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# Simultaneous Effects of Hydrostatic Pressure and External Electric Field on the Energy Spectra of Two Donors in a Strained Zinc Blende GaN/AlGaN Quantum Dot

Research Article

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**Abstract.** The energy spectrum of two donors in a strained GaN quantum dot embedded in $Al_xGa_{1-x}N$ has been investigated under the influence of hydrostatic pressure and external electric field. Our calculations are carried out using variational principle within the single band effective mass approximation by means of dot radius, hydrostatic pressure, and electric field. The numerical results show that the binding energy of two donors increase, attains a maximum value, and then decreases as the quantum dot radius increases for any electric field. Moreover, the binding energy of two donors increases with the pressure for any size of dot. Our results are compared with existing literature.

**Keywords.** Strained quantum dot; Variational method; Hydrostatic pressure; Electric field

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## 1. Introduction

The present decade is seeing remarkable activities on the physics of low-dimensional system both experimentally and theoretically [1]. The subject of low-dimensional semiconductors is an penetrating electric field and quantum size effects is that they exhibit some physical properties such as optical and electronic transport qualities which are totally not quite the same as those of the bulk semiconductor constituents has been a point of incredible enthusiasm for quite a while

[2,3]. The study of optical properties of three-dimensionally confined electrons and holes in QDs in external fields is vital in view of their potential application to novel quantum devices [4]. Consequently, GaN/$Al_xGa_{1-x}N$ is truly appropriate for the optoelectronic devices working in the short wavelengths of visible and ultraviolet spectral regions [5]. An external electric field along the progress path of *quantum dots* (QDs) can be utilized to control and modify the output intensity of the optoelectronic devices, so the function of the electric effect has been broadly contemplated for quantum well [6] and QDs [7,8].

The study of hydro-genic impurity states is one of the foremost difficulties in semiconductor low-dimensional systems because their occurrence impacts greatly the electronic mobility and optical properties. In this way, in the past several years, theoretical researching by applying external perturbations, such as applied electric field and hydrostatic pressure on the impurity states in semiconducting nanostructures [9, 10]. These outcomes exposed that the applied electric field and hydrostatic pressure clearly affected the impurity states in semiconducting nanostructures. Be that as it may, as far as anyone is concerned, few papers are associated with examining the impurity states in ZB nitrides-based nanostructures, such as ZB GaN/AlN quantum dot QD, by applying external perturbations to date.

The investigation on confined donors or acceptors in QDs low-dimensional semiconductor heterostructures have been made by several authors [11–14]. There has been no report of the calculation of simultaneous effects of hydrostatic pressure on the energy spectra of two donors in a strained zinc quantum dots in the presence of an electric field. The study of the behavior of simultaneous effects of hydrostatic pressure and energy levels in strained quantum dots in the presence of an electric field will prompt to a superior comprehension of their properties and is the subject of this article. In this paper, we will investigate theoretically the energy spectra of two donors in a strained Zinc Blende GaN/AlGaN QD, as the effects of the applied hydrostatic pressure and electric field.

## 2. Modal and Theory

The Hamiltonian for two donors confined in the strained ZB GaN/GaAlN QD, under the influence of the hydrostatic pressure and applied electric field along the growth direction, within the framework of effective-mass approximation may be written as

$$H = H_0 - \frac{e^2}{4\pi\varepsilon_0\varepsilon(P)|r_1 - r_2|} \tag{2.1}$$

with

$$H_0 = \sum_{j=1}^{2}\left[\frac{1}{2m^*}\left(\bar{p}_j + \frac{e}{c}\bar{A}_j\right)^2 + V_D(\bar{r}_j) + eF.r_j\right] \tag{2.2}$$

where $F$ is external electric field along $Z$ axis

$$V_D = \frac{V_{0B}r^2}{R^2} \quad \text{for } |r| \le R \text{ and } V_D = V_{0B} \text{ for } |r| > R$$

$V_{OB}(\bar{r})$ is the barrier height given by $V_{OB}(\bar{r}) = Q_c\Delta E_g(x)$. $Q_c$ is the conduction band off-set parameter, which is taken to be 70% of the conduction band and $m^*$ is the effective mass of

the electron which is equivalent to $0.19\,m_e^*$ and $\varepsilon_o$ is the effective dielectric constant of the quantum dot, and $\varepsilon(P)$ is the pressure-dependent effective mean relative dielectric constant of the zinc blende GaN material.

