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BROKEN REFLECTION SYMMETRY AND DIAMAGNETIC COEFFICIENT OF CARRIERS CONFINED IN SEMICONDUCTOR LATERAL QUANTUM DOT MOLECULES

UDC 539

The theoretical study of the reflection asymmetry impact on the electron and hole localizations in self-assembled InGaAs/GaAs semiconductor lateral quantum dot molecules is made. The previously proposed mapping method is used to simulate the ground-state electron (hole) wave function and the energy in molecules. The description is suited to clarify the important questions of the control and the stability of the wave functions and the diamagnetic coefficient of carriers confined in molecules with broken reflection symmetry. Our simulation results demonstrate that, in a reflection symmetric (balanced) molecule, the carrier ground-state wave function is distributed equally over two potential valleys corresponding to the actual positions of the dots combined into the molecule. However, even a very small reflectional imbalance in the geometry of molecules destroys the symmetric distribution of the wave function. This causes the localization of the function in the potential valley of only one of the dots and leads to a rapid decrease of the diamagnetic coefficient. We have found that the hole wave function is more sensitive to the imbalance in the reflection symmetry than the electron wave function, and the localization effect is getting stronger, when the interdot distance in the molecule increases.

K e y w o r d s: quantum dot molecule, semiconductor, wave function, modeling, diamagnetic response.

1. Introduction

The recent development of semiconductor technologies allows us to fabricate semiconductor quantum dots (and molecules combined from dots) within wide ranges of geometrical shapes and material parameters, to study their properties in detail, and to use them for various applications in quantum information processing, nano-optics, nano-biology, nanomedicine (see, e.g., [1–6] and references therein). The manipulation and the reconfiguration of wave functions of electrons and holes confined in quantum dot molecules (QDMs) are regarded as "isospin" operations. The isospin is a mark to the actual localization of a particle, and its properties in QDMs can be used in quantum information processing in a complete analogy to the properties of a particle spin [7, 8]. Therefore, the control and the manipulation of a wave function configuration of carriers confined in QDMs are key targets for the application of semiconductor quantum dots in quantum information technology.

In a weak external magnetic field B, the ground-state energy of an electron (hole) confined in a QDM can be written as $E_{\mathrm{e(h)}}(B) = E^0_{\mathrm{e(h)}} + s\mu_{\mathrm{B}} g_{\mathrm{e(h)}} B + + \alpha_{\mathrm{e(h)}} B^2$ [9], where $E^0_{\mathrm{e(h)}}$ stands for the electron (hole) energy at $B = 0$ T, μ_{B} is the Bohr magneton, $g_{\mathrm{e(h)}}$ is the electron (hole) Landé factor, $s = \pm 1/2$ presents the particle spin value and the polarization along the magnetic field direction, and $\alpha_{\mathrm{e(h)}}$ is the electron (hole) diamagnetic coefficient. The diamagnetic coefficient is obviously connected to the second derivative of the carrier energy with respect to the magnetic field magnitude and, therefore, to the single particle differential magnetic susceptibility of the QDM $\chi_{\mathrm{e(h)}}(B) = -d^2 E_{\mathrm{e(h)}}(B)/dB^2$ in the weak-field limit at the absolute zero temperature ($\alpha_{\mathrm{e(h)}} = -\frac{1}{2}\chi_{\mathrm{e(h)}}(0)$) [10, 11].

When the magnetic field is applied along a QDM growth direction (z axis), the coefficient can be evaluated, by using the effective radius (the characteristic lateral confinement length) of the electron – ρ_{e} (hole – ρ_{h}) in the plane perpendicular to the magnetic field (x-y plane): $\alpha_{\mathrm{e(h)}} = e^2 \rho^2_{\mathrm{e(h)}}/8m_{\mathrm{e(h)}}$ [9]. Here, e is the electronic charge, and $m_{\mathrm{e(h)}}$ stands for the electron

