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**THE EFFECT OF SHALLOW
IMPURITIES ON THE LIGHT ABSORPTION
BY THE NANOCRYSTALS CdS**

The energy of quantum transitions of exciton-impurity states in a heterosystem with nanocrystals is calculated. The absorption spectra associated with the indicated transitions are analyzed. It is qualitatively shown that broad luminescence bands in the red region are related to the impurity acceptor states, and the high narrow ones in the violet region to pure excitonic states and excitonic states interacting with the ion of a donor. The satisfactory quantitative agreement of our calculations with experimental data for high energy luminescence bands is obtained.

Keywords: acceptor and donor impurities, exciton, light absorption coefficient, nanocrystal.

1. Introduction

Important tasks of scientists and technologists in materials science are the search for new materials that can be applied in nanoelectronics. The most productive way in this direction is the use of heterosystems with various nanoobjects: quantum dots (QDs), quantum wires, quantum wells, and their combination. Based on these systems, there is a significant number of devices, whose main characteristic is the low power consumption and high performance.

The main task of physicists is to develop effective models for forecasting and managing the properties of QD, detecting and fixing these properties, as well as the development of a methodology that will allow one to get the assigned high-quality objects with predefined characteristics.

Today, high-quality QDs can be produced, but there is no guarantee of the absence of various defects in them. In a single nanocrystal, at least one impurity atom can be present. Moreover, the impurities can

passivate the torn ties on the QD surface. In addition, the impurities can be purposefully injected into a nanoobject by the doping. Therefore, the impurities may be in the QD and affect its properties. In this connection, there are a number of theoretical works [1–9], in which the energy spectra of donors and acceptors are determined as functions of the nanocrystal parameters.

The most informative and relatively simple methods that give a possibility to study the electronic structure of QDs in practice are experiments dealing with the photoluminescence and absorption of light. These data are the basis, on which we can test the theoretical models relating to the energy structure of nanocrystals and to the linear or nonlinear absorption of electromagnetic waves.

There is a significant number of experimental works on the luminescence and the absorption of electromagnetic waves by nanocrystals [10–15]. The authors of these and other papers obtained the dependences of the luminescence intensity on the average size of nanocrystals and the wavelength. Many researchers are attracted by the heterostructures of CdS QD. It

turned out that they can be used in biological indicators, in light-emitting diodes with a high coefficient of usefulness actions, *etc.*

The aims of this work are

- calculation of the electron transition energy into the exciton and exciton-donor states and the determination of the light absorption coefficient connected with those transitions;
- analysis of obtained theoretical results and their comparison with experimental data on the photoluminescence in the visible spectral range for the heterosystem with nanocrystals CdS.

2. Formulation of the Problem. The Solution of the Schrödinger Equation for an Exciton and Exciton-Impurity Complexes in the QD

The heterosystem with a spherical semiconductor nanocrystal with radius a , which is placed in a dielectric matrix, is considered. Let the size of a nanocrystal be such that, to solve the Schrödinger equation for electrons or holes, we can use the effective mass method. We suppose that the effective masses of quasiparticles are isotropic in each component of the heterosystem. The electron and heavy hole effective masses in the nanocrystal are $m_{e;1}$, $m_{h;1}$; and $m_{e;2}$, $m_{h;2}$ in the matrix, respectively. The dielectric permittivity of the QD and matrix are ε_1 and ε_2 , respectively. We suppose that, at the center of the QD, charged or neutral impurities of the donor or acceptor type can be present. Those impurities can cause the formation of impurity-exciton complexes of various kinds: $D^+ - X$ (positive charged ion of the donor impurity D^+ and exciton X); $A^- - X$ (negative charged ion of the acceptor impurity A^- and exciton); $D^0 - X$ (neutral donor impurity D^0 and exciton X); and $A^0 - X$ (neutral acceptor impurity and exciton). Those complexes are manifested in the optical spectra.

