperature to higher values. Our evaluated results of FWHM broadening increase with temperature. This is due to many types of relaxations processes involved in line- width broadening. The dominant contributions come from exciton-phonon coupling and ionized impurity scattering process<sup>22</sup>. Our theoretically evaluated results are in good agreement with the other theoretical workers<sup>23-25</sup>.

## MATHEMATICAL FORMULAE USED IN THE EVALUATION

**Evaluation of optical properties of CdS quantum dots :**One considers quantum dots as an isolated spherical nanoparticles containing N atoms confined in a face-centred cubic (fcc) structure or in a hexagonal closed packed (hcp)structure. When photon strikes CdS nanoparticle, electrons in a valence band state absorbs photons and go to the excited conduction band state of S. The total energy may be written in the form<sup>26</sup>

$$E[\rho] = C_{K} \int \rho(r)^{\frac{5}{3}} dr + \frac{\eta}{8} \int \frac{\left|\nabla \rho(r)\right|^{2}}{\rho(r)} dr + \int \rho(r) v(r) dr + \frac{1}{2} \iint \frac{\rho(r)\rho(r')}{|r-r'|} dr dr' - C_{e} \int \rho(r)^{\frac{4}{3}} dr \quad ..(1)$$

The Euler equation has been presented in terms of functional derivatives:

$$\frac{5}{3}C_{K}\int\rho(r)^{\frac{2}{3}}dr + \frac{\eta}{8}\left[\frac{|\nabla\rho(r)|^{2}}{\rho(r)^{2}} - 2\frac{\nabla^{2}\rho(r)}{\rho(r)}\right] + v(r) + e^{2}\frac{\rho(r)}{|r-r'|}dr - \frac{4}{3}C_{e}\int\rho(r)^{\frac{1}{3}}dr = \mu \qquad \dots (2)$$

Here r is the displacement coordinates of the electrons from the centre of a sphere and is dependent on the quantum numbers n, 1 and s. For a completely degenerate electron gas at absolute zero temperature,  $\mu$  is the Fermi energy. V(r)=v<sub>1</sub>(r<sub>1</sub>)+v<sub>2</sub>(r<sub>2</sub>) is the summation of nuclear potentials of each atomic element of the QDs. The density of conduction electrons  $\rho(r)$  of an atom is a function of atomic number Z and absorption  $\sigma(r)$ . Since both  $\rho(r)$  and  $\sigma(r)$  are continuous functions, the

transformation of density functional energy E will be absorption functional energy  $E[\rho]$ . This can be achieved by algebraically substituting the electron density function with the absorption function in the Euler-Lagrangian equation (2). The absorption function  $\sigma(r)$  is derived in terms of electronic density  $\rho(r)$ . For QDs, the highly occupied state orbital electrons in the valence band absorb photons and transit to the higher energies of unoccupied state orbital in the conduction band. Hence the coordinate r of the electron is dependent on the principal quantum number n, angular quantum number 1 and spin quantum number s.

**Determination of optical band gap and radius of CdS nanoparticles:**The formation of CdS nanoparticles can be observed using powder X ray diffraction studies. XRD patterns of CdS nanoparticles are synthesized with sodium sulphide and thioacetamide as sulphur source. One uses UV-Vis spectroscopy in this study. The optical band gap of CdS nanoparticles is determined from the absorption spectra. In high absorption region the absorption spectra is due to interband transition among extended states in both valence and conduction bands. The optical absorption coefficient depends on optical band gap given by

$$\alpha(v) = K(hv - E_{p})^{n} / hv \qquad \dots (3)$$

Here E<sub>g</sub> represents the optical band gap, K is a constant and n depends on the nature of transitions. N has values of 1/2, 3/2, 2 and 3 for allowed direct transitions, forbidden direct transitions, allowed indirect transitions and forbidden indirect transitions respectively<sup>27,28</sup>. The energy band gap E<sub>g</sub> can be determined from UV-Vis spectra by obtaining  $d(Ln(\alpha hv))/d(hv)$  as a function of hv at ( $E_{a} - hv = 0$ )<sup>29,30</sup>

$$d(Ln(\alpha h\nu)) / d(h\nu) = n/(h\nu - E_g) \qquad \dots (4)$$

The results obtained for nanoparticles prepared with sodium sulphide and thioacetamide are given in table T3 and T4 for different irradiation times.