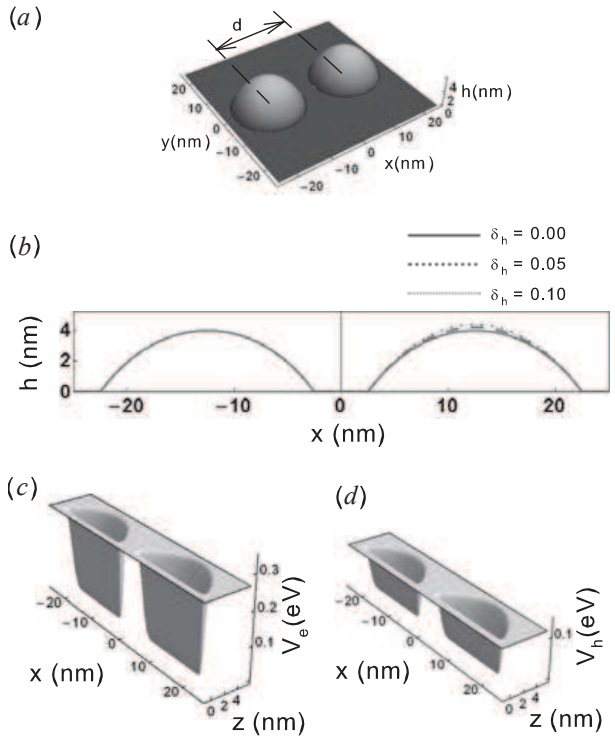

Fig. 1. QDM's geometrical and potential characteristics: (*a*) General shape of the QDM structure ($R_{\rm B}$ = 10 nm, $h_{\rm D}$ = 4 nm, d = 25 nm, δ_h = 0.00); (*b*) Cross section by the $(x, 0, z)$ plane of the QDM structure for different values of the parameter δ_h; (*c*) Projection of the electron confinement potential on the $(x, 0, z)$ plane (δ_h = 0.10); (*d*) Projection of the hole confinement potential on the $(x, 0, z)$ plane (δ_h = 0.10)

(hole) effective mass. Therefore, the actual value of the particle diamagnetic coefficient can be used for a preliminary estimation of the electron (hole) lateral confinement length and the actual localization in a QDM.

In this paper, we theoretically study the impact of the broken reflection symmetry on the actual localization of the ground-state wave functions and on the diamagnetic coefficients of electrons and holes confined in an $In_cAs_{1-c}Ga/GaAs$ laterally coupled lens-shaped double quantum dot structure (lateral QDM) [12, 13]. Deploying our mapping method [14], we reproduce three-dimensional geometrical and material characteristics of the QDM and simulate electronic properties of the QDM with the reflection symmetry and when the symmetry is broken. We demonstrate that, for the QDM with the reflection symmetry with respect to the reflection in the y-z plane (see Fig. 1), the ground-state electron and hole wave functions are equally distributed (balanced) between two potential valleys of the QDM. But, a very small imbalance in the geometrical characteristics of the dots in the x direction (see Fig. 1, *a*) can lead to the localization of the wave functions in one of the potential valleys of the QDM, which causes a significant decrease of the diamagnetic coefficient. We have investigated the localization effect for different distances between the centers of the quantum dots in the QDM on the x-y plane and have found that the localization effect is getting stronger when the distance increases.

2. Theoretical Model and Method of Calculation

We describe single electron and hole energy states in $In_cAs_{1-c}Ga/GaAs$ laterally coupled semiconductor quantum dots in the presence of an external magnetic field $\mathbf{B}$ using the effective one electronic (hole) band Hamiltonian with the position-dependent effective mass [14, 15]

$$\hat{\rm H}_{\rm e(h)} = \hat{\Pi}_{\rm e(h)} \frac{1}{2m_{\rm e(h)}(\mathbf{r})} \hat{\Pi}_{\rm e(h)} + V_{\rm e(h)}(\mathbf{r}), \qquad (1)$$

