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Original Article

Modeling and Simulation of Emission Wavelength of The CdSe, CdS and ZnS Semiconductor Nanostructures for Device Applications

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Abstract *- This work focuses on the theoretical modeling and simulation of emission wavelengths in semiconductor Quantum Dots (QDs), particularly those composed of CdSe, CdS, and ZnS. The formulated model clearly demonstrates a direct quadratic dependence between the quantum dot size and its corresponding emission wavelength: as the QD size increases, the emission shifts toward longer wavelengths. In contrast, reducing the size intensifies quantum confinement effects, resulting in a wider bandgap and shorter emission wavelengths, commonly called a blue shift. The tunable emission ranges observed are approximately deep red to green for CdSe (As a result, CdSe quantum dots are widely used in optical displays due to their tunable emission across the visible spectrum), yellow to blue for CdS (These emission properties make CdS quantum dots suitable for use in visible-light LEDs, particularly in the blue-green range) and blue to ultraviolet for ZnS (As a result ZnS QDs are used in solid-state lighting for blue and ultraviolet emission and photodetectors due to their wide band gap). These optical properties stem from the discrete energy levels introduced by quantum confinement, contrary to the continuous bands in bulk semiconductors. Notably, ZnS displays the most pronounced confinement effects and emits at the shortest wavelengths among the three materials, attributed to its relatively large intrinsic bandgap, making it an excellent candidate for high-power devices and can operate at high temperatures, making them suitable for applications in harsh vicinities.*

Keywords *- Nanostructures, Quantum dots, Emission wavelength, Confinement effect, Blue shift, Charge carriers.*

1. Introduction

Quantum Dots (QDs), semiconductor nanostructures derived from group II-VI materials such as CdSe, CdS, and ZnS, have garnered significant attention due to their exceptional optical and electronic properties. These unique behaviors stem from quantum confinement effects, which lead to discrete energy levels and size-dependent emission wavelengths that can be precisely tuned by adjusting the confinement dimensions. This tunability underscores the broad applicability and versatility of QDs in a wide range of fields, including bioimaging, display technologies, solar energy conversion, sensing, environmental remediation, and biomedical applications [1][2].

Quantum Dots (QDs) are semiconductor particles at the nanometer scale that exhibit quantum confinement in all three spatial directions, effectively trapping an exciton (a pair consisting of an electron and a hole) [3][4]. These structures generally have dimensions ranging from approximately 1 to 10 nanometers. At such a small scale, their optical and electronic characteristics differ markedly from those observed in bulk semiconductors [5][6]. In bulk form, charge carriers like electrons and holes are relatively free to move, resulting in a continuous valence band and the conduction band distribution. However, this behavior changes dramatically as the material dimensions shrink to the nanoscale [7][8][9].

When the size of a semiconductor crystal is reduced to the nanometer scale, particularly to dimensions comparable to the exciton Bohr radius, as shown in Figure 1.1, quantum confinement effects become increasingly dominant [10][11]. This spatial restriction limits the free movement of charge carriers (electrons and holes), resulting in the formation of discrete, quantized energy levels rather than continuous energy bands [12][13]. Consequently, electrons can only occupy specific electronic energy states, much like the

behavior observed in atoms. This atom-like behavior is why quantum dots are often described as "artificial atoms." The energy gap between these discrete levels and the optical bandgap of the material is strongly dependent on the size of the quantum dot; with smaller dots generally exhibit larger energy gaps and higher energy emissions, while larger dots tend to have narrower gaps and lower energy transitions [14][15][16].

