GROUND AND EXCITED STATES OF D^0 AND D^- DONORS IN A SPHERICAL QUANTUM DOT

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For the spherical nanoheterostructure Si/SiO_2 in the approximation of effective mass for nondegenerated bands, we calculated the energies of the ground and excited states of the electrons of neutral (D^0) and negatively charged (D^-) donors as functions of the radius of a quantum dot, on the basis of the exact solution of the Poisson and Schrödinger equations. The singlet and triplet states for D^- donor are determined, and the dependence of the energies of the ground states of D^0 and D^- donors on the dielectric permittivity of the matrix is studied.

1. Introduction

Admixture states in various bounded systems such as quantum wells (QW), quantum threads (QT), and quantum dots (QD) are a subject of intense studies in fundamental and applied works. To describe the main properties of QD, most of the works use the continual model of quantum dot, whose results are in good agreement with experimental data. In the frame of this model, the first theoretical studies of admixture states in QD were carried out in [1–8]. The solutions of the Schrödinger equation were obtained for a hydrogen-like neutral admixture with the Coulomb interaction between particles without regard for the fact that the dielectric permittivity is different for separate components of the heterosystem. In calculations, we used the mean value of this quantity. The calculation showed that the energy of the 1S ($n_r = 0$, $l = 0$) state at great radii tends to the value which is determined by the effective Rydberg energy ($-\mathrm{Ry}^*$) like in a hydrogen-like atom. It was also shown that the states 2S ($n_r = 1$, $l = 0$) and 2P ($n_r = 1$, $l = 1$) which are degenerate in a free hydrogen atom split in QD, if the radius of QD becomes less than $8a_0^*$, where a_0^* is the effective Bohr radius. But if the radius of QD is greater than $10a_0^*$, then the indicated states have the same energy ($-0.25\mathrm{Ry}^*$) which equals the excited state energy for the free hydrogen atom. For very small values of the radius of QD ($a < 0.5a_0^*$), the energies of states tend to values which are the sum of hydrogen-like energies and the confinement potential.

The ground and excited levels of donors D^0 and D^- in the heterostructure with a quantum well in a magnetic field were studied in [9] by using the variation method. In [10], it was experimentally shown that the binding energy of a D^- donor in a two-dimensional QW is significantly greater than that in the three-dimensional case. The dependence of the ground energy levels of donors D^0 and D^- in a spherical QD on the radius and the various confining potentials (rectangular, parabolic, and triangular ones) was determined in [11]. The interaction between charged particles was presented in the form of the Coulomb interaction in a dielectric homogeneous medium.

The influence of polarization charges of the surface of a nanoheterostructure on the energy of a quasiparticle is studied in works [12–15]. In those works with the use of the force potential of electrostatic images, the presence of bound surface charges on the interface was taken into account for heterosystems of different nature. In heterostructures, where the dielectric permittivity of the matrix is less than that in QD, the account of the polarization increases the effective bandgap [16]. In addition, it was proved that the successive account of polarization effects allows one to explain a significant increase in the binding energy of an exciton in the given heterostructures.

The use of the mean value of the dielectric permittivity in calculations allows one to describe the properties of heterostructures only approximately. This approximation is not valid for a heterosystem with a great difference between the dielectric permittivities of QD and the matrix. In [8], various values of the dielectric permittivity were chosen in calculations, but the Coulomb energy of interaction of an admixture ion with an electron possesses a discontinuity on the surface of a heterosystem. In further comprehensive studies of donors, it is also important to determine the ground and excited energy states of a negatively charged donor and to find theoretically their dependence on the size of QD.

In the present work on the basis of the solution of the Poisson equation, we obtained the potential energy of interaction of an admixture ion with an electron, with regard for different values of the dielectric permittivities of QD and the matrix. With the use of this potential energy, we exactly solved the Schrödinger equation for a D^0 donor at the center of QD. Moreover, on the basis of the solutions obtained, we determined the ground and excited energies of the S-states of a D^- donor. Specific calculations were performed for the nanoheterosystem Si/SiO_2.

2. Statement of the Problem and Its Solution

We consider a quantum dot with radius a. The dielectric permittivity of QD equals ε_1. It is positioned in the matrix with dielectric permittivity ε_2. At the center of this spherical quantum dot, an admixture is located.