where $\mathbf{r} = (x, y, z)$ is the three-dimensional radius vector, $\hat{\Pi}_{\rm e(h)} = -i\hbar\nabla_{\mathbf{r}} - q_{\rm e(h)}\mathbf{A}(\mathbf{r})$ is the electron (hole) momentum operator, $\nabla_{\mathbf{r}}$ is the spatial gradient, $q_{\rm e(h)} = -(+)e$, and $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{B} = \nabla_{\mathbf{r}} \times \mathbf{A}(\mathbf{r})$. For the QDMs with and without reflection symmetry, we use a gauge-origin-independent definition for the vector potential (see Ref. [16] and references therein) $\mathbf{A}(\mathbf{r}) = \mathbf{B} \times (\mathbf{r} - \bar{\mathbf{r}})/2$, where $\bar{\mathbf{r}}$ stands for the expectation value of the position of a carrier in the ground state. Using this gauge in Hamiltonian (1), we can write the diamagnetic coefficient for the electron (hole) confined in a QDM (when the magnetic field is applied along the z direction) as [16]

$$\alpha_{\rm e(h)} = \frac{e^2}{8} \left\langle \frac{(\mathbf{r}_{\perp,{\rm e(h)}} - \bar{\mathbf{r}}_{\perp,{\rm e(h)}})^2}{m_{\rm e(h)}(\mathbf{r})} \right\rangle \Bigg|_{B=0}, \qquad (2)$$

where $\mathbf{r}_\perp = (x, y)$ is the two-dimensional radius vector on the x-y plane, $\langle f \rangle_{\rm e(h)}$ stands for the expectation value of a quantity f in the electron (hole) ground state with the wave function

$$\langle f \rangle_{\rm e(h)} = \int \psi^*_{\rm e(h)}(\mathbf{r})\, f(\mathbf{r})\, \psi_{\rm e(h)}(\mathbf{r})\, d\mathbf{r}, \qquad (3)$$

and $\bar{\mathbf{r}}_{\perp,\mathrm{e(h)}} = \langle \mathbf{r}_{\perp} \rangle_{\mathrm{e(h)}}$ is the expectation value of the electron (hole) position on the x-y plane.

To describe comprehensively all position-dependent geometrical and material parameters of a QDM, we map the realistic geometry of the QDM on the smooth three-dimensional quantum confinement potential. First, noting that a self-assembled lens-shaped lateral quantum dots are grown, by starting from a flat substrate parallel to the x-y plane, we model the QDM shape profile by a function $h(x,y)$. The function reproduces the local height of the QDM (along the z direction) at the actual position on the x-y plane. For the lens-shaped circular quantum dots where the distance separating the centers of the dots along the x direction is d (see Fig. 1), we can write this function as [17]

$$h(x,y) = [h_{-}(x,y) + h_{-}(x,y)]F(x,y),$$

$$h_{\mp}(x,y) = \sqrt{R_0^2 - [(x \pm d/2) + y^2]} - R_0 + h,$$

when $(x \pm d/2) + y^2 \leq R_{\mathrm{B}}^2$;

$$h_{\mp}(x,y) = 0,$$

when $(x \pm d/2) + y^2 < R_{\mathrm{B}}^2$;

$$F(x,y) = 1 + \delta_{\mathrm{h}} \exp\left[-\frac{(x - d/2)^2 + y^2}{b^2}\right],$$

$$R_0 = \frac{R_{\mathrm{B}}^2 + h_{\mathrm{D}}}{2h_{\mathrm{D}}}, \tag{4}$$

where R_{B} and h_{D} are dots' base radius and maximal height. The reflection asymmetry (with respect to the reflection in the y-z plane) is described by the function $F(x,y)$, where the range of the reflection asymmetry in dots' heights is presented by a parameter b. Therefore, deviations from the reflection symmetry in QDM's shape are controlled by a dimensionless parameter δ_h as [16, 17]

$$\delta_{\mathrm{h}} = \frac{h(d/2,0)|_{\delta_{\mathrm{h}} \neq 0} - h(d/2,0)|_{\delta_{\mathrm{h}}=0}}{h(d/2,0)|_{\delta_{\mathrm{h}}=0}}, \tag{5}$$

Figure 1 shows the shape of a QDM and its cross section by the $(x,0,z)$ plane for different deviations from the reflection-symmetric configuration.

