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Original research article

Mathematical modelling of optical properties of CdSe/ZnS core shell quantum dot

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ABSTRACT

In this paper, the electron and hole energies are computed for core/shell quantum dots (CSQDs) using two ways. First, we have resolved the three dimensional Schrödinger equation in the spherical coordinate system. The second approach is based on a combination of coordinate transformation and the finite difference method. The carrier energy levels of CdSe/ZnS CSQD are investigated, then the transition energies and the oscillator strength are deduced.

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1. Introduction

The last decade has been marked by great progress on the synthetic chemistry of semiconductor nanocrystals (NCs). Among these, the core-shell NCs [1], obtained with II-VI semiconductors, such as CdS/CdSe [2,3], CdSe/ZnS [4,5] and CdTe/ZnS [6]. These hetero-structures present a large mismatch and the band gap of the shell material encloses the band gap of the core and the electrons and holes are confined within the width of semiconductor quantum dot. The CSQDs have been used in many applications, in the optical domain such as QD lasers [7], solar cells [8,9], optical communication [10] and recently for several biological purposes [11].

The different existing shapes for the nanostructures are a consequence of different techniques of growth. For III–V compound semiconductors, we can find pyramidal and lens shapes profile quantum dot [12,13] and due to their complex forms, the calculation of electronic and optical properties of these structures require an extensive theoretical and numerical effort [14,15]. For II–VI quantum dots, the transmission electron microscopy, have shown spherical shapes as shown in Fig. 1 [16] and we also can remark that the CSQDs are not perfectly sphere-shaped. Many theoretical investigations on these structures have been reported and the majority of these authors used the effective mass approximation and have resolved the Schrödinger equation with the spherical coordinates [17–19]. In the present work we have used for modelling CdSe/ZnS CSQDs, both, this method and a mathematical model based on coordinate transformation. The latest model, used in our previous works for modeling different geometrical forms of quantum wires and dots, has given results in agreement with experiment [20–22].

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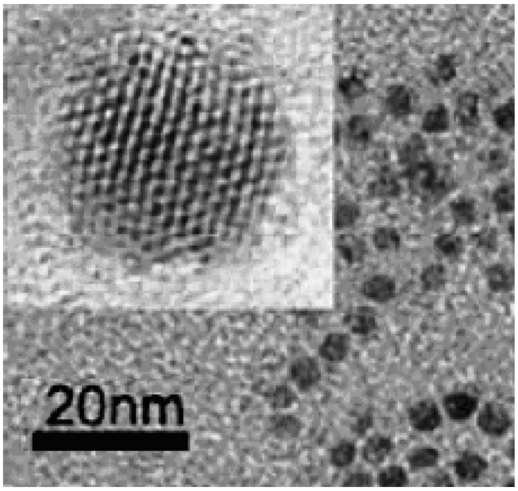

Fig. 1. High-resolution TEM images of CdSe/ZnS nanocrystals. Size of the inset is 5.4 nm × 5.1 nm.

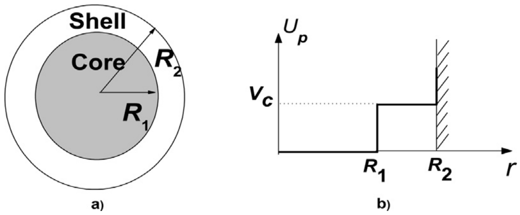

Fig. 2. The model for core-shell QD**a)** and corresponding schematic of potentials **b)**.

This paper is organized as follows. In Section 2, the details of different methods will be presented. The appropriate choice of coordinate transformation will be also discussed. In Section 3, the electron and hole energy levels, transition energies as well as oscillator strengths are investigated. Finally, conclusions will be presented in Section 4.

2. Theoretical methods

2.1. First mathematical method

We consider a spherical quantum dot with a central semiconductor core coated with a larger bandgap semiconductor material acting as a shell. In this core-shell structure the inner radius is denoted by R_1 and outer radius by R_2 like is shown in Fig. 2a).

The first method consists to resolve the Schrödinger equation of the electron (hole) in the spherical coordinates [23]:

$$\left\{-\frac{\hbar^2}{2m_i^* r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]+U_p(r)\right\}\psi_{nlm}(r,\theta,\phi)=E\psi_{nlm}(r,\theta,\phi) \tag{1}$$

The expression of effective mass $m_i^*$and the confined potentials $U_p(r)$(Fig. 2b)) of particles is:

$$m_i^* = \begin{cases} m_1^* & r \le R_1 \\ m_2^* & R_1 < r \le R_2 \end{cases} \tag{2}$$

$$U_{p_i}(r) = \begin{cases} 0 & r \le R_1 \\ V_c & R_1 < r \le R_2 \\ \infty & R_2 < r \end{cases} \tag{3}$$

As the mass and the potential are symmetric spherically, the separation of radial and angular coordinates leads to:

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi) \tag{4}$$

$R_{nl}(r)$ is the radial wave function, and $Y_{lm}(\theta,\phi)$is the spherical harmonic, where n is the principal quantum number, l and m are the angular momentum quantum numbers.

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