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Theoretical investigation of single dopant in core/shell nanocrystal in magnetic field

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ABSTRACT

The control of single dopant or "solitary dopant" in semiconductors constitute a challenge to achieve new range of tunable optoelectronic devices. Knowing that the properties of doped monocrystals are very sensitive to different external perturbations, the aim of this study is to understand the effect of a magnetic field on the ground state energy of an off-center ionized donor in a core/shell quantum dot (CSQD). The binding energies with and without an applied magnetic field are determined by the Ritz variational method taking into account the electron-impurity correlation in the trial wave function deduced from the second-order perturbation. It has been found that the external magnetic field affects strongly the binding energy, and its effect varies as a function of the core radius and the shell thickness. We have shown the existence of a threshold ratio $(a/b)_{crit}$ which represents the limit between the tridimensional and the spherical surface confinement. In addition our analysis demonstrates the important influence of the position of ionized donor in the shell material.

1. Introduction

Due to their surprising optoelectronic properties, the nanomaterials made in semiconductors (quantum wells, wires, and dots) continue to attract extensively experimental and theoretical interest [1–3]. In such structures the confinement effect restricts the motions of charge carriers (electrons and holes) in one, two or three dimensions leading to a partial or total quantization of the energy levels where some new photoluminescent transitions appears and new applications become possible [4,5].

In recent years, the progress in chemical growth process have permit to fabricate a new class of coated spherical quantum dots called core/shell quantum dots (CSQD). They are composed by two semiconductor materials with different band alignment: the core with a large band gap which play the role of substrate is coated by a spherical shell with a small band gap or vice versa (Fig. 1). These manufacturing processes allowed to manipulate several combinations of II–IV, III–V or IV–VI semiconductors [6–10]. The originality of these double layer structures is that their physical properties can be controlled by changing the nature or the size of the core or shell and consequently manipulated in advance by tuning the electron and hole

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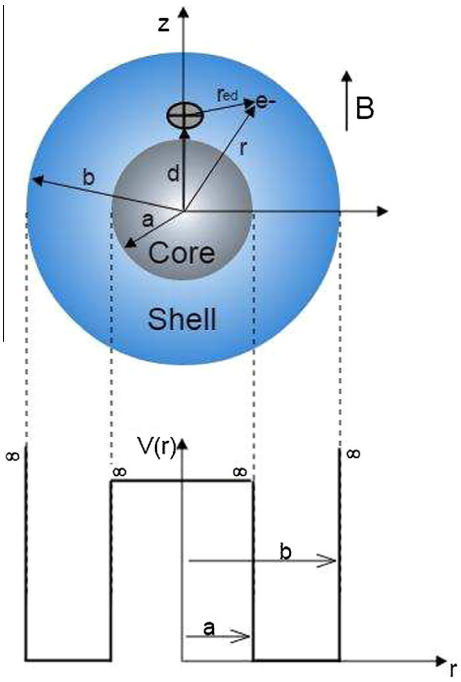

Fig. 1. Simplified potential energies representation of a core/shell quantum dot.

energy levels. This technical process so-called "wave function engineering" offers more emergent opportunities for large optoelectronic applications in different domains: solar cells [11,12], optical encoding [13], high resolution cellular imaging [14], quantum computing [15], tumor targeting [16] and biosensors [17].

During the growth process, it is possible to willingly add impurities into nanodots [18]. The control of nature and number of dopant atoms provides extensive tunable optoelectronic properties. It is well known that the binding of both ionized donors or acceptors with excitons plays a key role in the interpretation of photoluminescence spectrum [19–22]. Some remarkable properties are attributed to these complex systems such as the origin of UV in ZnO [20,21] or low-threshold lasing in ZnSe [23]. The inclusion of a single dopant or "solitary dopant" in a nanocrystal constitute a challenge for several scientists. The systematic explorations using a combination of optical measurements and scanning tunnelling spectroscopy in the control of the band gap and Fermi energy of doped semiconductor nanocrystals reveal that the properties due to solitary dopant lead to a new generation of optoelectronic devices such as solar cells and thin-film transistors [24]. We note that other breakthrough applications of the single dopant in confined medium are now possible or about to emerge; for more details we refer the reader to Refs. [25,26].

Generally speaking, the engineering of optoelectronic devices based on single dopant depends on several external perturbations (electric field, magnetic field, strain, temperature) and on the impurity position. Many theoretical and experimental studies have been devoted to the impurities in different configurations. In a series of papers, Cristea and Niculescu [27–29] have exposed some interesting theoretical results concerning the electronic properties of CdSe/ZnS and ZnS/CdSe CSQD taking into account the dielectric mismatch and the photoionization charges. Their investigation of the photoionization have shown a pronounced red shift for low dielectric constant. In addition, they have found that the binding energy of donor states in ZnS/CdSe under an electric field is blue shifted due to the dielectric confinement. On the other hand the theoretical studies of linear and nonlinear optical properties of ZnO/ZnS and ZnS/ZnO core–shell dots [30] have shown that in both structures the increasing of the shell thickness reinforces the nonlinear absorption coefficients and provokes a change in refractive index independently on the dielectric environment. The theoretical investigation of the oscillator strength of intra and interband quantum transitions in $GaAs/Al_xGa_{1-x}As$ spherical QD with an ionized donor placed at the center has shown that the existence of the impurity in the center of the core prevents the possibility to fabricate light source with multicolor emission [31]. The linear and third-order nonlinear optical absorption and refractive index have been studied using the compact density approach and show that the impurity transition is strongly affected by the shell thickness and the transitions between orbital with bigger l value shift to a higher photon energy region [32]. The position and electric field effects on single dopant has been subject of some of our last works in which we have attempted to explain the behavior of an off-center single dopant in thin quantum disk submitted to electric field [33]. The binding energy depends on disk size, donor position, strength and orientation of the field. We have also analyzed the interactions of a single ionized donor with an exciton [34], our theoretical prediction shows that the polarizability of the exciton bound to an ionized donor is proportional to $R^{3.5}$ and the Haynes rule remains valid even in the presence of electric field. In core/shell structures we have investigated the effect of dielectric