Vol 12 No 11, November 2003
1009-1963/2003/12(11)/1296-05

Chinese Physics

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Electron self-energy and effective mass in a single heterostructure*

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(Received 10 February 2003; revised manuscript received 7 April 2003)

In this paper, we investigate the electron self-energy and effective mass in a single heterostructure using Green-function method. Numerical calculations of the electron self-energy and effective mass for GaAs/AlAs heterostructure are performed. The results show that the self-energy (effective mass) of electrons, which incorporate the energy of electron coupling to interface-optical phonons and half of the three-dimensional longitudinal optical phonons, increase (decrease) monotonically from that of interface polaron to that of the 3D bulk polaron with increasing the distance between the positions of the electron and interface.

Keywords: semiconductors, electron-phonon interactions
PACC: 7340, 7360F

1. Introduction

The heterostructure and superlattice of insulators and semiconductors have many potential electronic and optical properties, which continue to receive much attention in both the theoretical research and the application to electronic and optical devices.[1,2] The polaron effects of electron-interface-optical-phonon interaction result in some changes of the electron self-energy and the effective mass which are very different from those in three-dimensional (3D) systems, and have been investigated extensively. In the past years, many works on the properties of interface polaron were studied using the perturbation Theory,[3−5] the Lee–Low–Pines (LLP) variation method[6−8] and the Feynman path integral approach.[9−11] Recently, Jia *et al* have carried out theoretical research on the electronic structure of GaAs(311)A and GaAs(311)B[12] and an electronic structure investigation on Gan(0001) is reported.[13] Hai,[5] for example, investigated the polaron energy and effective mass in a quantum well by applying the perturbation theory, Li and Gu[7] investigated intermediate-coupling polaron in a polar-crystal slab by using LLP variation method. A few works, which include the study of many-body effects in the normal-state polaron system[14] and the investigation of exact ground-state properties of polarons in the limit of large dimensions,[15] have been done using the powerful Green-function method. Recently, Charrour presented a systematic study of the ground-state binding energy of hydrogenic impurity in a cylindrical quantum dot,[16] and the effect of electron-phonon interaction on an electron bound to an impurity in a spherical quantum dot is studied by Melinikov[17], etc.

In the past, many works were contributed to the investigation of the properties of interface polarons.[18,19] However, rather insufficient attention has been paid to the properties of polaron as a function of the distance between the positions of the electron and interface. In this paper, we apply the Green-function method to the study of the effect of electron-phonon interactions on the self-energy and the effective mass of an electron in a single heterostructure. We put Hamiltonian into the second quantization representation only on the area parallel to the interface. Our numerical results of the self-energy and effective mass using the GaAs/AlAs heterostructure as an example show that the electron self-energy and effective mass in a single heterostructure are strongly related to the distance of the electron to the interface. We

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find that the total electron self-energy, which incorporates the contribution of electron coupling to interface-optical phonons and half of the 3D bulk longitudinal optical (LO) phonons to electron self-energy, increases monotonically from that of interface polarons to that of 3D polarons with increasing the distance of the electron to the interface. We also find that the total effective mass, which incorporates the contribution of electron interaction with interface-optical phonons and half of the 3D bulk LO phonons to the effective mass, decreases monotonically from that of interface polarons to that of 3D polarons with increasing distance of the electron to the interface.

2. Hamiltonian and calculation

Let us consider a single heterostructure. The space for $z > 0$ is occupied by GaAs (crystal 1) and that for $z < 0$ by AlAs (crystal 2). Considering only the motion of an electron with mass m, the Hamiltonian for the coupling of an electron to the bulk and interface optical phonons in a single heterostructure can be given by

$$H = \frac{p^2}{2m} + V(z) + \sum_q \hbar\omega_{\mathrm{L}n} a_q^+ a_q + \sum_{q_\parallel} \hbar\omega_\pm a_{q_\parallel}^+ a_{q_\parallel} + H_{\mathrm{e-BO}} + H_{\mathrm{e-IO}}, \quad (1)$$

where p is the momentum operator of the electron, m is the band mass of the electron, $V(z)$ is the confining potential in the z direction, a_q^+ (a_q) is the creation (annihilation) operator of a bulk LO phonon with wavevector q and energy $\hbar\omega_{\mathrm{L}n}$ (n=1,2), $a_{q_\parallel}^+$ ($a_{q_\parallel}$) is the creation (annihilation) operator of an interface-optical (IO) phonon with wavevector $q_\parallel$ and energy $\hbar\omega_\pm$. $H_{\mathrm{e-BO}}$ is the electron-LO-phonon interaction Hamiltonian in half of the 3D bulk crystal, $H_{\mathrm{e-IO}}$ is the electron-IO-phonon interaction Hamiltonian. We regard the band mass to be homogeneous one.