The particle radius can be calculated using equation proposed by Brus<sup>31,32</sup>. The Brus equation is used to describe the emission energy of quantum dot semiconductor nanocrystals. The expression gives a relation between radius of the crystalline and the energy gap which explains the quantum size effect

$$E_g = E_{g0} + \frac{\hbar^2 \pi^2}{2R^2} \left[\frac{1}{m_e} + \frac{1}{m_h}\right] - 1.786 \frac{e^2}{\varepsilon R} - 0.248 E_{ry} \qquad \dots (5)$$

Here  $E_g$  is the band gap value of the nanopartcles.  $E_{g0}$  is the band gap value of the bulk material,  $m_e$ and  $m_h$  are effective masses of electrons and holes respectively.  $\varepsilon$  is the dielectric constant of the semiconductor, R is the radius of the particle, h is the Planck's constant and  $E_{ry}$  is the effective Rydberg energy<sup>33</sup>. The first term of equation (5) referred to as the quantum localization term (i.e Kinetic energy term) which shifts the energy  $E_g$  to higher energy proportional to R<sup>2</sup>. The second term of equation (5) arises due to screened coulomb interaction between electrons and holes. The third term is the size independent term. It is the salvation energy loss and is usually small and ignored. In case of semiconductors the effect of the second term which represents the Coulomb interaction is also very small and can be ignored. Study of temperature dependent photoluminescence (TDPL) spectra of CdS QDs: Temperaturedependent photoluminescence (TDPL) studies were carried out on CdS QDs. It enhances the band-toband luminescence. It also indicates the role of thermally activated surface –trap states. The studies also demonstrate that the main non-radiative processes are thermal escape of carriers associated by LO phonons (Longitudinal optical phonon) and thermally activated ionized impurity scattering. In this study CdS QDs have been synthesized using  $\gamma$ -irradiation technique.

The temperature dependent integrated PL-intensity is written as<sup>34</sup>

$$I_{PL}(T) = \frac{n_0}{1 + Ae^{-E_a/k_\beta T} + B(e^{E_{Lo}/k_\beta T} - 1)^{-m}} \qquad \dots (6)$$

Here  $n_o$  is integrated PL intensity at T=0.  $A = (\frac{\gamma_a}{\gamma_{rad}})$  and  $B = (\frac{\gamma_o}{\gamma_{rad}})$  are constants related to the strength of the involved process. m=no of LO phonons involved in the thermal process. E<sub>LO</sub> is the LO-

phonon energy=37.2meV. Activated energy  $E_a = 2.0 (meV)$ . The experimental value<sup>35</sup> of m=5.6 ± 0.5.

As the sample temperature increases the peak position of the central PL band correspond to band-toband transitions shift. This can be attributed to temperature dependent shift of band energy gap and is determined by empirically established Varshni relation<sup>36</sup>

$$E_g(T) = E_g(0) - \alpha \frac{T^2}{T + \beta} \qquad \dots \tag{7}$$

Here  $E_g(0)$  is the band gap at T=0.  $\alpha$  is temperature coefficient,  $\beta$  is a constant very close to Debye temperature  $\theta_D$  of the material. In the case of bulk semiconductor<sup>37</sup>, the values are given as  $\alpha = (2.6 \pm 0.06) \times 10^{-4} \text{ eV/K}$ ,  $\beta = 280 \pm 18 \text{K}$ ,  $\beta = \theta_D = 300 \text{K}$ 

The linewidth broadening with increasing sample temperature in the case of semiconductor QDs is given by<sup>37</sup>

$$\Gamma(T) = \Gamma_{inh} + \sigma T + \Gamma_{LO} (e^{E_{LO}/k_{\beta}T} - 1)^{-1} + \Gamma_{imp} e^{-E_a/k_{\beta}T} \qquad \dots (8)$$