The Hamiltonian of electrons (holes) for the complexes $D^+ - X$ and $A^- - X$ (in the atom system of units) takes the form

$$\hat{H}_{\{A^- - X\}} = \hat{H}_{\{A\}} + \hat{H}_{\{e\}} - \frac{1}{\varepsilon |\mathbf{r}_e - \mathbf{r}_h|} + \frac{1}{\varepsilon r_{\{e\}}}, \quad (1)$$

where $\varepsilon = (\varepsilon_1 + \varepsilon_2)/2$ (Table),

$$\hat{H}_{\{D\}} = -\frac{1}{2} \nabla \frac{1}{m_{\{e\}}} \nabla - \frac{1}{\varepsilon r_{\{e\}}} + U_{\{e\}}(r_{\{e\}}) \quad (2)$$

is the Hamiltonian of donors or acceptors,

$$U_{\{e\}}(r_{\{e\}}) = \begin{cases} 0, & r_{\{e\}} \leq a, \\ U_{\{e\},0}, & r_{\{e\}} > a \end{cases} \quad (3)$$

is the confinement potential,

$$\hat{H}_{\{e\}} = -\frac{1}{2} \nabla \frac{1}{m_{\{e\}}} \nabla + U_{\{e\}}(r_{\{e\}}) \quad (4)$$

is the Hamiltonian of one hole or electron. The Schrödinger equation with Hamiltonian (1) is solved by the variational method. The trial variational wave function is chosen as

$$\psi_{\{A^- - X\}}(\mathbf{r}_{\{h\}}, \mathbf{r}_{\{e\}}) = C_{\{A^- - X\}} \psi_{\{A\}}(\mathbf{r}_{\{e\}}) \times \psi_{\{e\}}(\mathbf{r}_{\{h\}}) \exp \left[-\alpha_{\{A^- - X\}} |\mathbf{r}_e - \mathbf{r}_h| \right], \quad (5)$$

where $C_{\{A^- - X\}}$ is the normalization constant, $\psi_{\{A\}}$ and $\psi_{\{e\}}$ are exact solutions of the Schrödinger equations

$$\hat{H}_{\{D\}} \psi_{\{A\}}(\mathbf{r}_{\{e\}}) = E_{\{e\}} \psi_{\{A\}}(\mathbf{r}_{\{e\}}), \quad (6)$$

$$\hat{H}_{\{e\}} \psi_{\{e\}}(\mathbf{r}_{\{h\}}) = E_{\{h\}} \psi_{\{e\}}(\mathbf{r}_{\{h\}}), \quad (7)$$

The solutions of Eq. (6) are expressed as the products of spherical functions and Coulomb or Whittaker functions [2–4, 7], and the solutions of Eq. (7) are the products of spherical functions and Bessel functions.

According to the variational Ritz method, the minimized functional is equal to the ground-state energy of each exciton-impurity complex.

The electron (hole) Hamiltonians of the heterosystem with the impurity complexes $D^0 - X$ and $A^0 - X$ can be written as

$$\hat{H}_{\{D^0 - X\}} = \hat{H}_{\{D^0\},1} + \hat{H}_{\{A^0\},2} + \hat{H}_{\{e\}} - \frac{1}{\varepsilon |\mathbf{r}_{\{h\},1} - \mathbf{r}_{\{e\}}|} - \frac{1}{\varepsilon |\mathbf{r}_{\{h\},2} - \mathbf{r}_{\{e\}}|} + \frac{1}{\varepsilon r_{\{e\}}}, \quad (8)$$

where

$$\hat{H}_{\{A^0\},i} = -\frac{1}{2} \nabla_i \frac{1}{m_{\{e\}}} \nabla_i - \frac{1}{\varepsilon r_{\{e\},i}} + U_{\{e\}}(r_{\{e\},i}), \quad (9)$$

$i = 1, 2$, and $\hat{H}_{\{h\}}$ is expressed by (4).