The Hamiltonian for D^- in the approximation of effective mass has the form

$$\mathbf{H} = \mathbf{H}_{0,1} + \mathbf{H}_{0,2} + W(r_1, r_2), \tag{1}$$

where

$$\mathbf{H}_{0,i} = -\frac{\hbar^2}{2}\nabla\frac{1}{m^*(r_i)}\nabla + W(r_i) + U(r_i) \tag{2}$$

is the Hamiltonian for the i-th electron,

$$m^*(r_i) = \begin{cases} m_1^*, & r_i < a, \\ m_2^*, & r_i \geq a \end{cases}$$

is the effective mass of an electron of the heterosystem. The potential energy of interaction of an electron with the admixture ion which is located at the center of QD has the form

$$W(r_i) = -Ze^2 \begin{cases} \dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1\varepsilon_2 a} + \dfrac{1}{\varepsilon_1 r_i}, & r_i < a \\ \dfrac{1}{\varepsilon_2 r_i}, & r_i \geq a. \end{cases} \tag{3}$$

At the same time, the potential energy which is due to the band gap (the confinement potential) of the heterostructure is given by the formula

$$U(r_i) = \begin{cases} -U_1, & r_i < a, \\ 0, & r_i \geq a, \end{cases} \qquad U_1 > 0. \tag{4}$$

On the basis of the solution of the Poisson equation, we can also get the following formula for the interaction of electrons:

$$W(r_1, r_2) = e^2 \times$$

$$\times \begin{cases} \frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1}\sum\limits_{n=0}^{\infty}\frac{n+1}{\varepsilon_1 n+\varepsilon_2(n+1)}\frac{r_1^n r_2^n}{a^{2n+1}}P_n(\cos\theta) + \\ +\frac{1}{\varepsilon_1}\sum\limits_{n=0}^{\infty}\frac{r_2^n}{r_1^{n+1}}P_n(\cos\theta), & \begin{array}{l} r_1 < a, \\ r_2 < a, \\ r_2 < r_1, \end{array} \\ \frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1}\sum\limits_{n=0}^{\infty}\frac{n+1}{\varepsilon_1 n+\varepsilon_2(n+1)}\frac{r_1^n r_2^n}{a^{2n+1}}P_n(\cos\theta) + \\ +\frac{1}{\varepsilon_1}\sum\limits_{n=0}^{\infty}\frac{r_1^n}{r_2^{n+1}}P_n(\cos\theta), & \begin{array}{l} r_1 < a, \\ r_2 < a, \\ r_1 < r_2, \end{array} \\ \sum\limits_{n=0}^{\infty}\frac{2n+1}{\varepsilon_1 n+\varepsilon_2(n+1)}\frac{r_1^n}{r_2^{n+1}}P_n(\cos\theta), & \begin{array}{l} r_1 < a, \\ r_2 > a, \end{array} \\ \sum\limits_{n=0}^{\infty}\frac{2n+1}{\varepsilon_1 n+\varepsilon_2(n+1)}\frac{r_2^n}{r_1^{n+1}}P_n(\cos\theta), & \begin{array}{l} r_1 > a, \\ r_2 < a, \end{array} \\ \frac{\varepsilon_2-\varepsilon_1}{\varepsilon_2}\sum\limits_{n=0}^{\infty}\frac{n}{\varepsilon_1 n+\varepsilon_2(n+1)}\frac{a^{2n+1}}{r_1^{n+1}r_2^{n+1}}P_n(\cos\theta) + \\ +\frac{1}{\varepsilon_2}\sum\limits_{n=0}^{\infty}\frac{r_2^n}{r_1^{n+1}}P_n(\cos\theta), & \begin{array}{l} r_1 > a, \\ r_2 > a, \\ r_2 < r_1, \end{array} \\ \frac{\varepsilon_2-\varepsilon_1}{\varepsilon_2}\sum\limits_{n=0}^{\infty}\frac{n}{\varepsilon_1 n+\varepsilon_2(n+1)}\frac{a^{2n+1}}{r_1^{n+1}r_2^{n+1}}P_n(\cos\theta) + \\ +\frac{1}{\varepsilon_2}\sum\limits_{n=0}^{\infty}\frac{r_1^n}{r_2^{n+1}}P_n(\cos\theta), & \begin{array}{l} r_1 > a, \\ r_2 > a, \\ r_1 < r_2, \end{array} \end{cases} \tag{5}$$

where $P_n(x)$ are the Legendre polynomials.