The polarizing electron cloud of the interface ions induces an image potential, which is

$$V(z) = \frac{e^2(\varepsilon_{\infty 1} - \varepsilon_{\infty 2})}{4z\varepsilon_{\infty n}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})}, \quad (2)$$

where $\varepsilon_{\infty 1}$ and $\varepsilon_{\infty 2}$ are the optical dielectric constants of crystals 1 and 2, respectively. n=1 and 2 denote crystals 1 and 2. For a single heterostructure, the electron-LO-phonon interaction Hamiltonian of an electron with half of the 3D bulk and interface optical phonons is given by[20]

$$H_{\mathrm{e-BO}} = \sum_{q_z>0} \sum_{q_\parallel} \mathrm{e}^{\mathrm{i}q_\parallel \cdot r_\parallel} \Gamma_{\mathrm{L}n}(q_\parallel, q_z, z)[a_{\parallel j} + a_{-q_{\parallel j}}^+] \quad (3)$$

and

$$H_{\mathrm{e-IO}} = \sum_{q_\parallel} \mathrm{e}^{\mathrm{i}q_\parallel \cdot r_\parallel} \Gamma_{\mathrm{IO}}^\pm(q_\parallel, z)[a_\parallel + a_{-q_\parallel}^+], \quad (4)$$

where $\Gamma_{\mathrm{L}n}(q_\parallel, q_z, z)$ and $\Gamma_{\mathrm{IO}}^\pm(q_\parallel, z)$ are the coupling functions that describe the coupling strengths of a single electron with half of the 3D bulk optical-phonon modes in crystals 1 and 2 and with the interface optical phonon modes at the position z, respectively. The expression of the coupling function in half of the 3D bulk crystal is given by

$$\Gamma_{\mathrm{L}n}(q_\parallel, q_z, z) = -\left[\frac{\omega_{\mathrm{L}n}e^2}{2V}\right]^{1/2}\left[\frac{1}{\varepsilon_{\infty n}} - \frac{1}{\varepsilon_{0n}}\right]^{1/2} \times \frac{1}{[q_\parallel^2 + q_z^2]^{1/2}}\theta_n(z)2\sin(q_z z), \quad (5)$$

where $\omega_{\mathrm{L}n}$ denotes the frequency of LO phonons in a polar crystal n (n=1 and 2), V denotes the volume of the polar crystal and

$$\theta_n(z) = \begin{cases} 1, \\ 0, \end{cases}$$

when the electron is in crystal n (n=1,2), $\theta_n(z)$ equals unity and elsewhere it is zero. $\Gamma_{\mathrm{IO}}^\pm(q_\parallel, z)$ is given by

$$\Gamma_{\mathrm{IO}}^\pm(q_\parallel, z) = -\left[\frac{\omega_\pm e^2}{2S}\right]^{\frac{1}{2}} \times \left[\frac{1}{\beta_1^{-1}(\omega_\pm) + \beta_2^{-1}(\omega_\pm)}\right]^{\frac{1}{2}} \times \frac{1}{\sqrt{2q_\parallel}}\mathrm{e}^{-q_\parallel|z|}, \quad (6)$$

where

$$\beta_n(\omega_\pm) = \left(\frac{1}{\varepsilon_{\infty n}} - \frac{1}{\varepsilon_{0n}}\right)\frac{\omega_{\mathrm{L}n}^2}{\omega_\pm^2}\left[\frac{\omega_\pm^2 - \omega_{\mathrm{T}n}^2}{\omega_{\mathrm{L}n}^2 - \omega_{\mathrm{T}n}^2}\right]^2, \quad n = 1, 2; \quad (7)$$

and $\omega_\pm$ is determined by

$$\begin{cases} \varepsilon_n(\omega) = \varepsilon_{\infty n}\dfrac{\omega^2 - \omega_{\mathrm{L}n}^2}{\omega^2 - \omega_{\mathrm{T}n}^2}, \\ \varepsilon_1(\omega) + \varepsilon_2(\omega) = 0. \end{cases} \quad (8)$$