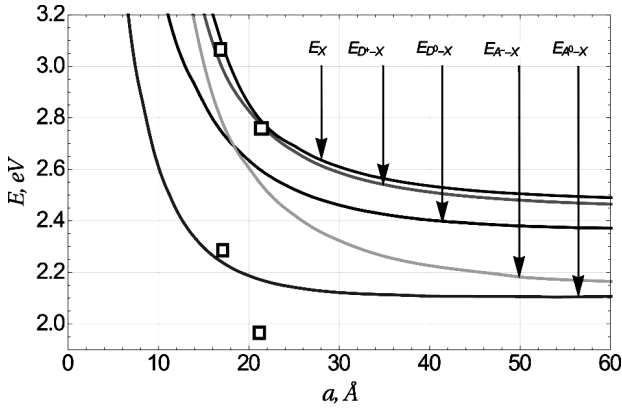


Fig. 1. Energies of the exciton and the exciton-impurity complexes in a QD. The squares represent experimentally defined [10, 13] energies of quantum transitions of CdS nanocrystals with average radii of 17 and 21.5 Å

Crystal parameters

Crystal	m_e	m_h	ε	$U_{0,e}$, eV	$U_{0,h}$, eV
CdS	0.2	0.74	5.5	2.70	3.42
SiO ₂	1.0	1.00	3.9	–	–

The Schrödinger equation with Hamiltonian (8) is also solved by the Ritz variational method. The trial wave function of the ground state is

$$\begin{aligned} \psi_{\{A^0-X\}}^{D^0-X}(\mathbf{r}_{\{e\}}, \mathbf{r}_{\{h\},1}, \mathbf{r}_{\{h\},2}) &= C_{\{A^0-X\}}^{D^0-X} \times \\ &\times \psi_{\{A^0\},1}^{D^0}(\mathbf{r}_{\{e\},1}) \psi_{\{A\},2}^{D^0}(\mathbf{r}_{\{e\},2}) \psi_{\{e\}}^h(\mathbf{r}_{\{e\}}) \times \\ &\times e^{\left[-\alpha_{\{A^0-X\},1}^{D^0-X} |\mathbf{r}_{\{h\}} - \mathbf{r}_{\{e\},1}| - \alpha_{\{A^0-X\},2}^{D^0-X} |\mathbf{r}_{\{h\}} - \mathbf{r}_{\{e\},2}| \right]}, \end{aligned} \tag{10}$$

where $\psi_{\{A^0\},i}^{D^0}(\mathbf{r}_{\{e\},i})$ and $\psi_{\{e\}}^h(\mathbf{r}_{\{e\}})$ are exact solutions of Eqs. (6) and (7), which concern with the electron and hole ground states, $\alpha_{\{A^0-X\},1}^{D^0-X}$ and $\alpha_{\{A^0-X\},2}^{D^0-X}$ are variational parameters.

If there are no impurities or their influence is insignificant in the QD, then the “pure” exciton states may occur in the heterosystem. In this case, the Hamiltonian of the system has the form:

$$\hat{H}_X = \hat{H}_e + \hat{H}_h - \frac{1}{\varepsilon |\mathbf{r}_e - \mathbf{r}_h|}, \tag{11}$$

where \hat{H}_e and \hat{H}_h are defined by (4), and the variational wave function for the ground state is chosen as

$$\psi_X(\mathbf{r}_e, \mathbf{r}_h) = C_X \psi_e(\mathbf{r}_e) \psi_h(\mathbf{r}_h) \exp[-\alpha_X |\mathbf{r}_e - \mathbf{r}_h|], \tag{12}$$

where α_X is a variational parameter.

The calculation of the corresponding energies is carried out for the QD heterosystem CdS/SiO₂, the parameters of which are given in the Table.

Figure 1 shows the results of calculations of the energies of the ground states of the exciton and the every exciton-impurity complexes for different radii of the QD. It can be seen that the Wannier–Mott exciton energy is close to the energy of the exciton-impurity complex $D^+ - X$ for the entire region of the change of the QD radius ($10 \text{ \AA} \leq a \leq 60 \text{ \AA}$).