Due to the mismatch of lattice constants and applied hydrostatic pressure, we consider the variations of parameters, such as dot size, dielectric constant and effective mass. The donor binding energy is affected by the variations. In present paper, we display the above parameters of GaN and AlN depends on strain and hydrostatic pressure. The corresponding parameter of $Al_xGa_{1-x}N$ can be obtained by linear interpolation method [15].

The pressure dependent lattice constant is expressed by Murnaghan state equation [16]:

$$a_j(P) = a_j(0)\left[1 - \frac{P}{3B_{oj}}\right] \tag{2.3}$$

where $a_j(0)$ is the $j$ material's lattice constant for zero pressure, and $B_{oj}$ is the $j$ material's bulk modulus of zinc-blende structure.

The variations of biaxial and uniaxial strain tensor ratio with pressure can be written as [17]

$$\varepsilon_{xx,j}(P) = \varepsilon_{yy,j}(P) = \frac{a_k(P) - a_j(P)}{a_j(P)}, \tag{2.4}$$

$$\varepsilon_{zz,j}(P) = -2\frac{C_{12,j}}{C_{11,j}}\varepsilon_{xx,j}(P), \tag{2.5}$$

where $j$ is GaN($Al_xGa_{1-x}N$) material, $k$ is $Al_xGa_{1-x}N$ (GaN) material, and $C_{11,j}$ and $C_{12,j}$ are elastic constants for $j$ material.

The hydrostatic pressure $P$ dependent band gap is given as [16]

$$E_{g,j}(P) = E_{g,j}(0) + bP + cP^2, \tag{2.6}$$

where $b$ and $c$ are the pressure coefficient of band gap for GaN or $Al_xGa_{1-x}N$ and the band gap of $Al_xGa_{1-x}N$ for zero pressure obtained by linear interpolation method.

In the strained zinc blende GaN quantum dot, the variation of band gap with the pressure and strain can be considered as [17]

$$E_{g,j}(P,\varepsilon) = E_{g,j}(P) + (\alpha_j^c - \alpha_j^v)[2\varepsilon_{xx,j}(P) + \varepsilon_{zz,j}(P)], \tag{2.7}$$

where $\alpha_j^c$ and $\alpha_j^v$ are the deformation potentials of conduction and valence band, respectively.

The pressure and strain dependent electronic effective mass is given by [18]

$$\frac{m_e}{m_j} = 1 + \frac{C_j}{E_{g,j}(P,\varepsilon)}, \tag{2.8}$$

where $C_j$ is a constant and can be determined by solving eq. (2.9) when $P = 0$. The hydrostatic pressure dependence of frequencies can be written by the Gruneisen parameter [16].

$$\gamma_{ij} = B_{0j}\frac{1}{\omega_{i,j}}\frac{\partial\omega_j(P)}{\partial P} \qquad [i = LO, TO]. \tag{2.9}$$

The modified phonon energy due to pressure can be written as,

$$\hbar\omega_{i,j}(P) = \hbar\omega_{i,j}\exp\left(\frac{r_{i,j}}{B_{o,j}}P\right) \qquad [i = LO, TO]. \tag{2.10}$$

The hydrostatic pressure dependence of high frequency dielectric constant can be written as [19]

$$\varepsilon_{\infty,j}(P) = 1 + [\varepsilon_{\infty,j} - 1]\exp\left[\frac{5}{3B_{0,j}}(f_{ion,j} - 0.9)P\right]. \tag{2.11}$$

Using the *Lyddane-Sachs-Teller* (LST) relationship [17], the static-dielectric constant with pressure effect can be given as,

$$\varepsilon_{0,j}(P) = \varepsilon_{\infty,j}(P)\left[\frac{\hbar\omega_{LO}}{\hbar\omega_{TO}}\right]^2. \tag{2.12}$$

Using the linear interpolation method, the other parameters with pressure for ternary mixed crystal $Al_xGa_{1-x}N$ can be obtained as follows:

$$Q_{Al_xGa_{1-x}N} = (1-x)Q_{GaN} - xQ_{AlN}, \tag{2.13}$$

where $Q_{GaN}$ and $Q_{AlN}$ are the corresponding parameters associated with GaN and AlN, respectively.

