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# The effect of intense laser field on the photoionization cross-section and binding energy of shallow donor impurities in graded quantum-well wire under an electric field

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## Abstract

The laser-field dependence of the impurity binding energy and donor-related photoionization cross-section in graded quantum-well wire under an external static electric field is calculated by a variational method and in the effective mass approximation. We have shown that, in the graded quantum-well wire structures, not only the ‘dressed’ potential but also the applied direction of the external electric field plays a very important role in the determination of the binding energy.

## 1. Introduction

In recent years many theoretical and experimental investigations have been performed on the issue of the hydrogenic binding of an electron to a donor impurity which is confined within low-dimensional heterostructures. The understanding of the electronic and optical properties of impurities in such systems is important because the optical and transport properties of devices made from these materials are strongly affected by the presence of shallow impurities. And the impurity-related photoionization cross-section is mainly used in semiconductors. In recent years, work has been done on the photoionization cross-section of hydrogenic impurities in structures of reduced dimensionality such as quantum wells, wires and quantum dots [1–9].

It is well known that the application of an intense laser field considerably affects the optical and electronic properties of semiconductors [10–16]. More recently, such studies have been extended to low-dimensional semiconductor heterostructures where intense electric fields are created by an applied ac voltage or a high-intensity THz laser [17–20]. It was reported that the binding energy of an impurity in low-dimensional systems decreases on increasing the laser-field amplitude [21, 22].

We have calculated the intense laser field and electric field effects on the donor–impurity-related photoionization cross-section and impurity binding energy in GaAs/GaAlAs graded quantum-well wire (GQWW) using a variational approach. To the best of our knowledge, this

is the first study on the effect of an intense laser field on the donor-related photoionization cross-section.

## 2. Theory

In low-dimensional electronic systems, the photoionization process is described as an optical transition that takes place from the impurity ground state as the initial state to the conduction subbands, which requires sufficient energy in order for the transition to occur. The excitation energy dependence of the photoionization cross-section associated with an impurity, starting from Fermi's golden rule in the well-known dipole approximation, as in the bulk case, is [1, 7]

$$\sigma(\hbar\omega) = \left[ \left( \frac{\xi_{\text{eff}}}{\xi_0} \right)^2 \frac{n_r}{\varepsilon(P)} \right] \frac{4\pi^2}{3} \alpha_{\text{FS}} \hbar\omega \sum_f |\langle \psi_i | \vec{r} | \psi_f \rangle|^2 \delta(E_f - E_i - \hbar\omega) \quad (1)$$

where  $n_r$  is the refractive index of the semiconductor,  $\alpha_{\text{FS}} = e^2/\hbar c$  the fine structure constant, and  $\hbar\omega$  the photon energy.  $\xi_{\text{eff}}/\xi_0$  is the ratio of the effective electric field  $\xi_{\text{eff}}$  of the incoming photon and the average field  $\xi_0$  in the medium [23].  $\langle \psi_i | \vec{r} | \psi_f \rangle$  is the matrix element between the initial and final states of the dipole moment of the impurity.

The method used in the present calculation is based upon a nonperturbative theory that has been developed to describe the atomic behaviour in intense high-frequency laser fields [21, 22]. We assume that the radiation field can be represented by a monochromatic plane wave of frequency  $\omega$ . For linear polarization, the vector potential of the field in the laboratory frame is given by  $A(t) = eA_0 \cos \omega t$ , where  $\mathbf{e}$  is the real unit vector of the polarization. By applying the time-dependent translation  $\mathbf{r} \rightarrow \mathbf{r} + \alpha(t)$  the semi-classical Schrödinger equation in the momentum gauge, describing the interaction dynamics in the laboratory frame of reference, was transformed by Kramers as follows [24]:

$$-\frac{\hbar^2}{2m^*} \nabla^2 \varphi(\mathbf{r}, t) + V(\mathbf{r} + \alpha(t)) \varphi(\mathbf{r}, t) = i\hbar \frac{\partial \varphi(\mathbf{r}, t)}{\partial t}. \quad (2)$$

