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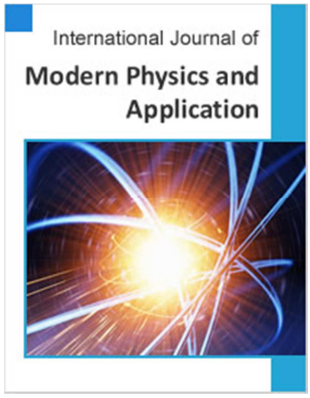

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The Influence of Quantum Dot Size on Confinement Energy: A Modified Single Band Toy Model Approach

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Abstract

The influence of Quantum Dot Size on Confinement Energy was investigated using the modified single band toy model (MSBTM) approach with three different semiconductor quantum dots (QD) (Cadmium Selenide (CdSe), Zinc Sulphide (ZnS), and gallium Arsenide (GaAs)) considered. This was aimed at computing the emission and confinement energies of different sizes of the QD's considered, and also comparing the degree of confinement of this study with other experimental works. It was observed that the sizes of semiconductor quantum dots considered are the same as the nano-size of the Bohr exciton radius of electron-hole pairs in solids. Due to this fact, they exhibit effects of quantum size as particles in a three dimensional box. The emission and confinement energies of electrons in semiconductor quantum dots considered increased exponentially with a decrease in the size of the nano-crystal. The graphs of the emission and confinement energies were plotted as a function of dot size for each of the three different semiconductor quantum dots. These exponential decay curves indicates that the lowest possible energy for a quantum dot sample is never zero as predicted using Brus equation.

1. Introduction

The concept of Quantum of (QD) has been a subject of research over a tangible period [1]. This is due to its lofty physical properties and exciting applications in various aspects of nanotechnology. We can attribute these properties to the size dependent band gap of the QD [2]. Several theoretical methods have been used to investigate this phenomenon. This includes the Tight-Binding Approach (TBA) [3], the *K.P.* method [4], Effective-Mass Approximation (EMA) [5] and most recently, the Finite-Depth Square-Well Effective-Mass Approximation (FWEMA) model [6], Potential-Morphing Method (PMM) [7] and Single Band Toy Model (SBTM) [8].

Baskoutas *et al.* [9] calculated the exciton energy of the narrow band gap colloidal PbS, PbSe and InAs QD using the PMM within the FWEMA, assuming a single dependent dielectric function.

Kumar *et al.* [10] also used *k.p.* model to calculate the shape and size dependent electronic properties of GaAs/AlGaAs QD's. They adopted this model due to its simplicity and accuracy for modelling the band structure near the first Brillouin zone [11].

Ekong and Osiele [12] employed a quantum confinement model to study different shapes of nanocrystalline silicon (nc–Si) QD, within the limits of an effective diameter of 3nm. This leads to different electronic energy based on the transitions from the quantum selection rule.

Using the Modified Single Band Toy Model (MSBTM) approach, the influence of QD size on confinement energy of certain nanocrystals has been investigated. Also, a strained magnetic field interacting with the electronic structure of the spherical QD has been considered within the framework of a confined radial potential. This led us to the determination of Confinement Energy using the MSBTM.

We have also obtained the emission energy of the QD in the absence of the magnetic field, thereafter comparing the confinement energy involved in the emission energy with the confinement energy model obtained by Brus [13]. This has led us to obtain an expression for the Confinement Potential Frequency (CPF). We have presented the theoretical framework of this paper in section 2, results and discussion in section 3 and finally conclusion in section 4.

2. Theoretical Framework

Zhang *et al.* [8] provided the basis for the Single Band Toy Model (SBTM) by consideringthe total Lagrangian of a coupled system aside the unperturbed cohesive energy given by:

$$\left(\mathrm{E_c}-\frac{\hbar^2}{2\mathrm{m}^*}\nabla^2\right)\psi(\mathrm{r})+\mathrm{a_c}.\mathrm{Tr}(\varepsilon)\psi(\mathrm{r})=\mathrm{E}\psi(\mathrm{r}) \quad (1)$$

where m^* is the effective mass of the electron, $\varepsilon=\frac{1}{2}(\nabla U+\nabla^{\mathrm{T}}\mathrm{U})$ is the elastic strain tensor (where U is the strain energy for linear elastic deformation and ∇^T is the local strain tensor), E_c is the energy of the band gap edge for the conduction of the valence band, E is the electronic spectrum of energies, $\psi(r)$ is the wave function and a_c is the deformation potential constant.

