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Ground state energy and wave function of an off-centre donor in spherical core/shell nanostructures: Dielectric mismatch and impurity position effects

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ABSTRACT

Ground state energy and wave function of a hydrogen-like off-centre donor impurity, confined anywhere in a ZnS/CdSe spherical core/shell nanostructure are determined in the framework of the envelope function approximation. Conduction band-edge alignment between core and shell of nanostructure is described by a finite height barrier. Dielectric constant mismatch at the surface where core and shell materials meet is taken into account. Electron effective mass mismatch at the inner surface between core and shell is considered. A trial wave function where coulomb attraction between electron and off-centre ionized donor is used to calculate ground state energy via the Ritz variational principle. The numerical approach developed enables access to the dependence of binding energy, coulomb correlation parameter, spatial extension and radial probability density with respect to core radius, shell radius and impurity position inside ZnS/CdSe core/shell nanostructure.

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1. Introduction

Quantum size effects are revealed through confinement in nanometer scale size systems. They have been reported, for the first time, in the early 1980s by Ekimov [1] and Brus [2,3]. Since this breakthrough, low-dimensional systems have been studied extensively both experimentally and theoretically. Quantum dots (QDs) are semiconductor droplets which may be precipitated by annealing in a semiconducting or in an isolating host matrix or synthesized chemically at low temperature as colloidal suspensions in organic solutions. QDs are exotic structures which are at the midway between solids and atoms. They are as compact as solids, but their emission and absorption spectra are close to those of isolated atoms. In fact, due to three-dimensional confinement, electrons and holes degrees of freedom are frozen in all directions of space. Because of their nanometer scale size, quantum characters of charge carriers are revealed, their energies are quantized and depend on dot size. Accordingly, the line corresponding to HOMO to LUMO transition is blue shifted and the absorption edge is reduced to a series of narrow and intense peaks. This property allows tuning, in advance, effective gap of a quantum dot which is known in literature under the name of '*band gap engineering*.'

Now, progress reached in experimental techniques of growth has made it possible to fabricate high-quality semiconductor QDs within a large range of sizes for different fields of applications such as optical encoding [4], multiplexing [5], energy harvesting [6], biology and medicine where QDs are used in the study of intracellular processes at single molecule level [7,8]. They are also used in high-resolution cellular imaging [9–12], in long term in vivo observation of cell trafficking, in tumor targeting and in diagnostics [13–16].

Since the mid-1990s, interest dedicated to QDs has begun to shift progressively to core/shell nanostructures. These onion-like

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nanostructures also named quantum dot–quantum well structures [17] involve essentially lattice-matched semiconductors. They are mostly obtained via chemical processes of growth by encapsulating a spherical quantum dot of a given semiconductor with a spherical shell of another semiconductor. The shell may also be coated by a spherical organic or inorganic thin layer to passivate the quantum dot surface and to deactivate dangling bonds. According to conduction and valence band profiles of the semiconductors involved, the final nanostructure may be of type I when charge carriers are confined in nanostructure core (CdSe/CdS [18], CdSe/ZnSe [19]), inverted type I when charge carriers are confined in nanostructure shell (CdS/CdSe [20], ZnSe/CdSe [21]), type II when electrons and holes are confined, respectively, in core and shell of quantum dot (CdTe/CdSe [22], CdS/ZnSe [23]) or vice versa. In core/shell nanostructures, electron and hole ground state energies as well as their probability densities depend on core and shell radii. This allows tuning, in advance, effective gap of nanostructure and single particles probability of presence inside core and shell, which is known in literature under the name of '*wave function engineering*.'

According to current state-of-the-art, solution processable semiconducting colloidal core/shell nanostructures exhibit attractive optical properties. Their photoluminescence spectrum depends on semiconductors involved and also on core size and shell thickness allowing synthesis of quantum dot size-tunable color colloidal solution, fabrication of electrically driven colloidal quantum dot light emitting devices (QD-LED) and electrically driven full-color QD-LED displays [24].

Hydrogenic impurities whose energy levels are close to conduction and valence band-edges are predisposed to play an important role in optical transitions occurring in core/shell nanostructures. Recently, some theoretical works were devoted to stark effect [25] and diamagnetic effect [26] on donor binding energy, respectively, in a spherical quantum dot and in a spherical quantum dot–quantum well. This year, diamagnetic susceptibility [27] and polarizability [28] of a donor impurity confined in a core/shell nanostructure were calculated in the framework of the envelope function approximation. It appears that application of an external magnetic field, which is equivalent to additional cylindrical confinement, implies a strengthening of attraction between opposite sign particles for all donor positions. However, effects of an external electric field on donor binding energy depend on donor position and field strength.

