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International Scientific Conference
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EFFECT OF ALUMINUM CONCENTRATION ON INTRADONOR TRANSITION AND NORMALIZED INTRADONOR TRANSITION ENERGIES IN InAs/$In_{1-x}Al_xAs$ SPHERICAL QUANTUM DOT

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Abstract
In the InAs/$In_{1-x}Al_xAs$ spherical quantum dot, the variation of the intradonor transation and normalized intradonor transition energies are calculated using the variational method under the effective mass approximation. It has been observed that when the quantum dot radius increases, the intradonor transition energy decreases, whereas the normalized intradonor transition energy increases when the impurity is located near the center of the quantum dot and remains constant when it is near the edge. In addition, we determined that when the aluminum concentration increases, the intradonor transition energy increases while the normalized intradonor transition energy decreases. However, when the position of the impurity changes from the center of the quantum dot to the edge, it is observed that the intradonor transition energy first decreases and then increases again after the minimum value, while the normalized intradonor transition energy decreases and does not change even if the aluminum concentration is increased after the position of the impurity where the intradonor transition energy is minimum. To our knowledge, this study has been the first to calculate the normalized intradonor transition energy for the InAs/$In_{1-x}Al_xAs$ structure for different aluminum concentrations.

Keywords: Intradonor transition energy, normalized intradonor transition energy, InAs/$In_{1-x}Al_xAs$ spherical quantum dot, variational method.

INTRODUCTION

Low-dimensional structures such as quantum wells, quantum wires, and quantum dots represent an important area of research in nanotechnology and condensed matter physics [1-9]. These structures are characterized by the confinement of electrons and other charge carriers in one or more dimensions, leading to a better understanding of their electronic, optical, and magnetic properties.

Quantum dots (QDs) are one of the semiconductor nanostructures that exhibit unique optical and electronic properties due to quantum confinement effects [7-9]. These effects occur when the size of the QD becomes comparable to the de Broglie wavelength of the charge carriers, giving rise to discrete energy levels similar to those found in atoms. Confining electrons within these nanostructures provides precise control over their energy states, making quantum dots extremely important for applications in fields such as optoelectronics, quantum computing, and biomedical imaging [10].

One of the important issues in QD research is understanding the energy transitions that occur within these nanostructures [11]. In particular, the intradonor transition energy refers to the energy difference between the ground state and the excited state of an electron within a donor impurity in a quantum dot. This transition is important because it affects the electronic and optical properties of the QD [12]. To better understand these transitions, it is important to consider the normalized intradonor transition energy, which provides a dimensionless measure of the energy levels within a QD. Normalization allows comparison of transition energies across different QD sizes, shapes, and material compositions, providing a better understanding of how these factors affect the electronic structure of QDs. Therefore, studying the intradonor transition energies in spherical QDs is crucial to better

doi: www.doi.org/10.70456/EYSP8852

understanding nanostructured materials. By studying these transitions and their normalized values, researchers can optimize QDs for specific applications and tailor their properties to achieve desired results in various technological areas.

In this study, the intradonor transition energy and normalized intradonor transition energy for different aluminum concentration values are calculated with respect to spherical quantum dot (SQD) radius and impurity location. We present the organization of the paper as follows: we present the theory in Section 2, the results and discussion in Section 3, and the conclusions in Section 4.

EXPOSITION

The Hamiltonian for a single electron system with hydrogenic impurity in a SQD is given by: [12, 13]

$$H = -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right) - \frac{A\,e^2}{4\pi\varepsilon_0\varepsilon r} + \frac{B\,\hbar^2}{2m^*}\frac{(l(l+1)}{r^2} + V(x,r) \quad (1)$$

Where, m^*, ε and $V(x,r)$ are electronic effective mass, dielectric constant and confining potential, respectively. A and B are arbitrary constants determined to make the theory more understandable. In Equation 1, A=0 and 1 indicate the absence of impurity and the presence of impurity, respectively, and similarly B=0 and 1 is used to indicate the ground state and the excited state.