In order to represent the Hamiltonian in the second quantization representation, we expand the electron wavefunction $\Psi(r)$ ($\Psi^+(r)$) in a basis set $\phi_k(r)$ ($\phi_k^+(r)$) with the well-known method

$$\Psi(r) = \sum_{k_\parallel} c_{k_\parallel}\phi_{k_\parallel}(r), \quad (9a)$$

$$\Psi^{+}(r)=\sum_{k_{\parallel}} c_{k_{\parallel}}^{+}\phi_{k_{\parallel}}^{*}(r), \tag{9b}$$

where

$$\phi_{k_{\parallel}}(r)=\frac{1}{2\pi}\mathrm{e}^{\mathrm{i}k_{\parallel}\cdot r_{\parallel}},$$

$$\phi_{k_{\parallel}}^{*}(r)=\frac{1}{2\pi}\mathrm{e}^{-\mathrm{i}k_{\parallel}\cdot r_{\parallel}}. \tag{10}$$

Here $k_{\parallel}$ is the wavevector of the electron in the x-y plane, $r_{\parallel}$=(x, y). Substituting Eqs. (9), (10) into Eqs. (1), (3) and (4), we obtain the second quantized effective Hamiltonian

$$\begin{aligned}H=&\sum_{k_{\parallel}}\frac{\hbar k_{\parallel}^{2}}{2m}c_{k_{\parallel}}^{+}c_{k_{\parallel}}+\frac{p_z^2}{2m}+V(z)\\&+\sum_{q}\hbar\omega_{\mathrm{LO}}a_q^{+}a_q\\&+\sum_{q_{\parallel}}\hbar\omega_{\pm}a_{q_{\parallel}}^{+}a_{q_{\parallel}}+H_{\mathrm{e-BO}}+H_{\mathrm{e-IO}},\end{aligned} \tag{11}$$

where

$$H_{\mathrm{e-BO}}=\sum_{k_{\parallel},q_{\parallel}}\Gamma_{\mathrm{L}n}(q_{\parallel},q_z,z)c_{k_{\parallel}+q_{\parallel}}^{+}c_{k_{\parallel}}[a_{q_{\parallel}}^{+}+a_{-q_{\parallel}}], \tag{12}$$

$$H_{\mathrm{e-IO}}=\sum_{k_{\parallel},q_{\parallel}}\Gamma_{\mathrm{IO}}^{+}(q_{\parallel},z)c_{k_{\parallel}+q_{\parallel}}^{+}c_{k_{\parallel}}[a_{q_{\parallel}}^{+}+a_{-q_{\parallel}}]. \tag{13}$$

In the following we will derive the self-energy and effective mass of an electron by using the standard Matsubara Green function method.[21] For a weak electron–phonon coupling system, it is a good approximation that we only take the first term in the perturbation series for the self-energy. The contribution of electron interaction with bulk optical phonons to the electron self-energy is

$$\begin{aligned}&\Sigma_{\mathrm{L}n}(k_{\parallel},\mathrm{i}k_n)\\=&-\sum_{q_z>0}\sum_{q_{\parallel}}[\Gamma_{\mathrm{L}n}(q_{\parallel},q_z,z)]^2(q_{\parallel},q_j)\frac{1}{\beta}\\&\times\sum_{\mathrm{i}q_n}g^{(0)}(k_{\parallel}+q_{\parallel},\mathrm{i}k_n+\mathrm{i}q_n)D^{(0)}(q_{\parallel},\mathrm{i}q_n)\\=&\sum_{q_z>0}\sum_{q_{\parallel}}\frac{2\pi\hbar\omega_{\mathrm{L}n}e^2}{SL_z}\left[\frac{1}{\varepsilon_{\infty n}}-\frac{1}{\varepsilon_{0n}}\right]\frac{\theta_n(z)\sin^2(q_zz)}{q_{\parallel}^2+q_z^2}\\&\times\left(\frac{n_{\mathrm{p}}+n_{\mathrm{F}}}{\mathrm{i}k_n+\hbar\omega_{\mathrm{LO}}-\varepsilon_{k_{\parallel}+q_{\parallel}}}+\frac{n_{\mathrm{p}}+1-n_{\mathrm{F}}}{\mathrm{i}k_n-\hbar\omega_{\mathrm{LO}}-\varepsilon_{k_{\parallel}+q_{\parallel}}}\right)\end{aligned} \tag{14}$$

