QUANTUM SIZE EFFECT ON THE ELECTRONIC PROPERTIES OF SOME TERNARY SEMICONDUCTOR QUANTUM DOTS

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Abstract

Quantum dots (QD) also known as semiconductor fluorescent nanoparticles has gain a lot of attention because it is among the nanomaterials family that holds great potential for variety of applications. In this study the quantum size effect on the electronic properties of some ternary quantum dots of AlGaAs, GaInP, GaInSb, GaInAs and GaAsSb were investigated using the particle in a box model as the basis. The confinement energy, Coulombic energy and energy band gap of these quantum dots were computed. The results obtained showed that as the dot size increases, the confinement energy, Coulombic energy and energy band gap of these quantum dot decreases. Among the quantum dots considered, GaInSb has the highest confinement energy AlGaAs quantum dot has the largest Coulombic energy while GaInP has the highest energy band gap. The result of this work reveals that suitable choices of the size of the quantum dot can enhance the electronic and optical properties of these quantum dots for suitable applications.

Keywords: Quantum dots**,** Quantum size, Quantum confinement, Electronic properties, Ternary Semiconductor

INTRODUCTION

Quantum dots (QD) are semiconductors particles of a few nanometres in size that exhibits three dimensional quantum confinements, resulting in distinctive electronic, optical and transport properties. Quantum confinement can be described as the arrangement of the electron-hole pairs inside a material in one or more dimensions, and is categorized as, one dimensional confinement as seen in quantum wells, two dimensional confinement in thin-films or Quantum wires, or three dimensional confinement as in quantum dots (Trindade et al., 2001, Alivisatos,1996). As a result of the size of the quantum dots, electrons that are confined possess greater energy than the electrons in the bulk materials. Quantum confinement gives rise to size dependent phenomenon. Quantum dots that are small in size have stronger confinement resulting in larger energy band gaps (Alivisatos, 1996). Consequently, quantum dots with various emission colors can be fabricated from similar material by varying their sizes (Dabbousi and Bawendi, 1995). In accordance with the variation in its size, any color of light can be emitted by a quantum dot from the same nanocrystal semiconductor and this makes effective control possible which can be tuned during synthesis processes in order to emit these colours (Yoffe, 2001). Consequently, the larger dots emit colours like red at longer wavelengths, while smaller dots emit colours like green at shorter wavelengths. Quantum dots find applications in single-electron transistors solar cells, Light emitting diode lasers (Huffaker et al., 1998), single-photon sources, (Senellartet et al., 2017) , Second-harmonic generation quantum computing, (Michalet et al., 2005). The minute size of quantum dots gives room for quantum dots to be dispersed in solution, making them useful in inkjet printing and Spin-coating (Xu et al., 2016). Quantum dots have outstanding electroluminescence and photoluminescence properties and this makes them very suitable for display systems. In comparison to organic luminescent substances that are employed in fabricating organic light emitting diodes (OLEDs), materials made from quantum dots have numerous advantages, such as longer lifetime, lower power consumption, purer colors and lower manufacturing cost. Another good property of quantum dots is that any substrate can be utilized for the deposition, making it possible in the manufacture of printable, flexible, even rollable quantum dot displays of different sizes. Group III–V compound semiconductor is an alloy originating from elements in group III (B, Al, P, Ga, and In) and group V (N, P, As, Sb, and Bi) in the periodic table. These classes of semiconductors have unique properties not found in silicon. For instance, most group III-V semiconductors have direct energy band gap. In addition by using ternary alloys of these semiconductors, the energy band gaps can be continuously varied over a wide range (Mićić and Nozik, 2002). The exclusion of toxic heavy metals like Cd and Pb makes III–V nanocrystals a compelling alternative material platform useful in biological imaging and optoelectronic devices. (Zhong and Scholes, 2011).

Using the particle-in-a-box model, Uduakobong (2017) investigated the effects of confinement energies on PbS and InP quantum dots using Brus equation. The results they got revealed that for PbS and InP studied, their ground state confinement energy is inversely proportional to the size of the quantum dots. Onyia et al., (2018) carried out a study of quantum confinement effects on ZnS ,CdSe, and GaAs quantum dots using particle in a box model. He found that discrete electronic states arose at the conduction and valance bands. Ekong and Osiele (2016) carried out a quantum confinement study of the electronic energy of some nanocrystalline silicon quantum dots of different shapes and found that quantum dots of different shapes exhibit different electronic energy based on the transitions from the quantum selection rules. Neeleshwar et al., (2005) carried out a study for size dependent properties of CdSe quantum dots and found that at room temperature, there is a blue shift of the energy band gap, change in magnetic susceptibility and a change in structure compared to the bulk CdSe. These changes were attributed to changes in size and surface effects. In this study, the particle in a three dimensional box model was used to develop the theoretical frame work used to investigate quantum size effect on the electronic properties of Aluminium Gallium Arsenide (AlGaAs), Gallium Indium Phosphide (GaInP), Gallium Indium Arsenide (GaInAs), Gallium Indium Antimonide (GaInSb), and Gallium Arsenide Antimonide (GaAsSb) quantum dots to provide an insight into the electronic properties of ternary quantum dots.