The confining potential, $V(x,r)$, is taken by [12]

$$V(x,r) = \begin{cases} 0 & r \le R \\ V_0(x) = Q_c\,\Delta E_g^{\Gamma}(x) & r \ge R \end{cases}, \quad (2)$$

where $Q_c = 0.5$ is the conduction band offset parameter, x shows the aluminum concentration. $\Delta E_g^{\Gamma}(x)$ is the band gap of heterostructure at the Γ point and, is defined as follows [12, 14]

$$\Delta E_g^{\Gamma}(x) = 0.360 + 2.012x + 0.698x^2 \quad \text{for} \quad InAs/In_{1-x}Al_xAs \quad (3)$$

The trial wave functions for the ground state ($1s(n=1,l=0)$) and excited state ($1p(n=1,l=1)$) of the SQD system in the presence of impurity are given by [15,16]

$$\psi_{1s}^{imp}(r,r_i) = \begin{cases} (N_{1si}\sin(k_{1si}r)/r)\exp\left(-\lambda_{1s}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r \le R \\ (N_{1so}\exp(-(k_{1si}r))/r)\exp\left(-\lambda_{1s}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r \ge R \end{cases} \quad (4)$$

and

$$\psi_{1p}^{imp}(r,r_i) = \begin{cases} N_{1pi}\left(\frac{\sin(k_{1pi}r)}{(k_{1pi}r)^2}-\frac{\cos(k_{1pi}r)}{(k_{1pi}r)}\right)\mathrm{r}\cos(\theta)\exp\left(-\lambda_{1p}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r \le R \\ N_{1po}\left(\frac{1}{(k_{1po}r)}+\frac{1}{(k_{1po}r)^2}\right)\exp(-k_{1po}r)\,\mathrm{r}\cos(\theta)\exp\left(-\lambda_{1p}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r \ge R \end{cases} \quad (5)$$

where λ_{1s} and λ_{1p} are variational parameters and N_{1si}, N_{1so}, N_{1pi} and N_{1po} terms denote normalization coefficients. In Eqs.(4 and 5), k_{1si}, k_{1so}, k_{1pi} and k_{1po} are given by,

$$k_{1si} = \sqrt{2m^*E_{1s}^{sub}/\hbar^2}$$
$$k_{1so} = \sqrt{2m^*\left(V_0(x)-E_{1s}^{sub}\right)/\hbar^2}$$
$$k_{1pi} = \sqrt{2m^*E_{1p}^{sub}/\hbar^2}$$
$$k_{1po} = \sqrt{2m^*\left(V_0(x)-E_{1p}^{sub}\right)/\hbar^2}. \quad (6)$$

In Eq. 6, E_{1s}^{sub} and E_{1p}^{sub} represent the subband energies of the 1s-ground state and 1p-excited state. These energies are

obtained from the transcendental equations for both the ground and excited states [12]. Energies are given as follows for 1s and 1p impurity state, respectively

$$E_{1s}^{imp} = min_{\lambda_{1s}} \langle \psi_{1s}^{imp} | H^{A=1,B=0} | \psi_{1s}^{imp} \rangle / \langle \psi_{1s}^{imp} | \psi_{1s}^{imp} \rangle \quad (7)$$

and

$$E_{1p}^{imp} = min_{\lambda_{1p}} \langle \psi_{1p}^{imp} | H^{A=1,B=1} | \psi_{1p}^{imp} \rangle / \langle \psi_{1p}^{imp} | \psi_{1p}^{imp} \rangle \quad (8)$$

,

The intradonor transition energy between ground state 1s and excited state 1p is defined as [17]

$$E_{imp1s1p}^{Trans} = E_{1p}^{imp} - E_{1s}^{imp} \quad (9)$$

To better understand intradonor transition energy $E_{imp1s1p}^{Trans}$, it is important to defined the normalized intradonor transition energy $NE_{imp1s1p}^{tran}$, which provides a dimensionless measure of the energy levels within a QD and described as [17];

$$NE_{imp1s1p}^{Trans} = E_{imp1s1p}^{Trans} / E_{1s}^{imp} = \left[E_{1p}^{imp} - E_{1s}^{imp}\right] / E_{1s}^{imp} \quad (10)$$

.

RESULTS AND DISCUSSIONS

In this section, the results of the intradonor transition energy and normalized intradonor transition energy for the InAs/$In_{1-x}Al_xAs$ SQD as a function of the dot radius and impurity location for different aluminum(Al) concentrations using the variational method under the effective mass approach are presented. In the calculations, the effective mass and dielectric constant for the InAs/$In_{1-x}Al_xAs$ SQD are taken as $m^* = 0.026m_0$ and $\varepsilon = 12.5$. In addition, it is seen that the obtained results are compatible with the intra-donor transition energy and intra-donor normalized transition energy results found in the literature for the aluminum concentration x = 0.35 in InAs/$In_{1-x}Al_xAs$ SQD [18]. For different aluminum concentrations, the results of the changes in intradonor transition energy and intradonor normalized transition energy depending on the SQD radius for different impurity positions are presented in Figures 1-2, and the changes depending on the impurity location for different quantum dot radii are presented in Figures 3-4.

