Effect of charge-carrier screening on the exciton binding energy in GaAs/Al_xGa_{1-x}As quantum wells

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(Received 18 June 1992)

Exciton binding energies of heavy- and light-hole excitons affected by charge-carrier screening in GaAs-Al_xGa_{1-x}As quantum wells are calculated by the variational-perturbation method. The exciton binding energies are found to decrease rapidly when the screening length is less than $30a_B^h$ (effective exciton Bohr radius). This screening length corresponds to a carrier density of 7.0×10^{13} /cm³ at T=10 K. In the calculation, the Debye screening model is used for charge carriers. The exciton binding energies as functions of the screening length, carrier density, and quantum-well parameters have been calculated. The critical carrier densities, above which no excitons can be formed, are obtained at different well thickness. The effects of charge-carrier screening to the exciton photoluminescence are also discussed.

I. INTRODUCTION

With the recent development in semiconductor artificial structures, such as quantum wells (QW's) and superlattices (SL's), many important physical properties have been explored.^{1,2} In fundamental physics, OW and SL structures have been used to explore the physical properties of low-dimensional systems and quantum effects. Many phenomena in QW's and SL's have been discovered. QW's and SL's are also very promising in many practical applications such as high-speed electronics, photoelectronics, and photonic devices exempted by quantum-well lasers,³ modulation-doped field-effect transistors,⁴ photodetectors,⁵ etc. For QW and SL optical properties, exciton binding energy in QW structure plays a crucial role and has been studied extensively both in theory and experiment.⁶⁻⁹ The most common method used to calculate exciton binding energy in QW's and SL's is the variational method. Another simple yet useful method, the variational-perturbation approach,¹⁰ has also been used and proved to be reliable.¹¹

Experimentally, one finds that electrons and holes form plasma instead of excitons when excitation light intensity is very high.¹² It is conceivable that at a certain range of light excitation, there will be a coexistence of excitons and free carriers. Such a coexistence of excitons and free carriers and the transformation between the form of excitons \iff electrons + holes have been used to explain the experimental results of exciton dynamics of photo-luminescence in QW's.¹³ Thus, exciton binding energy depends on charge-carrier density and the exciton binding energy becomes zero above a certain carrier density. The effects of free carriers to the exciton binding energy in QW's are especially important at high temperatures and under an external electric field, in which case the charge-carrier density is high.^{12,14} The carrier density can be much larger than 10^{14} /cm³ due to the high quantum efficiency of QW structure and hence the charge screening effect could be very important. It is known that the exciton binding energy is decreasing when an external electric field is applied along the direction perpendicular to the well which is a direct result of the separation of electron and hole wave functions in the presence of the field.⁸ The charge screening becomes more important in this case since the local density could be even higher due to the carrier and exciton localization. It is important to understand the exciton properties in the presence of free carriers.

In this paper, the effects of the charge screening on exciton binding energy have been calculated by the variational-perturbation method. The advantage here is that it is a simple, nevertheless, effective method. A rapid decrease of exciton binding energy has been obtained for the screening length less than $30a_B^h$, or equivalently, the carrier density larger than 7.1×10^{11} /cm³. In the calculation, the Debye screening model is used at temperature T = 10 K. Exciton binding energy as functions of the screening length and the carrier density are calculated. The critical carrier densities, above which no excitons can be formed, are obtained at different well thickness. These results are consistent with experimental observations. The effects of charge screening to the exciton photoluminescence are also discussed.

II. CALCULATIONS

When excitons and free carriers coexist in QW's, the Coulomb interaction between the electron and hole of an exciton will be affected, or screened by these charge carriers. Thus, the exciton binding energy will be changed. In the following, we solve the exciton binding energy with the existence of a free carrier of density n. Excitons in this case can be approximated by a screened Coulomb interaction between electron and hole. The interaction between excitons has been neglected. Also, we assumed that the carrier density is important for screening of the exciton; however, it is not high enough to cause the effect of energy-gap renormalization.

