EXCITONIC LUMINESCENCE IN SPHERICAL
CORE-MULTI-SHELL QUANTUM DOT
STRUCTURES

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ABSTRACT

EXCITONIC LUMINESCENCE IN SPHERICAL CORE-MULTI-SHELL QUANTUM DOT STRUCTURES

In this thesis, we studied excitonic light emission from core-multishell semiconductor hetero-nanocrystals having a spherically symmetric shape as a function of core size and shell thicknesses. Different combinations of semiconductors were considered in the core/shell/shell structure. The multilayer quantum dot structures that we considered were in A/B/A/B form, where A and B denote II-VI binary semiconductor crystals. We used method of finite differences to solve the Schrödinger equation of the confined exciton problem numerically. Several approximations including the effective mass approximation for the electron and hole masses, and treatment of Coulomb interaction as a perturbation, were employed. Normalized oscillator strengths for optical transitions and coexistence of multiple transitions from a single structure at several frequencies have been investigated. In this study, three different pairs of semiconductors are considered. One of them is (CdSe) ZnS) CdSe) ZnSe), other is (CdSe) CdS) CdSe) CdSe) and third one is (CdTe) ZnS) CdTe) ZnSe). According to our calculation, (CdSe)ZnS)CdSe)ZnSe) structure, when the core radius is 1.51 nm with some different shells combinations, has multi-color emissions from higher frequency to lower frequency in the visible spectrum. (CdSe) CdS) CdSe) CdSe) structure has multi-color emissions when the core radii are 2.02 nm and 2.52 nm yet this structure is the most inefficient structures which we analyse. Moreover, multi-color emissions are obtained from the structure (CdTe) ZnS) CdTe) ZnS) when the core radii are 1.29 nm, 1.93 nm, 2.58 nm and 3.23 nm. Also, this structure has nearly white light emission for 3.23 nm core radius with 3 ML ZnS shell and 1 ML CdTe shell, and with 4 ML ZnS shell and 1 ML CdTe shell.
ÖZET

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CHAPTER 1
INTRODUCTION

Nowadays the requiring faster and smaller devices forced to natural limits in microelectronics, for this reason, different approaches and studies are needed to achieve practical low dimensional systems. During the past years concern about nano scale systems highly increased therefore synthesis of functional nano-materials exhibited considerable developments with their controllable size, shape, electronic and optical properties.

One of these focused issues are nano-dimensional semiconductor structures at which quantum-size effects start to dominate as electron and hole motions are confined attwo particle reach to two particle reach to two particle reach to least one dimensions. In bulk semiconductors, electron at the valance band is excited by absorbed photon. The required energy for excitation is is indicated by energy band gap of semiconductor. The excited electron leaves behind positive charged particle (hole) at the valance band. Electron at the conduction band and hole at the valance band are attracted to each other by Coulomb force. Bound state of these electron and hole is named exciton. When an exciton recombine means electron back to valance band, it emits photon so the excitonic luminescence occurs. In quantum dot, energy levels in valance and conduction bands have discrete distribution and the band gap is larger than compared to bulk state because of Quantum confinement effects. Quantum confinement effects occur when the size of structure is comparable to Bohr radius of electron-hole pair (exciton). Bohr radius is smallest possible orbit radius which is about 10 nm for electron hole pair in semiconductors. Therefore, when the size of semiconductor crystal is comparable to 10 nm, excitonic luminescence has quantized energy levels and is possible to occur in visible spectrum.

The quantum confinement effects was first observed in the 1920’s that when the absorption and luminescence of heated glasses containing CdS colloids color shifts to smaller wavelengths. In the 1960’s, it was reported that there were differences between absorption spectra of colloidal semiconductor particles and spectra of the corresponding bulk materials [3–5]. Soon after the invention of Molecular Beam Epitaxy (MBE) [6, 7], quantized energy levels of confined charge carriers in 2D-structures were confirmed by experimental observation [8]. Afterward, this intresting effects were attracted considerable attention by theoretical and experimental studies [9–22]. Theoretical studies were started in the 1980’s for the effect of size on electronic structures. The first theoretical de-
scriptions about the nature of the 3D excitonic quantum confinement were given by Efros and Efros [10] and by Brus [9]. Progressive different theoretical studies and improvement in synthesis techniques allowed various works on nano-crystals [23–31]. These works were also extended to complex nano-structures like coated semiconductor particles which included layers of shells with different semiconductors surrounding core of quantum dot, so called core/shell quantum dot. The first effort on core/shell quantum dot was obtained by using HgS layer on CdS core and CdS layer on them in 1993 [31]. Then, (CdS)CdSe/CdS and (ZnS)CdS/ZnS structures were successfully synthesized, and some of them also theoretically investigated [32–36] These early core/shell or core/shell/shell quantum dots had light emissions in only mono color. But the there is a strong demand for multi-color emitting nanocrystal systems. To obtain different color or white light, different types of nanocrystals must be carefully combined. In stead of that, multi-color or white light emitting systems using only a single type of nanocrystal are more convenient for fabrication and for efficient emission.

On the other hand, quantum dots with specified properties are put to use on so many areas and on stand by many others.

First of all, today fluorescent quantum dots are successfully used for diagnostics in biology. Nanocrystal particles have tunable and distinct spectrum of emission and long life compared to conventional fluorophores. Semiconductor quantum dots are easily bound to proteins and DNA molecules so that biological reactions can be followed. Because of these properties, semiconductors quantum dots have promising future for further imaging techniques for the biological processes.

Another potential applications are opto-electronics devices such as light emitting diodes (LEDs), photovoltaic cells and lasers. Combination of optical and electronic properties of semiconductors quantum dots and white light emitting systems are the real achievements. In recent years, considerable progress has been made in this route [37, 38].

