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Intraband absorption of D^- center in CdSe/CdS/CdSe/CdS multilayer quantum dot

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ABSTRACT

Absorption characteristics of a D^- center in CdSe/CdS/CdSe/CdS multilayer quantum dot are studied within the framework of effective mass approximation. The energy eigen values and corresponding wave functions are obtained by solving the coupled Poisson-Schrondinger equations self-consistently, using finite difference matrix diagonalization method. Based on this, the effect of core radius, shell thickness and well width on absorption coefficient and absorption wavelength are investigated. This model predicts that, the D^- center has considerable intraband absorption, of the order of $10^3\ \mathrm{cm}^{-1}$, in the far infrared region. The absorption characteristics can be finely tuned by varying the layer thicknesses.

1. Introduction

Within the past few decades low dimensional systems are in the front line research areas in physics, because of their fundamental importance and wide range of applications [1–9]. Quantum dots(QDs) are zero dimensional nanostructures, exhibiting quantum confined effects, containing several hundred to several thousand atoms. The attracting features of QDs are that, their energy levels, wave functions, density of states, etc. can be controlled by the shape, size and composition of the structure [10–16].

Nanostructure systems consisting of two or more different materials are known as nano-heterostructures. They exhibits diverse functionalities within a single heterostructure, which we cannot expect from the nanostructures of their individual component materials. A donor impurity atom, which bounds an electron to it in a QD is known as hydrogenic(D^0),because of their similarities with hydrogen atom. Hydrogenic impurity in a QD is considered as one of the best models for understanding many of the electronic and optical properties of nano heterostructures. Hydrogenic impurity effects in QDs have attracted many researchers, and a large number of investigations are done on nano-heterostructures, hydrogenic impurity and their combinations [17,18].

A system of two electrons in the attractive electrostatic field of a donor impurity in a nanostructure is known as a D^- center. If we consider a D^- center in a semiconductor quantum dot, its electronic and optical properties strongly depend on the coulomb interaction between the electrons in it. Using variational method Zhu et al. [19] have observed binding energy of D^- as a function of dot radius and barrier height. With parabolic confinement Xie has calculated the energy spectrum of a D^- center in a disc shaped QD [20]. He also examined magnetic field effects on the electronic properties and the second bound state binding energy spectra of D^- center in QD [21]. Gu and Liang worked on D^- centers in QD with a Gaussian confining potential [22]. Photoionization cross section and inter-sublevel transitions in a one and two electron spherical quantum dot with a hydrogenic impurity were studied by Sahin et al. [26].

To the best of our knowledge, investigations are hardly being done on the optical properties of D^- center in core-shell-well-shell quantum dot. In the present work, we investigate the absorption properties of a D^- center in CdSe/CdS/CdSe/Cds core-shell-well-shell spherical quantum dot. Here, we study the variation of absorption coefficient as a function of incident photon wavelength by varying layer thickness of the QD heterostructure. Without any lose of generality, the many body interactions are introduced by the Hartree approximation [23]. The calculations are based on effective mass approximation, and poisson-schrodinger equations are solved numerically and self consistently for determining the energy eigen values and corresponding wavefunctions.

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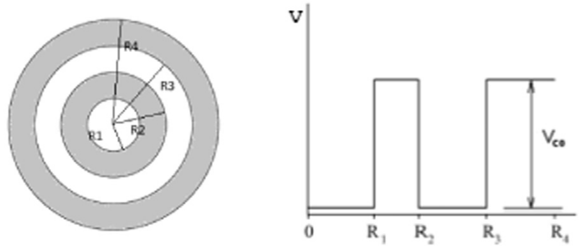

Fig. 1. Schematic representation of CdSe/CdS/CdSe/CdS core-shell-well-shell spherical quantum dot and its potential profile. V_{co} is the conduction band offset of the system.

2. Theoretical model

Consider a quantum heterostructure consisting of two electrons in the attractive potential of a positively charged impurity atom at its center. The Schrodinger equation for such a system, in effective mass approximation, has the following form,

$$\left(\frac{-\hbar^2}{2}\nabla_r\left(\frac{1}{m^*}\right)\nabla_r + V_e(r) - \frac{Ze^2}{kr} + \frac{l(l+1)\hbar^2}{2m^*r^2} - e\phi_{scf}\right)R_{nl} = E_{nl}R_{nl} \tag{1}$$

where, first term represents the kinetic energy of electron, $\hbar$ is reduced Planks constant, m^* is the effective mass of the electron. $V_e(r)$ is the position dependent confining potential and given by,

$$V_e(r) = \begin{cases} 0 & r \le R_1 \quad \text{and} \quad R_2 \le r \le R_3 \\ V_{co} & R_1 \le r \le R_2 \quad \text{and} \quad r > R_3 \end{cases} \tag{2}$$

Here, V_{co} is the conduction band offset of the system. The basic structure of spherical QD under consideration is shown in Fig. 1. R_1 is the core radius, $R_s = R_2 - R_1$ is taken as shell thickness and well width is $R_w = R_3 - R_2$.

Coulombic interaction between the electron and donor impurity is represented by third term, where Ze is the charge of impurity and k is the position dependent dielectric constant. Fourth term is the centrifugal term, where l is the angular momentum quantum number. E_{nl} is the single particle energy eigen value and $R_{n,l}(r)$ is the radial wave function for the electron. ϕ_{scf} is the self consistent Hartree potential between the interacting electrons. Here we consider that, each electron moves in the electrostatic potential of the other. Hence it is desirable to introduce Hartree approximation for determining the interaction potential between the electrons. This Hartree potential can be calculated by solving the corresponding Poisson equation.