The three-dimensional smooth quantum confinement potential $V_{\mathrm{e(h)}}(\mathbf{r})$ for the electrons (holes) in the QDM can be obtained by the composition- and geometry-dependent profile of the local conducting band offset [14, 16, 17]:

$$V_{\mathrm{e(h)}}(\mathbf{r}) = \Delta E_{\mathrm{e(h)}}\{1 - T_{+}(s-z)T_{-}[z - h(x,y)]\}. \tag{6}$$

Here, $T_{\pm}(t) = [1 \pm \tanh(t/a)]/2$, $\Delta E_{\mathrm{e(h)}} = E_{\mathrm{e(h)}}^{\mathrm{out}} - E_{\mathrm{e(h)}}^{\mathrm{in}}$ is the overall conducting (valence) band offset between the inner and outer semiconductor materials in the $\mathrm{In}_c\mathrm{As}_{1-c}\mathrm{Ga}/\mathrm{GaAs}$ heterostructure, and subscripts "in" and "out" denote the actual material parameters (the conducting (valence) band bottom (top) energy) inside and outside the dots. The effective substrate-dot interface is assigned to be at the plane $z = s$. The slope and the range (the degree of smoothness) of a potential change at the boundaries of the dots are controlled by a parameter a. The three-dimensional confinement potential (6) reflects, in a very obvious and natural way, smooth variations of the material parameters across the boundaries of the dots (see Fig. 1, c and d). Using (6), we define the dimensionless mapping function [14, 17]

$$M(\mathbf{r}) = 1 - \frac{V_{\mathrm{e(h)}}(\mathbf{r})}{\Delta E_{\mathrm{e(h)}}}. \tag{7}$$

This function accumulates information about the shape and the local material content of a QDM. Using the mapping, we can derive all position-dependent geometrical and material parameters of the structure. For instance, the position-dependent effective mass $m_{\mathrm{e(h)}}(\mathbf{r})$ of the electron (hole) is defined as $m_{\mathrm{e(h)}} = m_{\mathrm{e(h)}}^{\mathrm{in}} M(\mathbf{r}) + m_{\mathrm{e(h)}}^{\mathrm{out}}[1 - M(\mathbf{r})]$.

The confinement potentials and the position-dependent effective masses are used to obtain solutions of the Schrödinger equation corresponding to Hamiltonian (1). The solutions give us the electron (hole) ground-state energy $E_{\mathrm{e(h)}}$, wave functions, expectation values of particles' positions, mean (effective) lateral electron (hole) radius

$$\rho_{e(h)} = \sqrt{\left\langle \left(\mathbf{r}_{\perp,\mathrm{e(h)}} - \bar{\mathbf{r}}_{\perp,e(h)}\right)^2 \right\rangle},$$

and diamagnetic coefficients (2) in QDMs with various deviations from the reflection symmetry.

3. Simulation Results and Discussion

In our simulation of the electron (hole) ground-state energy and wave function for the QDMs, we