It is seen that the presence of impurities leads to a decrease in the electron-hole pair energy, as compared with the case of their absence. This means that, in the presence of such impurities, the creation of exciton-impurity complexes is more energy-efficient. The possible existence of such complexes in the CdS QD was indicated in the experimental works [10, 13].

In order to compare the theoretical results with the experimental data, we show the energy of quantum transitions during luminescence of the CdS QD, which was experimentally determined in [10, 13], in Fig. 1. Based on the calculations, we can conclude that the energies $E_1 = 3.05 \text{ eV}$ and $E_2 = 2.75 \text{ eV}$ can be interpreted as those corresponding to the electron-hole transition in case of their recombination in the presence of a charged donor or in the absence of it. The transition energy $E_3 = 2.25 \text{ eV}$ can be related to the presence of a neutral acceptor, which forms the exciton complex $A^0 - X$, in the QD. For the transition $E_4 = 1.95 \text{ eV}$, it is of importance to find a satisfactory theoretical explanation.

In order to determine the contribution of each of the impurity complexes to the optical parameters, the absorption coefficient of the heterosystem in the presence of various types of exciton-impurity complexes in the QDs is also calculated.

3. Light Absorption Coefficient of the Heterosystem with QDs

Let the heterosystem be irradiated by a monochromatic linearly polarized light at the frequency

$\omega = 2\pi c/\lambda$ and with weak intensity (insufficient for the manifestation of nonlinear effects). Accordingly, the absorption coefficient of a nanoheterosystem with QDs, which is due to interband direct transitions, is determined at low temperatures by the formula [16]:

$$\alpha_{\text{QD}}(\lambda) = \frac{A}{\hbar^2 \frac{2\pi}{\lambda}} \sum_{i,j} |\langle \psi_i | \psi_j \rangle|^2 \delta(E_j - E_i - \hbar\omega(\lambda)), \quad (13)$$

where $A = \frac{2\pi\hbar e^2}{m_0 \varepsilon_0 c} \frac{N}{n} E_p$, e is the electron charge, m_0 is the free electron mass, ε_0 is the electric constant, c is the speed of light, N is the concentration of QDs, $n = \sqrt{\varepsilon}$, $\hbar\omega$ is the light quantum energy, $E_p \approx 23$ eV is Kane's matrix element [16], and ψ_i and ψ_j are the envelope wave functions of the initial i and final j states. In what follows, we consider the two-level system: E_1 is the energy of the system provided that the electron is in the valence band, and $E_2 = E_1 + \hbar\omega$.

We consider the heterogeneous expansion of absorption bands, which is related to the dispersion of the dimensions of a QD in the matrix. In [17], it was shown that the account for such a dispersion determines the final half-width of the absorption band. Let the distribution of the QD dimensions be described by the Gauss function

$$g(s, \bar{a}, a) = \frac{1}{s\sqrt{2\pi}} \exp\left(-\frac{(a - \bar{a})^2}{2s^2}\right), \quad (14)$$

where a is the QD radius (variable), s is the half-width of distribution (14), which is defined by the mean radius \bar{a} and the value of σ expressed in percentages: $s = \bar{a}\sigma/100$. With regard for all the approximations described above, the absorption coefficient of a heterosystem with the QD takes the form:

$$\alpha(\lambda) = B\lambda \int g(s, \bar{a}, a) I_{2,1}(a) \delta(E_2(a) - E_1(a) - \hbar\omega(\lambda)) da, \quad (15)$$

where

$$I_{2,1}(a) = |\langle \psi_2 | \psi_1 \rangle|^2 \quad (16)$$

is the overlap integral, and $B = \frac{A}{2\pi\hbar}$. In view of the properties of the delta-function, we get