In Fig. 1, we give the dependence of the potential energy

$$\Pi(r_i) = U(r_i) + W(r_i) = \begin{cases} -\dfrac{Ze^2}{\varepsilon_1 r_i} - U_0(a), & r_i < a, \\ -\dfrac{Ze^2}{\varepsilon_2 r_i}, & r_i \geq a \end{cases} \tag{6}$$

of the i-th particle on the distance from the origin of the coordinate system. In formula (6), we introduced the notation

$$U_0(a) = \frac{Ze^2(\varepsilon_1 - \varepsilon_2)}{\varepsilon_1 \varepsilon_2 a} + U_1. \tag{7}$$

A change in the size of the nanocrystal varies the depth of the potential well for each electron. It is also seen from (6) that the change of the effective potential well ($U_0(a)$) depends on the dielectric permittivities inherent to the nanoheterostructure. If the dielectric permittivity of QD is greater than that of the matrix, then a decrease in the radius of QD will increase the depth of the potential well. But if the matrix has a greater dielectric permittivity, then the depth of the quantum well will decrease.

The Schrödinger equation with Hamiltonian (2) is solved exactly. The solutions are determined for the discrete spectrum. In view of the spherical symmetry of the system, the wave function can be represented in the form of a product of the radial and angular components as

$$\psi(r_i, \theta_i, \varphi_i) = R(r_i) Y_l^m(\theta_i, \varphi_i), \tag{8}$$

where $Y_l^m(\theta_i, \varphi_i)$ are the spherical functions. The domain of definition of radial wave functions is composed from two parts: the internal region ($r_i < a$) and the external one ($r_i \geq a$).

1. Internal region ($r_i < a$)

a. *Energy range* ($E_i < -U_0$). The radial Schrödinger equation has the form

$$\left\{ -\frac{\hbar^2}{2m_1^*}\left(\frac{d^2}{dr_i^2} + \frac{2}{r_i}\frac{d}{dr_i}\right) + \right.$$

$$\left. + \frac{\hbar^2 l(l+1)}{2m_1^* r_i^2} - \frac{Ze^2}{\varepsilon_1 r_i} - U_0(a) - E_i \right\} R_1(r_i) = 0. \tag{9}$$

Let us introduce the dimensionless quantities

$$\rho = \frac{r_i}{a_b^*},$$

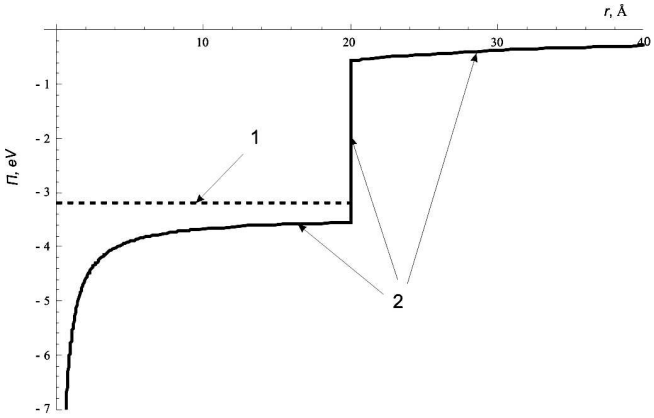

Fig. 1. Potential energies $U(r)$ (line 1) and $\Pi(r)$ (curve *2*)

$$a_b^* = \frac{\hbar^2 \varepsilon_1}{m_1^* Ze^2} = a_b \frac{\varepsilon_1}{Z\mu} = 0.5292 \times 10^{-10} \frac{\varepsilon_1}{Z\mu_1^*} \ \text{Å},$$

where $\mu_1 = m_1^*/m_0$ and m_0 is the free electron mass. Then Eq. (9) takes the form

$$\left\{ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} - k^2 \right\} R_1(\rho) = 0, \tag{10}$$