Here  $\Gamma_{inh}$  is temperature independent inhomogeneous broadening which represents fluctuations in size, shape, composition etc. Of QDs. The second and third terms are related to homogenous broadening due to exciton-phonon coupling.  $\sigma$  is the exciton-accoustic phonon coupling coefficient.  $\Gamma_{LO}$  is the exciton-phonon coupling strength.  $\Gamma_{imp}$  is the linewidth due to impurity scattering. The fourth term of equation (8) is related to FWHM (Full width at half maximum) broadening due to ionized impurity scattering. E<sub>a</sub> is the activation energy required for ionization. The experimental data<sup>38</sup> of the above quantities are the following:

 $\Gamma_{inh} = 46.4 \pm 0.3 \text{ meV}, \ \sigma = 48 \pm 4 \,\mu\text{eV/K}, \ \Gamma_{LO} = 15 \pm 3 \,\text{meV} \text{ and } E_{LO} = 37.2 \,\text{meV}.$ 

#### **DISCUSSION OF RESULTS**

Using the theoretical formalism of N. Soltani *et al.*<sup>18</sup>, N. Q. S. Sabir<sup>19</sup>, P. Ghosh *et al.*<sup>20</sup> and S. Baturay<sup>21</sup>, we have studied experimental and theoretical works of CdS QDs of face centered cubic (fcc) and hexagonal close packed (hcp) structure synthesized from Sulphur source of Sodium

Sulphide and thioacetamide respectively. The studies were performed via microwave-hydrothermal method, chemical participation method,  $\gamma$ -irradiation technique and spray pyrolysis method respectively. The QDs were characterized using X ray diffraction (XRD) method, transmission electron microscopy (TEM) and UV-Visible spectroscopy respectively. The band gap of the CdS QDs were derived from time independent Schrodinger equation with Density Functional theory (DFT)<sup>12</sup>, Brus equation<sup>31,32</sup>, D. Valerui etal<sup>34</sup> with empirically established Varshni relation<sup>36</sup> respectively. In **table T1**, we have shown the evaluated results of UV-Visible Absorbance (a.u.) as a function of wavelength (nm) of CdS nanoparticle synthesized using Sodium Sulphide as Sulphur source with the help of XRD studies for different irradiation times. Our theoretically obtained results show that Absorbance (a.u.) decrease with wavelength for each irradiation times.

Wavelength		Absorbance(a.u) of G	CdS nanoparticle –	
(nm)	t=10min	t= 15min	t = 20min	t= 25min
300	2.352	2.528	2.686	3.147
350	2.147	2.485	2.542	3.082
400	2.084	2.342	2.446	2.939
450	1.987	2.297	2.365	2.847
500	1.792	2.218	2.287	2.705
550	1.656	2.164	2.209	2.632
600	1.543	2.093	2.153	2.547
650	1.498	1.847	2.104	2.439
700	1.385	1.708	1.989	2.365
750	1.298	1.632	1.847	2.308
800	1.202	1.557	1.709	2.227
850	1.157	1.422	1.635	2.142
900	1.102	1.308	1.508	2.057
950	0.985	1.217	1.432	1.832
1000	0.847	1.143	1.305	1.705

**Table T1:** An evaluated result of UV-Visible Absorbance (a.u) as a function of wavelength (nm) of CdS nanoparticle synthesized using Sodium Sulphide as Sulphur source with XRD studies for different irradiation time

In **table T2**, we repeated the calculation for Absorbance (a.u.) for CdS nanoparticle synthesized using thioacetamide as Sulphur source as a function of wavelength (nm) with the help of XRD studies with different irradiation times. In this case also, the same results were observed where Absorbance (a.u) decreases with wavelength with each irradiation time. These results show that there is a shift of the absorbance edge compared to bulk CdS . This is due to quantum confinement effect. In **table T3 and T4**, we have shown the evaluated results of  $[d(\ln(\alpha hv))/d(hv)](eV)^{-1}$  as a function of hv (eV) for CdS nanoparticle synthesized using Sodium Sulphide as Sulphur source and thioacetamide as Sulphur source both using XRD studies for different irradiation times. Our evaluated results show that  $[d(\ln(\alpha hv))/d(hv)](eV)^{-1}$  increase, attain maximum value and then decrease with hv (eV) for each irradiation time. However the results show that peak value shifts as one increase the irradiation time to higher and higher values. These results are very useful in order to calculate the energy band gap of CdS nanoparticle.