In this thesis, multi-color light emission from core-multishell semiconductor quantum dots are treated. In the next chapter, the theoretical bases on which our numerical study is standing are given, then numerical representations are shown. Results of our computations are discussed last two chapters.
CHAPTER 2

METHOD

2.1. Theory

First of all, to solve our problem of electron-hole pair in spherical symmetric quantum dot heteronanocrystal structure, it is necessary to give general Hamiltonian,

\[ H = -\frac{\hbar^2}{2m_e} \nabla^2_e - \frac{\hbar^2}{2m_h} \nabla^2_h - \frac{1}{4\pi \varepsilon} \frac{e^2}{|r_e - r_h|} + V_e(r_e) + V_h(r_h) + E_g. \]  

(2.1)

Here \( \varepsilon \) is the dielectric constant of semiconductor material. \( E_g \) is the band gap energy of bulk semiconductor material. \( r_e, m_e, V_e(r_e) \) and \( r_h, m_h, V_h(r_h) \) are position, the effective mass, potential well height of electron and hole, respectively.

Figure 2.1. Left: Schematic of core-multishell semiconductor hetero-nanocrystal. Right: Radial energy diagram (not drawn to scale)[1]

The theoretical analysis starts with assuming strong confinement potential so that the Coulomb interaction between electron and hole is negligible comparatively. Also because
of the mass of electron and hole may depend on the position, we applied effective mass approximation which works well even for nano-dimensional structure [27, 39–43].

2.1.1. One Particle States

For single electron or hole, Schrödinger equation, without considering Coulomb interaction, can be written in the form of

\[
-\frac{\hbar^2}{2m(r)} \nabla^2 + V(r) \psi(r) = E\psi(r),
\]

(2.2)

\[
\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi).
\]

(2.3)

We consider a spherically symmetric heteronanocrystal structure, in order to separate the angular and the radial part of the equation. In Equation (2.2), \(\psi_{nlm}(r, \theta, \phi)\) represents the wavefunction of the corresponding particle in spherical coordinates \((r, \theta, \phi)\), \(R_{nl}(r)\) is radial wavefunction, \(Y_{lm}(\theta, \phi)\) is the spherical harmonics, \(n\) is the principal quantum number, \(m\) and \(l\) are the angular momentum quantum numbers.

\[
V(r) = \begin{cases} 
V_1 & \text{for } 0 \leq r < r_1 \\
V_2 & \text{for } r_1 \leq r < r_2 \\
& \vdots \\
V_N & \text{for } r_{N-1} \leq r < r_N 
\end{cases}
\]

(2.4)

The confinement potential written in Equation (2.3) is assumed stepwise constant value throughout distinct regions. At all regions, confinement potentials are spherically symmetric that means there is no angular dependence but there is only radial dependence. In the spherical symmetric case, \(m = 0\) and \(l = 0\), angular part of the wavefunction gives
constant factor of $1/\sqrt{4\pi}$ and radial eigenfunction $R_{nl}(r)$ in the $N$ regions is stated,

$$R_{nl}(r) = \begin{cases} R_{nl,1} & \text{for } 0 \leq r < r_1 \\ R_{nl,2} & \text{for } r_1 \leq r < r_2 \\ \vdots \\ R_{nl,N} & \text{for } r_{N-1} \leq r < r_N \end{cases} \quad (2.5)$$

Two cases are distinguished to find $R_{nl}(r)$; in regions where $E_{nl} > V_q$, the solution is a linear combination of spherical Bessel and Neumann functions as

$$R_{nl,q}(r) = A_{nl,q}j_l(k_{nl,q}r) + B_{nl,q}n_l(k_{nl,q}r), \quad (2.6)$$

with

$$k_{nl,q} = \sqrt{\frac{2m_q(E_{nl} - V_q)}{\hbar^2}}, \quad (2.7)$$

on the other hand, in the case of $E_{nl} < V_q$, the wave equation yields linear combination of Hankel functions $h_l^{(+)}$ and $h_l^{(-)}$ as

$$R_{nl,q}(r) = A_{nl,q}h_l^{(+)}(\kappa_{nl,q}r) + B_{nl,q}h_l^{(-)}(\kappa_{nl,q}r), \quad (2.8)$$

with

$$\kappa_{nl,q} = \sqrt{\frac{2m_q(V_q - E_{nl})}{\hbar^2}}, \quad (2.9)$$

At the crossing of regions, the general solution must satisfy the boundary conditions [44, 45],

$$R_{nl,q}(r_q) = R_{nl,q+1}(r_q) \quad (2.10)$$
\[
\frac{1}{m_q} \frac{dR_{nl,q}(r)}{dr} \bigg|_{r=r_q} = \frac{1}{m_{q+1}} \frac{dR_{nl,q+1}(r)}{dr} \bigg|_{r=r_q} \tag{2.11}
\]

After applying the requirements, \( R_{nl}(r) \) has to be regular at \( r = 0 \) and has to converge to zero when \( r \to \infty \). \( N \) regions means \( N - 1 \) boundaries, Equation (2.9) and (2.10) leads to \( 2N - 2 \) equalities and \( 2N - 2 \) unknown coefficients \( A_{nl,q}, B_{nl,q} \). To find the nontrivial solution of this linear equation system, the determinant of unknown coefficients have to be zero,

\[
D_l = D_l(E_{nl}) = 0. \tag{2.12}
\]

After finding the eigenvalue as a single zero of Equation (2.11), the linear equations can be solved as a function of \( A_{nl,q} \) or \( B_{nl,q} \) and last unknown coefficient is determined by the normalization of \( R_{nl}(r) \) [31, 40]. These calculations gives the wave function of single electron or single hole and corresponding energy of its state with no interaction.

### 2.1.2. The Coulomb Interaction

At the beginning of analysis, our first assumption is strong confinement potential therefore, by using the first order perturbation theory, the exciton binding energy due to Coulomb interaction between electron and hole is written as [31];

\[
E_c = -\frac{e^2}{4\pi} \int \int d\mathbf{r}_e d\mathbf{r}_h \frac{\psi_e^*(\mathbf{r}_e)\psi_h^*(\mathbf{r}_h)\psi_e(\mathbf{r}_e)\psi_h(\mathbf{r}_h)}{|\mathbf{r}_e - \mathbf{r}_h|} \frac{1}{\bar{\varepsilon}(\mathbf{r}_e, \mathbf{r}_h)} \tag{2.13}
\]

In Equation (2.12), \( e \) and \( h \) represent electron and hole, and \( \varepsilon \) is effective dielectric constant. \( 1/|\mathbf{r}_e - \mathbf{r}_h| \) is expended in the form of spherical harmonics by using cosine law with angle \( \theta_h \) which is the angle between \( \mathbf{r}_e \) and \( \mathbf{r}_h \) when \( \mathbf{r}_e \) is fixed on polar axis.

