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## ON THE THEORY OF THE BINDING ENERGY OF EXCITON QUASIMOLECULES IN GERMANIUM/SILICON DOUBLE QUANTUM DOTS

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A theory of exciton quasimolecules (formed from spatially separated electrons and holes) in a nanosystem consisting of double quantum dots (QDs) of germanium synthesized in a silicon matrix is presented. It is shown that the binding energy of the singlet ground state of the quasimolecule of an exciton is considerably larger than the binding energy of biexciton in a silicon single crystal by almost two orders of magnitude.

It is shown that the exciton quasimolecule formation is of the threshold character and possible in a nanosystem, where  $D$  is the distance between the surfaces of QD that satisfies the following condition:  $D_c^{(1)} \leq D \leq D_c^{(2)}$  (where  $D_c^{(1)}$  and  $D_c^{(2)}$  are some critical distances). Using the variational method, we obtain the binding energy of the exciton quasimolecule singlet ground state of the system as a function of the distance between the surfaces of QD  $D$ , and the QD radius  $a$ .

It is shown that the convergence of two QDs up to a certain critical value of the distance between the surfaces of QD  $D_c$  leads to the effective overlapping of the electron wave functions and the appearance of exchange interactions. As a result, the exciton quasimolecules can be formed from the QDs. It is shown that the existence of such a critical distance  $D_c$  arises from the quantum size effects. Dimensional quantization of electrons and holes motion leads to the following fact: as the distance between the surfaces of the QD  $D_c$  decreases, the decrease in the energies of interaction of the electrons and holes entering into the Hamiltonian of the exciton quasimolecule cannot compensate for the increase in the kinetic energy of the electrons and holes. At larger values of the distance between the surfaces of the QD  $D$ ,  $D \geq D_c^{(2)}$ , the exciton quasimolecule breaks down into two excitons (consisting of spatially separated electrons and holes), localized over the QD surfaces.

The fact that the energy of the ground state of singlet excitonic quasimolecule is in the infrared range of the spectrum, presumably, allows us to use a quasimolecule for the development of new elements of silicon infrared nanophotonics.

**Keywords:** *spatially separated electron and holes, quantum dots, binding energy, coulomb and exchange interaction*

### INTRODUCTION

At present, the optical properties of Ge/Si heterostructures with germanium quantum dots (QD) are a subject of the intense study. In Ge/Si heterostructures, the structures that have self-assembled Ge/Si nanoislands are promising for the implementation of effective sources of infrared radiations, since the photoluminescence signal of such nanostructures, is in the spectral range of

$$0.20\text{--}1.14 \text{ eV}, \quad (1)$$

and observable at room temperatures [1, 2]. In order to create new Ge/Si – based heterostructures with new effective optoelectronic devices, the mechanism of light

absorption in such nanoheterostructures must be studied [1–5]. The Ge/Si heterostructures with germanium QDs are classified as those of the second type. Such nanoheterostructures are characterized by the presence of significant gaps in the valence and conduction bands. The ground electron state therein is located in the silicon matrix, and the ground hole level is in the bulk of the germanium QD. The significant gap in the valence band causes hole localization in the QD bulk. A significant gap in the conduction band is the potential barrier for electrons (electrons move throughout the matrix and do not penetrate into the QD volume) [1–5]. In Ref. [1], the study of the optical properties of Ge/Si heterostructures with germanium QDs was the first to discover

the spatial separation between electrons and holes, as a result of which the electrons localized on the QD surface, and the holes moved through the QD bulk.

The energy of the Coulomb interaction of electron with hole form is a potential well, in which electron is localized above the surface of the QD. In the bulk of the QD, there is a hole, while the electron is localized above the spherical surface of the QD-matrix interface [6, 7].