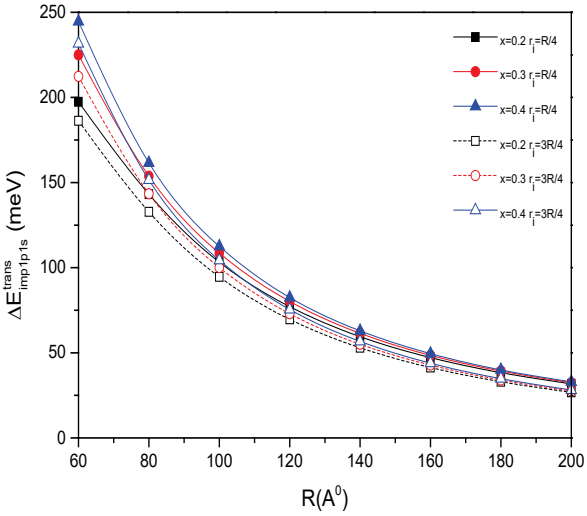

Figure 1. *Variation of the intradonor transition energy and normalized intradonor transition energy with quantum dot radius for different aluminum concentration and impurity positions.*

In Figure 1, the variation of the intradonor transition energy depending on the SQD radius is investigated for different aluminum concentrations and impurity positions. It is seen that the intradonor transition energy decreases when the radius of the SQD increases. In addition, it is seen that the intradonor transition energy increases when the aluminum concentration increases, while it decreases when the impurity position close to the edge of the SQD. This is because the increase in aluminum concentration increases the confinement potential defined in equation 2, which causes an increase in the intradonor transition energy. Moreover, the intradonor transition energy of the impurity at the position $r_i = \frac{3R}{4}$ is lower compared to the position $r_i = \frac{R}{4}$. This can be interpreted

as the opposite behavior of the binding energy at these values of the impurity.

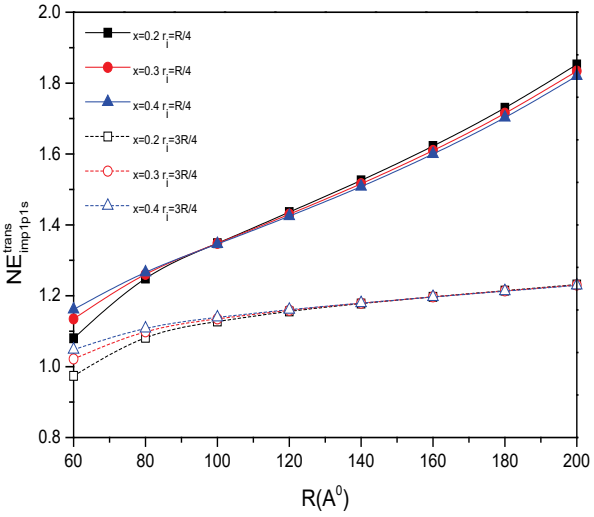

Figure 2. *Variation of normalized intradonor transition energy with quantum dot radius. The aluminum concentration and impurity positions are the same as Figure 1.*

The change of normalized intradonor transition energy depending on the radius of the SQD for different aluminum concentrations (x=0.2, 0.3 and 0.4) and impurity positions ($r_i = \frac{R}{4}$ *and* $\frac{3R}{4}$) is examined in Figure 2. It is observed that with increasing radius of SQD, normalized intradonor transition energy tends to increase almost in both positions of impurity. In addition, for values of SQD radius smaller than about $R=100A^0$, normalized intradonor transition energy also increases as aluminum concentration increases for both positions of impurity. On the other hand, for values of radius greater than $R=100A^0$, the normalized intradonor transition energy for impurity position $r_i = \frac{R}{4}$ decreases with increasing aluminum concentration, while for impurity position $r_i = \frac{3R}{4}$, the increase in aluminum concentration does not affect the normalized intradonor transition energy.

Therefore, by examining the change in normalized intradonor transition energy depending on the SQD radius, information can be obtained about the effect of impurity location and aluminum concentration on normalized intradonor transition energy, and it can be said that the obtained results will make a significant contribution to researchers in determining which values of impurity location and aluminum concentration to use in their studies.