$$\alpha(\lambda) = B\lambda \int g(s, \bar{a}, a) I_{2,1}(a) \times$$

$$\times \sum_n \frac{\delta(a - a_{0,n}) da}{\left| \frac{d}{da} (E_2(a) - E_1(a) - \hbar\omega(\lambda)) \right|_{a=a_{0,n}}}, \quad (17)$$

where $a_{0,n}$ are simple zeros of the function $F(a) = (E_2(a) - E_1(a) - \hbar\omega(\lambda))$. Hence,

$$\alpha(\lambda) = B\lambda \sum_n \frac{g(s, \bar{a}, a_{0,n}) I_{2,1}(a_{0,n})}{\left| \frac{d}{da} (E_2(a) - E_1(a) - \hbar\omega(\lambda)) \right|_{a=a_{0,n}}}. \quad (18)$$

Now, we set specific ψ_1 and ψ_2 in (18). If there is no impurity in the QD, and when an exciton is formed by the absorption of an electromagnetic wave, then $\psi_1 = \delta(\mathbf{r}_e - \mathbf{r}_h)$ and $\psi_2 = \psi_X(\mathbf{r}_e, \mathbf{r}_h)$. When there is the ion of a donor or acceptor impurity in the QD and when the light is absorbed, the complex $D^+ - X$ or $A^- - X$ is formed. Then $\psi_1 = \delta(\mathbf{r}_e - \mathbf{r}_h)$ and $\psi_2 = \psi_{\left\{ \begin{smallmatrix} D^+ - X \\ A^- - X \end{smallmatrix} \right\}}(\mathbf{r}_e, \mathbf{r}_h)$. Let a neutral donor (acceptor) impurity be in the QD and let, when light absorbed, a complex $D^0 - X$ ($A^0 - X$) be formed. Then $\psi_1 = \psi_{\left\{ \begin{smallmatrix} D \\ A \end{smallmatrix} \right\}, 1}(\mathbf{r}_{\left\{ \begin{smallmatrix} e \\ h \end{smallmatrix} \right\}, 1}) \delta(\mathbf{r}_{\left\{ \begin{smallmatrix} h \\ e \end{smallmatrix} \right\}} - \mathbf{r}_{\left\{ \begin{smallmatrix} e \\ h \end{smallmatrix} \right\}, 2})$, $\psi_2 = \psi_{\left\{ \begin{smallmatrix} D^0 - X \\ A^0 - X \end{smallmatrix} \right\}}(\mathbf{r}_{\left\{ \begin{smallmatrix} h \\ e \end{smallmatrix} \right\}}, \mathbf{r}_{\left\{ \begin{smallmatrix} e \\ h \end{smallmatrix} \right\}, 1}, \mathbf{r}_{\left\{ \begin{smallmatrix} e \\ h \end{smallmatrix} \right\}, 2})$. The overlapping integrals were calculated for all these QD models, and the absorption coefficients were determined according to formula (18).

Figure 2 shows the plots of the wavelength dependence of the relative light absorption coefficient for the CdS/SiO₂ heterosystem.

It is seen that each of the above-described light absorption mechanisms corresponds to different values

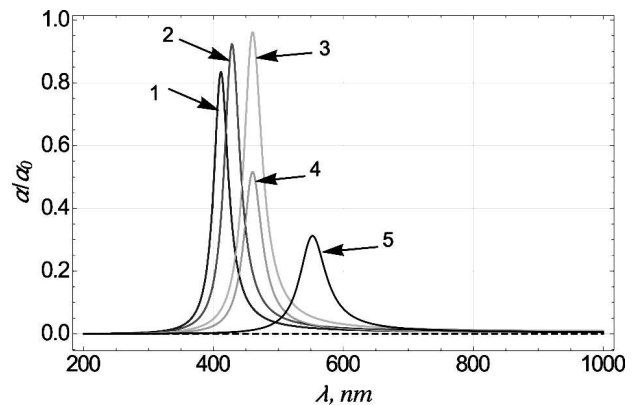


Fig. 2. Dependence of the relative absorption coefficient for each individual type of the exciton complex on the wavelength. Curve 1 corresponds to the exciton absorption X , 2 - $D^+ - X$, 3 - $A^- - X$, 4 - $D^0 - X$, 5 - $A^0 - X$. Average radius of the QD is 17 Å, $\sigma = 10\%$