with

$$n_{\mathrm{p}}=\frac{1}{\mathrm{e}^{\beta\hbar\omega_{\mathrm{LO}}}-1},\qquad n_{\mathrm{F}}=\frac{1}{\mathrm{e}^{\beta\varepsilon_{k_{\parallel}+q_{\parallel}}}-1},$$

where n_{p} and n_{F} are the phonon and fermion occupation factor, $g^{(0)}$ $(k_{\parallel},\mathrm{i}k_n)$ and $D^{(0)}(q_{\parallel},\mathrm{i}q_n)$ are the Green function of free electron and phonon, respectively. Set $\mathrm{i}k_n=E+\mathrm{i}\delta$ so that the real part of the retarded self-energy of electron interaction with LO phonons is

$$\begin{aligned}&\mathrm{Re}[\Sigma_{\mathrm{L}n}^{\mathrm{ret}}(k_{\parallel},E)]\\=&\frac{\hbar\omega_{\mathrm{L}n}e^2}{2}\left(\frac{1}{\varepsilon_{\infty n}}-\frac{1}{\varepsilon_{0n}}\right)\\&\times\sum_{q_z>0}\frac{1}{L_z}\int_0^{2\pi}\int_0^{q_m}\frac{\theta_n(z)\sin^2(q_zz)\mathrm{d}^2q_{\parallel}}{q_{\parallel}^2+q_z^2}\\&\times\left(\frac{n_{\mathrm{p}}+n_{\mathrm{F}}}{E+\hbar\omega_{\mathrm{LO}}-\varepsilon_{k_{\parallel}+q_{\parallel}}}+\frac{n_{\mathrm{p}}+1-n_{\mathrm{F}}}{E-\hbar\omega_{\mathrm{LO}}-\varepsilon_{k_{\parallel}+q_{\parallel}}}\right).\end{aligned}$$

At zero temperature, $n_{\mathrm{p}}=0$. The fermion occupation factors n_{F} are all zero, if there is only one particle in a band. After setting $k_{\parallel}$=0, one can obtain

$$\begin{aligned}\mathrm{Re}[\Sigma_{\mathrm{L}n}^{\mathrm{ret}}(0,E)]=&\frac{\hbar\omega_{\mathrm{L}n}e^2}{8\pi}\left(\frac{1}{\varepsilon_{\infty n}}-\frac{1}{\varepsilon_{0n}}\right)\\&\times\int_0^{q_m}\frac{\theta_n(z)(1-\cos(2q_zz))\mathrm{d}q_z}{2(\hbar\omega_{\pm}-E-E_{q_z})}\\&\times\ln\frac{(\hbar\omega_{\pm}+x_m-E)E_{q_z}}{(\hbar\omega_{\pm}-E)(x_m+E_{q_z})},\end{aligned} \tag{15}$$

where

$$E_{q_{\parallel}}=\frac{\hbar^2q_z^2}{2m}. \tag{16}$$

Considering the boundary of the first Brillouin zone, the upper integral limit in above equations can be written as

$$q_m=\frac{\sqrt{3}\pi}{a},\qquad x_m=\frac{\hbar^2q_m^2}{2m}=\frac{3\pi^2\hbar^2}{2ma^2}. \tag{17}$$

The self-energy of an electron interacting with interface optical phonons is

$$\begin{aligned}&\Sigma_{l'}^{\mathrm{IO}}(k_{\parallel},\mathrm{i}k_n)\\=&-\sum_{q_{\parallel}}[\Gamma_{\mathrm{IO}}^{2}(q_{\parallel},z)]^2(q_{\parallel},q_j)\frac{1}{\beta}\\&\times\sum_{\mathrm{i}q_n}g^{(0)}(k_{\parallel}+q_{\parallel},\mathrm{i}k_n+\mathrm{i}q_n)D^{(0)}(q_{\parallel},\mathrm{i}q_n).\end{aligned}$$

