

# Effect of dielectric environment on electronic and optical properties of spherical core/shell quantum dot: comparison of two models

Lj. Stevanović, V. Pavlović, M. Miladinović, M. Živković, S. Milenović, O. Stefanović and M. Perić

Department of Physics, Faculty of Sciences and Mathematics, University of Niš, Serbia

vladan.pavlovic@pmf.edu.rs



**Abstract:** The subject of this study is the influence of dielectric environment on the energies and wave functions of electron in conduction band of CdSe/ZnS spherical core/shell quantum dots (CSQD) and oscillator strength of  $1s \rightarrow 1p$  intraband transition. We use two common approaches to take into account the effect of dielectric matrix, which consist in adding corresponding terms to the electron Hamiltonian. We perform calculations using effective mass approximation by imposing the corresponding boundary conditions on the values of wave function and its first derivative for the cases when CSQD is embedded in SiO<sub>2</sub> and HfO<sub>2</sub> dielectric matrix. The effect of CSQD radius on results is discussed.

## Introduction

In the most general sense, quantum dots (QDs) are physical systems which can be used to confine electrons inside a small region of space, where the linear dimensions of that region are of the order of several nanometers. Quantum dots are usually practically realized as semiconductor nanocrystals. CSQDs are quantum dots whose central region (core) is filled with one type of semiconductor material (in our case CdSe), and the surrounding layer (shell) is filled with a different semiconductor material (in our case ZnS). The reason for studying CSQDs is their application in optoelectronics, bio-imaging, quantum computing [1].

## Theory

Energies and wave functions of electron in conduction band of CSQD were calculated in effective mass approximation. The electrons inside the QD induce bound charges on the surface of the material in which the QD is located, so in principle we have to consider such interactions as well. We first considered the case when this interaction was neglected. Therefore, we solve the Schrödinger equation in which the Hamiltonian has the form:

$$\hat{H} = -\frac{\hbar^2}{2m^*(\vec{r})}\Delta + V(r),$$

where  $m^*(\vec{r})$  is the effective mass of the electron:

$$m^*(\vec{r}) = \begin{cases} m_1^*, & 0 < r < R_1, \\ m_2^*, & R_1 < r < R_2, \end{cases}$$

and:

$$V(r) = \begin{cases} 0, & 0 < r < R_1 \\ V_0, & R_1 < r < R_2 \\ \infty, & r > R_2 \end{cases}$$

where  $R_1, R_2$  are respectively the radius of the core and radius of the shell, and  $V_0$  is a constant.

Due to the symmetry of the system, we can separate variables as follows:

$$\psi_{nlm}(\vec{r}) = P_{nl}(r)Y_{lm}(\theta, \phi),$$

where  $Y_{lm}(\theta, \phi)$  are the known spherical harmonics, and the problem is reduced to solving the radial Schrödinger equation for radial wave function  $P_{nl}(r)$  and corresponding energy  $E_{nl}$ .

After solving the equation, we apply boundary conditions for the continuity of the wave function, as well as the Ben Daniel-Duke condition [2]:

$$\begin{aligned} P_{nl}^{(1)}(R_1) &= P_{nl}^{(2)}(R_1), \\ P_{nl}^{(2)}(R_2) &= 0, \\ \frac{1}{m_1^*} \frac{dP_{nl}^{(1)}(r)}{dr} \Big|_{r=R_1} &= \frac{1}{m_2^*} \frac{dP_{nl}^{(2)}(r)}{dr} \Big|_{r=R_1}. \end{aligned}$$

Using these equations, we obtain energies and dipole matrix element numerically.

Next, we also took the interaction between the electron and the bound charges on the surface of the CSQD into account. There are two main methods used in the literature to describe this interaction, using either additional potential term  $\Sigma$  [3]:

