THE EFFECT OF PRESSURE ON EXCITED STATE BINDING ENERGY, EXPECTATION VALUE OF THE ELECTRON-IMPURITY AND IMPURITY SELF-POLARIZATION IN A GAAS-$GA_{1-X}AL_XAS$ SPHERICAL QUANTUM DOT

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Abstract
The excited state, 2p, energy of a hydrogenic impurity in GaAs-$Ga_{1-X}Al_XAs$ spherical quantum dot, is computed as a function of the donor positions and the pressure. In order to study the polarization dependency on the location of a donor ion, for the first time we define impurity self-polarization. We study how the impurity self-polarization depends on the location of the impurity and the pressure. We have also shown that expectation value of the electron-impurity is dependent on the impurity position and pressure.

Keywords: binding energy, impurity self-polarization, excited state.

INTRODUCTION

There is an increasing interest in the electronic and optical properties of the of the hydrogenic impurity which is confined in semiconductor quantum dots (QDs) recently [1-3]. Quantum dots confine charge carriers in all three space dimensions and their size, shape, and other properties can be controlled in experiments. Because of the simplicity, spherical shape quantum dot has been preferred. The spherical symmetry allows one to reduce the problem to that of the solving Schrodinger equation in the radial variable [4-5]. A donor impurity plays an important role in quantum dots. In recent years, increasing attention has been focused on the problem of donor impurity states in a single quantum dot under the influence of hydrostatic pressure.

There are many studies focused on the ground state binding energy [6]. In the present work, we calculate the binding energy for excited state 2p of a donor impurity in a spherical quantum dot, expectation value of the electron-donor impurity distance, and polarization of the donor impurity as a function of the impurity position and pressure, using the effective-mass approximation within a variational approach.

THEORY

In the effective mass approximation, in the presence of an off-centre hydrogenic impurity located at $\vec{r}_i = (0,0,z_i)$, the Hamiltonian in a spherical quantum dot is given by [7],

$$H = -\frac{\hbar^2}{2m^*(P)}\nabla^2 - \frac{e^2}{\epsilon(P)r} + V(r,P), \quad (1)$$

Where $V(r,P), \varepsilon(P) and\ m^*(P)$, are the hydrostatic pressure dependent confining potential, the electric constant and the effective mass of the electron, respectively. The explicit expressions of effective mass, radius and dielectric constant are defined as [8,9],

$$m^*(P) = m^*(0)\exp(0.078P) \quad (2)$$

$$R(P) = R(0)(1 - 1.5082 * 10^{-3}P) \quad (3)$$

$$\epsilon(P) = 13.13 - 0{,}088P \quad (4)$$

The confining potential is given by [3]

$$V(r,P) = \begin{cases} 0 \quad , & r < R \\ V_0(x,P) = 0.6 * (1.155x + 0.37x^2 + PD(x)), & r \geq R \end{cases} \tag{5}$$

Where $D(x) = -1.3 * 10^{-2}\, x \, \frac{eV}{GPa}$ and x is Al concentration and where we choose as $0.2 \leq x \leq 0.4$.

In the presence of the impurity for excited state($n = 2, l = 1, m = 0$), the trial eigen functions of the Hamiltonian for 2p-state are chosen to be [10],

$$\psi_{2p}(\vec{r}, V_o, R, r_i) = \begin{cases} N_{2pi}\left(\frac{sin(k_{1si}(P)r)}{r}\right) r\cos\theta \exp\left(-\lambda_p\sqrt{r^2 + r_i^2 - 2rr_i\cos\theta}\right) & ,r < R \\ N_{2po}(\,exp(-k_{1so}(P)r)/r)r\cos\theta\exp\left(-\lambda_p\sqrt{r^2 + r_i^2 - 2rr_i\cos\theta}\right), & r \geq R \end{cases} \tag{6}$$

where λ_p is the variational parameter. The binding energy of 2p-state binding energies of an off-centre hydrogenic impurity in the dot [10] is defined, as

$$E_{b2p}(V_o, R, P, r_i) = E_{2p}^0(V_o, P, R) - E_{im2p}(V_o, R, P, r_i)\,. \tag{7}$$

Where $E_{2p}^0(V_o, P, R)$, the excited state energy in the absence of the impurity of system(n=2,l=1) is obtained by solving radial Schrodinger equation.

The electron-impurity distance changes with the impurity position r_i, dot radius R and confining potential $V(r)$. The 2p-state expectation value $\langle|r\cos\theta - r_i|\rangle_{2p}$ is given by [11],

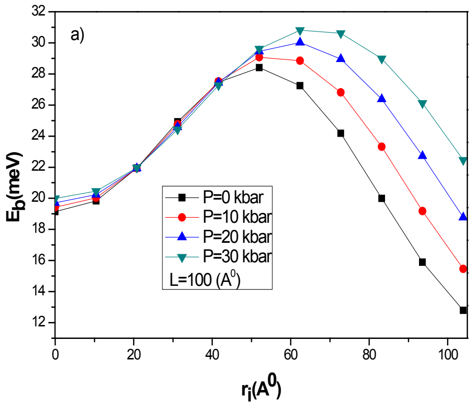
$$\langle|r\cos\theta - r_i|\rangle_{2p} = \frac{\langle\psi_{2p}(\vec{r},r_i,R)||r\cos\theta - r_i||\psi_{2p}(\vec{r},r_i,R)\rangle}{\langle\psi_{2p}(\vec{r},r_i,P,R)|\psi_{2p}(\vec{r},r_i,R)\rangle} \tag{8}$$