For an accurate solution for the Confinement energy for a low dimensional QD, we modify this model by assuming that a well known strain field exist that interacts with the electronic structure of the QD and perturbs it. The motion of the confined electron in a spherical QD confined by a radial potential of the form $\frac{1}{2}\mathrm{m_e^*}\omega_\mathrm{o}^2\mathrm{r}^2$, with the application of external magnetic field is given by:

$$\left[\mathrm{E_c}-\frac{1}{2}\mathrm{m}^*(\mathrm{p}-\mathrm{e}/\mathrm{c}\,\mathrm{A})^2\right]\psi(\mathrm{r})+\frac{1}{2}\mathrm{m}^*\omega_\mathrm{o}^2\mathrm{r}^2\psi(\mathrm{r})=\mathrm{E}\psi(\mathrm{r}) \quad (2)$$

where

$$\mathrm{E_c}=\mathrm{E}_{\mathrm{c,v}}^{\mathrm{o}}+\mathrm{a_c}\mathrm{r}\in_\mathrm{h}, \quad (3)$$

is the energy of the conduction band state, $E_{c,v}^o$ is the energy of the band edge for conduction or valence band, $\in_h$ is the hydrostatic strain, r is the radius of the QD and ω_o is the frequency of the QD confinement potential [14].

For the Confinement energy, the Modified Single Band Toy model becomes:

$$\mathrm{E_C}-\mathrm{E_g}=\frac{\mathrm{m}^{*3}\mathrm{r}^6(\omega_\mathrm{c}^2-\omega_\mathrm{o}^2)^2}{8\hbar^2} \quad (4)$$

where E_C is the emission energy of the QD, E_g is the Band gap of the bulk semiconductor, r is the radius of the dot, ω_c is the cyclotron frequency, ω_o is the confinement potential frequency, $\hbar$ is the modified Planck's constant and m^* is the exciton reduced mass.

Equation (4) is based on the assumption on space quantization of the orbital angular momentum, in which the direction of the orbital angular momentum vector is quantized with respect to the direction of the external magnetic field B.

For a zero magnetic field, $\omega_c^2=0$. Equation (4) now becomes:

$$\mathrm{E_C}=\mathrm{E_g}+\frac{4\pi^2\mathrm{m}^{*3}\mathrm{r}^6\omega_\mathrm{o}^4}{8\mathrm{h}^2} \quad (5)$$

where h is the Planck's constant. The second term in equation (5) is the confinement energy of the semiconductor QD.

Comparing the Confinement energy in Brus equation [15] and the Confinement energy in equation (5), we have that:

$$\omega_\mathrm{o}=\frac{\mathrm{h}}{\sqrt{2\pi}\mathrm{m}^*\mathrm{r}^2} \quad (6)$$

being the Confinement Potential frequency (CPF).

3. Results and Discussions

The material parameters utilized for the computation of the confinement energies at various radii is given in the tables below:

Table 1. *Material Parameters used for the computation of the confinement energies at various radii which is less than the Bohr Radius a_B [16].*

Quantum Dots	Band Gap Energy	Electron Effective Mass	Hole Effective Mass	Exciton Bohr Radius
	E_g(eV)	m_e^*/m_o	m_{eh}^*/m_o	a_B(nm)
GaAs	1.518	0.066	0.470	12.5
ZnSe	2.820	0.150	0.800	3.8
CdSe	1.840	0.130	0.450	4.9

Table 2. *Deformation Potential of Zincblende II-IV wide band gap semiconductors [17].*

Compound	a(eV)	b(eV)
CdSe	-3.664	-0.80
CdTe	-4.520	-1.10
ZnS	-4.000	-0.62
ZnSe	-4.530	-1.14
ZnTe	-5.800	-1.80
GaAs	-8.930	-1.76

Table 3. *Hydrostatic strain as it varies with different dot sizes [18].*

For Gallium Arsenide (GaAs)

R(nm)	0.50	1.00	1.50	2.00	3.00	4.50	6.00	8.50	10.00	11.50
$\in_h$	0.487	0.484	0.480	0.475	0.470	0.459	0.452	0.435	0.427	0.420