Wavelength	<b>←</b>	Absorbance(a.u) of (	CdS nanoparticle –	>
(nm)	t=10min	t= 15min	t = 20min	t= 25min
400	2.357	2.486	2.525	2.627
440	2.225	2.405	2.483	2.546
450	2.168	2.363	2.378	2.435
460	1.957	2.278	2.295	2.368
470	1.822	2.105	2.148	2.295
480	1.706	1.987	2.086	2.122
500	1.535	1.842	1.979	1.987
510	1.427	1.735	1.874	1.869
520	1.278	1.678	1.705	1.784
530	1.108	1.546	1.632	1.659
540	1.057	1.429	1.438	1.567
550	0.923	1.346	1.373	1.449
560	0.478	1.265	1.282	1.385
570	0.157	1.186	1.184	1.297
580	0.095	1.108	1.105	1.122

Table T2: An evaluated result of UV-Visible Absorbance (a.u) as a function of wavelength (nm) of
CdS nanoparticle synthesized using thioacetamide as Sulphur source with XRD studies for different
irradiation time

**Table T3:** An evaluated result of  $[d(\ln(\alpha hv))/d(hv)](eV)^{-1}$  as a function of hv (eV) for CdS nanoparticle synthesized using Sodium Sulphide as Sulphur source with the help of XRD studies with different irradiation times

Photon energy	$\longleftarrow \qquad [d(\ln(\alpha hv))/d(hv)](eV)^{-1} \longrightarrow$			
(eV)	t= 10min	t= 15min	t= 20min	t= 25min
2.0	1.844	2.056	2.165	2.274
2.1	1.987	2.167	2.247	2.358
2.2	2.095	2.279	2.323	2.435
2.4	2.216	2.355	2.438	2.546
2.5	2.326	2.487	2.578	2.635
2.6	2.294	2.538	2.659	2.704
2.7	2.267	2.509	2.602	2.657
2.8	2.148	2.435	2.584	2.602
2.9	1.987	2.367	2.478	2.576
3.0	1.884	2.316	2.392	2.495
3.1	1.753	2.274	2.316	2.382
3.2	1.628	2.209	2.243	2.323
3.3	1.567	2.127	2.184	2.276
3.4	1.486	1.956	2.106	2.212
3.5	1.355	1.873	1.989	2.144
3.6	1.309	1.753	1.842	2.085

Photon energy	<b>←</b>	$[d(\ln(\alpha h\nu))/d(h$	$(eV)^{-1}$	
(eV)	t= 10min	t= 15min	t= 20min	t= 25min
2.40	1.256	1.486	1.659	1.985
2.50	1.674	1.985	2.156	2.256
2.55	1.958	2.058	2.325	2.478
2.60	2.322	2.459	2.554	2.976
2.65	2.568	2.625	2.698	3.149
2.70	2.685	2.856	2.965	3.286
2.75	2.358	2.987	3.086	3.474
2.80	2.206	2.705	3.279	3.597
2.85	2.109	2.584	3.158	3.284
2.90	1.955	2.435	2.987	3.107
2.95	1.802	2.252	2.705	2.944
3.00	1.734	2.109	2.554	2.795
3.10	1.656	1.987	2.327	2.576
3.20	1.539	1.875	2.236	2.464
3.30	1.464	1.752	2.043	2.347
3.40	1.432	1.648	1.887	2.123

**Table T4:** An evaluated result of  $[d(\ln(\alpha h\nu))/d(h\nu)](eV)^{-1}$  as a function of  $h\nu$  (eV) for CdS nanoparticle synthesized using thiocetamide as Sulphur source with the help of XRD studies with different irradiation times

In **table T5**, we have repeated the calculation of Absorbance (a.u) as a function of wavelength (nm) for CdS nanoparticle synthesized using thermo spectronics , Genesis 20 spectrometer in the wavelength of 400-700nm at room temperature using the stable dispersion formed in DMSO after ultrasonication<sup>39</sup>. Here, our obtained results also show the same trend in which absorbance decreases with wavelength.