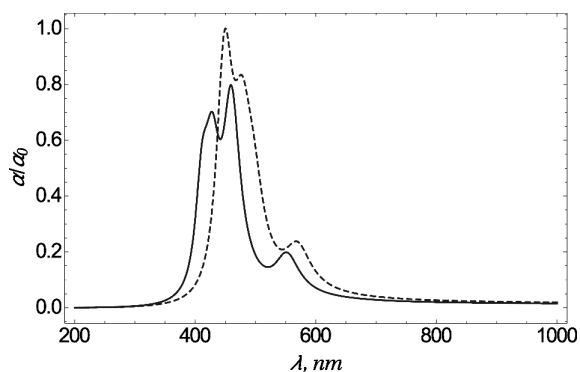


Fig. 3. Dependence of the relative absorption coefficient with regard for all the absorption mechanisms described above. The solid and dashed curves correspond to the average QD radii equal to 17 and 21.5 Å, respectively, $\sigma = 10\%$

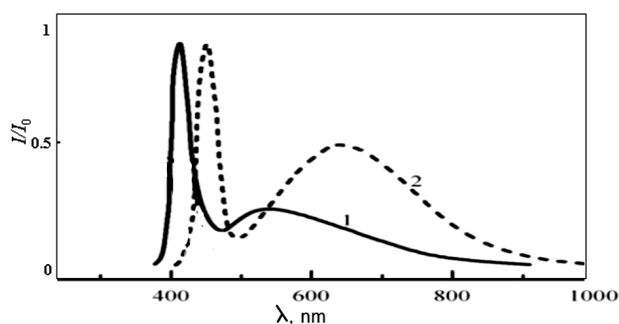


Fig. 4. Dependence of the relative luminescence intensity for CdS nanocrystals. The solid and dashed curves correspond to the QD average radii 17 and 21.5 Å [10, 13]

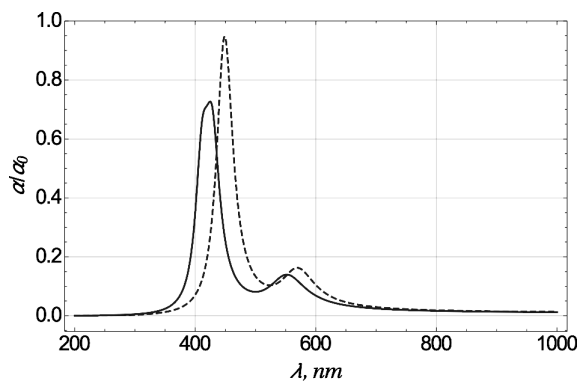


Fig. 5. Relative absorption coefficient of light for nanocrystals with an average radius of 17 Å (solid) and 21.5 Å (dashed); $\sigma = 10\%$

of absorption peaks and their positions on the scale of wavelengths. For an average QD radius 17 Å, the presence of impurities leads to the displacement of all absorption peaks toward long waves relative to the

exciton band (curve 1). The absorption peaks due to the presence of a neutral impurity D^0 or A^0 are approximately two times smaller than the absorption peaks responsible for the presence of D^+ or A^- ion impurity ions.

If we take into account that all the above-mentioned absorption mechanisms occur in the QD heterosystem, then the absorption coefficient will have the same form as in Fig. 3. The resulting graph is compared with the corresponding luminescence graphs of the experimental works [10, 13] (Fig. 4).