Here  $V(\mathbf{r})$  is the atomic binding potential, and

$$\alpha(t) = \mathbf{e} \alpha_0 \sin \omega t, \quad (3)$$

with the laser-dressing parameter  $\alpha_0 = eA_0/m^*c\omega$ , represents the quiver motion of a classical electron in the laser field and  $V(\mathbf{r} + \alpha(t))$  is the 'dressed' potential energy. In terms of the average intensity of the laser,  $I$ ,  $\alpha_0$  can be written as [17]

$$\alpha_0 = (I^{1/2}/\omega^2)(e/m^*)(8\pi/c)^{1/2} \quad (4)$$

where  $e$ ,  $m^*$ ,  $c$ ,  $A_0$  and  $\omega$  are the charge and effective mass of electron, velocity of the light, the amplitude of the vector potential, and the frequency of applied field in cgs units, respectively.

Following the Floquet approach [21, 22], the space-translated version of the Schrödinger equation, equation (2), can be cast in the equivalent form of a system of coupled time-independent differential equations for the Floquet components of the wavefunction  $\varphi$ , containing the (in general complex) quasi-energy  $E$ . For the zeroth Floquet component  $\varphi_0$  the system reduces to the time-independent Schrödinger equation [17, 21, 22].

$$\left[ -\frac{\hbar^2}{2m^*} \nabla^2 + V(\mathbf{r}, \alpha_0) \right] \varphi_0 = E \varphi_0, \quad (5)$$

where  $V(\mathbf{r}, \alpha_0)$  is the 'dressed' potential which depends on  $\omega$  and  $I$  only through  $\alpha_0$  [21]. For the Coulomb potential case  $V(\mathbf{r}) = -\frac{e^2}{\varepsilon|\mathbf{r}|}$ , the 'dressed' potential has the form [25]

$$V_c(\mathbf{r}, \alpha_0) = -(e^2/2\varepsilon) \left( \frac{1}{|\mathbf{r} + \alpha_0|} + \frac{1}{|\mathbf{r} - \alpha_0|} \right), \quad (6)$$

where  $\varepsilon$  is the dielectric constant.

Before proceeding further and applying the above-described dressed potential theory to our system, we write down the Hamiltonian of a system consisting of an electron bound to a donor impurity inside the graded quantum-well wire. We assume the presence of an intense high-frequency laser field as well as an external electric field applied along to the  $z$ -direction (the laser-field polarization is along the  $z$ -direction). The Hamiltonian is

$$H = \frac{p_y^2}{2m^*} + H_x + H_z + V_c(\mathbf{r}, \alpha_0) \quad (7)$$

where  $V_c(\mathbf{r}, \alpha_0)$  is the Coulomb potential between the electron and impurity ion and  $H_x$  and  $H_z$  are Hamiltonians for the electron in the  $x$ - and  $z$ -directions in the absence of the impurity, respectively:

$$H_x = \frac{p_x^2}{2m^*} + V(x) \quad (7a)$$

$$H_z = \frac{p_z^2}{2m^*} + V_b(z, \alpha_0) + eFz, \quad (7b)$$

where  $F$  is the applied external electric field strength,  $V(x)$  is the confinement potential in the  $x$ -direction, which is given by

$$V(x) = \begin{cases} V, & |x| \leq -L_x/2 \\ 0, & \text{otherwise} \end{cases} \quad (7c)$$

and  $V_b(z, \alpha_0)$  is the 'dressed' confinement potential which is given by the following expression:

$$\begin{aligned} V_b(z, \alpha_0) = & \frac{V}{2} [\Theta(|z| - (L_z/2 + \alpha_0)) + \Theta(|z| - (L_z/2 - \alpha_0))] \\ & + \frac{V}{8} \left[ \left( \frac{z}{L_z/2 - \alpha_0} + 1 \right) \Theta((L_z/2 - \alpha_0) - |z|) \right. \\ & \left. + \left( \frac{z}{L_z/2 + \alpha_0} + 1 \right) \Theta((L_z/2 + \alpha_0) - |z|) \right] \end{aligned} \quad (8)$$

where  $V$  is the conduction band offset at the interface, and  $\Theta$  is the step function.