In this study, we determine ground state energies and wave functions of an electron and a hole confined in a spherical core/shell nanostructure. We show that for a fixed dot radius R_S, there are two critical values R_{Ce} and R_{Ch} of core radius for which electron energy E_e^{1s} is equal to conduction band offset V_{0e} and hole energy E_h^{1s} is equal to valence band offset V_{0h}, respectively (see Fig. 2 (2) and (4)). So, for $0<R_C<R_{Ce}$, electron energy E_e^{1s} is lighter than conduction band offset V_{0e} while hole energy E_h^{1s} is lighter than valence band offset V_{0h}. Both electron and hole wave functions are standing in shell and are evanescent in core (see Fig. 2 (1)). For $R_{Ce}<R_C<R_{Ch}$, electron energy E_e^{1s} is larger than conduction band offset V_{0e} whereas hole energy E_h^{1s} is lighter than valence band offset V_{0h}. Electron wave function is standing throughout the nanostructure while hole wave function is standing in shell and evanescent in core (see Fig. 2(3)). For $R_{Ch}<R_C<R_S$, electron energy E_e^{1s} is larger than conduction band offset V_{0e} while hole energy E_h^{1s} is larger than valence band offset V_{0h}. Both electron and hole wave functions are standing throughout the nanostructure (see Fig. 2(5)). On the basis of single-particle wave function expressions, we construct trial wave functions for exciton and off-centre donor which take into account attractive coulomb correlation between opposite sign particles. We determine via the Ritz variational principle ground state energy and binding energy of exciton as functions of core and shell radii. We also determine ground state energy, binding energy, coulomb correlation parameter, spatial extension and radial probability density of a donor placed anywhere in ZnS/CdSe spherical core/shell nanostructure as functions of core radius, shell radius and ionized donor position.

2. Theory

We consider an off-centre donor confined in an inverted type I core/shell hetero-nanostructure (see Fig. 1). This kind of structure is composed of a spherical wide band gap semiconductor nanocrystal of radius R_C and a dielectric constant ε_1 playing the role of core, over-coated with a narrower band gap semiconductor layer of radius R_S, thickness $T=R_S-R_C$ and dielectric constant ε_2 playing the role of a shell. The whole nanostructure is immersed in an aqueous or organic solution. The bottom of the core conduction band is above the bottom of the shell conduction band (see Fig. 1). The top of the core valence band is below the top of the shell valence band (see Fig. 1). Due to this well-like band profiles, charge carriers are partially confined in the narrowest band gap semiconductor.

2.1. Electron and hole ground states

In the framework of the envelope function approximation and assuming isotropic, parabolic and non-degenerated bands, the Hamiltonians of confined electron (e) and hole (h) in CGS electrostatic units read as

$$H_i=(\hbar/j\nabla_i)1/2m_i^*(r_i)(\hbar/j\nabla_i)+V_{wi}(r_i) \quad (i=e,h) \tag{1}$$

The first term stands for hermitian kinetic energy operator for a position-dependent effective mass particle proposed for the first time by BenDaniel and Duke [29].

Electron and hole effective masses are given in unit of free electron mass m_0 by

$$m_i^*(r_i)=\begin{cases} m_{i1}^*, & r_i<R_C \\ m_{i2}^*, & R_C<r_i<R_S \end{cases} \quad (i=e,h) \tag{2}$$

R_C and R_S are, respectively, inner and outer radii of core/shell nanostructure (see Fig. 1).

Due to conduction and valence band offsets between core, shell and host medium, electron and hole confining potentials inside core/shell nanostructure $V_{wi}(r_i)$ $(i=e,h)$ are expressed as follows:

$$V_{wi}(r_i)=\begin{cases} V_{0i}, & 0<r_i<R_C \\ 0, & R_C<r_i<R_S \\ \infty, & R_S<r_i \end{cases} \quad (i=e,h) \tag{3}$$

The Schrödinger equations giving single-particle eigenvalues E_i $(i=e,h)$ and eigenfunctions$\Psi_i(\vec{r_i})$ $(i=e,h)$ are written as

$$H_i\,\Psi_i(\vec{r_i})=E_i\,\Psi_i(\vec{r_i}) \quad (i=e,h) \tag{4}$$

Separation of radial and angular variables in Eq. (4) leads to the following expressions of wave functions:

$$\Psi_i(\vec{r_i})=R_i^{n,l}(r_i)\;Y_{l,m}(\theta_i,\varphi_i) \quad (i=e,h) \tag{5}$$

$R_i^{n,l}(r_i)$ is the radial part of wave functions, $Y_{l,m}(\theta_i,\varphi_i)$ is a spherical harmonic, n is principal quantum number, l and m are orbital and magnetic quantum numbers.

Afterwards, we focus on single-particle ground states corresponding to the following quantum numbers: $n=1$, $l=0$ and $m=0$, namely, 1s states since nanostructure effective gap is

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