where

$$\frac{1}{\text{Ry}^*} = \frac{2m_1^*}{\hbar^2}(a_b^*)^2 = \frac{\varepsilon_1^2}{Z^2\mu_1^*}\frac{1}{\text{Ry}} = \frac{1}{13.598}\frac{\varepsilon_1^2}{Z^2\mu_1^*} \ \text{eV}^{-1},$$

$$k^2 = -\frac{E_i + U_0(a)}{\text{Ry}^*} > 0.$$

The solution of Eq. (10) which is bounded as $\rho \to 0$ has the form

$$R_1(\rho) = C_1 \rho^l e^{-k\rho} L_{-l-1+\frac{1}{k}}^{2l+1}(2k\rho), \tag{11}$$

where $L_b^a(x)$ is the generalized Laguerre polynomial.

b. *Energy range* ($0 > E_i > -U_0$). Analogous transformations lead to the equation

$$\left\{ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} + \eta^2 \right\} R_1(\rho) = 0, \tag{12}$$

where

$$\eta^2 = \frac{E_i + U_0(a)}{\text{Ry}^*} < 0.$$

The solution of Eq. (12) can be represented as

$$R_1(\rho) = C_1 \rho^l e^{-i\eta\rho} L_{-l-1-\frac{i}{\eta}}^{2l+1}(2i\eta\rho). \tag{13}$$

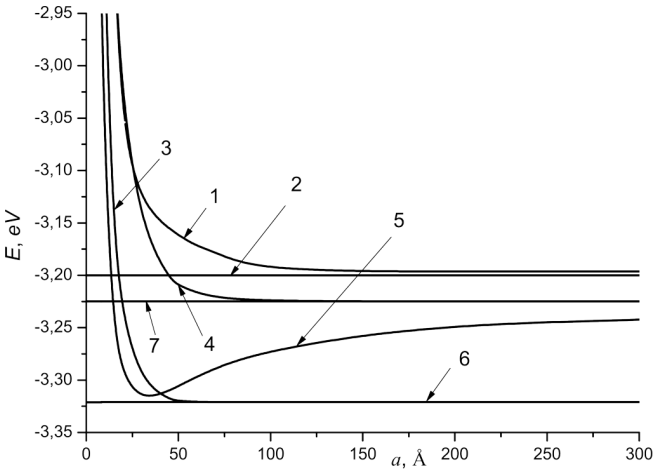

Fig. 2. Energy of the ground state of a D^0 donor as a function of the radius of QD

2. External region ($r_i \geq a$)

After the transformations and simplification, the Schrödinger equation is reduced to the equation

$$\left\{\frac{d^2}{d\rho^2}+\frac{2}{\rho}\frac{d}{d\rho}-\frac{l(l+1)}{\rho_i^2}+\frac{2M}{\varepsilon\rho}-M\chi^2\right\}R_2(\rho)=0, \tag{14}$$

where

$$M=\frac{m_2^*}{m_1^*},\quad \varepsilon=\frac{\varepsilon_2}{\varepsilon_1},\quad \chi^2=-\frac{E_i}{\mathrm{Ry}^*}.$$

The solution of Eq. (14) which is finite as $\rho\to\infty$ has the form

$$R_2(\rho)=C_2\rho^l e^{-\chi\sqrt{M}\rho}F\left(l+1-\frac{\sqrt{M}}{\varepsilon\chi},2l+2,2\sqrt{M}\chi\rho\right), \tag{15}$$

where $F(a,b,x)$ is the confluent hypergeometric function. The boundary conditions which are satisfied by the wave functions and the probability density flow yield the dispersion equation, from which we get the energy spectrum of the electron of a univalent admixture:

$$M\frac{\frac{d}{dr_i}R_1(r_i)}{R_1(r_i)}\bigg|_{r_i=a}=\frac{\frac{d}{dr_i}R_2(r_i)}{R_2(r_i)}\bigg|_{r_i=a}.$$

In order to calculate the energies of levels of D^- which possesses two electrons, it is necessary to choose a wave function which takes the spins of particles into account:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}\left[\psi_\alpha(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2)\pm\psi_\beta(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2)\right]. \tag{16}$$

In formula (16), the plus and minus signs are referred, respectively, to singlet (antiparallel spins) and triplet (parallel spins) states, and $\alpha=\{n_r,\,l,\,m\}$, where n_r=0, 1, 2, ..., l=0, 1, 2, ..., and m=0, ±1, ±2, ..., ±l are, respectively, the radial, orbital, and magnetic quantum numbers.