\[
|\mathbf{r}_e - \mathbf{r}_h| = \sqrt{r_e^2 + r_h^2 - 2r_e r_h \cos \theta_h}. \tag{2.14}
\]

For the effective dielectric constant \( \bar{\varepsilon}(r_e, r_h) \) in Equation (2.12), we make an approximation over volume of shells considering the boundary values to calculate mean dielectric
constant because materials have different dielectric constant. If the fractions of distance between electron and hole in different material is regarded, the calculation of effective dielectric constant so all calculation become exceedingly heavy.

\[
\bar{\varepsilon}(r_e, r_h) = \begin{cases} 
\varepsilon_1 & \text{for } r_{\text{max}} < r_1 \\
\varepsilon_{\text{rmax}} & \text{for } r_1 < r_{\text{max}} < r_2 \\
\varepsilon_3 \left( \frac{r_{e}^2 - r_2^2}{r_{\text{max}}} + \frac{r_2^2 - r_1^2}{r_{\text{max}}} + \varepsilon_3 r_1^2 \right) & \text{for } r_2 < r_{\text{max}} < r_3
\end{cases}
\]

(2.15)

In Equation (2.14), \(r_1, r_2, r_3\) are radius of core and shell boundaries, \(\varepsilon_1, \varepsilon_2, \varepsilon_3\) are dielectric constant at core, first shell and second shell, respectively. \(r_{\text{max}}\) refers to larger of \(r_e\) and \(r_h\). \(\varepsilon_{\text{rmax}}\) is the dielectric constant at the position where larger of \(r_e\) and \(r_h\) refers. Hereby, effective dielectric constant becomes free from angular dependence. After separating the variables of wave functions and conjugate wave functions in spherical coordinates, the Coulomb energy is expressed as

\[
E_c = -\frac{e^2}{4\pi} \int_0^{2\pi} \int_0^\pi d\theta_e d\phi_e \sin \theta_e |Y_e(\theta_e, \phi_e)|^2 \int_0^{2\pi} d\phi_h |Y_h(\theta_h, \phi_h)|^2 \\
\times \int dr_e dr_h r_e^2 r_h^2 \int_0^\pi d\theta_h \sin \theta_h \frac{|R_e(r_e)|^2 |R_h(r_h)|^2}{\sqrt{r_e^2 + r_h^2 - 2r_e r_h \cos \theta_h} \bar{\varepsilon}(r_e, r_h)}
\]

(2.16)

Here, \(\psi_e(r_e) = R_e(r_e)Y_e(\theta_e, \phi_e)\) and \(\psi_h(r_h) = R_h(r_h)Y_h(\theta_h, \phi_h)\).

\[
E_c = -\frac{e^2}{4\pi} \int_0^{2\pi} \int_0^\pi d\theta_e d\phi_e \sin \theta_e |Y_e(\theta_e, \phi_e)|^2 \int_0^{2\pi} d\phi_h |Y_h(\theta_h, \phi_h)|^2 \\
\times \int dr_e dr_h r_e^2 r_h^2 |R_e(r_e)|^2 |R_h(r_h)|^2 \frac{1}{\bar{\varepsilon}(r_e, r_h)} \left( \sqrt{r_e^2 + r_h^2 - 2r_e r_h \cos \theta_h} \right) \left| \frac{\pi}{0} \right|
\]

(2.17)
\( l = m = 0 \) because of spherical symmetry, and the angular part of the wavefunction is constant value, \( Y_{le,lm}(\theta_e, \phi_e) = Y_{lh,lm}(\theta_h, \phi_h) = 1/\sqrt{4\pi} \).

\[
E_c = -\frac{e^2}{4\pi} \int_0^{2\pi} \int_0^\pi d\theta_e d\phi_e \sin \theta_e |Y_e(\theta_e, \phi_e)|^2 \int_0^{2\pi} d\phi_h |Y_h(\theta_h, \phi_h)|^2 \\
\times \int \int d\rho_e d\rho_h \rho_e^2 \rho_h^2 \left[ \frac{|R_e(\rho_e)|^2 |R_h(\rho_h)|^2}{\varepsilon(\rho_e, \rho_h)} \frac{1}{\rho_e \rho_h} \right] \left[ (\rho_e + \rho_h) - |\rho_e - \rho_h| \right]
\]

(2.18)

After integration over the angular coordinates, the equation becomes;

\[
E_c = -\frac{e^2}{4\pi \varepsilon_0} \int_0^{\infty} d\rho_e \left[ \int_0^{\rho_e} d\rho_h \rho_e^2 \rho_h^2 |R_e(\rho_e)|^2 |R_h(\rho_h)|^2 \frac{1}{\varepsilon(\rho_e, \rho_h)} \right. \\
+ \left. \int_{\rho_e}^{\infty} d\rho_h \rho_e^2 \rho_h^2 |R_e(\rho_e)|^2 |R_h(\rho_h)|^2 \frac{1}{\varepsilon(\rho_e, \rho_h)} \right]
\]

(2.19)

For the simpler representation,

\[
E_c = -\frac{e^2}{4\pi \varepsilon_0} \int \int d\rho_e d\rho_h \rho_e^2 \rho_h^2 \left[ \frac{|R_e(\rho_e)|^2 |R_h(\rho_h)|^2}{\max(\rho_e, \rho_h)} \frac{1}{\varepsilon(\rho_e, \rho_h)} \right].
\]

(2.20)

After determining the Coulomb energy, the transition energy can be written as,

\[
E_{tr} = E_e + E_h + E_c + E_{sm},
\]

(2.21)

\( E_e \) and \( E_h \) are single particles eigen energy without interaction between them, \( E_c \) is Coulomb energy and \( E_{sm} \) is smallest band gap energy of materials that are used in structure. Transition energy is recombination energy of exciton so the energy of emitted light.
2.1.3. Oscillator Strength

In our analysis, oscillator strength of the excitons are also calculated. Oscillator strength is dimensionless quantity which expresses the transition ability of an exciton from one quantum state to another. This transition is the source of light from quantum dot, thus oscillator strength gives the idea about dominant color of emitted light. Simply, calculation overlapping of single electron and hole wavefunction and dividing by binding energy of corresponding energy gives the recombination probability [46]. The envelope function of exciton is;

\[ \Psi_{ex}(r) = \psi_e(r_e)\psi_h(r_h)\phi(|r_e - r_h|), \tag{2.22} \]

and the oscillator strength is written as;

\[ f_{ex} \propto \frac{1}{E_c} \left[ \int \Psi_{ex}(r = r_e = r_h) d\mathbf{r} \right]^2, \tag{2.23} \]

where \( E_c \) is the Coulomb interaction between electron and hole. Not the exact value of oscillator strength, we are interested in comparison of oscillator strengths values of states in related quantum dot.