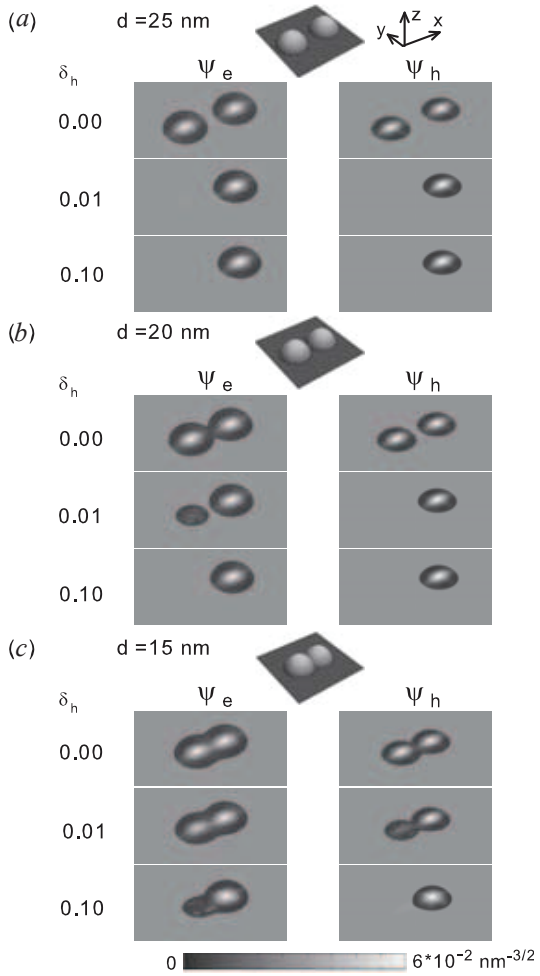

Fig. 2. Electron and hole ground-state wave functions for different δ_h and d: (a) 25 nm; (b) 20 nm; (c) 15 nm

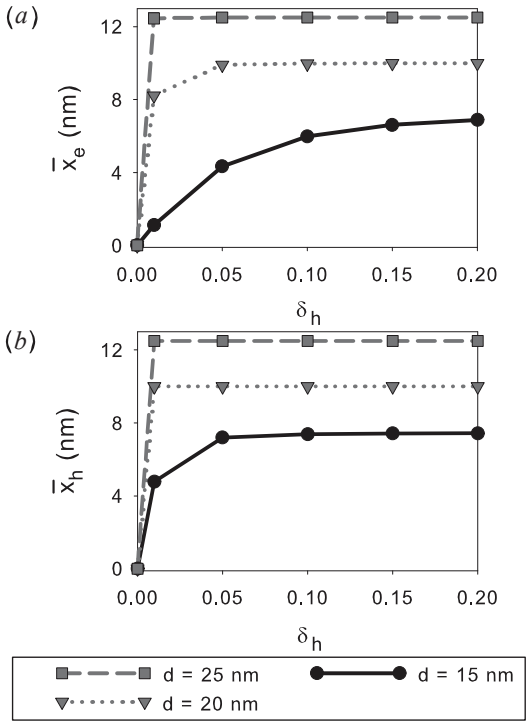

Fig. 3. Expectation value of the position of the electron (a) and the hole (b) in the ground state on the x axis in the QDMs with different geometrical parameters

use a realistic geometry and material parameters for $In_cAs_{1-c}Ga/GaAs$ nano-structures [11, 16, 18, 19]. The geometrical characteristics are chosen as $R_B = 10$ nm, $h_D = 4$ nm, $b = R_B$, $a = 0.4$ nm, and $s = 0.0$ nm.

We take material parameters from [18, 19] and adjust them according to the actual composition and strain inside the dots [11, 16]: $m_e^{InAs} = 0.044\ m_0$, $m_h^{InAs} = 0.074\ m_0$, $m_e^{GaAs} = 0.067\ m_0$, $m_h^{GaAs} = 0.5\, m_0$, $E_g^{InAs} = 0.842$ eV, $E_g^{GaAs} = 1.52$ eV, (m_0 is the free-electron mass). A material parameter $D^{in(out)}$ for the $In_cGa_{1-c}As$ compound is obtained according to the linear interpolation $D_c^{in(out)} = cD_{InAs}^{in(out)} + (1-c)D_{GaAs}^{in(out)}$.

The In concentration inside dots is taken to be $c = 0.6$, and we take 70% of the heterostructure gap difference to be the conducting band offset and 30% to be the valence band offset in the dot. The energy and the wave function of the electron (hole) confined in QDMs are obtained numerically by the iterative method with the use of the COMSOL MULTIPHYSICS package [20, 21]. We use the wave function to simulate the expectation values of particles' positions, effective lateral radii, and diamagnetic coefficients for QDMs with the reflection symmetry and when the symmetry is broken. We consider the QDMs with various interdot distances.