In order to calculate the ground state binding energy of two donor impurities in ZB GaN/AlGaN QD, the trial wave function may be written as,

$$\Psi_{1s}(\bar{r}_1,\bar{r}_2) = \begin{cases} N_1\frac{\sin(\alpha_1 r)}{r}(1+\nu Fr\cos\theta)e^{-\gamma r^2}e^{-\lambda r^2}e^{-\zeta_1 r_1}e^{-\zeta_2 r_2}, \\ N_2\frac{e^{-\beta_1 r}}{r}(1+\nu Fr\cos\theta)e^{-\gamma r^2}e^{-\lambda r^2}e^{-\zeta_1 r_1}e^{-\zeta_2 r_2}, \end{cases} \tag{2.14}$$

where $\lambda\gamma$, $\zeta_1$ and $\zeta_2$ are the variational parameters.

The confining potential energies of two interacting donors are calculated using the wave functions eq. (2.14) for $1s$ states is obtained by

$$H_{IE} = \left\langle \Psi_{1s}(\vec{r}_1,\vec{r}_2)\left|\frac{2}{|\vec{r}_1-\vec{r}_2|}\right|\Psi_{1s}(\vec{r}_1,\vec{r}_2)\right\rangle. \tag{2.15}$$

In the above equation $|\vec{r}_1 - \vec{r}_2|$ determines the role of inter donor distances in the Coulomb interaction energy of two donor systems.

The ground state energy of two donor impurities in ZB GaN/AlGaN QD, may be obtained by minimizing

$$E = \min_{\gamma,\zeta}\frac{\langle\Psi_{1s}(\bar{r}_1,\bar{r}_2)|H|\Psi_{1s}(\bar{r}_1,\bar{r}_2)\rangle}{\langle\Psi_{1s}(\bar{r}_1,\bar{r}_2)|\Psi_{1s}(\bar{r}_1,\bar{r}_2)\rangle}. \tag{2.16}$$

The ground state binding energy of two donors $E_b$ can be obtained as follows:

$$E_b = E_0 - E, \tag{2.17}$$

where $E_0$ is the ground state energy for the Hamiltonian of eq. (2.2).

## 3. Results and Discussion

We have calculated the ground state binding energy of two donors as functions of the dot radius, the hydrostatic pressure and applied electric field F in a strained ZB $GaN/Al_xGa_{1-x}N$ quantum dot. In our calculation, we use the band gap difference [20] of $E_{g,AlGaN} = E_{g,GaN}(1-x) + xE_{g,AlN} + 530(1-x)x$ (meV) and assuming 70% contribution to the conduction band, the value of $V_0$ is $V_0 = 0.6\,(E_{g,AlGaN} - E_{g,GaN})$. The concentration $x$ in the $Al_xGa_{1-x}N$ material is selected as 0.2.

The parameters used in the computations are got from references [16, 21–23].