2.2. Numerical Approach

2.2.1. Finite Difference Method

The finite difference method is a basic numerical method which is based on the approximation of derivatives of the function with respect to grids on the variable of the function and equal differences between these grids. Let \( f \) be the function of variable \( r \) which has finite steps of \( h \) (\( h \) refers to hole when it is used as subscript otherwise it is step size) stated in Equation (2.24) and (2.25),

\[ r_i = r_0 + ih \quad (i = 1, 2, 3, \ldots) , \tag{2.24} \]
\[ h = r_{i+1} - r_i. \]  

(2.25)

Taylor expansion of \( f \) around \( r_i \) is;

\[ f(r_i + h) = f(r_i) + hf'(r_i) + \frac{h^2}{2!} f''(r_i) + \frac{h^3}{3!} f'''(r_i) + ... \]  

(2.26)

Thus first derivative of \( f \) at point \( r_i \) is approximately written as

\[ f'(r_i) \approx \frac{f(r_i + h) - f(r_i)}{h}, \]  

(2.27)

Equation (2.27) is the forward difference derivative formula. Taylor expansion of \( f(r_i - h) \) and first derivative which is named as backward difference derivative formula;

\[ f(r_i - h) = f(r_i) - hf'(r_i) + \frac{h^2}{2!} f''(r_i) - \frac{h^3}{3!} f'''(r_i) + ... \]  

(2.28)

\[ f'(r_i) \approx \frac{f(r_i) - f(r_i - h)}{h}, \]  

(2.29)

Forward difference and backward difference derivative formulas have error order of \( h \). There is more consistent formula for first derivative. Subtracting Equation (2.28) from (2.26) gives first derivative formula as;

\[ f'(r_i) \approx \frac{f(r_i + h) - f(r_i - h)}{2h} \]  

(2.30)

This is named central deference derivative derivative formula which has error order of \( h^2 \). Similarly sum of Equation (2.28) and (2.26) yields second derivative formula as;

\[ f''(r_i) \approx \frac{f(r_i + h) - f(r_i - h) - 2f(r_i)}{h^2} \]  

(2.31)
Now Schrödinger equation for the single particle can be written by substituting the derivative formula.

### 2.2.2. Schrödinger Equation Numerical Form

In order to write the Schrödinger equation of our system in useful form for numerical calculation, simple operations such as reducing the equation in dimensionless form and applying the approximate derivative formula are applied. The eigen energies and the eigen functions of a single particle in the structure are determined by calculation of computer program after numerical form is coded.

Firstly, separated variables of \((r, \theta, \phi)\) and the spherical symmetry on the system gives the radial wave equation of single particle in the form of;

\[
\frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{\hbar^2} \left[ V(r) + E \right] R = l(l + 1)R. \tag{2.32}
\]

To simplify the Equation (2.32), variables are changed,

\[
U(r) \equiv rR(r), \tag{2.33}
\]

Radial equation transforms to one dimensional Schrödinger equation,

\[
EU = \frac{\hbar^2}{2} \left[ \frac{d}{dr} \left( \frac{1}{m(r)} \frac{d}{dr} U \right) \right] + \left[ V + \frac{\hbar^2}{2m(r)} l(l + 1) \frac{r^2}{r_i} \right] U. \tag{2.34}
\]

To write in numerical form, derivative formula defined by finite difference approximation, which is adverted before, is applied to Equation (2.34),

\[
EU_i = \frac{\hbar^2}{2} \left[ \left( \frac{1}{m_{i+1}} - \frac{1}{m_{i-1}} \right) \frac{(U_{i+1} - U_{i-1})}{2h} + \frac{1}{m_i} \frac{(U_{i+1} - U_{i-1} - 2U_i)}{h^2} \right] U_i
\]

\[
+ \left[ V + \frac{\hbar^2}{2m_i} \frac{l(l + 1)}{r_i^2} \right] U_i \tag{2.35}
\]
In the equation, $h$ refers size of steps. $i$ is indice which counts the $h$ on the position axis from zero to end of considered length say it is the radius of quantum dot. $U_i$ represents numerical value at the $i$'th step from zero. The equation needs derivation to be more convenient for computer programming. First of all, it has to be written in dimensionless form.

\[
EU_i = \frac{\hbar^2}{2\hbar^2} \left[ \left( \frac{1}{4m_{i+1}} - \frac{1}{4m_{i-1}} \right) (U_{i+1} - U_{i-1}) + \frac{1}{m_i} (U_{i+1} - U_{i-1} - 2U_i) \right]
+ \left[ V + \frac{\hbar^2}{2m_i} \frac{l(l+1)}{r_i^2} \right] U_i
\]  
(2.36)

To construct a factor in the unit of energy, the right side of the equation is multiplied and divided with $m_e$. Angular momentum quantum number, $\frac{\hbar^2}{2m_i} \frac{l(l+1)}{r_i^2}$ is zero.

\[
l = 0,
\]  
(2.37)

thus

\[
\frac{\hbar^2}{2m_i} \frac{l(l+1)}{r_i^2} = 0,
\]  
(2.38)

the equation takes a form as

\[
EU_i = \frac{\hbar^2}{2\hbar^2 m_e} \left[ \left( \frac{m_e}{4m_{i+1}} - \frac{m_e}{4m_{i-1}} + \frac{m_e}{m_i} \right) U_{i+1} + \left( - \frac{m_e}{4m_{i+1}} + \frac{m_e}{4m_{i-1}} + \frac{m_e}{m_i} \right) U_{i-1} \right]
+ \left[ - \frac{\hbar^2}{2\hbar^2 m_e} \frac{2m_e}{m_i} + V \right] U_i.
\]  
(2.39)