In the framework of the effective-mass approximation, the Hamiltonian of an exciton in a QW, in the presence of free charge carriers, is given by

$$H = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_{h(l)}} \frac{\partial^2}{\partial z_{h(l)}^2} - \frac{\hbar^2}{2\mu_{h(l)}} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right]$$
$$- \frac{e^2}{\epsilon |\mathbf{r}_e - \mathbf{r}_{h(l)}|} e^{-|\mathbf{r}_e - \mathbf{r}_{h(l)}|/s} + V_e(z_e)$$
$$+ V_{h(l)}(z_{h(l)}) + E_g , \qquad (1)$$

where \mathbf{r}_e and $\mathbf{r}_{h(l)}$ are the coordinates of electron and (light) hole, respectively, heavy and $(x,y) = (x_e - x_{h(l)}, y_e - y_{h(l)})$ is the relative distance between the electron and hole in the transverse plane. In Eq. (1), the Coulomb interaction between the electron and hole has been multiplied by a factor which describes the screening of the exciton due to charge carriers. In writing Eq. (1), we have assumed that the charge carriers are distributed uniformly in the QW and represented by a screening length s. m_e and $m_{h(l)}$ are the electron effective mass and the longitudinal effective mass of heavy (light) holes, which are functions of the coordinate $z_{e,h(l)}$. $\mu_{h(l)}$ is the transverse reduced heavy- (light-) hole exciton mass and ϵ is the static dielectric constant. The confinement potential wells for the electron and hole in the z direction are assumed to be square shape,

$$V_{e,h(l)}(z_{e,h(l)}) = \begin{cases} V_{0e,0h(l)}, & |z_{e,h(l)}| \ge L/2\\ 0, & |z_{e,h(l)}| \le L/2. \end{cases}$$
(2)

The Hamiltonian in Eq. (1) with the potential of Eq. (2) cannot be solved exactly. We therefore use the variational-perturbation method by solving, instead of Eq. (1) directly, the following Hamiltonian:

$$H_0(\lambda) = H_e + H_{h(l)} + H_{\mu_{h(l)}}(\lambda) + E_g$$
(3a)

with

$$H_e = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z_e^2} + V_e(z_e) , \qquad (3b)$$

$$H_{h(l)} = -\frac{\hbar^2}{2m_{h(l)}} \frac{\partial^2}{\partial z_{h(l)}^2} + V_{h(l)}(z_{h(l)}) , \qquad (3c)$$

and

$$H_{\mu_{h(l)}} = -\frac{\hbar^2}{2\mu_{h(l)}} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] - \frac{\lambda e^2}{\epsilon |\rho_e - \rho_{h(l)}|} , \qquad (3d)$$

where ρ_e and $\rho_{h(l)}$ are the polar coordinates of the electron and heavy (light) hole in the x-y plane, and λ is a variational parameter. Then we treat the difference of Hamiltonian H and $H_0(\lambda)$, $H'(\lambda)$, as a perturbation,

$$H'(\lambda) = H - H_0(\lambda) = \frac{\lambda e^2}{\epsilon |\boldsymbol{\rho}_e - \boldsymbol{\rho}_{h(l)}|} - \frac{e^2 e^{-|\mathbf{r}_e - \mathbf{r}_{h(l)}|/s}}{\epsilon |\mathbf{r}_e - \mathbf{r}_{h(l)}|} .$$
(4)

Equations (3a)-(3d) can be solved analytically and the solutions are,

$$\Psi_{g}^{(0)} = f_{e,h(l)}(z_{e,h(l)})\Psi_{n|l|}(\rho,\phi) , \qquad (5a)$$

$$f_{e,h(l)}(z_{e,h(l)}) = \begin{cases} A_{e,h(l)} \cos(\kappa_{e,h(l)} z_{e,h(l)}) \\ & \text{for } |z_{e,h(l)}| \le L/2 \\ B_{e,h(l)} \exp(-\eta_{e,h(l)} z_{e,h,(l)}) \\ & \text{for } |z_{e,h(l)}| \ge L/2 \end{cases},$$

and

$$\Psi_{n|m|}(\rho,\phi) = \left[\frac{1}{2\pi}\right]^{1/2} e^{i|m|\phi} \frac{2}{a_B(n+\frac{1}{2})} \\ \times \left[\frac{(n-|m|)!}{(n+|m|)!(2n+1)}\right]^{1/2} \\ \times \rho^{|m|} e^{-\rho/2} L_{n+|m|}^{2|m|}(\rho) , \qquad (5c)$$