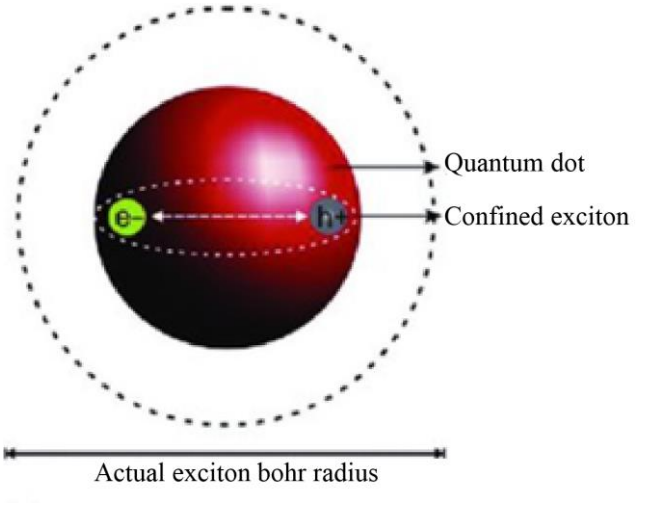

Fig. 1.1. Bohr exciton radius

Thus, as the size of a QD decreases, the band gap energy increases. This effect arises from the spatial confinement of electrons and holes, which leads to an elevation in their kinetic energy [17][18]. A commonly used approximation to describe this behavior is the "particle-in-a-box" model, in which the energy levels are inversely proportional to the square of the confinement length, in this case, the quantum dot's size. As the dimensions shrink, the energy separation between levels increases [19][20]. This shifts both absorption and emission spectra toward shorter wavelengths or higher photon energies, a phenomenon known as the optical blue shift, as illustrated in Figure 1.2. Such size-dependent spectral tunability enables control over the emission color of quantum dots, making them exceptionally valuable in optical and photonic technologies [21][22][23].

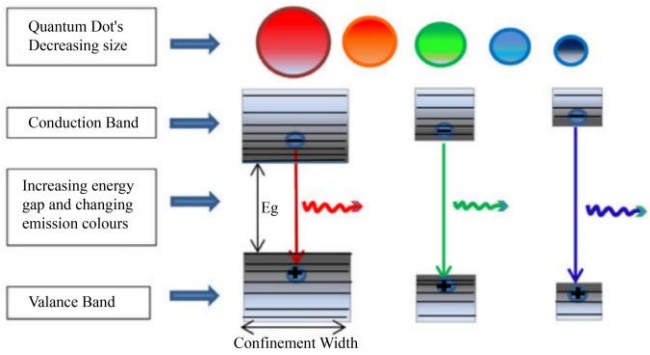

Fig. 1.2. Emission colors of QD with decreasing size

This research, an overview of emission wavelength for CdSe, CdS, and ZnS QDs, focusing on their characteristics, quantum confinement effects, and applications, are studied using the 3D potential well model.

2. Mathematical Formulation

To develop a model for the emission wavelength of Quantum Dots (QDs), the Schrödinger equation is solved within a three-dimensional potential well to determine the discrete energy states. These quantized energy levels are then used to calculate the corresponding emission wavelengths. A 3D potential well is appropriate for this model because, like QDs, it imposes confinement in all three spatial dimensions. However, unlike a simple potential well that typically confines a single particle, QDs confine an exciton (a bound pair of an electron and a hole), as illustrated in Figure 2.1. To more accurately represent the physical system, the masses of electron and hole are replaced by effective mass to account for the interaction between the charge carriers and the crystal lattice, in contrast to the idealized 3D potential well model that assumes a particle with a constant mass and neglects the complexities introduced by the material's electronic structure.

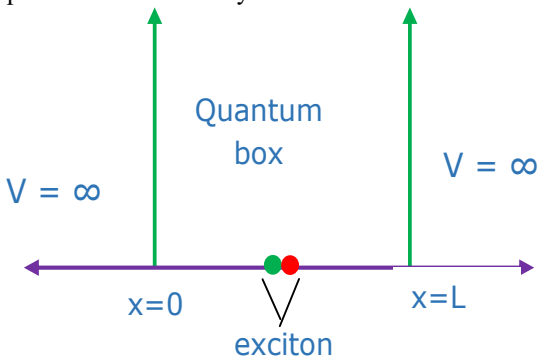

Fig. 2.1. Confined exciton in QDs

The time-independent Schrödinger equation for a particle of mass m in a 3D potential $V(r)$ is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r) \quad (1)$$