The investigation of the photoionization cross-section first needs to know the envelope functions of the initial ground state and the final state. In order to get the binding energy, we follow a variational method and we take the following trial wavefunction:

$$\psi_i(r) = \chi(x)\chi(z)\phi(y, \lambda) \quad (9)$$

where the wavefunction in the  $y$ -direction  $\phi(y, \lambda)$  is chosen to be Gaussian-type orbital function [26–30]

$$\phi(y, \lambda) = \frac{1}{\sqrt{\lambda}} \left( \frac{2}{\pi} \right)^{1/4} e^{-y^2/\lambda^2} \quad (10)$$

in which  $\lambda$  is a variational parameter. With the choice of  $\phi(y, \lambda)$ , the degrees of freedom are limited to one dimension along the axis of the wire. Our experience with variational calculations of the hydrogenic binding energy in quantum wells and quantum wires suggests that very simple Gaussian-type function gives quite accurate results in the case of moderate and strong fields ([28] and references therein).  $\chi(x)$  and  $\chi(z)$  are the first subbands' wavefunctions of the electron, which are exactly obtained from the one-dimensional Schrödinger equation in the  $x$ - and  $z$ -directions, respectively. The ground-state impurity binding energy is given by

$$E_B = E_x + E_z - \min_{\lambda} \langle \psi_i | H | \psi_i \rangle \quad (11)$$

where  $E_x$  and  $E_z$  are the lowest donor electron subband energies related to the  $\chi(x)$  and  $\chi(z)$  wavefunctions, respectively.

Because the electron motion along the  $y$ -axis is free, without the impurity potential the eigenstates associated with the Hamiltonian (7) of an electron emitted to the subbands  $n_x, n_z$  relative to the  $x$ - and  $z$ -directions of the quantum-well wire are given by

$$\psi_f(r) = \frac{1}{\sqrt{L_y}} \chi_{n_x}(x) \chi_{n_z}(z) e^{ik_y y} \quad (12)$$

where  $L_y$  is the length of the wire and  $k_y$  is the one-dimensional wavevector of the electron along the axis of the wire.  $\chi_{n_x}(x)$  and  $\chi_{n_z}(z)$  are chosen to be solutions of the one-dimensional Hamiltonian for an electron in the  $x$ - and  $z$ -directions. The final-state energy corresponding to the wavefunction equation (12) is

$$E_f = \frac{\hbar^2}{2m_e^*} k_y^2 + E_{n_x} + E_{n_z}. \quad (13)$$

For incident light polarized along the axis of the wire,  $y$ -direction, the transition to the first subbands  $n_x = 1, n_z = 1$  is dipole allowed. Thus in that case,  $\chi_{n_x}(x)$  and  $\chi_{n_z}(z)$  are taken to be the same as in the initial ground state, i.e., the first subbands' wavefunctions relative to the  $x$ - and  $z$ -directions of the wire, respectively. The photoionization cross-section for incident light polarized along the axis of the wire is given by

$$\sigma(\hbar\omega) = \left[ \left( \frac{\xi_{\text{eff}}}{\xi_0} \right)^2 \frac{n_r}{\varepsilon(P)} \right] \frac{\alpha_{\text{FS}} \lambda^5}{3} \left( \frac{\pi m^* E_S}{\hbar^2} \right)^{3/2} x \sqrt{x-1} \exp[-m^* (\lambda/\hbar)^2 E_S (x-1)] \quad (14)$$