In Fig. 2, we present the ground-state wave functions of the electron and the hole for QDMs with various interdot distances. When the parameter δ_h changes from 0 (reflectional symmetric QDM) to 0.10, the wave functions change from the reflectional symmetric profile (equally distributed in two dots) to reflection non-symmetric profiles: the wave function is localized in the potential valley of only one dot near

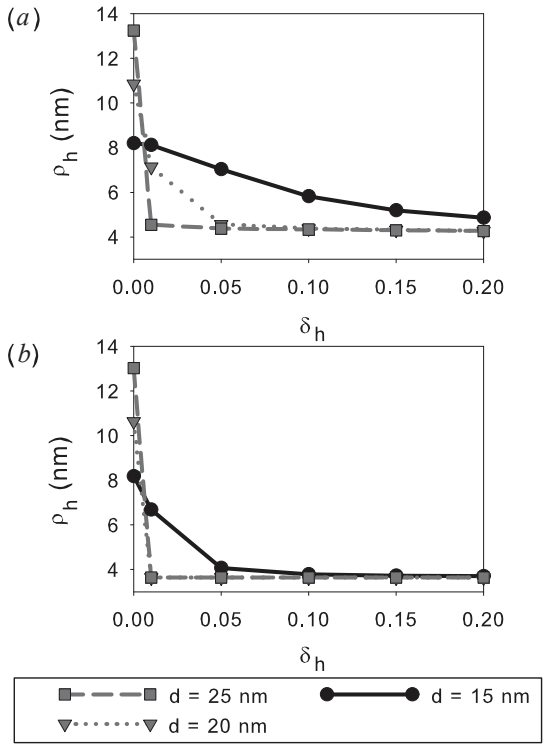

Fig. 4. Effective lateral radius of the electron (a) and the hole (b) in the ground state in the QDMs with different geometrical parameters

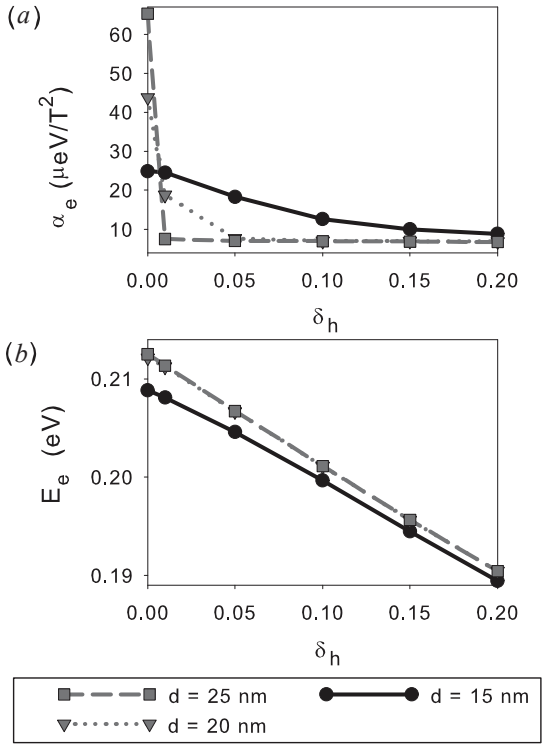

Fig. 5. Electron diamagnetic coefficient (a) and ground-state energy (b) for the QDMs with different geometrical parameters