with $k_{e,h(l)}$, $\eta_{e,h(l)}$ being

$$k_{e,h(l)} = \left[\frac{2m_{e,h(l)}^{w}E_{e,h(l)}}{\hbar^{2}}\right]^{1/2},$$

$$\eta_{e,h(l)} = \left[\frac{2m_{e,h(l)}^{b}(V_{0e,0h(l)} - E_{e,h(l)})}{\hbar^{2}}\right]^{1/2},$$
(6)

and $[\rho = 2\lambda r / a_B(n + \frac{1}{2}), \varphi]$ being the polar coordinates in the x-y plane. $a_B = \epsilon \hbar^2 / \mu_{h(l)} e^2$ is the three-dimensional exciton Bohr radius calculated with transverse effective reduced mass of $\mu_{h(l)}$. $L_{n+|m|}^{2|m|}(\rho)$ is the associated Laguerre polynomials. The eigenvalues of Eq. (5b) are determined by the equation

$$\frac{\eta_{e,h(l)}}{k_{e,h(l)}} = \frac{m_{e,h(l)}^{b}}{m_{e,h(l)}^{w}} \tan \left[\frac{k_{e,h(l)}L}{2} \right],$$
(7a)

with $m_{e,h(l)}^{w}$ and $m_{e,h(l)}^{b}$ being the masses of the electron and heavy (light) hole in the well and barrier regions, respectively. The eigenvalues of Eq. (5c) are

$$E_n = -\frac{\lambda^2 R}{(n+\frac{1}{2})^2}$$
, $n = 0, 1, 2, ...,$ (7b)

with $R = \mu_{h(l)}e^4/2(\epsilon\hbar)^2$ being the three-dimensional effective Rydberg calculated with the transverse effective reduced mass of the exciton.

The first-order perturbation energy for the ground state is

$$|\Delta E_{g}^{(1)}(\lambda)| = |\langle \Psi_{g}^{(0)}|H'(\lambda)|\Psi_{g}^{(0)}\rangle| = \left|\frac{4\lambda^{2}e^{2}}{\epsilon a_{B}}\int_{-\infty}^{\infty} dz_{e}|f_{e}(z_{e})|^{2}\int_{-\infty}^{\infty} dz_{h(l)}|f_{h(l)}(z_{h(l)})|^{2} \times \left[1 - \frac{4s}{a_{B}}e^{-|z_{e} - z_{h(l)}|/s} + \frac{4s}{a_{B}}\int_{0}^{\infty} dt \exp\left\{-t - \left[\frac{t^{2}a_{B}^{2}}{16s^{2}\lambda^{2}} + \left(\frac{z_{e} - z_{h(l)}}{s}\right)^{2}\right]^{1/2}\right\}\right\}\right|.$$
(8)

In the variational-perturbation scheme, ¹¹ the exciton binding energy is then given by

$$E_b = 4\lambda_0^2 R \quad , \tag{9}$$

where λ_0 is determined with the condition that $\Delta E_g^{(1)}(\lambda)$ in Eq. (8) equals zero.

III. RESULTS AND DISCUSSIONS

Equations (8) and (9) have been used to calculate the exciton binding energy for $Al_xGa_{1-x}As/GaAs$ quantum wells with the following parameters: potential wells for electrons and heavy (light) holes $V_{0e}=0.6\times(1.115x + 0.37x^2)$ and $V_{0h(l)}=0.4\times(1.115x + 0.37x^2)$, respectively, which corresponds to a band offset of 60%; $m_e^w=0.067m_0$, $m_e^b=(0.067+0.083x)m_0$; $m_l^w=0.45m_0$, $m_b^b=(0.45+0.2x)m_0$; $m_l^w=0.082m_0$, $m_l^b=(0.082+0.068x)m_0$ for the longitudinal masses of heavy (h) and light (l) holes in the well (w) and barrier (b) regions. The transverse masses for the heavy and light holes have been taken as $0.051m_0$ and $0.04m_0$,⁷ respectively, with m_0 being the free-electron mass. The dielectric constant ϵ is taken as 12.9.