By substituting the wave function (16) in the Schrödinger equation with Hamiltonian (1), we can obtain the energy of D^- as

$$E=E_\alpha+E_\beta+Q\pm A,$$

where $E_{\left\{\begin{smallmatrix}\alpha\\ \beta\end{smallmatrix}\right\}}$ is the energy of a hydrogen-like admixture,

$$Q=\int d\mathbf{r}_1 d\mathbf{r}_2\left|\psi_\alpha(\mathbf{r}_1)\right|^2 W(r_1,r_2)\left|\psi_\beta(\mathbf{r}_2)\right|^2,$$

$$A=\int d\mathbf{r}_1 d\mathbf{r}_2\psi_\alpha^*(\mathbf{r}_1)\psi_\beta^*(\mathbf{r}_2)W(r_1,r_2)\psi_\alpha(\mathbf{r}_2)\psi_\beta(\mathbf{r}_1).$$

3. Analysis of the Results Obtained

By using the above-presented formula, we determined the energies of the ground and several excited states of D^0 and D^- donors in a spherical QD, whose parameters are as follows:

$$\mu_1=0.25,\ \ \mu_2=0.5,\ \ \varepsilon_1=11.7,\ \ \varepsilon_2=2.4,\ \ U_1=3.2\ \text{eV}.$$

The obtained solutions for a D^0 donor in a spherical QD are analogous by their form to those in [1, 2, 7, 8] but are different quantitatively and, to a significant extent, qualitatively, because we are based on the exact solution of the equation Poisson and take the difference of the dielectric permittivities of QD and the matrix into account.

Let us substitute the mean value of the dielectric permittivity, $\varepsilon_c=\sqrt{\varepsilon_1\varepsilon_2}$, into all the above-obtained formulas instead of ε_1 і ε_2. Then our results pass into the corresponding solutions given in [1, 2, 7]. Moreover, if we drop the term $-Ze^2(\varepsilon_1-\varepsilon_2)/(\varepsilon_1\varepsilon_2 a)$ in formula (3), then we get the solutions of work [8].

In Fig. 2, we show the energy of the ground state of an electron in a spherical QD without an admixture (curve *1*) and the depth of the potential well of the electron which is due to the band gap (line *2*). As seen, the increase in the radius of QD leads to a smooth change of the energy of the ground state of the electron. We also present the energy of the ground state of a D^0 donor in

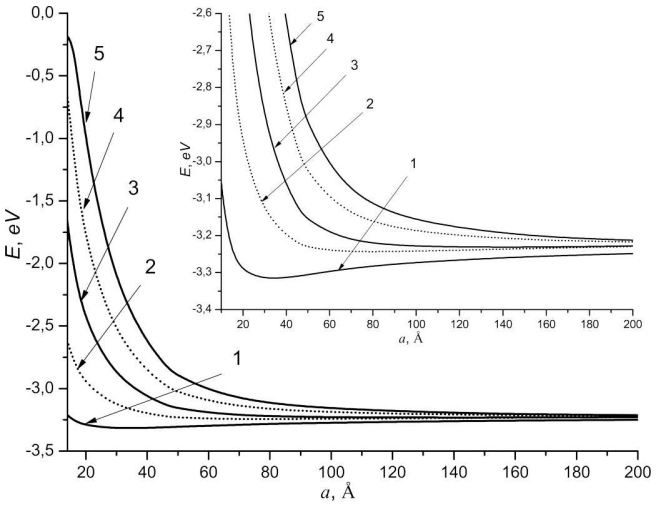

Fig. 3. Energy S-states (continuous curves) and P-states (dotted curves) of a D^0 donor. Numbers denote the following states: *1* – 1S, *2* – 2P, *3* – 2S, *4* – 3P, *5* – 3S