The impurity self-polarization along the $\vec{r}_i$ direction for the 2p excited state can be defined as [11]

$$sP_{i2p}(V_0, R, r_i) = \left[\frac{\langle\psi_{2p}(\vec{r},r_i,R)|-e(r\cos\theta - r_i)|\psi_{2p}(\vec{r},r_i,R)\rangle}{\langle\psi_{2p}(\vec{r},r_i,R)|\psi_{2p}(\vec{r},r_i,R)\rangle_{r_i\neq 0}}\right] - \left[\frac{\langle\psi_{2p}(\vec{r},r_i,R)|-e(r\cos\theta - r_i)|\psi_{2p}(\vec{r},r_i,R)\rangle}{\langle\psi_{2p}(\vec{r},r_i,R)|\psi_{2p}(\vec{r},r_i,R)\rangle_{r_i=0}}\right] \tag{9}$$

RESULTS

We have investigated the 2p state binding energy of hydrogenic impurity in spherical quantum dot under the influence of hydrostatic pressure. Calculations have been carried out to calculate binding energy and self- polarization of the spherical quantum dot. The parameters used in calculation are $m^*=0.067m_0$ and $\varepsilon_0 = 12.5$. The results are presented in Figs. 1-2.



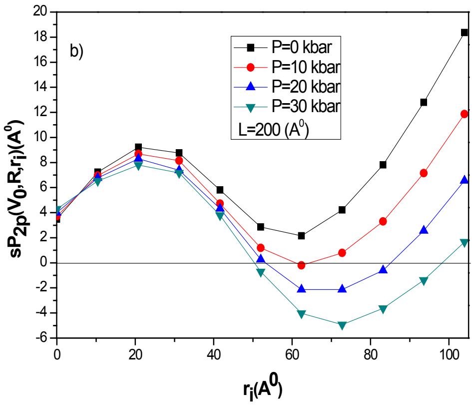
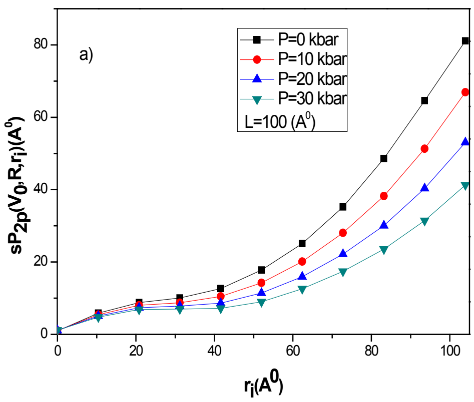


Figure 1. *The binding energies of 2p excited state of a donor impurity as a function of the impurity position confined in the spherical quantum dot for radii (a) L=100A^0 and b) L=200A^0.*

In figure 1(a and b) show that variation of impurity binding energy with impurity position varies from the center to a position in of the dot for the different values of four hydrostatic pressures P=0kbar, 10kbar, 20kbar and 30kbar. In fig.1a, it is clearly seen that the character of the binding energy variation with the impurity position under hydrostatic pressure is similar to without pressure. For the small dot radius, the effect of the pressure on the binding energy is more dominant. The hydrostatic pressure is not very important for the large dot radius [10].



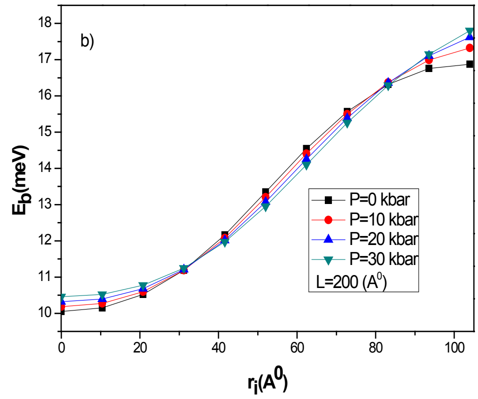


Figure 2*. The impurity self-polarizations of 2p excited state as a function of the impurity position confined in the spherical quantum dot for radii L=100A^0 and b) L=200A^0.*

In Figure 2 (a and b), we investigated the excited state impurity self-polarization as a function of impurity position for different values of dot radius and pressure. In Fig.2a, it is seen that the excited state impurity self-polarization decreases for any impurity positon when the dot radius and pressure increase [11].

CONCLUSIONS

In this study, the effects of hydrostatic pressure on the binding energy of the excited state of an off-center hydrogenic impurity, excited state 2p impurity self- polarization and the expectation values of the 2p electron-impurity was investigated. The result showed that binding energies increase to a maximum point and then decrease as the impurity position increase for L=100 A^0. The hydrostatic pressure also decreases impurity self-polarization when impurity position increases.

REFERENCES

[1] G Bastard Phys. Rev. B 24 4714 (1981)
[2] R L Greene and K K Bajaj Phys. Rev. B 31 4006 (1985)
[3] I Erdogan, O Akankan and H Akbas Superlattices Microstruct. 59 13 (2013)
[4] S Baskoutas and A F Terzis Eur. Phys. J. B 69 237 (2009)
[5] E Sadeghi Phys. E 41 1319 (2009)
[6] N P Montenegro and S T P Merchancano Phys. Rev. B 46 9780 (1992)
[7] B.H. Bransden, C.J. Joachain, Quantum Mechanics, second ed., Pearson, Harlow, 2000.
[8] A.J. Peter, Physica E 28 (2005) 225.
[9] Sr. G. Jayam, K. Navaneethakrishnan, Solid State Commun. 126 (2003) 681.
[10] P Bulut, I Erdogan and H Akbas Phys. E 63 299 (2014)
[11] A. I. Mese et al., Indian J Physics 91 263 2017)