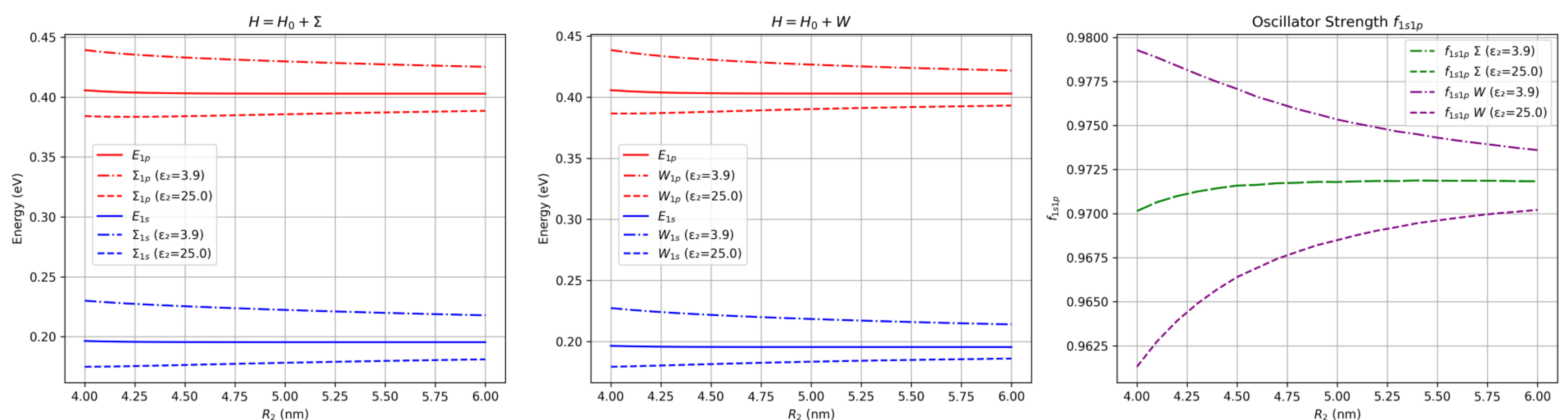
$$\Sigma = \frac{e^2}{8\pi\epsilon_0 R_2} \left( \frac{1}{\epsilon_{out}} - \frac{1}{\tilde{\epsilon}_r} \right) + \frac{0.47e^2}{4\pi\epsilon_0 \tilde{\epsilon}_r R_2} \left[ \frac{\tilde{\epsilon}_r - \epsilon_{out}}{\tilde{\epsilon}_r + \epsilon_{out}} \right]$$

or additional potential term  $W(r)$  [4]:

$$W(r) = \frac{e^2(\epsilon_1 - \epsilon_2)}{8\pi\epsilon_1 R_1} \sum_{k=0}^{\infty} \frac{k+1}{k\epsilon_1 + (k+1)\epsilon_2} \frac{r^{2k}}{R_2^{2k}}.$$

Here,  $\epsilon_1$  and  $\epsilon_2$  are dielectric constants of CSQD material and dielectric environment, respectively.

First, we include the  $\Sigma$  potential in the Schrödinger equation, and we solve it analytically. The required energies and the dipole matrix element of the transition are again determined by the same numerical methods as in the previous case. Finally, in the case of the  $W(r)$  potential, we use first order perturbation theory and solve the integrals numerically.



**Figure 1:** Energies of  $1s$  and  $1p$  states and oscillator strength of  $1s \rightarrow 1p$  intraband transition in CdSe/ZnS spherical CSQD as functions of quantum dot radius.

## Results and discussion

The following values of the parameters were used in calculation [5]:  $m_1^* = 0.13m_0$ ,  $m_2^* = 0.28m_0$ ,  $V_0 = 1.05$  eV,  $\epsilon_r(\text{CdSe}) = 9.7$ ,  $\epsilon_r(\text{ZnS}) = 8.4$ ,  $\epsilon_r(\text{SiO}_2) = 3.9$  and  $\epsilon_r(\text{HfO}_2) = 25$ .

First, we include the  $\Sigma$  potential in the Schrödinger equation, and we solve it analytically. The required energies and the dipole matrix element of the transition are again determined by the same numerical methods as in the previous case. Finally, in the case of the  $W(r)$  potential, we use first order perturbation theory and solve the integrals numerically.

We found that wave functions are the same in both models as for the plane CdSe/ZnS spherical CSQD. The model with term  $\Sigma$  in the Hamiltonian gives energy levels that are shifted up or down depending on dielectric constant of dielectric matrix and predicts the same value for the oscillator strength as for the plane quantum dot. On the other hand, inclusion of term  $W$  into Hamiltonian gives different energies and oscillator strength in comparison with the plane CdSe/ZnS spherical CSQD. Moreover, both models give the very similar energy values.

Finally, in our comparison of the two methods we can conclude that it is more precise to use the  $W(r)$  potential than the  $\Sigma$  potential. Instead of looking at first order perturbation theory, it would also be preferable to numerically solve the Schrödinger equation with the  $W(r)$  potential from the start.

## References

- [1] A. Sahu, D. Kumar, J. Alloys Compd. 924, 166508 (2022)
- [2] D. J. BenDaniel, C. B. Duke, Phys. Rev. 152, 68392 (1966)
- [3] K. Hasanirrok, A. Naifar, Plasmonics 19, 2317 (2023)
- [4] N. Yahayaoui, N. Zeiri, P. Baser, M. Said, S. Saadaoui, Plasmonics 18, 1489 (2023)
- [5] J. W. Haus, H. S. Zhou, I. Honma, H. Komiyama, Phys. Rev. B 47, 135965 (1993)