If we say

\[
\frac{\hbar^2}{2\hbar^2 m_e} \equiv \epsilon,
\]  
(2.40)
and divide both sides with $\epsilon$ and edit the equation, then the dimensionless eigenvalue equation is constructed as

$$
\frac{E}{\epsilon} U_i = \left( \frac{m_e}{4m_{i+1}} - \frac{m_e}{4m_{i-1}} + \frac{m_e}{m_i} \right) U_{i+1} + \frac{1}{\epsilon} \left[ \frac{V}{\epsilon} - \frac{2m_e}{m_i} \right] U_i + \left( \frac{-m_e}{4m_{i+1}} + \frac{m_e}{4m_{i-1}} + \frac{m_e}{m_i} \right) U_{i-1}
$$

(2.41)

This form of equation is ready to compute as $N \times N$ tridiagonal matrix where $N$ is the considered number of steps on the radius of quantum dot. The matrix is specified with entering the core and shell sizes, band gap energies, effective mass of electron and hole, and dielectric constants with respect to indice that counts the steps on the radius.

### 2.2.3. The Coulomb Interaction in Numerical Form

After determining the eigen states, we write down the effective dielectric constant and the Coulomb interaction in proper form for numerical computation as

$$
\bar{\varepsilon}(r_a, r_b) = \begin{cases} 
\varepsilon_1 & \text{for } r_{\text{max}} < r_1 \\
\varepsilon_{r_{\text{max}}} & \text{for } r_1 < r_{\text{max}} < r_2 \\
\varepsilon_3 (r_{\text{max}}^3 - r_2^3) + \varepsilon_2 (r_2^3 - r_1^3) + \varepsilon_3 r_2^2 \left( \frac{r_{\text{max}}}{r_{\text{max}}} - 1 \right)^2 & \text{for } r_2 < r_{\text{max}} < r_3
\end{cases}
$$

(2.42)

Here, $a$, $b$ and $c$ is the dummy indices from zero to $N$ for electron and hole, respectively. $r_a = ah$, $r_b = bh$ and $r_c = ch$ ($h$ refers to hole when it is used as subscript otherwise it is step size), $\text{max}$ is present the larger of $r_e$ and $r_h$. $r_1$, $r_2$, $r_3$ are radius of core and shell boundaries. $\varepsilon_1$, $\varepsilon_2$, $\varepsilon_3$ are dielectric constant at core, first shell and second shell, respectively.

$$
E_c = -\frac{e^2}{4\pi\varepsilon_0} \sum_{a=1}^{N} \left[ \sum_{b=1}^{a} \hbar^2 (ah)(bh)^2 |R_e(a)|^2 |R_h(b)|^2 \frac{1}{\bar{\varepsilon}(r_a, r_b)} + \sum_{c=a}^{N} \hbar^2 (ch)(bh)^2 |R_e(c)|^2 |R_h(b)|^2 \frac{1}{\bar{\varepsilon}(r_c, r_b)} \right]
$$

(2.43)
In Eqn.(2.44), $h$ is the step size and $a$ is the integer number so $ah$ refers a length as $bh$ does. If $N$ is sufficiently high means $h$ is small, the calculation is more accurate.

### 2.2.4. Oscillator Strength in Numerical Form

Another required value that we represented before is oscillator strength after computing the Coulomb interaction. The summation which is used for Coulomb interaction is also convenient for calculation the oscillator strength. Angular parts of the wave functions of electron and hole give constant value so we do not consider. After that, integration over radial part of the envelope function is formed as,

$$f_{ex} = \frac{1}{E_c} \left[ \sum_{a=b=1}^{N} (ah)(bh)R_e(a)R_h(b)h \right]^2,$$

(2.44)

$a$, $b$ are dummy indices again, $h$ is step size($h$ refers to hole when it is used as subscript), $R_e(r_a)$ is the value of electron radial wavefunction at the position of $ah$ and $R_h(r_b)$ is the value of hole radial wavefunction at the position of $bh$. 
Before giving the results, we would like to provide some information on the stages of calculation. In our analysis, we take two types of semiconductors spherically layered in the form of (core) shell) shell) shell). Core and the second shell are of the same material whereas the first shell and the last shells are of the other semiconductor. Firstly, a spherical core is considered with a radius of \( n \) mono-layer thickness, then another material is layered on the core as a shell with \( m \) mono-layer thickness, and then the core material is layered again on the first shell as second shell with a thickness of \( k \) mono-layers. Last shell covering the quantum dot is considered infinitely thick. In order to engineer the excitonic properties of the multi-layered quantum dots, the core radii are varied from 2 mono-layer to 5 mono-layer and shells thicknesses are varied from 1 mono-layer to 4 mono-layer (\( n = 2..5, m = 1..4, k = 1..4 \)). First three eigenfunctions of single electron and single hole, Coulomb energies, transition energies between electron and hole for all three states which means nine couples and oscillator strength of these couples are computed for all combinations of core-shell sizes.

In our investigation, three different pairs of semiconductors are considered. One of them is (CdSe) ZnS) CdSe) ZnSe), other is(CdSe) CdS) CdSe) CdSe) and third one is (CdTe) ZnS) CdTe) ZnSe). One of the reasons to choose these pairs is the difference between their band gap energies. Electron and hole are expected to be localized in the regions of the quantum dot with the smaller band gap energy. Variations in electron and hole localization regions and variation in eigenenergies are desired so that result to have different transition energies and different colors of emitted light can be obtained. Also, presence of alternative localization regions for electron and hole is important for achieving multi-color emission from the same dot.

In Table 3.1, we list bulk energy band gap value, effective masses of the electron and hole, mono-layer thickness and dielectric constant of the bulk materials material that we considered.

In the tables of results section, some specific configurations which show multi-color emission are given. First three columns inform the core and shell sizes, column of \( (n_e, n_h) \) gives the states of single particles which form an exciton, transition energy column gives the emission energies from recombination of those excitons, and column
of oscillator strength gives the ratio of relatively high oscillator strengths for those core-shell-shell sizes. Also probability distributions of single electron and hole, which create exciton with a relatively high oscillator strength, are shown in corresponding figures.