In [8], it is theoretically analyzed the exciton transitions in double vertically conjugated QD of germanium, separated by silicon layer of thickness  $d$ . The QD of germanium was in the form of pyramids with the ratio of the height  $h$  to the lateral dimension  $l = 10, 15, 20$  nm equals approximately to 0.1. The spatial structure of excitons and the oscillator is studied theoretically in Ref. [8]. The ground state of the exciton in a single germanium QD corresponded to the configuration in which the hole was in the ground state in germanium QD, and an electron moving in the silicon matrix was localized near the apex of the pyramidal QD. It is shown that for small distances ( $D < 3$  nm) between QDs, the electron configuration is analogous to the case of single QDs. It is found that with the increase in the distance  $D$  up to the values of 3.0–3.5 nm for  $l = 10, 15$  nm, the oscillator strength for the interband transition with the formation of the ground state of the exciton can be much larger (up to a factor of 5) than the analogous value in single QD. In [8], in contrast to the present work, when studying the occurrence of exciton states between the QD surfaces, the exchange interaction between electrons was not taken into account. Such exchange interaction, as it will be shown in the present paper, gives the main contribution to the binding energy of the exciton quasimolecule.

In [6], the theory of the exciton formed by spatially separated electron and hole is developed (the hole moves in the bulk of a germanium QD and the electron is localized above the spherical interface between the QD and the silicon matrix). It was found that the binding energy of an exciton in such a nanosystem is much higher (almost an order of magnitude) than the binding energy of an exciton in the silicon single crystal. In [6], in the framework of classical electrodynamics, an expression was obtained that describes the

Coulomb interaction between an electron and hole. In [6], the exciton appeared as a result of the Coulomb interaction between the electron and hole, which, in contrast to [1, 2, 8], was dependent on the dielectric permittivities of the QD and the matrix. The energy spectrum of the exciton, as a function of the radius of the germanium QD, was obtained in [6] for radii of QDs exceeding 3 nm. This is due to the fact that the study of exciton states in the nanosystem containing germanium QD with radii  $a$  less than 3 nm is incorrect in the framework where the expression for the Coulomb interaction between the electron and hole was obtained by the methods of classical electrodynamics.

The convergence of two QDs up to the certain critical value  $D_C$  between surfaces of QD leads to overlapping of the electron wave functions and the emergence of exchange interactions [9]. As a result, the conditions for the formation of quasimolecules from QDs can be appeared [1, 2, 8, 9]. One can also assume that the above conditions of formation of quasimolecules can be provided by external physical fields. This assumption is evidenced by results of [10, 11], in which the occurrence of the effective interaction between QDs at considerable distances under conditions of electromagnetic field was observed experimentally. In [12, 13], the energies of the ground state of “vertical” and “horizontal” located pair of interacting QDs (“molecules” from two QDs) were determined as a function of the steepness of the confining potential and the magnetic field strength. The quantum part of nanocomputer, which was implemented on a pair of QDs (“molecules” from two QDs) with charge states is  $n$  qubits [14]. The first smoothly working quantum computer has been on QDs with two electron orbital states as qubits, described by a pseudospin ( $1/2$ ). As a single cell was taken as a couple of asymmetric pair QDs with different sizes and significantly different energy. The electron is injected into the heterostructure from the channel occupied the lower level. That is, it was located in a QD with larger size.

In [3], the heterostructures which are linear chains of QDs germanium on Si substrates were obtained by electron-beam lithography method. The average sizes of the QD Ge is less than 60 nm. With increasing concentration of Ge QDs linear chains in the average distance between the

surfaces decreases QDs [3]. In such nanostructures at distances  $D_C$  between the surfaces of QD (which is about the Bohr radius of the electron in a silicon matrix,  $a_e = 0.63$  nm) the interaction between them must be taken into account. In this case, the overlap integral of the electron wave functions takes a significant value. As a result, the conditions for the formation of the excitonic quasi-molecules from of double QDs can be created.

Therefore, in the present paper, which is a continuation of the research [6], using the variational method, we obtain the binding energy of the excitonic quasimolecule singlet ground state in the system as a function of the spacing between the QD surfaces and the QD radius. We show that the excitonic quasi-molecule formation is of the threshold character and possible in a nanosystem, where the distance  $D$  between the surfaces of QD is given by the condition  $D_C^{(1)} \leq D \leq D_C^{(2)}$  (where  $D_C^{(1)}$  and  $D_C^{(2)}$  are some critical distances). A significant increase in the binding energy of the singlet ground state of excitonic quasimolecule (of spatially separated electrons and holes) in a nanosystem that consists of germanium QDs grown in a silicon matrix has been predicted; the effect is almost two orders of magnitude larger than the binding energy of biexciton in a silicon single crystal. It is shown that the major contribution to the excitonic quasi-molecule binding energy is made by the energy of the exchange interaction of electrons with holes and this contribution is much more substantial than the contribution of the energy of Coulomb interaction between the electrons and holes.