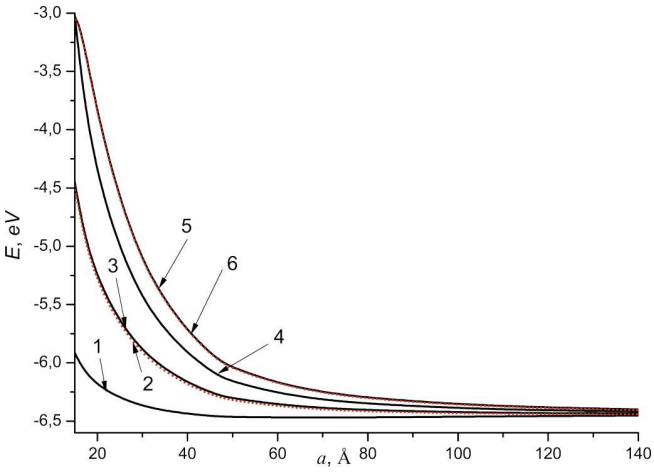

Fig. 4. Energy S-states of a negatively charged donor

a spherical QD calculated with the use of ε_c (curve *3*), formulas in [8] (curve *4*), and the potential energy (6) (curve *5*). It is seen from the figure that the energies of a donor obtained with the use of ε_c and formula (6) have close values, if the radius of QD $a \leq 40$ Å. If the radius of QD is more than 50 Å, then the difference between the energies increases with the radius. If we consider the great values of the radius of QD and use ε_c, then the energy tends to the value equal to the sum of the potential well depth $(-U_1)$ and the energy of a hydrogen-like atom which is determined by the effective Rydberg energy $\mathrm{Ry}_c^* = 13.598\ Z^2\mu_1^*/\varepsilon_c^2$ eV (line *6*). The calculations showed that the difference between the energies of the ground state, which are calculated with the use of ε_c and formula (6) (lines *6* and *7*), tends to the value $\mathrm{Ry}_c^* - \mathrm{Ry}^*$. For heterostructures, in which the dielectric permittivities of QD and the matrix are significantly different, the mentioned difference is essential.

In addition to the ground state of a D^0 donor in a spherical QD, we also considered the excited states. The results of calculations are given in Fig. 3. The solutions at fixed l are enumerated by the radial quantum numbers $n_r = 0, 1, 2, \ldots$ By analogy, like the case of a hydrogen-like atom, we can introduce a quantum number $n{=}n_r{+}l{+}1$. Respectively, we get the energy levels 1S ($n = 1$, $l = 0$, $n_r = 0$), 2S ($n = 2$, $l = 0$, $n_r = 1$), 3S ($n = 3$, $l = 0$, $n_r = 2$), 2P ($n = 2$, $l = 1$, $n_r = 0$), 3P ($n{=}3$, $l{=}1$, $n_r{=}1$).

The obtained order of quantum levels corresponds to that calculated in [1, 2, 7, 8]. But the consideration of the exact solution of the Poisson equation allows us to reveal such important specific feature of the dependence of two lowest energy states on the radius of QD as the presence of a minimum of energy at $a{\approx}35$ Å for 1S- and at $a{\approx}70$ Å for 2P-state. The minimum for the ground state is more clearly pronounced than that for the first excited state. The presence of such specific feature can be explained by the competition of two factors: the spatial confinement which increases the energy and the decrease of the energy due to the presence of the effective potential well $U_0(a)$.

We also determined the energy of a D^- donor at the center of a spherical QD as a function of the radius of QD. The results of calculations are shown in Fig. 4. The account of a symmetry of the wave function for the system of two electrons leads to the separation of the states into singlet (curves *1, 3, 4*, and *6*) and triplet ones (curves *2* and *5*). Curve *1* corresponds to the state, where two electrons are in 1S states (1S–1S), curves *2* and *3* – 1S–2S, curve *4* – 2S–2S, and curves *5* and *6* – 1S–3S states. Due to a small value of the exchange integral, the splitting between singlet and triplet levels is slight (Fig. 4), but it increases with decrease in the radius of QD (Fig. 5).

In order to determine the influence of the dielectric permittivity of the matrix on the spectrum of a donor, we calculated the energy of system as a function of ε_2 at the fixed radius of QD ($a = 25$ Å). The results are given in Fig. 6.