Figure 1 shows the heavy- and light-hole exciton binding energies in the GaAs/Al_{0.3}Ga_{0.7}As QW as functions of the screening length s for the cases of well thicknesses 50 and 100 Å. The exciton binding energies depend strongly on the screening length in all cases. For s larger than 5×10^3 Å, the effects of free carriers on the exciton binding are negligible. However, for the screening length less than 5×10^3 Å (or $30a_B^h$), the effects become significant. The exciton binding energies decrease by about 3 meV when s reduces from 5×10^3 to 2×10^2 Å for all the cases depicted in Fig. 1. The decreasing rates of exciton binding energy on the screening length are slight-



FIG. 1. The heavy- and light-hole exciton binding energies in GaAs/Al_{0.3}Ga_{0.7}As QW's as functions of the screening lengths for well thickness 50 and 100 Å.

ly different for different well thicknessess. The calculated exciton binding energy at the limit $s \rightarrow \infty$ is consistent with other calculations for a pure exciton system, which demonstrates the reliability of the present calculation. Table I lists the values of heavy- and light-hole exciton binding energies without charge screening $(s \rightarrow \infty)$ for x = 0.3 and 0.15 at three different well thicknesses of the present $(E_{bh(l)})$ and the previous calculation¹¹ $(E_{bh(l)}^*)$. The units for the well thickness w and the exciton binding energy are angstrom and meV, respectively. The results in Table I are in good agreement except in the case of w = 50 Å, where the different results are attribute to (a) a different band offset that has been used and (b) the contribution of wave functions of electrons and holes outside the well region in Eq. (8) which have also been included in our calculation. In fact, the integration terms of Eq. (8) outside the well cannot be neglected compared to the terms inside the well for small well thickness. Or equivalently speaking, the leakage of the wave function out of the well cannot be neglected. This wave-function leakage reduces the binding between the electron and hole of an exciton. Therefore, the infinity confinement approximation used in Ref. 11 overestimates the exciton binding energies, especially in the case of narrow wells. In the present calculation, the effects of finite barriers have also been included, as they should.

Figure 2 is the plot of the heavy- and light-hole exciton binding energies as functions of carrier density for well thickness 50 and 100 Å with x = 0.3. The relationship between the screening length s and carrier density has been assumed to follow the Debye screening length form,¹⁵

$$s = \left(\frac{\epsilon k T N_c}{e^2 n p}\right)^{1/2} = 2^{14} T^{5/4} / n , \qquad (10)$$

where *n* and *p* are the densities of electrons and holes, and N_c is the effective density of states of the conduction band. Here, we concentrate on the case that both excitons and free carriers are photoexcited, which implies n = p. From Fig. 2, the effects of the charge screening on the exciton binding energy are small for carrier density less than 7.0×10^{13} /cm³ which corresponds to an area density of 7.0×10^7 /cm² for a QW with a well thickness of 100 Å. However, the screening effects become very important as $n > 10^{14}$ /cm³. The rapid variation of exciton binding energy occurs at a carrier density of about 5×10^{14} /cm³ for both heavy- and light-hole excitons with all QW parameters investigated here.

The results in Fig. 2 may have some connection with exciton photoluminescence experiments in QW's, especially for the case of high excitation intensity, high temperatures, and under an external electric field. All of these conditions will enhance the carrier density, or equivalently the amount of charge screening to the binding of an exciton. Under these conditions, the charge screening could affect the shape of the exciton luminescence. If we define ΔE as the energy difference between the exciton binding energy for carrier densities of 7.1×10^{13} /cm³ and 3.7×10^{14} /cm³, we can investigate how the charge screening affects the exciton binding energy

TABLE I. Comparison of the calculated binding energy of heavy- (E_{bh}) and light-hole (E_{bl}) excitons at different well thicknesses with previous results $(E_{bh}^*, E_{bl}^*, \text{from Ref. 11})$. The units for well thickness and binding energy are angstrom and meV, respectively.