#### THE BINDING ENERGY OF THE SINGLET GROUND STATE OF EXCITON QUASIMOLECULE

Let us consider a model nanosystem that consists of two spherical germanium quantum dots: QD(A) and QD(B) with radius  $a$ , grown in a matrix of silicon with a dielectric constant ( $\epsilon_1 = 11.7$ ) ( $D$  is the distance between the surfaces of the QD). The QDs contain germanium with the dielectric constant of ( $\epsilon_2 = 16.3$ ) in their bulk. For simplicity, we assume that holes  $h(A)$  and  $h(B)$  with the effective mass ( $(m_e^{(1)}/m_0) = 0.39$ ) are located at the centers of QD (A) and QD(B), and electrons  $e(1)$  and  $e(2)$  with effective mass

( $(m_e^{(1)}/m_0) = 0.98$ ) are localized above the surfaces of QD(A) and QD(B) in a matrix of silicon, respectively, ( $m_0$  is the electron mass in free space;  $r_{A(1)}$  is the distance of the electron  $e(1)$  from the QD(A) center;  $r_{B(2)}$  is the distance of the electron  $e(2)$  from the QD(B) center;  $r_{A(2)}$  is the distance of the electron  $e(2)$  from the QD(A) center;  $r_{B(1)}$  is the distance of the electron  $e(1)$  from the QD(B) center). Let us assume that there is an infinitely high potential barrier on a spherical interface (QD – matrix). Therefore, in such a nanosystem, the holes do not escape from the volume of the QD as well as the electrons do not enter the QD. Thus, we can make the assumption that the holes  $h(A)$  and  $h(B)$  are located at the centers of QD(A) and QD(B).

Let us now use this model to consider the possibility of the formation of excitonic quasimolecule from spatially separated electrons and holes (the holes are located at the centers of QD(A) and QD(B) and electrons are localized near their spherical surfaces). Using adiabatic approximation and the effective mass approximation, the Hamiltonian of the excitonic quasimolecule (of spatially separated electrons and holes) can be written in the following form [9]:

$$\hat{H} = \hat{H}_{A(1)} + \hat{H}_{B(2)} + \hat{H}_{int} \quad (2)$$

where  $\hat{H}_{A(1)}$  and  $\hat{H}_{B(2)}$  are the Hamiltonians of the excitons of spatially separated hole  $h(A)$  and electron  $e(1)$  and hole  $h(B)$  and electron  $e(2)$ , respectively.

The contribution of the energy of polarization interaction with the surface of QD to the Hamiltonians of the excitons  $\hat{H}_{A(1)}$  can be and  $\hat{H}_{B(2)}$ , as the first approximation is neglected [6, 7]. Thus, the exciton Hamiltonian  $\hat{H}_{A(1)}$  takes the form of [6, 7]:

$$\hat{H}_{A(1)} = -\frac{\hbar^2}{2\mu} \Delta_{(1)} + V_{e(1)h(A)}(r_{A(1)}, r_{h(A)}) + E_g, \quad (3)$$

where the first term is the exciton kinetic energy operator and the energy of Coulomb interaction  $V_{e(1)h(A)}$  between electron  $e(1)$  and hole  $h(A)$  is given by the following expression [6, 7]:

$$V_{e(1)h(A)} = -\frac{1}{2} \left( \frac{1}{s_1} + \frac{1}{s_2} \right) \frac{e^2}{r_{A(1)}} \quad (4)$$

and  $E_g$  is the bandgap energy of the germanium ( $E_g = 0.661 eV$ ). The Hamiltonian  $\hat{H}_{B(2)}$  is of the same form as  $\hat{H}_{A(1)}$  (2). In the first approximation we can neglect the contributions to the Hamiltonian  $\hat{H}_{int}$  of the interaction energies of the electrons  $e(1)$  and  $e(2)$  and the holes  $h(A)$  and  $h(B)$  with polarization fields induced by these charge carriers on the surfaces of QD(A) and QD(B) [6]. Thus, the Hamiltonian  $\hat{H}_{int}$  incorporates only the energies of Coulomb interaction of electron  $e(1)$  with hole  $h(B)$ , and electron  $e(2)$  with hole  $h(A)$ , as well as that between electrons  $e(1)$  and  $e(2)$ , and holes  $h(A)$  and  $h(B)$  [9].