Theoretical Framework

The particle in a box model is a common application of a quantum mechanical model to a simplified system consisting of a particle moving in a three dimensional box. The result gives possible values of energy and wave function that the particle can have. For a three dimensional well of length l, we solve the Schrodinger equation and the wave function of such a system is given by

$$\Psi(x,y,z) = \sqrt{\frac{8}{l^3}}\, sin\frac{n_x\pi}{l} sin\frac{n_y\pi}{l} sin\frac{n_z\pi}{l} \qquad (1)$$

For a particle in three dimensional box, The energy of the particle is

$$E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n^2{}_x}{l^2{}_x} + \frac{n^2{}_y}{l^2{}_y} + \frac{n^2{}_z}{l^2{}_z}\right) \quad (2)$$

In order to apply this particle in a box model to the quantum dot, the length of the box is replaced by the radius, R of the quantum dot and the electronic mass by the mass of the electron m_e and of the hole, m_h to get the confinement energy
The confinement energy becomes

$$E = \frac{n\hbar^2\pi^2}{2m_eR^2} + \frac{n\hbar^2\pi}{2m_hR^2} \quad (3)$$

The lowest confinement energy or the ground state confinement energy becomes

$$E = \frac{\hbar^2\pi^2}{2R^2}\left(\frac{1}{m_e} + \frac{1}{m_h}\right) \quad (4)$$

To account for the energy between the particles and the crystal structure, the mass of the electron and hole are replaced with the reduced mass

$$\therefore E = \frac{\hbar^2\pi^2}{2R^2}\left(\frac{1}{m_e{}^*} + \frac{1}{m_h{}^*}\right) = \frac{\hbar^2\pi^2}{2\mu R^2} \quad (5)$$

where, $m_e{}^*$ is the effective mass of the electron, $m_h{}^*$ is the effective mass of the hole, and

μ is the reduced mass of the exciton system.

Coulombic attractions usually occurs between the electrons and holes which results to an energy proportional to the Rydberg's energy, and inversely proportional to the dielectric constant squared. This term is relevant when the semiconductor crystal is smaller than the exicton Bohr radius

$$E_{exciton} = -\frac{1}{\varepsilon_r{}^2}\frac{\mu}{m_e}R_Y = -R_y{}^* \quad (6)$$

where ε_r is the size-dependent dielectric constant of the semiconductor and R_Y is the Rydberg energy.
The energy associated with the Coulombic attraction is

$$E_{coulombic} = -1.8\frac{e^2}{\epsilon R} = \frac{1{,}8e^2}{4\pi\varepsilon_0\varepsilon_r R} \quad (7)$$

The total energy of a quantum dot is the sum of the band gap energy, confinement energy and the bound energy of the exciton. This is expressed as (Ikeri et al,. 2020):

$$E_{total} = E_{bandgap} + E_{confinement} + E_{exciton} \quad (8)$$

$$E_{total} = E_{bandgap} + \frac{\hbar^2\pi^2}{2\mu R^2} - R_y{}^* \quad (9)$$

The energy gap of quantum dots is the energy gap of the bulk semiconductor and the confinement energy of both electrons and holes expressed as

$$E_g = E_{bulk} + \frac{h^2}{8R^2}\left(\frac{1}{m_{e^*}} + \frac{1}{m_{h^*}}\right) \quad (10)$$

where, E_g is band gap energy of quantum dot, E_{bulk} is energy band gap of bulk semiconductor; R is radius of quantum dot; m_e^* is effective mass of the electron; m_h^* is effective mass of the hole; h is Planck's constant. The parameters of the ternary semiconductors used for the computation were obtained from Levinshtein et al,. 1999.