Table T5: An evaluated result of absorbance (a.u) of CdS nanoparticle as a function of wavelength
(nm), CdS nanoparticle is synthesized by a simple chemical route

Wavelength (nm)	Absorbance (a.u)
400	1.954
420	1.902
440	1.847
460	1.724
480	1.607
500	1.089
520	0.986
540	0.574
560	0.322
580	0.237
600	0.184
620	0.122
640	0.096
660	0.047

In **Table T6**, we have shown the evaluated results of absorbance (a.u) as a function of energy hv (eV) for CdS nanoparticle which were dispersed in acetone by ultasonication and were placed on Carbon coated Copper grid<sup>40</sup>. In this case our evaluated results show that absorbance increase with photon energy hv very sharply. These results are very useful in order to calculate particle size and also energy band gap of CdS nanoparticle. From these results the particle size comes out to be equal to 3.304nm keeping Values of  $E_{go}$ ,  $m_e$  and  $m_b = 2.57 \text{eV}$ ,  $1.73 \times 10^{-19}$  and  $7.29 \times 10^{-19}$  respectively<sup>41</sup>. The calculated band gap energy comes out to be equal to 2.678 eV against the expt value<sup>42</sup> 2.42 eV.

Energy (eV)	Absorbance (a.u)
2.0	0.054
2.15	0.065
2.20	0.098
2.25	0.187
2.30	0.252
2.35	0.336
2.40	0.488
2.45	0.659
2.50	0.787
2.55	0.894
2.60	1.087
2.65	1.276
2.70	1.384
2.80	1.492
3.00	1.657
3.20	1.848

**Table T6:** An evaluated result of absorbance (a.u) as a function of energy (eV) for CdS nanoparticle,CdS nanoparticle is synthesized by simple chemical route

From table T7 to T10, we have shown the evaluated results of temperature dependent intensity of PL spectra as a function of photon energy for different temperature, integrated PL intensity as a function of  $(k_{\beta}T)^{-1}$ , PL peak position (eV) as a function of temperature (K) and FWHM broadening as a function of temperature respectively. In Table T7, we have shown the evaluated results of temperature dependent intensity of PL-spectra as a function of photon energy for different temperature. Our observed result show that temperature dependent intensity of PL-spectra increases attain maximum value and then decrease with each temperature of CdS QDs. Here also the peak value shifts to higher temperature side. In table T8, we have shown the integrated PL intensity (arb.u) as a function of  $(k_{B}T)^{-1}$  (eV)<sup>-1</sup>. Our obtained results show that integrated PL-intensity increase with  $(k_{\beta}T)^{-1}$  and increase becomes large for high value of  $(k_{\beta}T)^{-1}$ . In **Table T9**, we have shown the evaluated results of peak position of PL-intensity (eV) as a function of temperature (K). Our evaluated results indicate that PL-peak position decrease with temperature. In the last Table T10, we have presented the evaluated results of FWHM broadening as a function of temperature. Our evaluated results show that FWHM broadening increases with temperature. This is due to many relaxation processes but the exciton-phonon and ionized impurity scattering contribution is dominant from others. There is large number of recent results<sup>43-60</sup> which reveals the similar behaviour.