For a 3D potential well with side length L:

$$V(x,y,z) = \begin{cases} 0 & if\ 0 \le x,y,z \le L \\ \infty & \text{otherwise} \end{cases} \quad (2)$$

Inside the well, where $V(x,y,z) = 0$, the Schrödinger equation simplifies to:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\psi(x,y,z) \quad (3)$$

We can separate variables by assuming a solution of the form:

$$\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z) \quad (4)$$

Substituting this into the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{\psi_x}\frac{d^2\psi_x}{dx^2} + \frac{1}{\psi_y}\frac{d^2\psi_y}{dy^2} + \frac{1}{\psi_z}\frac{d^2\psi_z}{dz^2}\right) = E \quad (5)$$

Since each term depends on a different variable, we can set each part equal to a constant:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi_x}\frac{d^2\psi_x}{dx^2} = E_x \quad (6)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi_y}\frac{d^2\psi_y}{dy^2} = E_y \quad (7)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi_z}\frac{d^2\psi_z}{dz^2} = E_z \quad (8)$$

Where

$$E = E_x + E_y + E_z \quad (9)$$

Each of these equations is similar to the one-dimensional infinite potential well problem. Applying the boundary conditions, the energy associated with each dimension becomes:

$$E_x = \frac{\hbar^2}{2m}\left(\frac{n_x\pi}{L}\right)^2 \quad (10)$$

$$E_y = \frac{\hbar^2}{2m}\left(\frac{n_y\pi}{L}\right)^2 \quad (11)$$

$$E_z = \frac{\hbar^2}{2m}\left(\frac{n_z\pi}{L}\right)^2 \quad (12)$$

Therefore, the total energy is:

$$E = E_x + E_y + E_z = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad (13)$$

Hence, the energy levels of a particle in a quantum dot are given by:

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad (14)$$

n_x, n_y, n_z are positive integers (1, 2, 3, ...).

These quantized energy levels illustrate the confinement effects in quantum dots, leading to discrete energy states that depend on the size of the dot and the quantum numbers. n_x, n_y, n_z.

The energy of an electron in the conduction band can be written as:

$$E_c = E_c^0 + \frac{\hbar^2\pi^2}{2m_c^*L^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad (15)$$

where E_c^0 is the conduction band edge energy and m_c^* the effective mass of the electron.

Similarly, the energy of a hole in the valence band can be written as:

$$E_v = E_v^0 + \frac{\hbar^2\pi^2}{2m_h^*L^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad (16)$$

where E_v^0 the valence band edge energy and m_h^* the effective mass of the hole. The ground state, which is the commonly observed state, can easily be found and taken. $n_x = n_y = n_z = 1$; then we get

$$E_c = E_c^0 + \frac{3\hbar^2\pi^2}{2m_c^*L^2} \quad (17)$$

$$E_v = E_v^0 + \frac{3\hbar^2\pi^2}{2m_h^*L^2} \quad (18)$$

Therefore the bandgap E_g which is the energy difference between the conduction band minimum and the valence band maximum:

$$E_{gap} = E_c - E_v \quad (19)$$

$$E_{gap} = \left(E_c^0 + \frac{3\hbar^2\pi^2}{2m_c^*L^2}\right) - \left(E_v^0 + \frac{3\hbar^2\pi^2}{2m_h^*L^2}\right) \quad (20)$$

$$E_{gap} = E_g^0 + \frac{3\hbar^2\pi^2}{2L^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) \quad (21)$$

where $E_g^0 = E_c^0 - E_v^0$ is the bulk bandgap.