The points, at which the curves cross the vertical line *1*, correspond to the dielectric permittivity of the matrix SiO_2. The points where the vertical line *2* crosses the curves correspond to the case where the dielectric

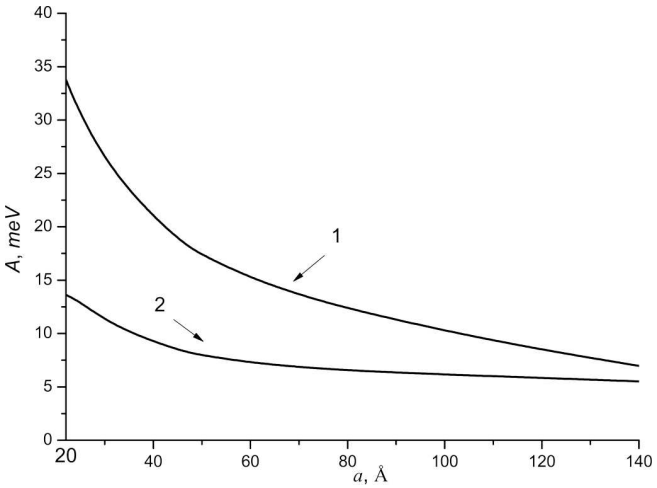

Fig. 5. Value of the exchange integral for 1S–3S (curve *1*) and 1S–2S (curve *2*) states of a D^- donor

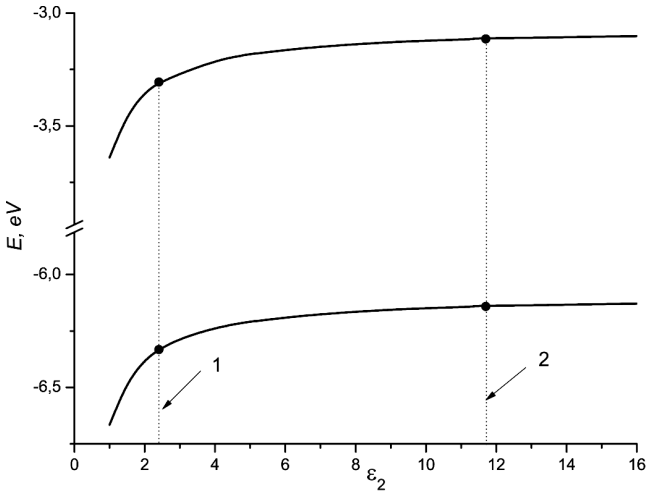

Fig. 6. Energy of the ground state of D^0 (upper curve) and D^- (lower curve) donors versus the dielectric permittivity of the matrix

permittivities of the matrix and QD are close to each other. It is seen from the figure that a decrease in the dielectric permittivity of the matrix leads to a decrease in the energies of D^0 and D^- donors in a spherical QD, whereas a growth of ε_2 causes an increase of the energy. At very great values of ε_2, the energy does not practically depend on it. The obtained dependence $E = E(\varepsilon_2)$ can be explained in the following way: a decrease in ε_2 increases the depth of the effective potential well (6), which causes a decrease in the energies of levels.

4. Conclusions

Thus, we have described the ground and excited states of a D^0 donor on the basis of the exact solution of the Poisson and Schrödinger equations. The calculations showed that these solutions differ from those obtained with the use of ε_c. We have also considered the ground and excited S-states of a D^- donor. It is established that the splitting into singlet and triplet states is small due to a small value of the exchange integral. We have also studied the behavior of the ground states of D^0 and D^- on a change of the dielectric permittivity of the matrix, which allows us to reveal a decrease in the energies of donors on a decrease in the dielectric permittivity of the matrix.

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ОСНОВНИЙ І ЗБУДЖЕНІ СТАНИ D^0 ТА D^- ДОНОРІВ У СФЕРИЧНІЙ КВАНТОВІЙ ТОЧЦІ

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Р е з ю м е

Для сферичної наногетероструктури Si/SiO_2 у наближенні ефективної маси для невироджених зон на основі точного розв'язку рівнянь Пуассона та Шредінгера обчислено енергію основного та збуджених станів електронів нейтрального (D^0) та негативно зарядженого (D^-) донорів як функцію радіуса квантової точки. Визначено синглетні та триплетні стани для D^- донора. Досліджено залежність енергії основного стану D^0 та D^- донорів від діелектричної проникності матриці.