### 3.1. CdSe-ZnS

One of the structures which we analyse is (CdSe) ZnS) CdSe) ZnSe). In Table 3.2, for 1.51 nm core radius, some significant multi-color emission cases. In Figure 3.1 and 3.2, it is shown that all the electrons are localized at the CdSe core and all the holes are localized at CdSe shell, in these cases. According to our calculation, (CdSe) ZnS) CdSe) ZnSe) structure with 1.51 nm core would emit various colors from higher frequency to lower frequency in the visible spectrum.

At first three rows of Table 3.2, structures have 3 ML ZnS shell(first shell) and at other three rows, structures have 4 ML ZnS shell. For both cases (with 3 and 4 ML ZnS shell), whatever the thickness of first shell is, the thickness of second shell determines the emission frequency. When structure have 3 ML ZnS shell with 1 ML CdSe shell has two different excitonic states which are created by electron and hole having single particle states of (1,2) and (2,2), and the case with 2 ML CdSe shell has the same excitonic states, but emission energies are different. But, when CdSe shell (second shell) thickness is with 1 ML, for both 3 ML and 4 ML ZnS shell, almost same transition energies are found. Also
Table 3.2. Some specific multi-color emission results for the structure (CdSe) ZnS) CdSe) ZnS) when core radius is 1.51 nm

<table>
<thead>
<tr>
<th>Core Radius (nm)</th>
<th>Shell Size (ML)</th>
<th>Shell Size (ML)</th>
<th>States (n_e, n_h)</th>
<th>Transition Energy (eV)</th>
<th>Oscillator Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.51</td>
<td>3</td>
<td>1</td>
<td>(1,2)</td>
<td>3.06</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>2.07</td>
<td></td>
</tr>
<tr>
<td>1.51</td>
<td>3</td>
<td>2</td>
<td>(1,2)</td>
<td>1.79</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>2.32</td>
<td></td>
</tr>
<tr>
<td>1.51</td>
<td>3</td>
<td>3</td>
<td>(2,1)</td>
<td>2.65</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,3)</td>
<td>3.16</td>
<td></td>
</tr>
<tr>
<td>1.51</td>
<td>4</td>
<td>1</td>
<td>(1,2)</td>
<td>3.10</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>2.14</td>
<td></td>
</tr>
<tr>
<td>1.51</td>
<td>4</td>
<td>2</td>
<td>(1,2)</td>
<td>1.72</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>2.55</td>
<td></td>
</tr>
<tr>
<td>1.51</td>
<td>4</td>
<td>3</td>
<td>(2,1)</td>
<td>2.62</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,3)</td>
<td>3.18</td>
<td></td>
</tr>
</tbody>
</table>

when the structure has 3 ML or 4 ML ZnS shell, they have almost same emission energies, if they have the same CdSe shell thickness. The reason of small increases in transition energies for structure with 4 ML ZnS shell is that 4 ML ZnS is a stronger barrier for an electron which is localized at core as shown in Figure 3.1, so the confinement effect is stronger. Thus, the emission energies are determined by the thickness of CdSe shell (second shell) for the 3 ML and 4 ML ZnS shell cases.

3.2. CdSe-CdS

One of the other structures that we investigate is (CdSe)CdS)CdSe)CdSe). In Table 3.3, for core sizes 2.02 nm and 2.52 nm, it is given that some shell sizes have multi-color emission. According to our calculation, for smaller core sizes, only mono-color emission is observed. Mono-color emission energy is changing from red to yellow with very little increasing frequency when we are increasing the core size. On the other hand, when structure have 2.02 nm core size, two different shell combination give multi-color emission. One of them is with 2 ML CdS shell(first shell) and 4 ML CdSe shell(second shell), and 4 ML CdS shell and 4 ML CdSe shell. For both cases, one of excitonic emissions is from (2,2) electron and hole state, despite being at same states, excitons have different emission energies. In Figure 3.3, it is shown that electron and hole are localized at core, but for the case with 4 ML CdS shell, hole have larger penetration to second shell,
Figure 3.1. Relative probability distribution of electron (blue) \(|R_e(r_e)|^2\), hole (red) \(|R_h(r_h)|^2\) and potential (green) \(V(r)\) of structure (CdSe ZnS) CdSe) ZnS) with core radius 1.51 nm. In our notation, x-y means x mono-layer first shell and y mono-layer second shell (for example ‘3-1’ indicates 3 mono-layer first shell and 1 mono-layer second shell). Also for (x,y) representation, x means \(n_e\) quantum number of electron and y means \(n_h\) quantum number of hole (for example (1,2) means electron is at ground state and hole is at first excited state). All peaks are normalized to 1.

which has larger volume to avoid confinement effect, therefore, The Coulomb energy is smaller because of difference in localization of electron and hole, and also 4 ML shell is stronger barrier and it makes the confinement effect is stronger for electron which is totally localized in core. So increasing the emission energy for same states of electron and hole from 2 ML CdS shell to 4 ML CdS shell is reasonable. In addition to this, for 2.02 nm CdSe core with 2 ML CdS shell and 4 ML CdSe shell, the highest excitonic emission energy is from (2,2) electron and hole states which are localized totally in CdSe core.

On the other hand, in Figure 3.4, it is shown that all multi-color excitonic emissions are from core of the quantum dot for the case of 2.52 nm CdSe core. Also, in the Table 3.3, there are three different excitonic emissions from the structure of 4 ML CdS shell with 1 ML CdSe shell, but the frequencies are very close to each other.
Figure 3.2. Relative probability distribution of electron (blue) $|R_e(r_e)|^2$, hole (red) $|R_h(r_h)|^2$ and potential(green) $V(r)$ of structure (CdSe) ZnS) CdSe) ZnS) with core radius 1.51 nm. In our notation, x-y means x monolayer first shell and y monolayer second shell (for example '4-1' indicates 4 monolayer first shell and 1 monolayer second shell). Also for (x,y) representation, x means $n_e$ quantum number of electron and y means $n_h$ quantum number of hole (for example (1,2) means electron is at ground state and hole is at first excited state). All peaks are normalized to 1.