RESULTS AND DISCUSSION

Fig. 1 shows the variation of confinement energy with radius for some ternary semiconductor quantum dots. The figure reveals that ground state confinement energy is inversely proportional to the radius of the quantum dot. That is, as the dot radius increases, the ground state confinement energy decays exponentially but never reaches zero, this is in agreement with the results of Ikeri et al., (2020) that studied confinement energy for single quantum dot. The figure further reveals that GaInSb quantum dot has the highest ground state confinement energy while AlGaAs and GalnP has the least confinement energy. This may be due the effective mass of electrons and holes in these semiconductor quantum dots, and their bulk energy band gap. The lowest possible energy in quantum dots is not zero irrespective of the fact that the confinement energy do not vary appreciably when the radius of the quantum dots is greater than 6 nm. The variation of the Coulombic energy with radius for some ternary quantum dots is shown in Fig.2. As revealed in the figure, the Coulombic energy decreases as the quantum dot size increases. The Coulomb energy in quantum dots has an inverse electron-hole separation which can be approximated to be the radius. Coulombic energy which is as a result of Coulombic interaction is an important property in localized energy levels (bound states) or electronic flat bands and results in many exotic quantum phases (Fu et al., 2020). *AlGaAs* quantum dot has the largest Coulombic energy, this means that it has small dot size, relatively large effective mass and small relative permittivity. Electrons and holes confined in semiconductor quantum dots are affected energetically by Coulomb charge interaction. The operating frequencies of photoemitters and detectors depend on these transition energies (Bose and Johnson, 2004). Figure 3 shows the variation of energy band gap of AlGaAs ,GaInP, GaInSb, GaInAs and GaAsSb quantum dots against radius. The figure shows that as the radius of the quantum dot is increasing, the energy band gap of the ternary semiconductor quantum dots decreases. This is in agreement with the result of Alivisatos, 1996 it is due to strong quantum confinement. This is due to the confinement of the electrons in the quantum dots. This suggests that the large quantum dots produce the shortest energy gap (reddish spectrum) and small quantum dots have long energy gap (bluish spectrum). The range of values of the energy band gap of the ternary semiconductor quantum dots is:GaInP: (2.90 – 2.07 eV) ,GaAsSb,: (2.28 – 0.56 eV), GaInAs : (2.17 – 0.67 eV), AlGaAs: (2.01 – 1.22 eV), and GaInSb: (1.88 – 0.12 eV). Fig. 3 further revealed that for ternary semiconductor quantum dots that have high energy band gap, the energy band gap do not vary so much as the radius of the quantum dot changes unlike quantum dots of ternary semiconductors that have small energy band gap. This shows that ternary semiconductor quantum dots of small energy band gap can emit light over a longer wavelength range when the radius of the quantum dot is varied.

Conclusion

The effect of quantum size on the electronic properties of ternary semiconductor quantum dots of AlGaAs, GaInP,GaInSb, GaInAs and GaAsSb were investigated using the particle in the box model. From the results we can infer that quantum confinement affects the Culombic energy, confinement energy and energy band gap. This confinement effect is more pronounced in the quantum dots of ternary semiconductors that are small in size. The energy band gap varies inversely with size and large energy band gap ternary semiconductor quantum dots emits light over a smaller range of wavelength compared to small energy band gap ternary semiconductor quantum dots that emits light over a longer wavelength range when their sizes are varied. This shows that suitable choices of the size of the quantum dot can enhance the electronic and optical properties of the dots.

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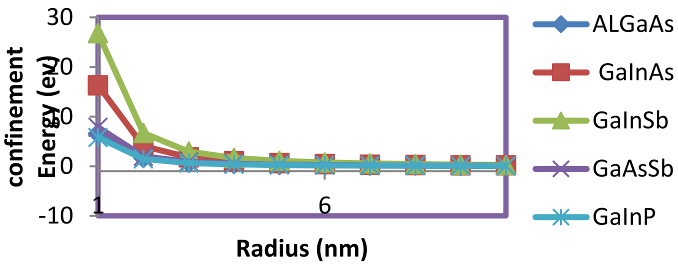

Fig. 1: Variation of confinement energy with radius for some ternary semiconductor quantum dots

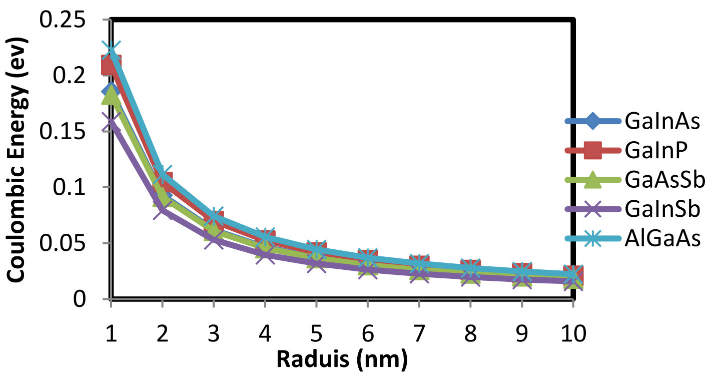

Fig. 2: Variation of Coulombic Energy with radius for some ternary semiconductor quantum dots

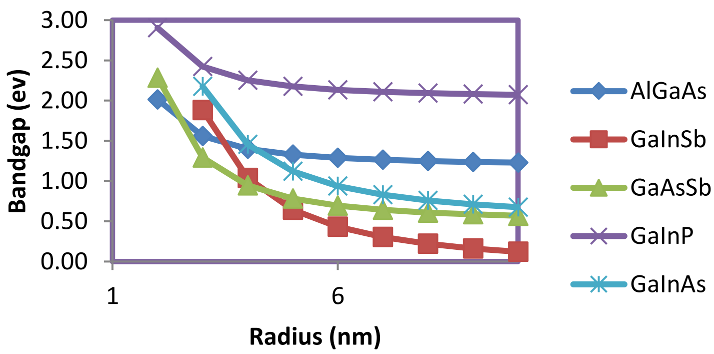

Fig.3: Variation of energy band gap with radius for some ternary semiconductor quantum dots