Under the assumption that the spins of the electrons  $e(1)$  and  $e(2)$  are antiparallel, let us write down the normalized wave function of the ground singlet state of the exciton quasimolecule as a symmetric linear combination of wave functions  $\Psi_1(r_{A(1)}, r_{B(2)})$  and  $\Psi_2(r_{A(2)}, r_{B(1)})$  [9]:

$$\begin{aligned} \Psi_s(r_{A(1)}, r_{A(2)}, r_{B(1)}, r_{B(2)}) = \\ = [2(1 + S^2(D, a))]^{-1/2} [\Psi_1(r_{A(2)}, r_{B(1)}) + \\ + \Psi_2(r_{A(2)}, r_{B(1)})] \end{aligned} \quad (5)$$

where  $S(D, a)$  is the overlap integral of single-electron wave functions. Assuming that the electrons  $e(1)$  and  $e(2)$  move independently from each other, let us represent the wave functions  $\Psi_1(r_{A(1)}, r_{B(2)})$  and  $\Psi_2(r_{A(2)}, r_{B(1)})$  (5) as a product of single-electron wave functions  $\varphi_{A(1)}(r_{A(1)})$  and  $\varphi_{B(2)}(r_{B(2)})$ , as well as  $\varphi_{A(2)}(r_{A(2)})$  and  $\varphi_{B(1)}(r_{B(1)})$ , respectively [9]. Let us also represent the single-electron wave functions as variational functions of Coulomb type [9]:

$$\begin{aligned} \varphi_{A(1)}(r_{A(1)}) &= \tilde{A} \exp\left(-\bar{\mu}(\tilde{a})\left(r_{A(1)} / a_{ex}^{2D}\right)\right), \\ \varphi_{B(2)}(r_{B(2)}) &= \tilde{A} \exp\left(-\bar{\mu}(\tilde{a})\left(r_{B(2)} / a_{ex}^{2D}\right)\right), \\ \varphi_{A(2)}(r_{A(2)}) &= \tilde{A} \exp\left(-\bar{\mu}(\tilde{a})\left(r_{A(2)} / a_{ex}^{2D}\right)\right), \\ \varphi_{B(1)}(r_{B(1)}) &= \tilde{A} \exp\left(-\bar{\mu}(\tilde{a})\left(r_{B(1)} / a_{ex}^{2D}\right)\right), \end{aligned} \quad (6)$$

where  $\bar{\mu}(\tilde{a})$  is a variational parameter,  $\tilde{a} = (a / a_{ex}^{2D})$  where  $a_{ex}^{2D} = (2\varepsilon_1\varepsilon_2 / (\varepsilon_1 + \varepsilon_2)) \cdot (\hbar^2 / \mu_0 e^2)$  is the Bohr radius of two-dimensional (2D) exciton localized over the flat interface between the germanium and the matrix of silicon,  $\mu_0 = m_e^{(1)} m_h / (m_e^{(1)} + m_h)$  is the reduced mass of

the 2D exciton (of spatially separated electrons and holes) [6, 7].

In the framework of the variational method, the energy of the excitonic quasimolecule ground singlet state, as a first approximation, is given by the mean value of the Hamiltonian  $\hat{H}$  (2) over the states described by the wave functions of the zeroth approximation  $\Psi_s$  (5) [9]:

$$\begin{aligned} E(\tilde{D}, \bar{\mu}(a, D), a) = \\ = \left\langle \Psi_s(r_{A(1)}, r_{A(2)}, r_{B(1)}, r_{B(2)}) \left| \hat{H} \right| \Psi_s(r_{A(1)}, r_{A(2)}, r_{B(1)}, r_{B(2)}) \right\rangle. \end{aligned} \quad (7)$$

With the explicit form of the wave functions (5), (6), the energy functional of the exciton quasimolecule singlet ground state takes the form

$$\begin{aligned} E_0(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a}) = 2E_{ex}(\tilde{a}, \bar{\mu}(\tilde{a})) + \\ + \frac{J(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a}) + K(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a})}{1 + S^2(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a})}. \end{aligned} \quad (8)$$