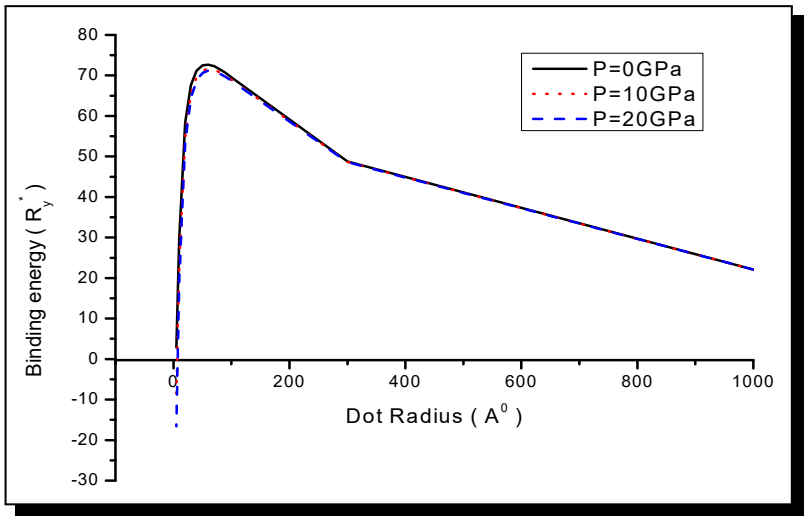
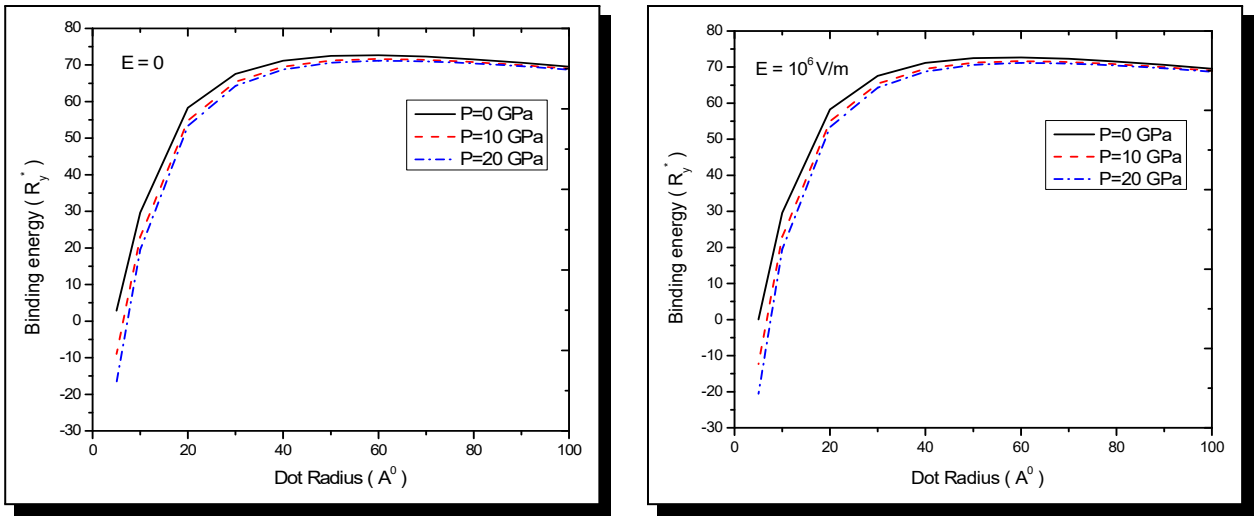



**Figure 1.** Variation of binding energy with dot radius as a function of pressure for without electric field

The ground-state binding energy of two donors in a strained ZB GaN/$Al_xGa_{1-x}N$ is displayed in Figure 1 as a function of the dot radius for different hydrostatic pressures ($P = 0, 10$ and 20 GPa) without electric field. It can be observed that the binding energy of donor linearly increases when the hydrostatic pressure increases. This is because the electron inside the quantum dot is much more localized when the hydrostatic pressure is increased. We also found that firstly, the donor binding energy increases until a maximum value, and then it begins to drop quickly in all the cases with the decrease of the dot radius. Thus, the increase in hydrostatic pressure enhances the Coulomb interaction between the electron and the impurity and the donor binding energy. In particular, it is also shown that the donor binding energy is much more sensitive to the hydrostatic pressure when the dot size is small.




