



Energy spectrum of an exciton in a CdSe/ZnTe type-II core/shell spherical quantum dot

A. Chafai^a, F. Dujardin^{b,*}, I. Essaoudi^a, A. Ainane^{a,b,c}

^a Laboratoire de Physique des Matériaux et Modélisation des Systèmes, (LP2MS), Unité Associée au CNRST-URAC 08, University of Moulay Ismail, Physics Department, Faculty of Sciences, B.P. 11201, Meknes, Morocco

^b LCP-A2MC, Institut de Chimie, Physique et Matériaux, Université de Lorraine, Metz, France

^c Max-Planck-Institut für Physik Complexer Systeme, Nöthnitzer Str. 38, D-01187, Dresden, Germany

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ABSTRACT

The binding energy of an exciton inside a CdSe/ZnTe core/shell spherical quantum dot was theoretically examined taking into account the dependence of the dielectric constant and charge carriers effective mass on radius, and using the envelope function approximation. Such a structure presents original optical and electronic properties because of the spatial separation of electrons and holes caused by the type-II alignment of energy states. The mean distance between the electron and hole was calculated variationally using a trial function taking into account the coulomb interaction between charge carriers. Our numerical results provide a description to the size dependence of the binding energy of an exciton inside a core/shell nanoheterostructure type-II. Indeed, by controlling the inner and outer radii, we can precisely control the energy spectrum of the exciton.

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1. Introduction

The increasing need to improve the electronic and optical properties of materials has allowed the nanomaterials to occupy a very important place in the world of scientific research. Because of the spatial size reduction, this class of materials, unlike the bulk materials, exhibits a quantum confinement effect which is qualified as a major feature of nanosized materials. If the motion of the charge carriers is free only in two spatial directions, then we talk about the quantum well [1–4] which is qualified as a quasi-two-dimensional nanomaterial. We can also talk about one-dimensional nanomaterial, quantum wire [5] or quantum rod [6], when the charge carriers are confined over two spatial directions. In addition to the two categories of nanomaterials already cited we can achieve zero-dimensional nanomaterial also known as quantum dot [7] by the confinement of the charge carriers within the three spatial directions. In such a system the motion of the charge carriers is limited to a very small spatial region leading to a strong overlap between the wave functions of the electron and hole and consequently their light emitting efficiency is remarkably improved compared to that in bulk materials. Indeed the exciton in these latter is not confined in space, and because of its very small binding energy can rapidly dissociate, increasing the probability of nonradiative relaxation events associated with crystalline defects and charge carrier traps on crystal surfaces.

Another significant advantage of nanomaterials is the ability to control their electronic and optical properties by changing their shape. For example, Arsoski et al. [8] have investigated the exciton states in a nanocup under a perpendicular magnetic

* Corresponding author.

E-mail address: francis.dujardin@univ-lorraine.fr (F. Dujardin).

field, Kazaryan et al. [9] have examined the case of two electron states inside a quantum ring on a sphere, Slachmuylders et al. [10] presented the energy spectrum of exciton and trion in a cylindrical nanowire. The effect of impurity position on optical properties of a pyramid and a cone-like quantum dot was studied by Khordad et al. [11]. Feddi et al. [12,13] studied the excitonic Stark effect in a quantum disk, while the investigation of the spherical shape can be found in Refs. [14–17].

The tunability of nanomaterial properties by lattice strain was also largely studied by several authors [18–20]. From the point of view of applications, a detailed knowledge of the response of nanomaterials to strain is fundamentally important. Because of lattice strain, the properties of nanostructures can be dramatically improved leading to technologically important electronic and optoelectronic devices [21].

The intriguing and valuable attributes of quantum dots make them the subject of much research. Indeed, the confinement of the charge carriers in this type of structure dramatically improves the optical properties and, unlike their bulk counterparts, leads to new optical properties such as carrier multiplication [22–24], spectral diffusion and single-particle blinking [25]. However, because of their very large surface/volume ratio, semiconductor quantum dots can also lose some of their desirable properties due to, for example, corrupted surfaces. Thus, the protection and passivation of the quantum dots surface is of major importance for almost all of their possible applications [26].