Here,  $E_{ex}(\tilde{a}, \bar{\mu}(\tilde{a}))$  is the energy functional of the exciton ground state (for the exciton formed from an electron and a hole spatially separated from the electron):

$$E_{ex}(\tilde{a}, \bar{\mu}(\tilde{a})) = \left\langle \varphi_{A(1)}(r_{A(1)}) \left| \hat{H}_{A(1)} \right| \varphi_{A(1)}(r_{A(1)}) \right\rangle. \quad (9)$$

The second term in (8) is a functional  $E_e(D, a)$  representing the binding energy of singlet ground state of excitonic quasimolecule. In the functional determined by formula (8),  $J(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a})$  is determined by the expression (here  $(\tilde{D} = (D / a_{ex}^{2D}))$ ):

$$\begin{aligned} J(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a}) = \\ = \left\langle \varphi_{A(1)}(r_{A(1)}) \varphi_{B(2)}(r_{B(2)}) \left| H_{int} \right| \varphi_{A(1)}(r_{A(1)}) \varphi_{B(2)}(r_{B(2)}) \right\rangle. \end{aligned} \quad (10)$$

The functional  $J(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a})$  (10) can be represented as the algebraic sum of the functionals of the average energies of Coulomb interaction [9]. In the functional described by (8),  $K(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a})$  is determined by the formula

$$K(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a}) = \left\langle \varphi_{B(1)}(r_{B(1)}) \varphi_{A(2)}(r_{A(2)}) \left| \hat{H}_{\text{int}} \right| \varphi_{A(1)}(r_{A(1)}) \varphi_{B(2)}(r_{B(2)}) \right\rangle. \quad (11)$$

The functional  $K(\tilde{D}, \bar{\mu}(\tilde{a}, \tilde{D}), \tilde{a})$  (11) can be represented as the algebraic sum of the functionals of the average energies of the exchange interaction [9].

Within the framework of the variational method at the first approximation the total energy of ground singlet state of excitonic quasimolecule is determined by average value of the Hamiltonian  $\hat{H}$  (2) for states, which are described by wave functions of the zero approximation  $\Psi_s(r_{A(1)}, r_{A(2)}, r_{B(1)}, r_{B(2)})$  (5) [9]:

$$E_0(\tilde{D}, \tilde{a}) = 2E_{\text{ex}}(\tilde{a}) + E_e(\tilde{D}, \tilde{a}), \quad (12)$$

where  $E_e(\tilde{D}, \tilde{a})$  is the binding energy of the ground singlet state of the excitonic quasimolecule and  $E_{\text{ex}}(\tilde{a})$  is the binding energy of the ground state of the exciton (consisting of spatially separated electron and hole) localized over the surface of QD, which was worked out in [6, 7].

## RESULTS AND DISCUSSION

Fig. presents the results of the variational calculations of the binding energy  $E_e(\tilde{D}, \tilde{a})$  studied in [1–3, 8] of the excitonic quasimolecule ground state in a nanosystem with germanium QD of the mean radius  $\bar{a}_1 = 12.8$  nm, grown in a matrix of silicon (the Bohr radius of the 2D exciton  $a_{\text{ex}}^{2D} = 2.6$  nm). The variational method that we used for the calculation of the excitonic quasimolecule ground state binding energy  $E_e(\tilde{D}, \tilde{a})$  is applicable provided that it is much smaller than the binding energy of the exciton ground state  $E_{\text{ex}}(\tilde{a})$ , i.e. the following condition must be fulfilled [9]:

$$\left( E_e(\tilde{D}, \tilde{a}) / E_{\text{ex}}(\tilde{a}) \right) \ll 1. \quad (13)$$

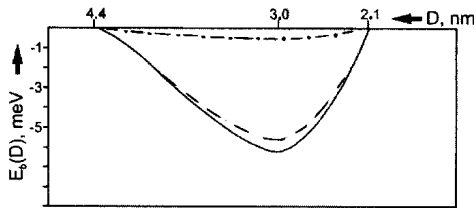
The binding energy  $E_e(\tilde{D}, \tilde{a})$  of the excitonic quasimolecule ground state in a nanosystem with QD germanium of the mean radius  $\bar{a}_1 = 12.8$  nm has a minimum