$(x = +d/2, y = 0)$ on the $x - y$ plane. The wave functions are localized in one of the potential valleys, when the imbalance in the QDM potential profile is really small. The hole wave function is more sensitive to the imbalance in the reflection symmetry: as the hole has a larger effective mass, the effect of the imbalance is stronger. Only when the dots overlap ($d = 15$ nm), some distribution of the wave functions between two dots remains up to $\delta_{\rm h} \sim 0.10$. But, as the distance between dots increases, the wave functions are localized in one of the dots already for $\delta_h \sim 0.01$. Accordingly, as it is shown in Fig. 3, the expectation value of particles' position in the ground state (when the parameter δ_h increases) rapidly moves from the center of the structure toward the imbalanced potential valley at $(x = +d/2, y = 0)$ on the $x - y$ plane. The mean position of the hole is almost stabilized in the valley, when the parameter $\delta_h \sim 0.10$ even for the overlapping dot configurations. We note that, for all configurations, the expectation value of the electron (hole) position on the y axis remains unchanged: $\bar{y}_{e(h)} = 0$. From Fig. 4, we see that the effective lateral radii of the electron and the hole follow the same tendency: electron's radius decreases gradually and hole's radius shrinks rapidly. The "one-valley" localization occurs in the reflection asymmetric configurations almost immediately, as the interdot distance reaches 25 nm.

In Fig. 5, a and Fig. 6, a, we show the dependence of the electron and hole diamagnetic coefficients on the parameter δ_h for various interdot distances. It is clear that the above-described sensitivity of the electron and hole wave functions' localizations and distributions to the imbalance in the reflection symmetry leads to a rapid decrease of the diamagnetic coefficients (a few times) already for small values of $\delta_{\rm h}$. For relatively large interdot distance ($d = 25$ nm), the diamagnetic coefficient drops by a factor of 10, when $\delta_h \sim 0.01$. However, for the "overlapping dots" molecules with $d < 2R_B$ (e.g., $d = 15$ nm), the same change in the diamagnetic coefficient magnitude can be achieved only when $\delta_h \sim 0.05$. The coefficients de-

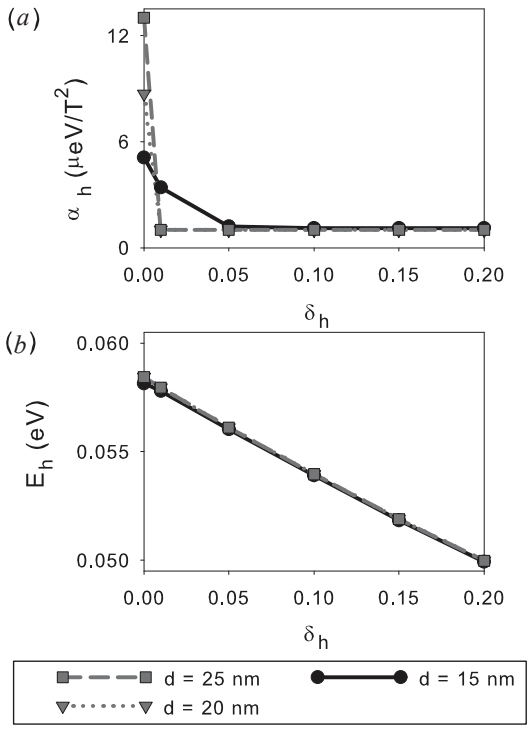

Fig. 6. Hole diamagnetic coefficient (*a*) and ground-state energy (*b*) for the QDMs with different geometrical parameters

crease only gradually, when the QDM geometry becomes more imbalanced along the x direction.

Contrary to the diamagnetic coefficient, the electron (hole) ground-state energy decreases slowly (about $10 \sim 15\%$) within the whole range of the imbalance growth (as it is shown in Fig. 5, *b* and Fig. 6, *b*). Therefore, we can conclude that the monitoring of the carrier energy characteristics can give very limited hints about the actual wave function configurations of the electron (hole) confined in QDMs. At the same time, the actual value of the diamagnetic coefficient can provide us with clear and direct information about the electron (hole) localization in the lateral QDMs with broken reflection symmetry.

4. Conclusions

Using the effective one-band Hamiltonian and the mapping method, we have simulated the localizations of electrons and holes in the semiconductor lateral QDMs with and without reflection symmetry. We have found that a small imbalance in the geometry of the QDM (small deviations in the dots height) leads to the collapse of the electron (hole) ground-state function into one of the dots. This generates a rapid decrease of the diamagnetic coefficient of carriers. We stress that the actual magnitude of the diamagnetic coefficient obtained from experiments can give an important insight on the wave function configurations for the carriers confined in the QDMs with uncertain symmetry.