When $k_{\parallel}$=0, we obtain the real part of $\Sigma_{l'}^{\mathrm{IO}}(k_{\parallel},\mathrm{i}k_n)$ in the zero-temperature case

$$\begin{aligned}\Sigma_{\mathrm{IO}}^{(1)}(0,E)=&\frac{\hbar\omega_{\pm}e^2}{4\pi}\frac{1}{\beta_1^{-1}(\omega_{\pm})+\beta_1^{-1}(\omega_{\mathrm{LO}})}\\&\times\int_0^{q_m}\frac{\mathrm{e}^{-2q_{\parallel}z}\mathrm{d}q_{\parallel}}{E-\hbar\omega_{\pm}-\varepsilon_{q_{\parallel}}},\end{aligned} \tag{18}$$

where

$$\varepsilon_{q_\parallel} = \frac{\hbar^2 q_\parallel^2}{2m_1}. \tag{19}$$

The approximation result of the effective mass can be obtained using

$$\frac{m}{m^*} = \lim_{k_\parallel \to 0} \frac{1 + \dfrac{\partial}{\partial \varepsilon_{k\parallel}} \mathrm{Re}[\Sigma^{\mathrm{ret}}(k_\parallel, E)]}{1 - \dfrac{\partial}{\partial E} \mathrm{Re}[\Sigma^{\mathrm{ret}}(k_\parallel, E)]} \tag{20}$$

and

$$\mathrm{Re}[\Sigma^{\mathrm{ret}}(k_\parallel, E)] = \mathrm{Re}[\Sigma^{\mathrm{ret}}_{\mathrm{BO}}(k_\parallel, E)] + \mathrm{Re}[\Sigma^{\mathrm{ret}}_{\mathrm{IO}}(k_\parallel, E)], \tag{21}$$

3. Results and discussions

In this paper, we select the GaAs/AlAs heterostructure as an example to study the polaron effect. The characteristic parameters concerned for the GaAs/AlAs heterostructure are taken as:

Table 1. Material parameters of GaAs and AlAs.

Material	Lattice constant	ε_0	ε_∞	$m_{\mathrm{b}}/m_{\mathrm{e}}$	$\hbar\omega_{\mathrm{LO}}$/meV	$\hbar\omega_{\mathrm{TO}}$/meV
GaAs	0.5654	13.18	10.89	0.0656	36.25	33.29
AlAs	0.5654	10.06	8.16	0.147	50.09	44.88

In the above table, m_{e} is the mass of a free electron and the lattice constant unit is nm.

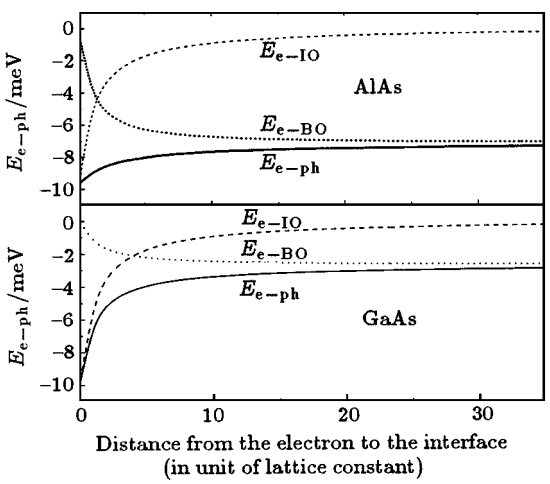


Fig.1. The self-energy of the polaron in a GaAs/AlAs heterostructure as a functions of the distance between the positions of the electron and the interface for E and $k_\parallel$=0.