**(a)** **(b)**

**Figure 2.** Variation of binding energy with dot radius as a function of pressure for $E = 0$ V/m and $E = 106$ V/m respectively

Figure 2a and 2b shows that the binding energy of donor impurity states as a function of the dot radius for different values of the electric field with the applied hydrostatic pressure. It is obviously seen that the donor binding energy hardly changes with respect to the applied electric field in the regime of strong geometric confinement. The binding energy diminishes when the quantum dot confinement decreases and the behavior becomes stronger in applied field increases. Thus, the electron wave function is more firmly localized inside the QD with decreasing the dot radius by the simultaneous application of electric field and hydrostatic pressure, and the Coulomb interaction between the electron and the impurity ion is increased, so the donor binding energy enhances correspondingly. However, below a certain value of the dot radius, the donor binding energy starts decreasing due to leakage of the electron wave function into the barrier region as shown in Figure 2.

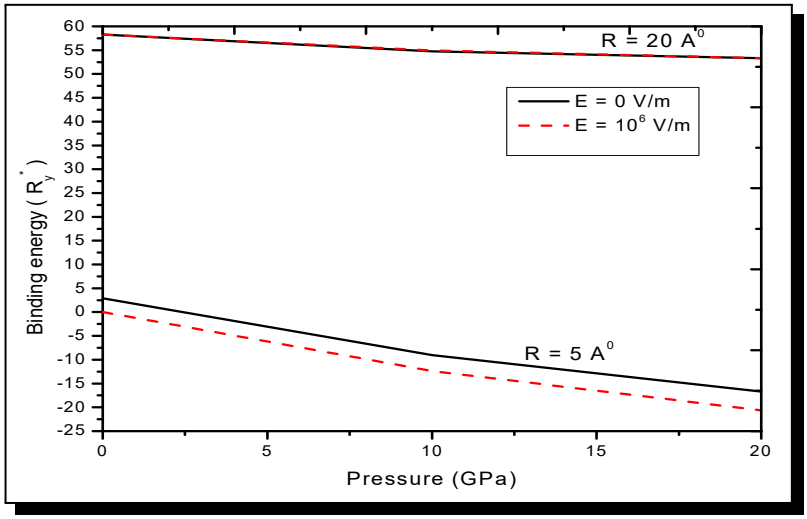



**Figure 3.** Binding energy as a function of pressure for different electric fields

In Figure 3, the binding energy is plotted as a function of the hydrostatic pressure for different quantum dot radii for different electric field. It shows that the impurity binding energy increases nearly linearly with the increasing pressure. In particular, the donor binding energy is much more sensitive to the hydrostatic pressure when the applied electric field is larger. Due to the simultaneous influence of electric field and hydrostatic pressure, the relative distance between the electron and the impurity is decreased, and then the Coulomb interaction is increased, when the dot size is reduced. However, below a certain value of dot radius, tunneling comes to play due to simultaneous effect of pressure and electric field.

In Figure 4 the variation of binding energy is shown as a function of electric field for various pressure for a particular dot of radius of $R = 20\,\mathrm{A}^\circ$. The increase of applied electric field leads to an enhancement of the binding energy linearly. We also observe that the influence of pressure is more appreciable for the strong confinement. It is also observed from the fact that the smaller external electric field along with hydrostatic pressure enhances the localization effect of the electron wave function in the dot. The distance between the electron and the impurity ion decreases, which causes the increase of the donor binding energy. When the applied electric

field is increases to a certain value, the probability of the electron in the dot leaking into barrier layer, which leads to the decrease of the donor binding energy.