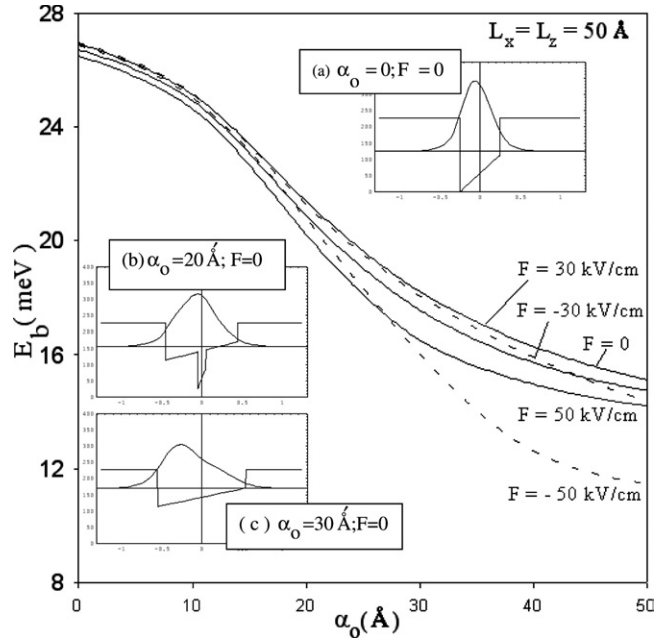
where  $x = \frac{\hbar\omega}{E_S}$  and  $E_S = E_{n_x} + E_{n_z} - E_i = E_B$ ,  $(\xi_{\text{eff}}/\xi_0) = 1$ . In producing the  $\sigma(\hbar\omega)$  expression, we accounted for all  $k_y$  values in the final state by converting the summation to a one-dimensional integral along the axis of the quantum-well wire of length  $L_y$ .

### 3. Results and discussion

For numerical calculations, we take  $m^* = 0.0665m_0$  (where  $m_0$  is the free electron mass),  $\varepsilon = 12.58$  and the barrier height  $V = 228$  meV.

The binding energy of a donor impurity localized at the centre of a GQWW as a function of the laser-field amplitude  $\alpha_0$  for wire dimensions  $L_x = L_z = L = 50$  Å according to different values of electric field- $F$  applied in the  $\pm z$ -directions is given in figure 1. The insets show the potential profile of the graded quantum wells in the  $z$ -direction and the amplitude of subband wavefunction of electron  $|\psi(z)|^2$  versus the position  $z$  in the absence of electric field for (a)  $\alpha_0 = 0$ , (b)  $\alpha_0 = 20$  Å and (c)  $\alpha_0 = 30$  Å. These insets are given in order to see how the geometric shape of the graded quantum well and the localization of the electron in the  $z$ -direction changes as  $\alpha_0$  increases in the absence of the electric field.

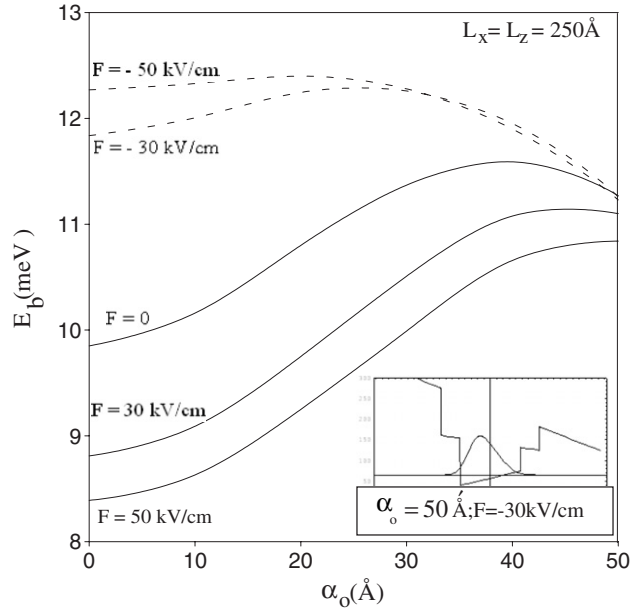
With small values of the laser-field magnitude,  $\alpha_0$ , the binding energy for an on-centre impurity is independent of both electric field strength and direction. As  $\alpha_0$  increases, the impurity binding energy decreases rapidly, since the Coulombic interaction between the electron and impurity ion decreases. For  $\alpha_0 \geq L_z/2$ , the GQW in inset (a) in figure 1 becomes a GQW with width  $2L_z$  and with height  $V/2$ , as seen in inset (c). So the probability of finding the electron and impurity in the same plane decreases, as does the binding energy. As is known, an electric field applied in different directions ( $-z$  or  $+z$  direction) to the GQW leads to the distortion in different directions of the graded well potential, and so the impurity binding energy increases or decreases, depending on the Coulombic interaction between the electron and impurity. The field dependence of the binding energy in narrow wire dimensions