In the last thirty years, particular attention was awarded to the study of core/shell semiconductor nanomaterials due to their exceptional properties. In this fashion, both the electron and hole can be confined in the core material (type-I) [27] or in shell material (inverted type-I) [28]. If the electron is confined in the shell material and the hole in the core material or vice-versa, then this type of confinement is known as type-II core/shell nanostructure [29]. In recent past, Kim et al. [30] have engineered a quantum dot heterostructure where the distribution of the hole probability density is maximum near the center of the dot, while the distribution of the electron probability density is maximum at the border, or vice versa. They have found that, because of the spatial separation of charge carriers, these heteronanostructures have a photoluminescence quantum yield (PL QY) lower than 4%. They have also found that the PL QY can be enhanced by the encapsulation of the core/shell nanomaterials, CdTe/CdSe in their paper, by a ZnTe layer. Using the first-order perturbation theory and taking into account the interface-polarization effects, Piryatinski et al. [29] have performed a theoretical study of the biexciton binding energy inside heteronanostructure with type-II band gap alignment. Their model shows that there is a strong exciton-exciton repulsion resulting from the simultaneous effects of quantum confinement and dielectric mismatch on charge carriers. Leontiadou et al. [31] presented calculations of the band-gap and radiative lifetime for various inner and outer radii of a CdSe/CdTe core/shell nanodot using a combination of $\mathbf{k}\cdot\mathbf{p}$ theory and configuration interaction (C.I.) method. The authors have shown that the properties of a CdSe/CdTe core/shell nanodot are size controlled, and that the increasing of shell thickness increases the exciton radiative lifetime, which is very useful to enhance the efficiency of photovoltaic devices. A theory of an exciton with spatially separated electron and hole inside a quasi-zero-dimensional nanodot was developed by Pokutnyi [32]. He has shown that the binding energy of an exciton is governed by the electron–hole Coulomb interaction and the spatial confinement. Type-I to type-II transition in AlInAs/AlGaAs semiconductor quantum dots was studied by Testelin and co-workers [33]. They have found that the type-I to type-II transition can be controlled by altering the concentration x of Aluminium in the $\text{Al}_x\text{Ga}_{1-x}\text{As}_{1-x}$ matrix. Using time-resolved and temperature-dependent photoluminescence techniques, Thuy et al. [34] have studied the photoluminescence properties of type-I and type-II CdTe/CdS core/shell semiconductor nanodots. Their comparative study of photoluminescence properties provides that type-I CdTe/CdS core/shell nanodots reveal a strong luminescence (QY = 60%) peaking at 550 nm with a short decay time of 20 ns, while type-II CdTe/CdS core/shell nanodots present a strong luminescence (QY = 20%) in the near-infrared region of 700–830 nm with a very long decay time of 190 ns.

The theoretical study of the binding of spatially separated electron and hole has also attracted significant interest of many authors. For example, Rorison [35] has calculated the binding energy of an exciton inside a spherical dot of semiconductor over-coated by another semiconductor. He has shown that the binding energy can be enhanced by choosing a finite potential barrier and, due to the wave function leakage, that the exciton binding energy increases more than that of the infinite barrier case for the same size of dot. He has also found that the exciton binding energy of type-II quantum well is significantly smaller than that of type-II quantum dot. Using a variational approach, Laheld et al. [36] have performed a theoretical model of exciton binding energy for different sets of electron and hole effective masses. Their study was essentially focused on the dependence of the exciton binding energy on the dot size and the offsets. In Ref. [37] a simulation of excitons and biexcitons in core/shell nanodots with Type-I, Type-I₂ and Type-II band alignments are presented. The authors have used the path integral quantum Monte Carlo method to examine the impact of the shell thickness on the electron-hole and the exciton-exciton interaction energies. They have found that the exciton correlation energy increases by decreasing the size of the nanostructures, or by decreasing the shell thickness for a fixed core radius. The binding energy of an exciton in a type-II CdSe/CdTe quantum dot was the subject of the study of Miloszewski et al. [38]. In their paper, they have calculated the eigenfunctions and eigenenergies of the confined electrons and holes, using a 8-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, after what they have found the exciton states using the C.I. method. They have shown that the exciton binding energy is large for a pure CdSe dot and that the addition of a CdTe shell decreases significantly this energy for thickness less than 1.5 nm, otherwise it is still constant.

In this paper, we deal with the spatial control of an exciton confined inside a spherical core/shell nanodot with type-II band gap alignment. To this end, we determine variationally the binding energy of an exciton as function of the spatial parameters (inner and outer radii). The average distance between the electron and hole is also examined. In the next section we introduce the model and the applied theory, while Section 3 is devoted to the presentation and discussion of our numerical results.

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