In Figs.1 and 2, we show the electron self-energy and effective mass in a single heterostructure as functions of the distance of the electron to the interface. Here the parameters E and $k_\parallel$ are set to 0. Figure 1 shows that the contribution of electron interaction with half of the 3D bulk LO-phonons to the electron self-energy makes the electron self-energy decrease monotonically, starting from zero to that in the bulk 3D GaAs(AlAs) as the distance of the electron to the interface increases. Figure 1 also shows that the contribution of electron interaction with interface-optical (IO)-phonons to the electron self-energy makes the electron self-energy increase monotonically, starting from that(about –9.68meV) in the GaAs/AlAs interface to near zero as the distance of the electron to the interface increases. If we incorporate the contribution of electron interaction with the IO- and half of the 3D bulk LO-phonons to the electron self-energy, we find that the electron self-energy increases monotonically, starting from that(about –9.68meV) in the GaAs/AlAs interface to that in the 3D bulk GaAs(AlAs) as the distance of the electron to the interface increases.

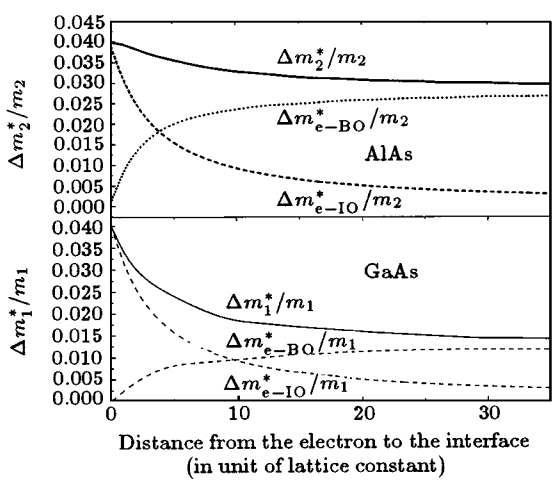


Fig.2. The effective mass of the polaron in a GaAs/AlAs heterostructure as a function of distance between the positions of the electron and the interface for E and $k_\parallel$=0. m_1 and m_2 are the electron band masses in the GaAs and AlAs bulk materials, respectively.

Figure 2 shows that the contribution of electron interaction with half of the 3D bulk LO-phonons to

the effective mass makes the effective mass increase monotonically, starting from zero to that in the 3D bulk GaAs(AlAs) as the distance of the electron to the interface increases. Figure 2 also shows that the contribution of electron interaction with IO-phonons to the effective mass makes the effective mass decrease monotonically, starting from $\Delta m^*/m_1$ equal to about 0.04 in the GaAs/AlAs interface to near zero with increasing the distance of the electron to the interface. If we incorporate the contribution of electron interaction with the IO- and half of the 3D bulk LO-phonons to the effective mass, we find that the effective mass decreases monotonically, starting from $\Delta m^*/m_1$ equal to about 0.04 in the GaAs/AlAs interface to that in the 3D bulk GaAs(AlAs) crystal with increasing the distance between the positions of the electron and interface. When the distance of an electron to the interface is equal to 30 times of the lattice constant, the correction to the effective mass is about 25% larger than that in the 3D bulk material.

4. Summary

We have studied the self-energy and effective mass of the electron in a single heterostructure using the Green's function method. In this theory, we expand the wavefunction in terms of a basis set which is only on the plane parallel to the interface so as to put Hamiltonian into the second quantization representation only on the plane parallel to the interface. Numerical calculations using a GaAs/AlAs heterostructure as an example are performed. The results show that the total self-energy, which incorporates the contribution of electron interaction with IO phonons and bulk LO phonons to the electron self-energy, increases monotonically, starting from that in the GaAs/AlAs interface to that in the 3D bulk GaAs(AlAs) as the distance between the electron and interface increases. The results also show that the band mass, which incorporates the contribution of electron interaction with the IO phonons and the 3D bulk LO phonons to the band mass, decreases monotonically, starting from that in the GaAs/AlAs heterostructure to that in the 3D bulk GaAs(AlAs) as the distance of the electron to the interface increases. One point the authors want to make clear is that in the present paper we aim at studying the polaron effect on the electron mass and self-energy. The potential in the z direction consists of $V(z)$ and the electron-phonon interaction induced parts $\Sigma_{\rm BO}(k_\parallel, E)$ and $\Sigma_{\rm IO}(k_\parallel, E)$. The z-direction–electron wavefunction is a rather complicated problem, which needs further investigation. One can also see that the one-phonon process electron self-energy includes the recoil part of the electron, which is the advantage of Green function method over the second perturbation theory (for instance compared with Ref. [19]).

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