Our approach can be useful for the realistic modeling of the magnetic response of semiconductor nanoobjects with realistic and non-symmetric geometry.

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О. Воскобойніков

ПОРУШЕНА СИМЕТРІЯ ДЗЕРКАЛЬНОГО ВІДОБРАЖЕННЯ ТА ДІАМАГНІТНИЙ КОЕФІЦІЄНТ НОСІЇВ, ЗАХОПЛЕНИХ ЛАТЕРАЛЬНИМИ НАПІВПРОВІДНИКОВИМИ МОЛЕКУЛАМИ З КВАНТОВИМИ ТОЧКАМИ

Р е з ю м е

У цій роботі теоретично досліджено вплив асиметрії дзеркального відображення на локалізацію електрона і дірки в самоорганізованих латеральних молекулах з InGaAs/GaAs квантовими точками. Використовується запропонований раніше метод відображення для моделювання хвильової функції основного стану електрона (дірки) та їх енергії в молекулах. Подібний підхід є зручним для з'ясування важливих питань, пов'язаних з контролем та стабільністю хвильових функцій і діамагнітного коефіцієнта носіїв, обмежених в латеральних напівпровідникових молекулах з квантовими точками з порушеною симетрією відбиття. Наші результати моделювання показують, що в симетричній (збалансованій) молекулі хвильова функція основного стану носія розподілена порівну між двома потенціальними ямами відповідно до місць локалізації квантових точок, що утворюють молекулу. Тим не менш, навіть дуже невеликий дисбаланс (асиметрія) дзеркального відображення в геометрії молекул руйнує симетричний розподіл хвильової функції. Наслідком цього є локалізація хвильової функції у потенціальній ямі тільки однієї з точок, що приводить до швидкого зменшення діамагнітного коефіцієнта. Ми виявили, що хвильова функція дірок є більш чутливою до дисбалансу в дзеркальному відображенні, ніж хвильова функція електрона, і ефект локалізації зростає, коли відстань між квантовими точками в молекулі збільшується.

А. Воскобойников

НАРУШЕННАЯ СИММЕТРИЯ ЗЕРКАЛЬНОГО ОТОБРАЖЕНИЯ И ДИАМАГНИТНЫЙ КОЭФФИЦИЕНТ НОСИТЕЛЕЙ, ЗАХВАЧЕННЫХ ЛАТЕРАЛЬНЫМИ ПОЛУПРОВОДНИКОВЫМИ МОЛЕКУЛАМИ С КВАНТОВЫМИ ТОЧКАМИ

Р е з ю м е

В этой работе теоретически исследовано влияние асимметрии зеркального отображения на локализацию электрона и дырки в самоорганизующихся латеральных молекулах с InGaAs/GaAs квантовыми точками. Используется предложенный ранее метод отображения для моделирования волновой функции основного состояния электрона (дырки) и их энергии в молекулах. Подобный подход является удобным для выяснения важных вопросов, связанных с контролем и стабильностью волновых функций и диамагнитного коэффициента носителей, ограниченных в латеральных полупроводниковых молекулах из квантовых точек с нарушенной симметрией отражения. Наши результаты моделирования показывают, что в симметричной (сбалансированной) молекуле волновая функция основного состояния носителя распределена поровну между двумя потенциальными ямами в соответствии с местами локализации квантовых точек, образующих молекулу. Тем не менее, даже очень небольшой дисбаланс (асимметрия) зеркального отображения в геометрии молекул разрушает симметричное распределение волновой функции. Следствием этого является локализация волновой функции в потенциальной яме только одной из точек, что приводит к быстрому уменьшению диамагнитного коэффициента. Мы обнаружили, что волновая функция дыр является более чувствительной к дисбалансу в зеркальном отображении, чем волновая функция электрона, и эффект локализации возрастает, когда расстояние между квантовыми точками в молекуле увеличивается.