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Electronic and Optical Properties of Quantum Dot Semiconductor Heterostructures

Shevchuk I.S.

email: i.s.shevchuk@ukr.net

Department of Theoretical and Applied Physics & Computer Simulation,

Ivan Franko Drohobych State Pedagogical University,

3 Stryis'ka St., Drohobych,UA–82100, Ukraine

In the article physical properties of semiconductor quantum dots and possibilities of their change through variation of size and occasionally shape are discussed. Modern techniques of fabricating quantum dots and their using in different electronic and optoelectronic devices are described. The comparison of a number of experimental and theoretical studies focused on studies of quantum-size effects, exchange electron-hole and electron-phonon interaction, Stokes shift, oscillator strength, light absorption coefficient and luminescence of semiconductor nanoheterosystems has been performed. The interaction of quantum dots with external electric and magnetic fields depending on quantum dot size and presence of hydrogenic impurities also has been analyzed.

Key words: quantum dot, nanoheterostructure, confined phonons, interface phonons, optical transitions, optical absorption, Stokes shift, impurity.

Quantum dots are frequently referred to as artificial atoms to emphasize that the charge carriers confined in these single objects exhibit discrete energy levels (subbands) similar to electrons in naturally occurring atoms in contrast with Bloch energy bands in crystals. Quantum dot semiconductor heterostructures (based on CdS, CdSe, HgS, ZnS, etc.) demonstrate unique size-dependent physical properties and appear to have great perspectives of practical use in streaming progress of nanoscale device technology, such as single-electron transistors, single-photon emitters, solar cells, lasers, LEDs, memory devices, fluorescent tags in biotechnology applications, etc. [1]. Both experimental and theoretical researches show that semiconductor quantum dots possess deterministic properties superior to those of quantum wells and wires for optoelectronic applications. In addition, semiconductor nanocrystals are useful in checking the validity of current theories of electron-hole interaction in confined nanoscale systems. Their electronic structure is defined by level splitting, Coulomb and exchange interaction as well as spin-orbit coupling. The first three factors increase significantly but demonstrate different behavior in the nanoscale limit. In this view size selection and control become a powerful tool of modifying different parameters

A number of techniques are effectively developed to fabricate quantum dots: colloidal growth, plasma synthesis, molecular beam epitaxy, embedding into the glass matrix by melting, quenching and successive nanocrystal growing, electrochemichal assembly, lithography technique, etc. Significant success is observed in the study of optical spectra of quantum dots and their behavior in the presence of the electric and magnetic fields. A variety of studies focuses on the observed electronic and optical properties in order to give an adequate theoretical description of the physical processes in quantum dots.

Most researches exploit certain simplifying approaches to study different properties in quantum dots, such as:

1. An effective mass approximation, which allows simplifying band structures by using theoretical techniques constructed for bulk semiconductor materials.
2. An infinite barrier potential model, in which particle and exciton wave functions are localized inside a small quantum dot space and vanish beyond QDs boundary due to impenetrable barriers.
3. A strong confinement approximation, which permits to neglect the Coulomb interaction and assume the electron-hole interaction as a perturbation to their kinetic energy. In this regime the individual motions of electrons and holes are separately quantized. It allows one to present exciton wave functions in the form of a product of electron and hole parts. Applicability of the strong confinement approximation is restricted by the QD radius less than the exciton Bohr radius. When the quantum dot radius is larger than the exciton radius, the exciton translation motion is confined. This is a case of the weak confinement regime.
4. An assumption of identical dielectric constants for a QD and a surrounding medium that ignores creation of induced image charges at the interface.
5. A dominant number of researches deal with quantum dots of spherical shape, which allows simpler computation and analytical presentation of the results.

In recent studies more realistic models are generally considered in order to get beyond the mentioned simplifications, but to succeed in overcoming even one or two of them is not an effortless procedure.

The effect of quantum confinement in both strong and weak confinement regimes leads to the blue shift of the absorption edge. It is nearly proportional to the quantum dot square radius. However, some important electronic properties can undergo modification only in the strong confinement approximation. In Ref. [2] it is shown that the electron-hole exchange interaction is significantly enhanced in comparison with the bulk due to the confinement effect. This effect is attributed to the spatial overlap of electron and hole functions which strongly increases with reducing size. The photoluminescence of CdSe quantum dots obtained with size-selective spectroscopic techniques exposes the presence of a fine structure. The calculations reveal the degree of linear polarization of the photoluminescence light under linearly polarized excitation.

Rapid progress in quantum dot fabricating makes it possible to obtain nanoscale multishell structures made of concentric layers of different materials. The shell material (with thickness of the order up to one monolayer) with a smaller bulk band gap (e.g., HgS) is placed between a core material with a larger bulk band gap (e.g., CdS) and a host non-polar material (a silicate medium or an organic compound). Such a core-shell structure is used to localize charge particle states within the core and passivate dangling bonds of the core surface. In addition to electronic and optical properties, the vibrational spectra are of vital importance in contributing to the physical characteristics of these heterostructures. In Ref. [3] for a semiconductor quantum-dot heterostructure of spherical geometry polar optical phonons are considered in the dielectric continuum approach, with the derivation of the internal longitudinal optical (LO) phonon electric potential and the electron-LO phonon interaction Hamiltonian. The electron-LO phonon interaction plays a significant role in defining the physical properties of quantum dot heterosystems. The influence of this interaction on electronic energy levels is discussed in the framework of the effective mass approximation. The calculations are carried out for the CdS/HgS quantum dot quantum well heterostructure. A detailed study of the strength of electron-phonon coupling and a perturbative estimation of polaronic energy corrections for both ground and excited states within the adiabatic approximation is performed. Interesting results concerning the size dependence of polaronic corrections are analyzed.