### 3.3. CdTe-ZnS

In this study, the other structure that is analyzed is (CdTe) ZnS) CdTe) ZnSe). According to our calculation, it is remarkable that for many different core radii with different shell sizes, (CdTe) ZnS) CdTe) ZnSe) structure have multi-color light emission. Consequently, (CdTe) ZnS) CdTe) ZnSe) quantum dot is more efficient than (CdSe) CdS) CdSe) CdS) quantum dot and (CdSe) ZnS) CdSe) ZnS) quantum dot to obtain multi-color emission.

Firstly, in Table 3.4, some specific multi-color emissions are given for 1.29 nm core radius. According to our calculations, when the structure has 3 ML ZnS with 1 ML CdTe shell, it gives different colors which are orange, green and blue. (1,2),(2,2) and (3,1) are states of electrons and holes, respectively. For 4 ML ZnS shell with 1 ML CdTe shell case gives nearly same colors of emissions and also (1,2), (2,2) which are states of emitting electron and hole couple are same with 3 ML ZnS with 1 ML CdTe shell case. For 3 ML ZnS shell with 2 ML CdTe shell, quantum dot have almost same colors of emissions with 4 ML ZnS shell with 2 ML CdTe shell but emissions are from
Table 3.3. Some specific multi-color emission results for the structure (CdSe) CdS) CdSe) CdS) when core radius is 2.02 and 2.52 nm

<table>
<thead>
<tr>
<th>Core Radius (nm)</th>
<th>Shell Size (ML)</th>
<th>Shell Size (ML)</th>
<th>States ($n_e, n_h$)</th>
<th>Transition Energy (eV)</th>
<th>Oscillator Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.02</td>
<td>2</td>
<td>4</td>
<td>(2,3)</td>
<td>2.02</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>2.88</td>
<td></td>
</tr>
<tr>
<td>2.02</td>
<td>4</td>
<td>4</td>
<td>(2,3)</td>
<td>2.26</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,1)</td>
<td>2.06</td>
<td></td>
</tr>
<tr>
<td>2.52</td>
<td>4</td>
<td>1</td>
<td>(2,2)</td>
<td>1.81</td>
<td>7</td>
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<tr>
<td>2.52</td>
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<td>4</td>
<td>(2,2)</td>
<td>1.86</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3,3)</td>
<td>2.17</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.4. Some specific multi-color emission results for the structure (CdTe) ZnS) CdTe) ZnS) when core radius is 1.29 nm

<table>
<thead>
<tr>
<th>Core Radius (nm)</th>
<th>Shell Size (ML)</th>
<th>Shell Size (ML)</th>
<th>States ($n_e, n_h$)</th>
<th>Transition Energy (eV)</th>
<th>Oscillator Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.29</td>
<td>3</td>
<td>1</td>
<td>(1,2)</td>
<td>2.02</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>2.36</td>
<td></td>
</tr>
<tr>
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<td></td>
<td></td>
<td>(3,2)</td>
<td>2.67</td>
<td></td>
</tr>
<tr>
<td>1.29</td>
<td>3</td>
<td>2</td>
<td>(2,1)</td>
<td>2.59</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,2)</td>
<td>3.02</td>
<td></td>
</tr>
<tr>
<td>1.29</td>
<td>4</td>
<td>1</td>
<td>(1,2)</td>
<td>2.10</td>
<td>1</td>
</tr>
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<td></td>
<td>(2,2)</td>
<td>2.40</td>
<td></td>
</tr>
<tr>
<td>1.29</td>
<td>4</td>
<td>2</td>
<td>(2,1)</td>
<td>2.63</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,3)</td>
<td>3.06</td>
<td></td>
</tr>
</tbody>
</table>

different states of electron-hole couples. Thus, for (CdSe) ZnS) CdSe) ZnS) nanocrystal, it is possible to say that when nanocrystal have 1.29 nm radius with 3 or 4 ML ZnS shell, colors of emissions are determined by thickness CdTe shell (second shell).

In edition to this, in Table 3.5, it is given that for structure having 1.93 nm core, despite varying the ZnS shell from 2 ML to 4 ML, emission energies do not change also the states of electron hole pairs are same if CdTe shell is 3 ML. So CdTe shell thickness determines multi-emission colors.

According to our calculations, some other multi-color emissions are obtained from the structure (CdTe) ZnS) CdTe) ZnS) when the core sizes are 2.58 nm and 3.23 nm. In Table 3.6, first 4 rows list the results for 2.58 nm core radius. It is shown that 3 ML ZnS shell with 1 ML CdTe shell and 4 ML ZnS shell with 1 ML CdTe shell structures have
Figure 3.3. Relative probability distribution of electron (blue) $|R_e(r)|^2$, hole (red) $|R_h(r)|^2$ and potential(green) $V(r)$ of structure (CdSe)CdS)CdSe)CdS) with core radius 2.02 nm. In our notation, x-y means x mono-layer first shell and y mono-layer second shell (for example ‘2-4’ indicates 2 mono-layer first shell and 4 mono-layer second shell). Also for (x,y) representation, x means $n_e$ quantum number of electron and y means $n_h$ quantum number of hole (for example (2,3) means electron is at first excited state and hole is at second excited state). All peaks are normalized to 1.

almost same emission energies. Those emissions are from the same states of which are (1,3) and (2,3). In Figure 3.5, it is shown that, for both pair of states ((1,3),(2,3)), electrons are localized at CdTe core and holes are localized at CdTe shell. Emission energies from the state (1,3) are exactly the same but for 4 ML ZnS shell, emission energy from the state (2,3) is a little bit larger than for 3 ML ZnS shell because of stronger barrier.