Poisson equation [24] can be written as,

$$\nabla k(r)\nabla\phi_{scf} = e\frac{\rho_e(r)}{\epsilon_0} \tag{3}$$

where, ϵ_0 is the dielectric permitivity of the vacuum and ρ_e is the density of the electron [25].

$$\rho_e(r) = \frac{1}{4\pi}\sum_{l=0}^{p} 2(2l+1)\sum_{n=1}^{np}\left|R_{n,l}\right|^2 + \frac{1}{4\pi}N_e\left|R_{n,l}\right|^2 \tag{4}$$

Here, contribution from fully occupied states to electron density is represented by the first term, in which spin and magnetic degeneracies are represented by $2(2l + 1)$. Angular momentum and principal quantum numbers are represented using p and n_p respectively. Contribution of the partially filled states is given by the second term. N_e is the number of remaining electrons in the last state. The Poisson-Schrodinger equations are solved in a self-consistent iterative method.

Electron makes a transition from a lower energy level to higher one, when it absorbs a comparable photon energy. Such a transition within the same band is known as intra-band transition. If the transition occur in between the valence and conduction bands they are known as inter-band ones. The absorption calculations for intra band transitions are based on Fermis golden rule. The absorption coefficient for intra-band transition is given by [26],

$$\alpha(\hbar\omega) = \frac{16\pi^2\beta_{FS}N_{fi}}{n_r V_c}\hbar\omega\left|Z_{fi}\right|^2\delta(E_f - E_i - \hbar\omega) \tag{5}$$

where, $\hbar\omega$ is the incident photon energy, β_{FS} is the fine structure constant, n_r is the refractive index of the semi conductor and E_i and E_f are the energy eigen values of initial and final states. Volume of the confinement regions is represented by V_c. $N_{fi} = N_i - N_f$ is the difference between number of electrons in initial and final states. The line shape function δ is given as,

$$\delta(E_f - E_i - \hbar\omega) = \frac{\hbar\Gamma}{\pi[(\hbar\omega - (E_f - E_i))^2 + (\hbar\Gamma)^2]} \tag{6}$$

in which, $\hbar\Gamma$ is the line shape broadening factor and its value is taken as 30 meV [27].

Z_{if} is the dipole matrix element between initial and final states. These states are determined by selection rules $\Delta l = \pm 1$. For transition between 1s-1p levels,

$$\left|Z_{if}\right|^2 = \frac{1}{3}\left|\int_0^\infty R_f(r)r^3R_i(r)dr\right|^2 \tag{7}$$

where,$R_i(r)$ and $R_f(r)$ are the radial wave functions of the initial and final states.

3. Results and discussion

In our calculation atomic units are used, where Planck constant $\hbar = 1$, the electronic charge e=1 and the bare electron mass $m_0 = 1$. The effective Bohr radius and Rydberg energy are $a_0 \approx 37.84A^0$ and $R_y \approx 20.44$ meV, respectively. The material parameters have been taken as $m_{CdSe} = 0.13m_0$, $m_{CdS} = 0.21m_0$, $k_{CdSe} = 9.3$, $k_{CdS} = 8.9$ [28]. The conduction band offset is taken as 0.32 eV [29,27]. The position dependent effective mass and dielectric constant are given by [30],

$$m^*(r) = \begin{cases} 1 & ; r \le R_1 \quad \textit{and} \quad R_2 \le r \le R_3 \\ \dfrac{m_2^*}{m_1^*} & ; R_1 < r < R_2 \quad \textit{and} \quad r > R_3 \end{cases} \tag{8}$$

$$k(r) = \begin{cases} 1 & ; r \le R_1 \quad \textit{and} \quad R_2 \le r \le R_3 \\ \dfrac{k_2}{k_1} & ; R_1 < r < R_2 \quad \textit{and} \quad r > R_3 \end{cases} \tag{9}$$

where, m_1^* is the effective mass of electron inside the CdSe material and k_1 is the dielectric constant of CdSe. In CdS these are m_2^* and k_2 respectively. Since the total radius of QD is 3a_0, the system is in the weak confinement region.

3.1. Absorption spectrum

3.1.1. Effect of core radius

Fig. 2 shows the variation of absorption coefficient as a function of incident photon wavelength for various core radii having a constant shell thickness ($R_s = 0.2a_0$) and well width ($R_w = 0.2a_0$). Here, we study the absorption of D^- center in the region $0.2a_0$ to $0.4a_0$ of core radius, since the absorption coefficients in the other regions are negligibly small. The highest absorption is observed for the core radius $0.2a_0$, implying the maximum probability of absorption of the system with change in core radius. We observe a subsequent decrease in the value of absorption coefficient as the core radius increases.

The value of absorption coefficient is proportional to the factor Z_{if}^2/V_c. Where, Z_{if} the dipole matrix element represents the overlapping of wave functions in the ground and excited states, while V_c is the confinement volume. Maximum overlapping of electronic wave functions cause a higher transition probability. When $R_1 = 0.2a_0$, the overlapping is maximum and the confinement volume is minimum