x = 0.3					x = 0.15			
w	E_{bh}	E_{bl}	E_{bh}^*	E_{bl}^{*}	E_{bh}	E_{bl}	E_{bh}^{*}	E_{bl}^{*}
50	8.75	9.67	9.34	10.87	8.05	8.47	9.18	10.70
100	7.53	8.39	7.75	8.75	7.22	7.86	7.57	8.52
200	5.94	6.58	6.04	6.71	5.80	6.36	5.92	6.50

ergies at different QW's. In Fig. 3 we plot ΔE as a function of well thickness with x = 0.3. A systematic decrease of ΔE is obtained as the well thickness increases. Figure 3 indicates that the charge screening effects are most important for narrower wells. This conclusion is consistent with the experimental observations of well-size dependence of exciton blueshift in QW's under high excitation intensities.^{16,17} Experimentally, the magnitude of the blueshift was found to depend predominantly upon the GaAs layer thickness, increasing at smaller well size.¹⁶ Also, the effects of the charge screening on heavy-hole excitons are more significant than that of light-hole excitons.

In Fig. 4 we plot the heavy- and light-hole exciton binding energies as functions of well thickness for two 3.6×10^{15} / cm³ different carrier densities, and 2.7×10^{14} /cm³. Similar behavior is obtained for these two carrier densities. However, a slightly slower decreasing of exciton binding energy for higher carrier densities is seen. In the case of high carrier density, we expect a higher reduction in the exciton binding energy. For example, in a coupled double quantum well subjected to an external electric field, electrons and holes are confined in different wells (bar exciton) and their local charge densities are now a function of the applied electric field due to interface roughness as well as exciton and carrier locali-



FIG. 2. The heavy- and light-hole exciton binding energies in $GaAs/Al_{0.3}Ga_{0.7}As$ QW's as functions of carrier density for well thickness 50 and 100 Å.

zations. The binding between the electron and hole of an exciton is expected to be much weaker, which implies an increase in the carrier density at a fixed temperature. This high carrier density then again reduces further the exciton binding energy.

Figure 5 is the plot of heavy- and light-hole exciton binding energy difference ΔE for two carrier densities $n=3.6\times10^{15}/\mathrm{cm}^3$ and $2.4\times10^{14}/\mathrm{cm}^3$ as a function of composition x with well thickness 100 Å. ΔE decreases as composition x decreases. Therefore, the effects of the charge-carrier screening on the exciton binding energy are more pronounced for QW's with larger Al composition. It is interesting to notice that for x < 0.2, ΔE for light-hole excitons is smaller than that for heavy-hole excitons. We attribute this to the fact, in this case, that the wave function of the light-hole exciton leaks out of the well region more severely than that of the heavy-hole exciton.

It is important to realize that no excitons can be formed in QW's under a high light excitation. There is only an electron-hole (e-h) plasma state. This has been confirmed by many experimental observations.^{12,18,19} This indicates that there exists a phase transition from a state of coexistence of carriers and excitons to an e-h



FIG. 3. The exciton binding-energy difference ΔE , for carrier densities 3.7×10^{14} /cm³ and 7.1×10^{13} /cm³ in GaAs/Al_{0.3}Ga_{0.7}As QW's as a function of well thickness.



FIG. 4. The heavy- and light-hole exciton binding energies as functions of well thickness for carrier densities 3.6×10^{15} /cm³ and 2.7×10^{14} /cm³.

plasma state with the increasing of excitation light intensity. It is widely referred to as a Mott transition. The exciton binding energy is an important parameter to characterize this transition. Equation (9) tells us that the exciton binding energy is zero when λ_0 is zero. From Refs. 10 and 11, we know that the variationalperturbation method may not be appropriate when λ_0 becomes very small. However, we can still use this method



FIG. 5. The heavy- and light-hole exciton binding energy difference ΔE for carrier densities 3.6×10^{15} /cm³ and 2.4×10^{14} /cm³ as a function of composition x in GaAs/Al_xGa_{1-x}As QW's with well thickness 50 Å.

to estimate the behavior of the phase transition between the e-h plasma and the exciton states. We calculated the exciton binding energy at high carrier densities, then extrapolated to the case of $E_b = 0$. Figure 6 plots the critical carrier density n_c versus well thickness for heavy- and light-hole excitons with x = 0.3. These two curves correspond to the coexistence curves which separates the two phases. The phase above the coexistence curve corresponds to an e-h plasma phase, while the phase below the curves corresponds to the coexistence of free electrons, holes, and excitons, with reduced exciton binding energy. The results in Fig. 6 can be understood by the fact that the mean distance between carriers decreases as the carrier density increases. There is no physical meaning any more to define an exciton when the Bohr radius for excitons becomes comparable with the mean distance between electrons and holes. In this case, electrons and holes form a plasma. This phase diagram indicates the limitation of the QW devices if one uses excitonic transition as an optical process.