Similar relation ship between the structures which have 3 ML ZnS shell with 4 ML CdTe shell and 4 ML ZnS shell with 4 ML CdTe shell. For both structures, energies of emissions and also the states of those emissions are the same. And electrons of emitting

Table 3.5. Some specific multi-color emission results for the structure (CdTe) ZnS) CdTe) ZnS) when core radius is 1.93 nm

<table>
<thead>
<tr>
<th>Core Radius (nm)</th>
<th>Shell Size (ML)</th>
<th>Shell Size (ML)</th>
<th>States ($n_e$, $n_h$)</th>
<th>Transition Energy (eV)</th>
<th>Oscillator Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.93</td>
<td>2</td>
<td>3</td>
<td>(2,1)</td>
<td>2.18</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3,3)</td>
<td>2.63</td>
<td></td>
</tr>
<tr>
<td>1.93</td>
<td>3</td>
<td>3</td>
<td>(2,1)</td>
<td>2.23</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3,3)</td>
<td>2.60</td>
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</tr>
<tr>
<td>1.93</td>
<td>4</td>
<td>3</td>
<td>(1,2)</td>
<td>2.23</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3,3)</td>
<td>2.59</td>
<td></td>
</tr>
</tbody>
</table>
states are localized at CdTe core and holes are localized at 4 ML CdTe shell which is shown in Figure 3.5.

For 2.58 nm core radius, multi color emission is determined by the CdTe shell thickness which means that increasing the ZnS shell thickness from 3 ML to 4 ML does not change the multi color emission energies as it is observed and reported in this study for smaller core radii.

Remarkable results are obtained from the structure with 3.23 nm core. In Table 3.6, last 4 row list the results of multi color emitting cases which have 3.23 nm CdTe core, ZnS shell with thickness from 1 ML to 4 ML and CdTe shell with thickness 1 ML. The structures with 1 ML and 2 ML ZnS shell, have the same emitting states which are (2,3) and (3,3). Those states have different emission energies but for both, electrons and holes are localized at CdTe core. On the other hand, the structures with 3 ML and 4 ML ZnS shell, have three different color of emissions. Both have nearly the same energies and the same states of electrons and holes have emissions. One of those emission energies is at range of color green, the other one is at the range of blue, and the last one, which have smallest oscillator strength, isn’t at the range of red. So these combination of color is very close to white light which is the real achievement. In addition to this, the structures with 3 ML and 4 ML ZnS shell have same CdTe shell with 1 ML thickness. Thus, it is possible to say that also for those structures, CdTe shell determines the emission as all
Table 3.6. Some specific multi-color emission results for the structure (CdTe) ZnS) CdTe) ZnS) when core radius is 2.58 and 3.23 nm

<table>
<thead>
<tr>
<th>Core Radius (nm)</th>
<th>Shell Size (ML)</th>
<th>Shell Size (ML)</th>
<th>States ((n_e, n_h))</th>
<th>Transition Energy (eV)</th>
<th>Oscillator Strength</th>
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<tbody>
<tr>
<td>2.58</td>
<td>3</td>
<td>1</td>
<td>(2,3)</td>
<td>1.77</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(1,3)</td>
<td>2.26</td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>(3,3)</td>
<td>2.17</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2,1)</td>
<td>1.96</td>
<td></td>
</tr>
<tr>
<td>2.58</td>
<td>3</td>
<td>4</td>
<td>(3,3)</td>
<td>2.22</td>
<td>3</td>
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<td></td>
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<td>(2,1)</td>
<td>1.96</td>
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<tr>
<td>2.58</td>
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<td>1</td>
<td>(1,3)</td>
<td>2.26</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(2,3)</td>
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<td>1.91</td>
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<tr>
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<td>(2,3)</td>
<td>2.29</td>
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<td>1.68</td>
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<td></td>
<td>(2,2)</td>
<td>1.83</td>
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(CdTe) ZnS) CdTe) ZnS) multi-color emitting structures.
Figure 3.5. Relative probability distribution of electron (blue) $|R_e(r)|^2$, hole (red) $|R_h(r)|^2$ and potential (green) $V(r)$ of structure (CdTe) ZnS) CdTe) ZnS) with core radius 2.58 nm. In our notation, x-y means x mono-layer first shell and y mono-layer second shell (for example ’3-1’ indicates 3 mono-layer first shell and 1 mono-layer second shell). Also for (x,y) representation, x means $n_e$ quantum number of electron and y means $n_h$ quantum number of hole (for example (2,3) means electron is at first excited state and hole is at second excited state). All peaks are normalized to 1.
Figure 3.6. Relative probability distribution of electron (blue) $|R_e(r_e)|^2$, hole (red) $|R_h(r_h)|^2$ and potential (green) $V'(r)$ of structure (CdTe) ZnS CdTe) ZnS) with core radius 3.23 nm. In our notation, x-y means x mono-layer first shell and y mono-layer second shell (for example ‘1-1’ indicates 1 mono-layer first shell and 1 mono-layer second shell). Also for (x,y) representation, x means $n_e$ quantum number of electron and y means $n_h$ quantum number of hole (for example (2,3) means electron is at first excited state and hole is at second excited state). All peaks are normalized to 1.
CHAPTER 4

CONCLUSION

Localizations of electron and hole, and the resulting excitonic light emission are calculated in multishell spherical quantum dot structures under several approximations. It is demonstrated that the emitted light color and transition rates can be engineered by changing core size shell thicknesses, and material combinations. We showed that in some specific quantum dots multi color emission can be obtained.

Three different pairs of semiconductors are considered in this study. One of them is (CdSe) ZnS) CdSe) ZnSe), other is (CdSe) CdS) CdSe) CdSe) and third one is (CdTe) ZnS) CdTe) ZnSe). According to our calculation, (CdSe)ZnS)CdSe)ZnSe) structure, when the core radius is 1.51 nm with some different shells combinations, has multi-color emissions from higher frequency to lower frequency in the visible spectrum. (CdSe) CdS) CdSe) CdSe) structure has multi-color emissions when the core radii are 2.02 nm and 2.52 nm yet this structure is the most inefficient structures which we analyse. Moreover, multi-color emissions are obtained from the structure (CdTe) ZnS) CdTe) ZnS) when the core radii are 1.29 nm, 1.93 nm, 2.58 nm and 3.23 nm. Also, this structure has nearly white light emission for 3.23 nm core radius with 3 ML ZnS shell and 1 ML CdTe shell, and with 4 ML ZnS shell and 1 ML CdTe shell.
REFERENCES


[29] H.S. Zhou, I. Honma, H. Komiyama, and J.W. Haus. Coated semiconductor nanoparticles...