For Zinc Selenide (ZnSe)

R(nm)	0.50	1.00	1.40	1.70	2.20	2.80	3.10	3.50	3.60	3.75
$\in_h$	0.490	0.485	0.484	0.480	0.476	0.472	0.469	0.465	0.464	0.462

For Cadmium Selenide (CdSe)

R(nm)	0.40	0.90	1.50	1.80	2.50	3.00	3.50	3.90	4.30	4.70
$\in_h$	0.489	0.487	0.482	0.480	0.477	0.470	0.466	0.462	0.460	0.458

The ground state confinement energy, emission energy and radius of QD for GaAs, ZnSe, and CdSe are shown in tables 4, 5 and 6 below respectively:

Table 4. *Ground State Confinement Energy, Emission Energy and Radius of Dot for GaAs.*

Radius of Dot(nm)	Ground State Confinement Energy (eV)	Emission Energy (eV)
0.50	26.0513	27.5693
1.00	6.5144	8.0324
1.50	2.8944	4.4124
2.00	1.6278	3.1624
3.00	0.7273	2.2417
4.50	0.3216	1.8396
6.00	0.1809	1.6989
8.50	0.0901	1.6081
10.00	0.0651	1.5831
11.50	0.0492	1.5672

Table 5. *Ground state Confinement Energy, Emission Energy, and radius of Dot for ZnSe.*

Radius of Dot(nm)	Ground State Confinement Energy (eV)	Emission Energy (eV)
0.50	11.9150	14.7350
1.00	2.9843	5.8043
1.40	1.5223	4.3423
1.70	1.0321	3.8521
2.20	0.6166	3.4366
2.80	0.3806	3.2006
3.10	0.3105	3.1305
3.50	0.2435	3.0635
3.60	0.2305	3.0503
3.75	0.2121	3.0321

Table 6. *Ground State Confinement Energy, Emission Energy, and Radius of Dot for CdSe.*

Radius of Dot (nm)	Ground State Confinement Energy (eV)	Emission Energy (eV)
0.60	266.0563	267.8963
0.90	4.6138	6.4150
1.50	1.6608	3.5008
1.80	1.1535	2.9935
2.50	0.5980	2.4380
3.00	0.4152	2.2552
3.50	0.3050	2.1450
3.90	0.2459	2.0859
4.30	0.2020	2.0420
4.70	0.1691	2.0091

