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Effect of Dot Size on Exciton Energy States Confined in a Spherical Gallium Arsenide Quantum Dot

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Here, we report the effect of dot size on exciton energies confined in a spherical Gallium Arsenide (GaAs) quantum dot and found that exciton energy is purely dependent on the dot size. The results showed that, by increasing the dot size, both the ground state energy and the first excited state energy decrease, and, at a given dot radius, the first excited state exciton energy is found to increase by 5 orders of magnitude more than the ground state exciton energy. In addition, we calculated and plotted the dependence of probability density on the exciton dot size in a GaAs quantum dot, and the results reveal that the probability of the exciton in the ground state is zero, whereas it is maximal in the first excited state. The present work significantly explains the exciton energies in a GaAs quantum dot, and their dependences on size of the semiconducting quantum dot that will find a number of applications in the modelling of future nanosize electronic devices.

Тут ми повідомляємо про вплив розміру точки на енергії екситонів, що містяться у сферичній точці арсеніду ґалію (GaAs), виявивши, що енергія екситона істотно залежить від розміру точки. Результати показали, що, зі збільшенням розміру точки як енергія основного стану, так і енергія першого збудженого стану зменшуються, і за заданого радіюса точки виявляється, що енергія екситона першого збудженого стану збільшується на 5 порядків величини понад енергію екситона основного стану. Крім того, нами було розраховано та побудовано залежність густини ймовірности від розміру екситонної точки у квантовій точці GaAs, а результати показують, що ймовірність екситона в основному стані дорівнює нулю, тоді як вона є максимальною в першому збудженому стані. Дана робота істотно пояснює енергії екситонів у квантовій точці GaAs та їх залежності від розміру напівпровідникової квантової точки, що знайде низку прикладних застосувань при моделюванні майбутніх нанорозмірних електронних пристроїв.

Здесь мы сообщаем о влиянии размера точки на энергии экситонов, которые содержатся в сферической точке арсенида галлия (GaAs), обнаружив, что энергия екситона существенным образом зависит от размера точки. Результаты показали, что с увеличением размера точки как энергия основного состояния, так и энергия первого возбуждённого состояния уменьшаются, и при заданном радиусе точки оказывается, что энергия екситона первого возбуждённого состояния увеличивается на 5 порядков величины свыше энергии екситона основного состояния. Кроме того, нами была рассчитана и построена зависимость плотности вероятности от размера экситонной точки в квантовой точке GaAs, а результаты показывают, что вероятность экситона в основном состоянии равняется нулю, тогда как она является максимальной в первом возбуждённом состоянии. Данная работа существенным образом объясняет энергии экситонов в квантовой точке GaAs и их зависимости от размера полупроводниковой квантовой точки, что найдёт ряд прикладных применений при моделировании будущих наноразмерных электронных устройств.

Key words: exciton energy, GaAs quantum dot, probability density, variational method, effective mass approximation.

Ключові слова: енергія екситона, квантова точка GaAs, густина ймовірности, варіяційна метода, наближення ефективної маси.

Ключевые слова: энергия экситона, квантовая точка GaAs, плотность вероятности, вариационный метод, приближение эффективной массы.

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1. INTRODUCTION

Synthesis of semiconductor quantum dots invites for theoretical approach, which can predict the effect of dot size on exciton electronic structure. Generation of bound electron–hole pairs called excitons in semiconductor quantum dots (QDs) are important factors and have significant role in determining the optical and electronic properties of QD system. Semiconductor QDs play an important role in optoelectronic and nanodevices because of their indirect band gap nature [1]. Excitons confined in QDs have remarkable properties which allow many applications in the fabrication of electronic nanodevices such as quantum dot lasers, single electron transistors *etc*. [2]. In past several years, authors were successful in explaining the quantum confinement of excitons in QDs, for example, Gan *et al*. [3] and Takagahara *et al*. [4] reported the exciton energy states in QDs, Brus *et al*. [5] used variational approach and calculated size-dependent exciton energy states, whereas Nair *et al*. [6] calculated the lowest exciton energy in semiconductor microcrystals, taking into consideration the size of the quantum dot. However, to the best of our knowledge, effect of dot size on exciton energies in GaAs QDs is not reported until date, and this article is aimed in that direction.

Here, in the present work, the exciton quantum state energies have been theoretically calculated for GaAs QD within the framework of effective mass approximation. Effects of GaAs QD size on the ground state and first excited state for exciton is examined. The results revealed that decrease in the exciton energy states is more profound up to a dot radius of approximately 100 nm, and, for larger GaAs quantum dots (> 100 nm), the exciton energy remains almost constant. Furthermore, the exciton probability density in the first excited state and ground state energy is inversely proportional to each other. The obtained results are consistent with the previously reported results in the literature.

The paper is organized as follows: Section 2 discusses the theoretical formulations and Section 3 presents the results and discussions. The conclusion remarks are presented in Section 4.

2. THEORETICAL FORMULATIONS

To calculate the exciton quantum state energies in GaAs quantum dot, we confine an exciton in a spherical GaAs quantum dot of radius R. The potential chosen for a particle is infinite potential well written as

$$v(r) = \begin{cases} 0, & r \le R, \\ \infty, & r \ge R. \end{cases} \tag{1}$$

The above potential is a central potential, so, the wave function may be written as follows:

$$\phi(r, \theta, \varphi) = f(r) Y_{lm}(\theta, \varphi) , \tag{2}$$

where $Y_{lm}(\theta, \varphi)$ are spherical harmonics, and $f(r)$ is the radial wave function.