Photon	Temperature dependent intensity PL-spectra(arb.u)			
energy(eV)	T=100K	T=150K	T=200K	T=300K
1.00	0.986	0.783	0.705	0.684
1.50	1.167	1.102	1.192	0.986
1.70	1.325	1.296	1.327	1.209
2.00	1.677	1.584	1.539	1.512
2.20	1.759	1.703	1.678	1.634
2.40	1.842	1.816	1.786	1.758
2.50	1.634	1.584	1.515	1.496
3.00	1.509	1.432	1.394	1.389
3.20	1.386	1.376	1.307	1.294
3.40	1.209	1.229	1.198	1.176
3.50	1.435	1.478	1.486	1.508
4.00	1.668	1.686	1.692	1.932
4.20	1.786	1.802	1.848	1.645
4.40	1.512	1.497	1.535	1.428
4.50	1.376	1.355	1.378	1.307
5.00	1.229	1.214	1.247	1.262

# Table T7:An evaluated result of temperature dependent intensity of PL-spectra as a function of photon energy (eV) at different temperature of CdS QDs

**Table T8:** An evaluated result of integrated PL-intensity as a function of  $(k_{\beta}T)^{-1}(eV)^{-1}$  of CdS

QDs

$(k_{\beta}T)^{-1}(eV)^{-1}$	Integrated PL-intensity (arb.u)
100	2.126
150	2.348
200	2.679
250	3.182
300	3.478
350	3.825
400	3.986
450	4.124
500	4.276
550	4.383
600	4.475
650	4.539
700	4.586
750	4.622
800	4.693
900	4.746
1000	4.822

# Table T9: An evaluated result of PL-intensity peak position (eV) as a function of temperature (K) of CdS QDs

Temperature (K)	PL-intensity peak position (eV)
50	3.269
100	3.202
150	3.165
200	3.128
220	3.109
240	3.112
250	3.086
270	3.072
300	3.054
320	3.008
340	2.986
350	2.874
370	2.853
400	2.708
500	2.634

# **Table T10:** An evaluated result of FWHM (Full width at half maximum) broadening $\Gamma$ (meV) as a<br/>function of temperature (K)

Temperature (K)	FWHM broadening $\Gamma$ (meV)
50	0.489
100	0.503
150	0.514
200	0.522
220	0.546
240	0.587
250	0.605
270	0.622
300	0.645
320	0.678
340	0.697
350	0.734
370	0.755
400	0.787
500	0.854

# CONCLUSION

From the above theoretical analysis and investigations, we have come across the following conclusion:

(1) We have studied the CdS quantum dots which were synthesized by microwave hydrothermal method. In this synthesis, one obtains face centred cubic (fcc) and hexagonal close packed (hcp) structure using Sodium Sulphide and thioacetamide as Sulphur source. We evaluated absorbance (a.u) as a function of wavelength (nm) for both

type of synthesized CdS nanoparticle with different irradiation times. The obtained results indicate that absorbance decrease with wavelength for both type of synthesized CdS nanoparticle for each irradiation time.

- (2) We have evaluated the band energy gap and size of particle from these evaluations. Our theoretically obtained results show that particle size increases with irradiation time whereas band energy gap decreases with increase of irradiation time. Our theoretical results also indicate that particle size obtained for hcp structure is large compared to fcc structure.
- (3) The entire evaluation is based on time independent Schrodinger equation with density Functional method (DFT). We have also used Brus equation to calculate particle size. The obtained results of band gap energy and particle size is in good agreement with the experimental data.
- (4) We have studied the temperature dependent intensity of PL-spectra as a function of photon energy for CdS QDs, integrated PL-intensity as a function of  $(k_{\beta}T)^{-1}$  and FWHM broadening  $\Gamma$  as a function of temperature. Our theoretically obtained results show that temperature dependent PL-intensity increase attain maximum value and then decrease with photon energy for each temperature. FWHM broadening  $\Gamma$  increases with temperature. These results show that in FWHM broadening large number of relaxation processes are involved in which exciton-phonon and ionised impurity scattering contribution are dominant. Our obtained theoretical results are in good agreement with other theoretical workers.
- (5) In this paper we have studied basically the optical properties of synthesized CdS nanoparticle using time independent Schrodinger equation with Density Function Theory (DFT), Brus equation and empirically established Varshni relation. The obtained results will be quite useful and helpful in order to understand the different relaxation processes involved in light emission from CdS nanoparticle. The results are very important for future applications in photonic and optoelectronic devices.

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