And the term,

$$\frac{3\hbar^2\pi^2}{2L^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) \quad (22)$$

represents the confinement energy contribution to the bandgap

Where

E_{gap} is bandgap of the QDs., E_g^0 is the bulk bandgap of the material, $\hbar$ is the reduced Planck's constant, L is the size of the QDs, m_e^* is the effective mass of the electron, m_h^* the effective mass of the hole. The derived expression of equation 21 shows that the bandgap of QDs increases as the size of the QDs decreases, illustrating the quantum confinement effect. The energy (E) of a photon is related to its wavelength (λ) by the equation:

$$E = \frac{hc}{\lambda} \quad (23)$$

Rearranging this equation to solve for the wavelength (λ) we get:

$$\lambda = \frac{hc}{E} = \frac{hc}{E_g^0 + \frac{3\hbar^2\pi^2}{2L^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)} \quad (24)$$

Equation 24 is the simplified model for the emission wavelength of QDs

3. Materials and Methods

In this study, a simplified model, represented by equation 24, is employed to calculate the emission wavelengths of group II-VI quantum dots, specifically CdSe, CdS, and ZnS, across different sizes. The relationship between quantum dot size and corresponding optical wavelength is analyzed by plotting emission wavelengths against varying sizes, allowing for the investigation of quantum confinement effects and their practical implications. The computation utilizes empirically derived parameters from published scientific literature, as detailed in Table 1.

Table 1. The Group II-IV QDs material parameters used for the study

Quantum dots	M_e^x	M_h^x	$E_{g(bulk)}$ at 300k
CdSe	$0.13m_o$	$0.45m_o$	1.74Ev
ZnS	$0.34m_o$	$0.23m_o$	3.68Ev
CdS	$0.21m_o$	$0.80m_o$	2.42Ev

4. Results and Discussion

The emission wavelength versus quantum dot size plots for CdSe, ZnS, and CdS, shown in Figure 4.1, clearly demonstrate an inverse quadratic relationship. As the size of the quantum dots decreases, the emission shifts toward shorter wavelengths, resulting in blueshift (emission or absorption shifts to shorter wavelengths). This shift is attributed to the increased energy separation between the quantized electronic levels under strong quantum confinement. In contrast, when the dot size increases, the emission moves toward longer wavelengths in the red region of the spectrum, as illustrated in Figure 4.2.

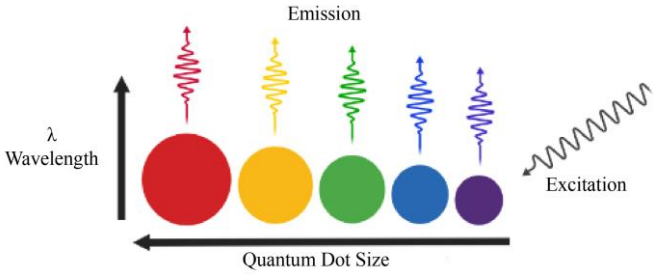

Fig 4.2. Redshift in the emission wavelength with increasing size

Observed redshift in quantum dots primarily illustrates a reduction in the optical band gap, often due to increased size or electronic interactions. It is a key signature of how the quantum dot's structure influences its optical behaviors.

Figure 4.1 illustrates the relationship between emission wavelength and quantum dot size for CdSe, CdS, and ZnS and demonstrates distinct size-dependent optical behaviors. As the QD size decreases for CdSe, the energy gap increases, causing the emission to move toward shorter wavelengths resulting in a visible color shift from deep red (~650 nm) to red, orange, yellow, and finally green (~510 nm) as the dot size reduces from approximately 6 nm to 2 nm. As a result, CdSe quantum dots are widely used in optical displays due to their tunable emission across the visible spectrum. They also find applications in photodetector devices for detecting visible light with fast response times.