The radial part of the Schrödinger equation is given by

$$\frac{-\hbar^2}{2m^*}\frac{d^2\rho}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2m^*} - E\right]\rho = 0 . \tag{3}$$

Here in the above expression, $m^* = \dfrac{m_e^* m_h^*}{m_e^* + m_h^*}$ is the reduced mass of the electron–hole pair (exciton), and $\rho(r) = r f(r)$.

The solutions to the Eq. (3) are the spherical Bessel functions, given by

$$\rho(r) = ArJ_l(kr)\,. \quad (4)$$

The spherical Bessel function $J_l(kr)$ has different functional forms for different values of l. Thereby, for each value of l, we get a series of values of E. The energy Eigen values of exciton confined in a spherical GaAs quantum dot and the radial wave function corresponding to $l = 0$ are obtained as follow:

$$J_0(kr) = \frac{\sin(kR)}{kR}\,, \quad (5)$$

$$\rho(r) = ArJ_0(kr)\,. \quad (6)$$

3. RESULTS AND DISCUSSIONS

Figure 1 shows the variation of exciton ground state and first excited state energy in GaAs spherical QD as a function of dot radius. It is note worth from Fig. 1 that the exciton energy decreases as the dot radius increases. This is due to increase in the exciton localization area and increase of overlap integral of electron and hole wave functions, which is consistent with the result reported in Ref. [7]. Moreover, from Figure 1, it is clear that the first excited state exciton energy is approximately by 5 orders of magnitude more than the ground state energy.

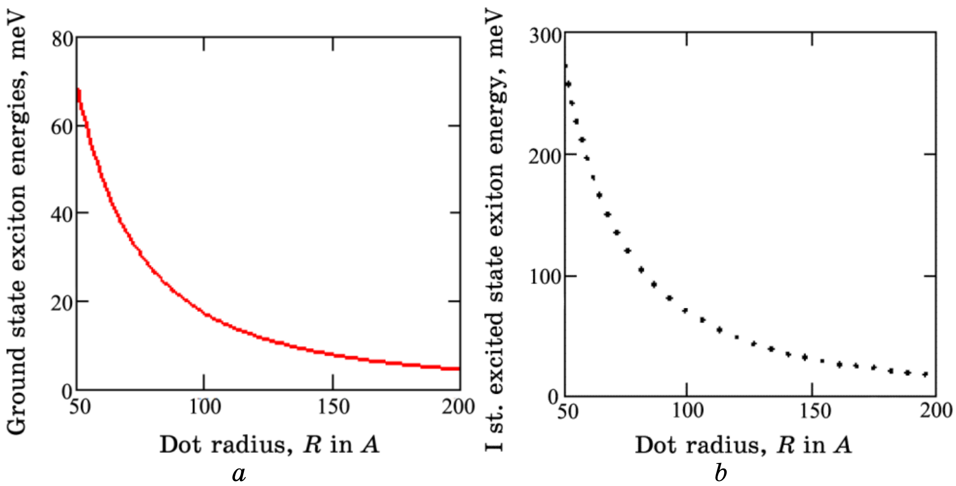

Fig. 1. Variation of exciton energy with the GaAs QD radius for (*a*) ground state or (*b*) first excited state ($A \equiv$ Å).

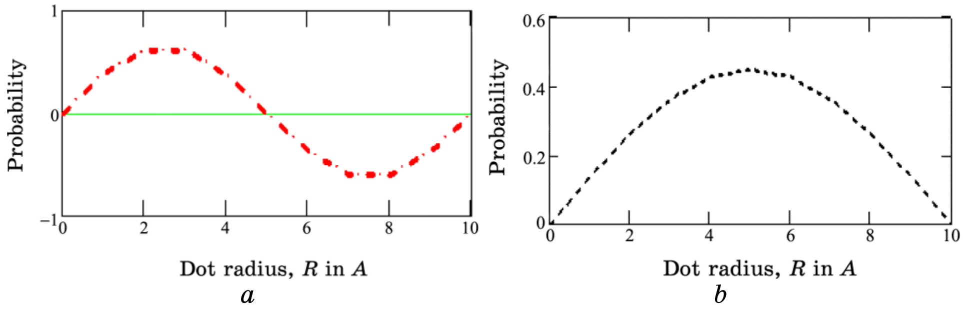

Fig. 2: Variation of probability of exciton with the GaAs QD radius for (*a*) ground state or (*b*) first excited state (*A* ≡ Å).

4. CONCLUSIONS

In this paper, we theoretically studied the effect of dot size on ground state and first excited state of an exciton confined in a GaAs spherical quantum dot. The results show that the exciton energy decreases as the dot radius increases. At a given dot size, the first exciton energy is found to increase 5 orders of magnitude more than the ground state exciton energy. Moreover, the exciton probability at a dot radius of 10 Å in both the first excited state energy and the ground state energy is zero, whereas it is maximal at a dot radius of 5 Å in the case of first excited state (Fig. 2). These results are important from both the basic points of view and the applied one and will find various applications in nanoelectronics.

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