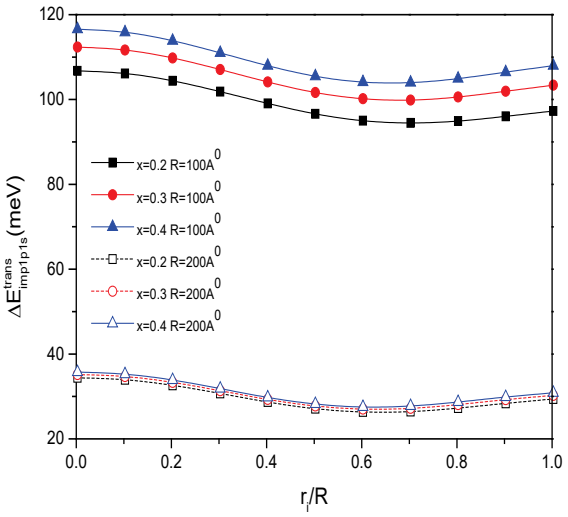

Figure 3*. Dependence of the intradonor transition energy on impurity position for different aluminum concentrations and dot radius R=100, 200A^0.*

In Figure 3, the change of intradonor transition energy depending on the impurity position is investigated for different aluminum concentrations and SQD radius. While the intradonor transition energy increases with the increase in aluminum concentration, it decreases with the increase in the SQD radius and the obtained results are in accordance with Figure 1. Additionally, the intradonor transition energy first decreases, becomes minimum at the impurity location around $r_i/R=0.5$, and then starts to increase again. This is because the probability of finding an electron in a SQD in an excited state is maximum around the impurity position $r_i/R = 0.5$, and at this value of the impurity position the intradonor transition energy is expected to be minimum.

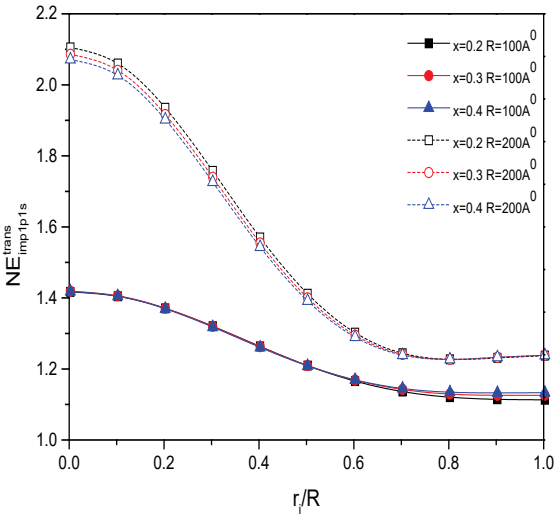

Figure 4. *The change of normalized intradonor transition energy depending on the position of the impurity. The aluminum concentration and dot radius values are taken as the same as in Figure 3.*

The change of normalized intradonor transition energy depending on the impurity position for different aluminum concentrations and SQD radius is presented in Figure 4. It is observed that at both values of the SQD radius, the normalized intradonor transition energy first decreases with the increase of the impurity position, and remains almost constant after the impurity position $r_i/R=0.8$. In addition, the effect of aluminum concentration on the normalized intradonor transition energy is more pronounced before the impurity location at approximately ri/R=0.8 for the radius $R=100A^0$ value, while it is more pronounced after the impurity location at approximately ri/R=0.8 for the radius $R=200A^0$ value. Moreover, at the value of radius $R=100A^0$, the normalized intradonor transition energy decreases with the increase of aluminum concentration until the value of the impurity location approximately ri/R=0.8 and then remains constant, while at the value of radius $R=200A^0$, the normalized intradonor transition energy remains constant until the value of the impurity location approximately ri/R=0.8 and then increases with the increase of aluminum concentration. Thus, by examining the normalized intradonor transition energy, it provides information to researchers about the importance of choosing the aluminum concentration, SQD radius and impurity location that they will use in future studies.

CONCLUSION

In this study, the variations of the intradonor transition energy and normalized intradonor transition energy of an electron in the SQD with respect to the radius and impurity location are investigated. First of all, the calculation of intradonor transition energies is of great importance in determining the optical properties of the $InAs/In_{1-x}Al_xAs$ SQD considered in the study. Secondly, the calculation of normalized intradonor transition energy shows more clearly the importance of the selection of factors such as aluminum concentration, SQD radius and impurity location, which have significant effects on determining the physical and electronic properties of the structures. According to the literature, this study calculates changes in electron intradonor transition energy and normalized intradonor transition energies based on different aluminum concentrations in $InAs/In_{1-x}Al_xAs$ SQD for the first time.

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