Authors in Ref. [4] investigate exciton states in cubic quantum dots with finite potential barrier height taking account of dielectric mismatch. The dependences of charge particles ground states in addition to the exciton bound energy and oscillator strength are obtained versus quantum dot size and dielectric constant of quantum dot and surrounding material. The characterization of exciton spectra in CdTe quantum dots placed in different dielectric matrices is presented.

In Ref. [5] the researchers study the character of the states involved in optical transitions in CdS quantum dots synthesized by colloidal solution chemistry using the *ab initio* accuracy charge patching method in combination with the folded electronic spectrum calculations of thousand atom nanostructures. They also investigate electron-hole exchange splitting in CdS quantum dots. Their results indicate that the top of the valence band is bright contrary to the numerous $\mathbf{k}\cdot\mathbf{p}$ calculations. The nature of a large value of the observed resonant Stokes shift, being one of the most common characteristics of quantum dots, is discussed. The phenomenon of the Stokes shift in III-V (InAs) and II-VI (CdSe) semiconductor quantum dots is addressed in Ref. [6]. Authors investigate excitonic states taking into account dielectric mismatch between the dot and surrounding matrix, and the electron-hole exchange interaction in the finite potential barrier model. The Stokes shift is calculated as a size-dependent function and compared to relevant experimental data. The mechanism of the Stokes shift is explained by splitting of excitonic states due to the electron-hole exchange interaction in accordance with the results of Ref. [5].

Ref. [7] presents the study on CdTe/CdS core-shell quantum-dot heterostructure synthesized by water-based route. The optical spectra measurements showed that the band gaps of the core and shell materials can be tuned by changing the molar proportion. The Stokes shift declines as a result of increasing the core-shell proportion. It is attributed to the subsequent increase of the electron-phonon interaction strength with the core-shell ratio rising.

Researchers in Ref. [8] study optical characterization of quantum dots made by the Stransky-Krastanov technique and dots in the apex of pyramidal structures. It is shown that the transportation of carriers depends on the magnitude of an imposed electric or magnetic field as well as the value of temperature. It allows one to control the charge state of the quantum dot. The authors showed that it can also be done by optical means only – by changing photoexcitation conditions. In addition, the interaction of the exciton with optical phonon modes was investigated.

The interaction of an electron (a hole, an exciton) with polar optical phonon modes is found to be strong in materials with high ionicity. The bound states of charge particles and optical phonons resulting from this strong interaction are characterized by lowering of energy in comparison with the non-interacting system and are called polarons. Ref. [9] deals with effects of polarons of large radii on optical spectra in quantum nanostructures including spherical dots. The authors used the electron-phonon interaction Hamiltonian of the form which takes into account a probable polarization of both the quantum dot and surrounding medium materials. They considered both confined and interface optical phonons and showed that contribution of interface phonons in polaron binding energy can exceed that of confined phonons.

Efficient carrier multiplication as a consequence of optical excitation could have a considerably wider application in the field of solar energy conversion (Ref. [10]). The effective carrier multiplication process makes it possible to enhance the peak theoretical power conversion efficiency and widen the choice of perspective materials for new solar technologies. It involves previously neglected narrow-gap semiconductors. Strongly confined semiconductor quantum dots are seen as prospective structures for efficient carrier multiplication in view of the discreet electronic structure. The authors determined the efficiency of carrier multiplication yields in CdSe and CdTe quantum dots by transient photoluminescence.

The author of Ref. [11] considers optical absorption of excitons in a disc-like quantum dot. Calculations are carried out in the effective mass approximation and compact density-matrix approach. Optical absorption coefficients and refractive index changes are found both with and without account of the exciton-phonon interaction. It is concluded that the effect of longitudinal optical phonons in estimation of the absorption coefficients and refractive index is quite significant.

Optical transitions in a quantum dot of lens shape are studied taking into account a hydrogenic impurity in Ref. [12]. Lens-shaped quantum dots are interesting from the point of view of their use in laser applications and high-performance laser diodes fabrication. The attention is paid to such an interesting characteristic of a quantum dot as possible intersubbands optical transition. The density matrix approach with the intersubband relaxation is employed to analytically estimate the linear and third-order nonlinear changes in the absorption coefficient and refractive indices in the presence of a hydrogenic impurity. It is obtained that the absorption coefficient and refractive indices are heavily influenced by optical intensity and the dot size.

CONCLUSIONS

The studies outlined in the present article are systematic investigations of electronic and optical properties of semiconductor quantum dot heterostructures to advance understanding of these systems as well as modeling of their optical properties in order to fabricate high-performance optoelectronic devices.

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