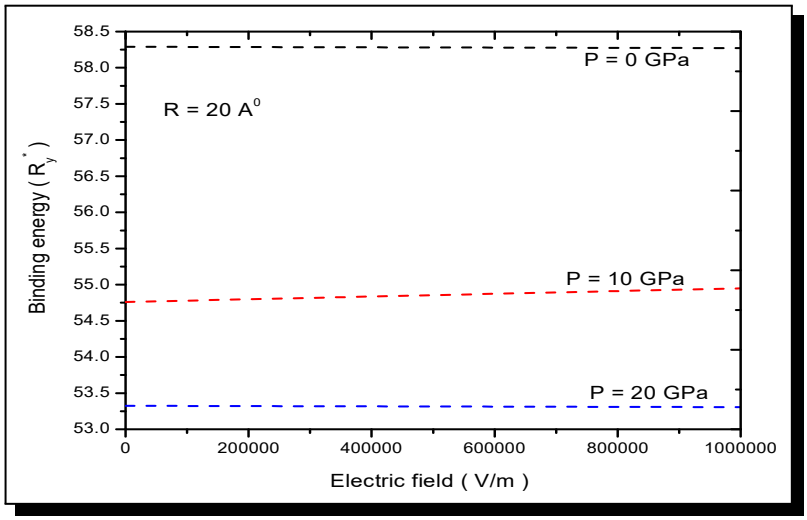



**Figure 4.** Variation of binding energy as a function of electric field for various pressure for a particular dot of radius $R = 20$ A°

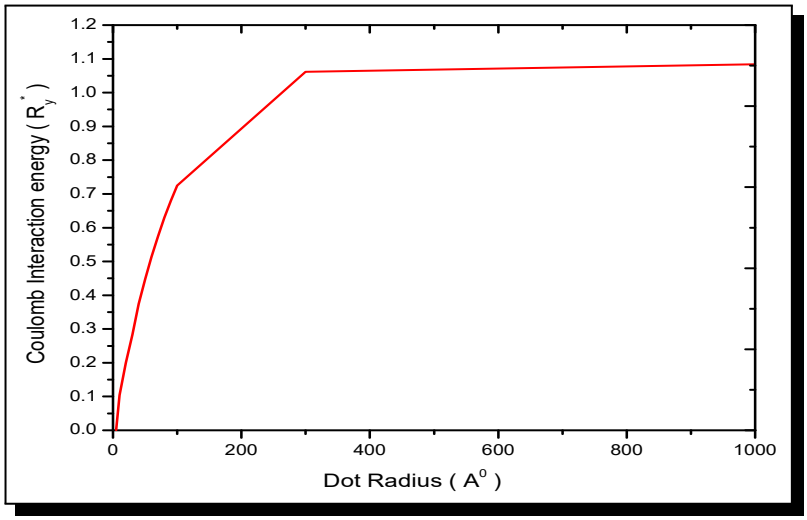



**Figure 5.** Variation of Coulomb interaction energy as a function of dot radius for high electric field ($10^6$ V/m) and high pressure ($P = 20$ GPa)

The variation of Coulomb interaction energy as a function of dot radius for high electric field and high pressure is as shown in Figure 5 for a constant inter donor distances ($r_1 - r_2 = 50$ A°). We observed that the interaction energy significantly increases the donor binding energy. It also noticed that Coulomb interaction energy increases with increase in dot size and reaches a constant value when approaching the bulk limit. It can be understood in a simple way that there is a rich competition between three physical phenomena such as geometric confinement, applied electric field and applied hydrostatic pressure. It results that, the geometric confinement

plays a predominant role over the three physical phenomena which is well known as quantum confinement effect. It is shown that the interaction energy strongly depends on inter donor distances and the interaction energy is appreciable when approaching the inter donor distances.

## 4. Conclusion

In conclusion, the binding energy of two donors in a strained zinc-blende GaN/$Al_xGa_{1-x}N$ spherical QD is discussed with a variational method by considering the simultaneous effect of hydrostatic pressure and applied electric field. Our results show that the binding energy of two donor impurities increases with pressure for any dot radius and decreases with electric field. The influence of strain effects on the binding energy for small dot radius is stronger compared to that of larger dot radius. We also hope that our results can stimulate further investigations of the related physics, as well as device applications in strained ZB GaN/AlGaN QD.

### Competing Interests

The authors declare that they have no competing interests.

### Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

## References

[1] K.-F. Berggren, *Int. J. Quant. Chem.* **33** (1988) 217, DOI: 10.1002/qua.560330306.

[2] G. Bastard, E. E. Mende, L. L. Chang and L. Esaki,

[3] G. Bastard, *Phys. Rev. B* **24**, 4714 (1981), DOI: 10.1103/PhysRevB.24.4714.