The above calculations were done by treating the Debye screening effects in three dimensions. The calculation for the two-dimensional screening effect is much more complicated. We discuss briefly the screening effects of free carriers to exciton binding energy in two dimensions (2D) here. Following Ref. 15, the equation determining the screened potential in 2D is written as

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left| \rho \frac{\partial V(\rho)}{\partial \rho} \right| = \frac{V(\rho)}{s^2} , \qquad (11)$$



FIG. 6. The critical carrier density n_c as a function of well thickness in GaAs/Al_{0.3}Ga_{0.7}As QW's. Here, n_c corresponds to the critical carrier density above which no excitons can be formed. In the region below this curve, there coexist free electrons, holes, and excitons with the exciton binding energy being reduced. However, there is only an electron-hole plasma state above this curve.

where s is the screening length in 2D. A change of the variable $x = \rho / s$ leads to the following equation:

$$\frac{d^2V}{dx^2} + \frac{1}{x}\frac{dV}{dx} - V = 0.$$
 (12)

The solution of Eq. (12) under the conditions that $V(\rho) \rightarrow 0$ as $\rho \rightarrow \infty$ and $V(\rho) \rightarrow \infty$ as $\rho \rightarrow 0$ is the modified Bessel function $K_0(x)$.²⁰ The asymptotic forms for $K_0(x)$ are

$$V(x) = K_0(x) = \begin{cases} -\ln\left[\frac{x}{2}\right], & x \to 0\\ \left[\frac{1}{2\pi x}\right]^{1/2} e^{-x}, & x \to \infty \end{cases}$$
(13)

A weaker screening effect would be expected in 2D if we compare Eq. (13) with the three-dimensional form $e^{-r/s}/r$. In the quantum-well case, electrons and holes are confined within the well region, so the screened potential for a quantum well should have a form that is in between the two- and three-dimensional cases. A suitable approach is to solve Poisson and Schrödinger equations simultaneously as done previously in Ref. 12.

It was shown by Ekenberg and Altarelli²¹ that the mixing of the light- and heavy-hole excitons in GaAs- $Al_xGa_{1-x}As$ is important. The mixing could cause a large change in exciton binding energy, especially for the light-hole exciton. Our calculation, which does not include this mixing, indicates that the binding energies of both light- and heavy-hole excitons decrease approximately in the same fashion as the screening length. Implicatively, the mixing of the light- and heavy-hole excitons could either increase or decrease the difference of the binding energy between the light- and heavy-hole excitons for high carrier density. These two cases will lead to different experimental observations, for example, in the photoluminescence measurement. In the former case, the peak of the light-hole exciton will shift toward the peak of the heavy-hole exciton and its height relative to the heavy-hole exciton will also increase due to the increasing transfer rate of the heavy hole to the light hole assisted by the mixing. Another effect that may be caused by mixing is the changing of the critical carrier density. Our calculation without considering the mixing shows that the critical carrier density for the light-hole exciton is larger than that for the heavy-hole exciton. The mixing could affect this behavior. If the mixing is in favor of increasing the difference of the heavy- and light-hole exciton binding energies, a larger carrier density is needed to screen the light-hole exciton.

IV. CONCLUSIONS

In conclusion, we calculated the charge-carrier screening effects on the heavy- and light-hole exciton binding energies in GaAs-Al_xGa_{1-x}As QW's by the variationalperturbation method. The effects of the charge screening on the exciton binding energy at different well thickness, composition x, and carrier density have been obtained. The effects of charge screening on the exciton photoluminescence are also discussed. The critical carrier density above which no excitons can be formed is also calculated at different well thickness. The calculated results here are consistent with experimental observations.

ACKNOWLEDGMENT

This work was supported by the National Science Foundation under Grant No. DMR-9118818.

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