If we compare the calculated values (Fig. 3) and the experimental ones (Fig. 4), then it is evident that not all of the types of impurity-exciton complexes mentioned above were obviously observed in the experiment. In this connection, we think that, in the experimental work dealing with the QD heterosystem, there are impurities of the acceptor type that interact with excitons. There are also pure homogeneous QDs, where the exciton transitions are observed. To compare experimental data, we calculated the absorption in the case of a pure exciton X and an exciton that interacts with the neutral acceptor $A^0 - X$. The results are presented in Fig. 5.

As one can see, we obtained a qualitative agreement of the energies and half-widths for long-wave bands and the quantitative agreement of these quantities for exciton bands. The main maxima on the experimental curves are due to the recombination of pure excitons, and the recombination with the participation of a neutral acceptor gives a contribution to the broad band. It should be noted that the luminescence causes a Stokes shift [17–19]. Experimentally, the luminescence maxima were observed at 435 nm (average radius 17 Å) and 480 nm (average radius 21.5 Å). The maxima of the main exciton absorption in our work for similar sizes correspond to 420 nm and 450 nm. In other words, the experimental peaks of luminescence are shifted to the long-wave region in comparison with our absorption results of 15 nm and 30 nm, respectively. The resulting energy differences are consistent with the Stokes shift data for QDs in CdS [13, 14, 18, 19].

As to the quantitative coincidence of the theory and experiment in the region of 550–650 nm, certain differences can be explained by the fact that the theory did not involve the surface defect states that could also contribute to a wide luminescence band. Along with this, there may be other causes (in particular,

phonon origin), which lead to the obtaining of wide radiation bands of light.

4. Conclusions

Experimental works devoted to the study of the absorption and luminescence spectra of impurity CdS nanocrystals [11–13] put a number of unresolved problems before the researchers. In the proposed theoretical work, the influence of impurity atoms and their ions of the donor and acceptor types on the exciton excitation energy is studied. Thus, we consider five types of the QD excitation: with the formation of the Wannier–Mott exciton and four types of exciton-impurity complexes ($D^+ - X$, $D^0 - X$, $A^- - X$, $A^0 - X$).

The calculations have shown that, for the mean CdS QD radii $a = 17 \text{ \AA}$ and 21.5 \AA , which appear in [13], the energies of the exciton formation and the exciton-impurity complex with the donor ion ($E_{D^+ - X}$) are quite close in magnitude. The energies of the $D^0 - X$ and $A^- - X$ complexes for the same QD radii are similar as well. For these energies, the condition $E_{D^0 - X} \approx E_{A^- - X} < E_X \approx E_{D^+ - X}$ holds. The energy of the formation of the complex $A^0 - X$ is the smallest.

The dependence of the total absorption coefficient of light on the wavelength for a heterosystem with such types of electron excitation shows that the main absorption band is characterized by two maxima (“humps”). It is formed by the quantum transitions of an electron with the formation of X , $D^+ - X$, $D^0 - X$, and $A^- - X$. The long-wave wing of this band appears during the formation of the complex $A^0 - X$. It is worth noting that the wavelength of light, at which the maximum absorption coefficient is realized at $a = 17 \text{ \AA}$, is close to the corresponding wavelength of the maximum of the luminescence intensity in work [13]. For QDs with an average radius of 21.5 \AA , the discrepancy between theory and experiment is greater. This problem will be discussed in our next work.

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ВПЛИВ МІЛКИХ ДОМІШОК НА СПЕКТР
ПОГЛИНАННЯ СВІТЛА НАНОКРИСТАЛАМИ CdS

Р е з ю м е

У роботі обчислено енергії квантових переходів екситонно-домішкових станів у гетеросистемі з нанокристаллами. Визначено енергії цих переходів та проаналізовано спектри поглинання, що пов'язані із зазначеними переходами. Якісно показано, що широкі смуги люмінесценції у червоній області пов'язані з домішковими акцепторними станами, а високі вузькі у фіолетовій області – з чистими екситонними станами та екситонними станами, що взаємодіють з іоном донора. Отримано задовільне кількісне узгодження наших обчислень з експериментальними даними для високоенергетичних смуг люмінесценції.