[4] U. Hohenester and E. Molinari, *Phys. Status Solidi* (A) **178** (2000) 277, DOI: 10.1002/1521-396X(200003)178:1%3C277::AID-PSSA277%3E3.0.CO;2-A.

[5] E. T. Yu, G. J. Sullivan, P. M. Asbeck, C. D. Wang, D. Qiao and S. S. Lau, *Appl. Phys. Lett.* **71**, 2794 (1997), DOI: 10.1063/1.120138.

[6] N. Wuritu and G. Jian, *Journal of Optoelectronics Laser* **21**, 1102 (2010) (in Chinese).

[7] C. I. Mendoza, G. J. Vazquez, M. Del Castillo-Mussot and H. Spector, *Phys. Rev. B* **71**, 075330 (2005), DOI: 10.1103/PhysRevB.71.075330.

[8] C. Dane, H. Akbas, S. Minez and A. Guleroglu, *Physica E: Low-dimensional systems and Nanostructures* **41**, 278 (2008), DOI: 10.1016/j.physe.2008.07.016.

[9] S. S. Li and J. B. Xia, *J. Appl. Phys.* **101**, 093716 (2007), DOI: 10.1063/1.2734097.

[10] N. Raigoza, A. L. Morales, A. Montes, N. Stress effects on shallow-donor impurity states in symmetrical GaAs/$Al_xGa_{1-x}As$ double quantum wells, *Phys. Rev. B* **69**, 045323 (2004), DOI: 10.1103/PhysRevB.69.045323.

[11] S. T. Perez-Merchancano, H. Paredes-Gutierrez and J. Silva Valencia, *J. Phys: Condens. Matter* **19**, 026225 (2007), DOI: 10.1088/0953-8984/19/2/026225.

**[12]** Y.-F. Huangfu and Z. W. Yan, *Journal of Inner Mongolia University* **39**, 18 (2008).

**[13]** W. Hui-Ting, W. Hai-Long and J. Li-Ming, *Acta Physica Sinica* **58**, 465 (2009) (in Chinese), DOI: 10.7498/aps.58.465.

**[14]** E. Sadeghi, *Physica E: Low-dimensional Systems and Nanostructures* **41**, 1319 (2009), DOI: 10.1016/j.physe.2009.03.004.

**[15]** S. Adachi, *J. Appl. Phys.* **58**, R1 (1985), DOI: 10.1063/1.336070.

**[16]** Z. W. Yan, S. L. Ban and X. X. Liang, *The Eur. Phys. J. B : Condensed Matter and Complex Systems* **35**, 41 (2003), DOI: 10.1140/epjb/e2003-00254-8.

**[17]** L. Shi and Z. W. Yan, *Phys. Stat. Sol. C* **8**, 42 (2011), DOI: 10.1002/pssc.201000625.

**[18]** D. Z.-Y. Ting and Y.-C. Chang, *Phys. Rev. B* **36**, 4359 (1987), DOI: 10.1103/PhysRevB.36.4359.

**[19]** J.-M. Wagner and F. Bechstedt, *Phys. Rev. B* **66**, 115202 (2002), DOI: 10.1103/PhysRevB.66.115202.

**[20]** H. Wang, G. A. Farias and V. N. Freire, *Phys. Rev. B* **60**, 5705 (1999), DOI: 10.1103/PhysRevB.60.5705.

**[21]** I. Vurgaftman, J. R. Meyer and L. R. Ram-Mohan, *J. Appl. Phys.* **89**, 5815 (2001), DOI: 10.1063/1.1368156.

**[22]** A. R. Goñi, H. Siegle, K. Syassen, C. Thomsen and J.-M.Wagner, *Phys. Rev. B* **64**, 035205 (2001), DOI: 10.1103/PhysRevB.64.035205.

**[23]** N. E. Christensen and I. Gorczyca, *Phys. Rev. B* **50**, 4397 (1994), DOI: 10.1103/PhysRevB.50.4397.