$E_e^{(1)}(D_1, \bar{a}_1) \approx -6.1$  meV (at the distance  $D_1 \cong 3.1$  nm) (Fig.) ( $E_e^{(1)}$  corresponds to the critical temperature  $T_c \approx 71$  K). As it follows from Fig., the excitonic quasimolecule appears in the nanosystem at distances  $D \geq D_c^{(1)} \cong 2.1$  nm between the surfaces of QD. The formation of such excitonic quasimolecule has of the threshold character and can occur in a nanosystem with quantum dots of the mean radius  $\bar{a}_1$ , where the distance  $D$  between the surfaces of QD exceeds a certain critical value  $D_c^{(1)}$ . The existence of such distance  $D_c^{(1)}$  arises from quantum size effects in which the decrease in the energies of interaction of the electrons and holes entering into the Hamiltonian (Eq. (2)) of the excitonic quasimolecule with decrease in the distance  $D$  between the surfaces of the QD cannot compensate for the increase in the kinetic energy of the electrons and holes.

The binding energy of the exciton  $E_{\text{ex}}(\tilde{a})$  amounts to  $E_{\text{ex}}(\bar{a}_1) \cong -64$  meV [6], with the energy of the excitonic quasimolecule ground state (12) taking the value of  $E_0(\tilde{D}_1, \bar{a}_1) \approx -134.1$  meV. It should be emphasized that the criterion (13) of the applicability of the variational method for the calculation of the exciton quasimolecule binding energy  $E_e(\tilde{D}, \tilde{a})$  is fulfilled ( $(E_e^{(1)}(D_1, \bar{a}_1) / E_{\text{ex}}(\bar{a}_1)) \cong 0.09$ ). At larger distances  $D$  between the surfaces of QD:  $D \geq D_c^{(2)} \cong 4.4$  nm, the excitonic quasimolecule breaks down into two excitons (consisting of spatially separated electrons and holes), localized over QD surfaces (Fig.). Thus, the excitonic quasimolecule can be formed in a nanosystem where  $D_c^{(1)} \leq D \leq D_c^{(2)}$  (see Fig.). Furthermore, a excitonic quasimolecule can exist only at temperatures lower than the critical temperature  $T_c \approx 71$  K. In the germanium monocrystal with the binding energy  $E_e = 0.34$  meV [15] (which corresponds to the temperature 4 K) the exciton binding energy  $E_e^{(1)}$  is almost two orders of magnitude.

As follows from the results of the variational calculations, the major contribution to the excitonic quasimolecule binding energy is from the energy of exchange interaction of electrons and holes, which

by far surpasses that from their Coulomb interaction (i.e. the ratio  $\leq 0.08$ ) (see Fig.). Since the calculations of the excitonic quasimolecule ground state binding energy  $|E_e(\tilde{D}, \tilde{a})|$  in the nanosystem are variational, the values of  $|E_e(\tilde{D}, \tilde{a})|$  and  $|E_e^{(1)}|$  can be somewhat underestimated.



**Fig.** The dependence of the binding energy of the ground singlet state  $E_e(D, \bar{a}_1)$  of the excitonic quasimolecule (continuous line) in a nanosystem made up of two spherical germanium quantum dots QD(A) and QD(B) with the mean radius  $\bar{a}_1 = 12.8$  nm, on the distance  $D$  between the surfaces of QD(A) and QD(B). Dependence of the exchange interaction energy of the electrons and holes (dashed line) and the energy of the Coulomb interaction between electrons and holes (dot dashed line) at the distance  $D$  between the surfaces of the quantum dots

As such, the interband electron electron transitions between the quantum-level of the hole located in the valence band of the germanium QD, and the quantum-level of the excitonic quasi-molecule located in the conduction band of the silicon matrix cause a significant absorption of radiation in the infrared wavelength region. In the considered energy intervals, located in the spectral range (1), where the absorption in the experiments from Refs. 1, 2 was observed, the indicated transitions ensure the significant experimentally-observed blurring of the absorption edge, all the way up to room temperatures.