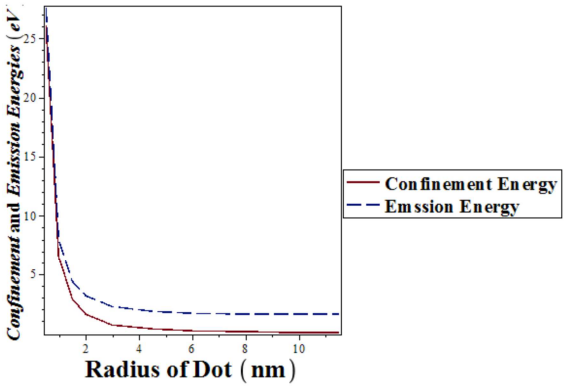

Figure 1. *Confinement and Emission Energies Vs Radius of Dot for GaAs.*

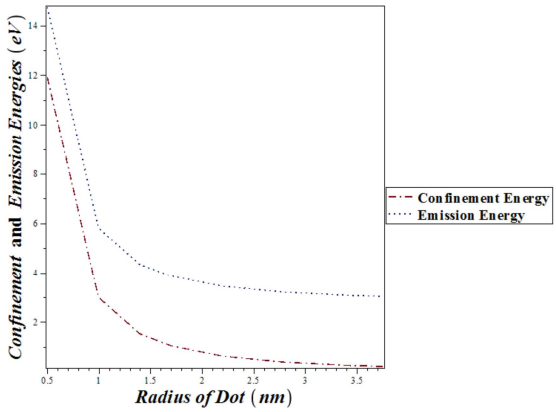

Figure 2. *Confinement and Emission Energies Vs radius of Dot for ZnSe.*

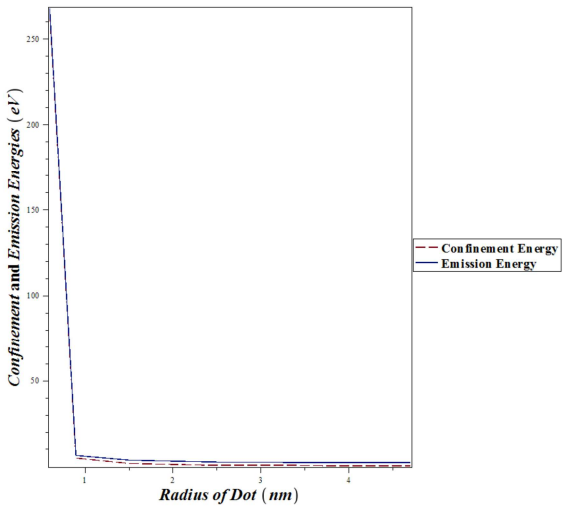

Figure 3. *Confinement and Emission Energies Vs Radius of Dot for CdSe.*

Results of the confinement and emission energies as they relate with the sizes of GaAs, ZnSe and CdSe are displayed in figure 1, 2 and 3 respectively. These graphs show an exponential dependence of the energies on the dot size, which is in agreement with the theoretical observations of [19].

The size of the dot becomes smaller as the confinement and emission energies increases. This indicates that confinement effect dominates [20]. This indicates that the strength of the confinement effect depends strongly on the confinement and emission energies of the quantum dots. In figure 1, the strong confinement energy and emission energy of about 26.05eV and 27.56eV respectively is obtained at dot radius below 1.0nm for GaAs. For ZnSe, we observed that the strong confinement energy and emission energy of 11.9eV and 14.7eV respectively at dot radius below 1.0nm. This is shown in figure 2. In figure 3 with the consideration of CdSe at a dot radius of about 0.6nm, confinement energy and emission energy of 266.05eV and 267.89eV respectively was obtained. The discrepancy between the confinement energies and the emission energies for GaAs and CdSe is not much, but there is a tangible difference between the emission energy and confinement energy for ZnSe. The exponential decay curves seen in these figures can be said to be asymptotic to the dot radius axis. It is seen here that the confinement energy and the emission energy of carriers (electron and hole) and the spacing of the energy levels in these QDs increase as the size decreases at nano-scale due to quantum size effect.

It can be observed that as the radius of the QD becomes smaller, the Bohr radii of the charge carrier become larger than the dot sizes, and their confinement to the dot causes their energy to increase.

Fundamentally, the perturbed electrons moves into excited states with an overall non-zero momentum. This is as a result of the existed strained field that interacts with the electronic structure of the QD. Due to that fact that the first excited state is very close to the ground state, small excitation can lift the electrons into the excited states. As such, the excited electrons move in the mostly empty conduction band and the unexcited electrons move in the slightly empty valence band. The movement of the unexcited electrons can be seen as the movement of the positive charged holes [21].

We have used effective mass approximations for the electrons and holes in our calculations for the purpose of small momenta. The Exciton Bohr radius used provides a convenient length scale to evaluate the impact of quantum confinement on the properties of QD considered [22]. In our model, the inverse quadratic dependence of dot radius in the confinement energy means that in the limit of small dot radius, the confinement term dominates.

This model is in agreement with the experiment work carried out by Vachaspati [21] on the unperturbed finite well approximation on Cadmium Selenide with different dot sizes. It is worthy to note that this model is likely to break down for narrow band dots (e.g. Indium Arsenide), in which its conduction band is highly non-parabolic.

4. Conclusions

We have studied the Influence of Quantum Dot Size on Confinement Energy using the Modified Single Band Toy Model approach. The modified single band toy model obtained for the three different semiconductor quantum dots exhibit the size dependence predicted by Brus Equation. It was also observed that the sizes of semiconductor quantum dots considered are the same as the nano-size of the Bohr exciton radius of electron-hole pairs in solids. Due to this fact, they exhibit effects of quantum size as particles in a three dimensional box. The results obtained, analyzed and compared with already existing experimental results are in good agreement with the experimental observation of the size dependence on the band gap energy. The decrease in the confinement and emission energies as a function of the dot size suggests that quantum confinement effect exist in the QD considered.

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