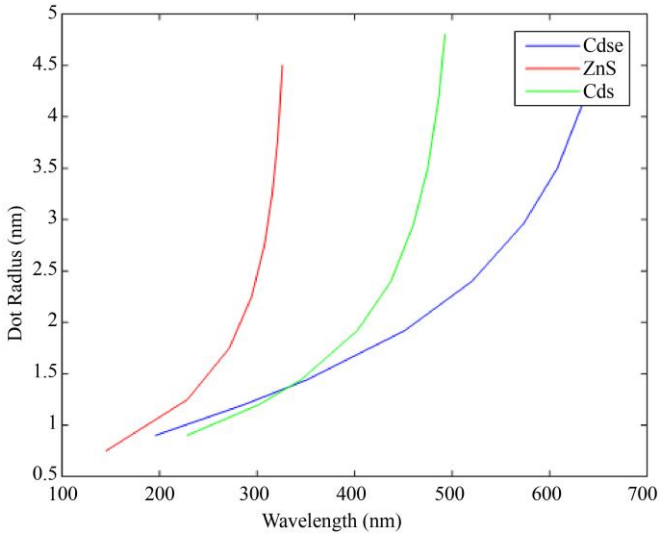

Fig. 4.1. Emission wavelength as a function of different sizes for CdSe, CdS, and ZnS QDs

As the size of CdS QDs decreases, the energy gap widens, resulting in emission at shorter wavelengths. This causes a visible shift in color from yellow-orange (~580–600 nm) to green and ultimately blue (~450 nm) as the dot size reduces from 5–6 nm to below 2 nm. These emission properties make CdS quantum dots suitable for use in visible-light LEDs, particularly in the blue-green range. They also serve as light-absorbing materials or sensitizers in QD solar cells, where their tunable energy gap helps capture a broader portion of the solar spectrum.

As the ZnS QDs size decreases, the energy gap increases dramatically, causing the emission to move to shorter wavelengths, leading to a shift from blue (~450 nm) to violet and near-ultraviolet (<400 nm) as the dot size decreases from

5 nm to below 2 nm. As a result, ZnS QDs are used in solid-state lighting for blue and ultraviolet emission and photodetectors due to their wide band gap. In addition, they are used to convert high-energy ultraviolet photons into visible light, improving photovoltaic efficiency via photon down-conversion.

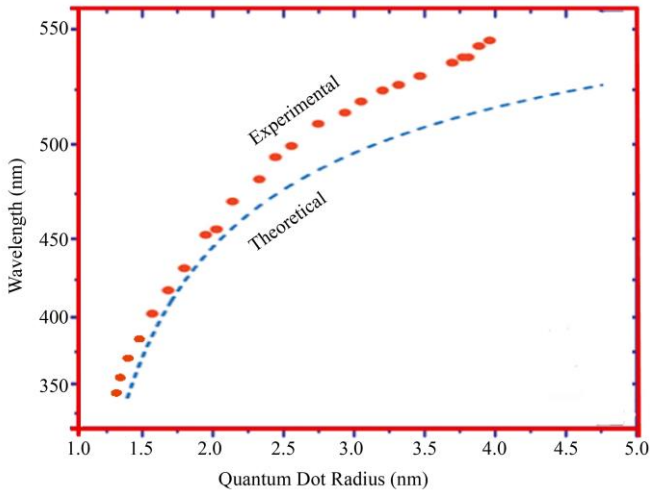

Fig. 4.3. Computed//experimental emission wavelength versus QD size

These observations clearly highlight the strong influence of quantum confinement on the optical output of QDs, allowing for precise tuning of their emission properties by simply adjusting their size. The emission wavelengths calculated using our model are compared with experimental data, as illustrated in Figure 4.3.

There is a strong agreement between our theoretical calculation and experimental values

5. Conclusion

The impact of quantum confinement on the emission wavelengths of CdSe, CdS, and ZnS quantum dots has been thoroughly examined using the formulated model. The results demonstrate clear size-dependent emission characteristics driven by quantum confinement, which leads to a blue emission shift as the quantum dots' size decreases. Specifically, CdSe quantum dots emit across the visible spectrum from red to green, CdS spans from yellow to blue, and ZnS primarily emits in the blue to ultraviolet. Ultimately, by controlling the size of these quantum dots, researchers and engineers can fine-tune their optical and electronic properties to meet specific application requirements. These unique properties make Group II-VI quantum dots highly versatile and valuable for applications in bioimaging, medical diagnostics, display technologies, solar cells, and sensors.

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