In [8], the energy of the Coulomb interaction between electron and hole decreased (from 28.8 to 24.4 meV) with increasing the lateral size  $l$  (from  $l = 10$  nm to  $l = 20$  nm) of pyramidal germanium QD. In [6], the exciton from spatially separated electron and hole (the hole was moving in QD, and the electron was localized over spherical surface

seperataion (QD - matrix)) arose as a result of the Coulomb interaction  $V_{eh}$  (4) between electron and hole, which, in contrast to [1, 2, 8], was dependent on the dielectric permittivities of the QD and matrix. In [6], the nanosystem consisting of spherical shape germanium QD was studied as well. It was shown in [6] that the energy of the Coulomb interaction between electron and hole decreased (from 94 to 26 meV) with increasing the radius of germanium QD  $a$  (from  $a = 3$  nm to  $a = 5$  nm). Since in [6] the expression  $V_{eh}$  (4), which describes the Coulomb interaction between electron and hole, was obtained in the framework of classical electrodynamics, the study of exciton states in nanosystem containing a QD with radii  $a$  less than 3 nm is incorrect.

## CONCLUSIONS

Thus, it has been shown that the exciton quasimolecule formation is of the threshold character and possible in a nanosystem, where the distance  $D$  between the surfaces of QD is given by the condition  $D_c^{(1)} \leq D \leq D_c^{(2)}$  (where  $D_c^{(1)}$  and  $D_c^{(2)}$  are some critical distance). A significant increase in the binding energy of the singlet ground state of excitonic quasi-molecule (of spatially separated electrons and holes) in a nanosystem that consists of germanium QDs grown in a silicon matrix has been predicted; the effect is almost two orders of magnitude larger than the binding energy of biexciton in a silicon single crystal. It is shown that the major contribution to the exciton quasi-molecule binding energy is made by the energy of the exchange interaction of electrons with holes and this contribution is much more substantial than the contribution of the energy of Coulomb interaction between the electrons and holes (see Fig.).

The fact that the energy of the ground state singlet excitonic quasi-molecule is in the infrared range of the spectrum, presumably, allows the use of a quasi-molecule to create new elements of silicon infrared nano-optoelectronics [12–14].

## Теорія енергії зв'язку екситонних квазімолекул у германій/кремнієвих подвійних квантових точках

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Розвинуто теорію екситонних квазімолекул (утворених із просторово розділених електронів і дірок) у наносистемі, що складається з подвійних квантових точок (КТ) германію, синтезованих у кремнієвій матриці. Показано, що енергія зв'язку основного синглетного стану екситонної квазімолекули значно більша (майже на два порядки) за енергію зв'язку біекситону в монокристалі кремнію. Установлено, що утворення екситонної квазімолекули має пороговий характер і можливе в наносистемі, в якій відстань  $D$  між поверхнями КТ визначається умовою  $D_C^{(1)} \leq D \leq D_C^{(2)}$  (де  $D_C^{(1)}$  і  $D_C^{(2)}$  – деякі критичні відстані). Використовуючи варіаційний метод, отримано енергію зв'язку основного синглетного стану екситонної квазімолекули в такій системі, як функцію відстані  $D$  між поверхнями КТ та радіуса  $a$  КТ. Показано, що зближення двох КТ до певного критичного значення  $D_C$  між поверхнями КТ, призводить до ефективного перекриття хвильових функцій електрона та виникнення обмінних взаємодій. В результаті можуть бути створені умови для виникнення екситонних квазімолекул з КТ. Установлено, що існування критичної відстані  $D_C^{(1)}$  було наслідком квантових розмірних ефектів. Розмірне квантування руху електронів і дірок призводило до того, що зі зменшенням відстані  $D$  між поверхнями КТ зменшення енергій взаємодії електронів і дірок, які входили в гамільтоніан екситонної квазімолекули, не змогло компенсувати збільшення кінетичної енергії електронів та дірок. На більших відстанях  $D$  між поверхнями КТ, таких що  $D \geq D_C^{(2)}$ , екситонна квазімолекула розпадалась на два екситони (що склались з просторово розділених електронів і дірок), локалізованих над поверхнями КТ. Той факт, що енергія основного стану синглетної екситонної квазімолекули знаходиться в інфрачервоному діапазоні спектра, імовірно, дозволяє використовувати квазімолекули для створення нових елементів кремнієвої інфрачервоної нанооптоелектроніки.

**Ключові слова:** просторово розділені електрони і дірки, квантові точки, енергія зв'язку, кулонівська та обмінна взаємодії

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