**Figure 1.** Binding energy of a donor impurity localized at the centre of a GQWW as a function of the laser-field amplitude  $\alpha_0$  for wire dimensions  $L_x = L_z = L = 50$  Å according to different values of electric field  $F$  applied in the  $\pm z$ -directions. The insets show the potential profile of the graded quantum wells in the  $z$ -direction and the amplitude of subband wavefunction of electron  $|\psi(z)|^2$  versus the position  $z$  in the absence of electric field for (a)  $\alpha_0 = 0$ , (b)  $\alpha_0 = 20$  Å and (c)  $\alpha_0 = 30$  Å.

is very weak, since the geometric confinement is predominant. However, the binding energy in narrow wire dimensions becomes sensitive to the electric field with the effect of intense laser field and the electric field applied in  $-z$ -direction, due to the geometric shape of the GQW. The dependence of the donor binding energy to direction of the electric field and intense laser field will lead to important consequences for optical studies and for transport measurements on GQWWs.

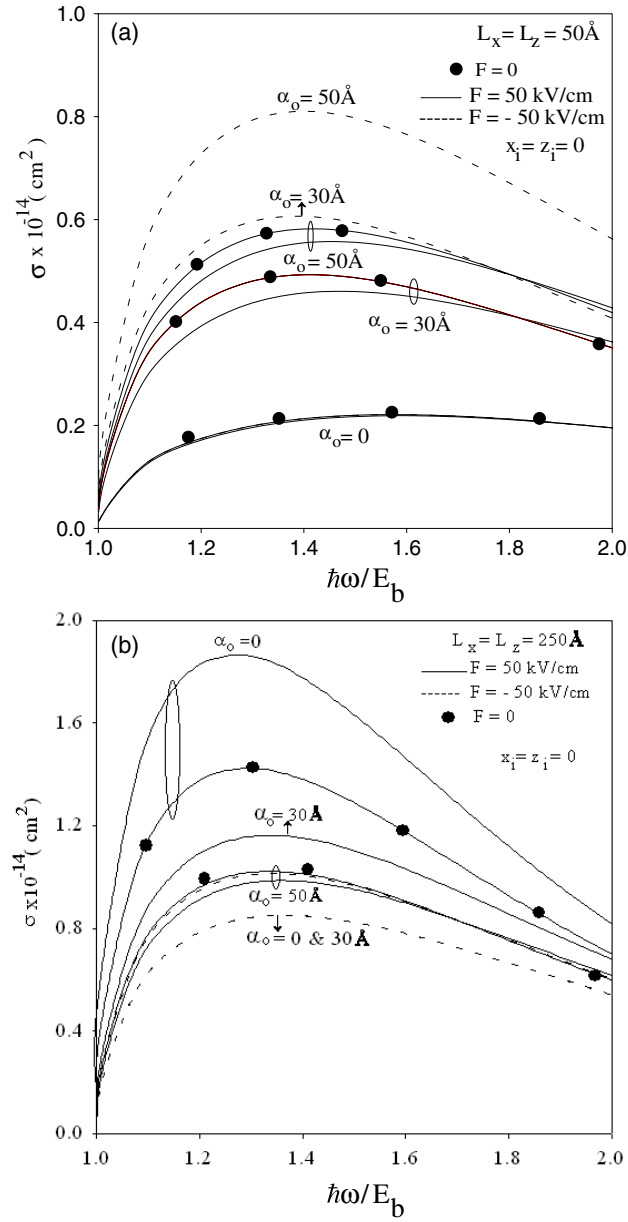
In figure 2 we show the variation of the impurity binding energy in the GQWW for wire dimensions  $L_x = L_z = L = 250$  Å as a function of the laser-field amplitude  $\alpha_0$  for several values of the external electric field applied in the  $\pm z$ -directions. The inset shows the potential profile of the graded quantum well in the  $-z$ -direction ( $-F$ ) and the amplitude of the subband wavefunction of the electron,  $|\psi(z)|^2$  versus the position  $z$ . For the wider QWWs, the binding energy is more sensitive to the external electric field for small values of  $\alpha_0$ . However, as  $\alpha_0$  increases, the binding energy is independent of both the electric field strength and applied electric field direction due to the geometric confinement of the structure, as is seen at the inset in figure 2. So, both the electric field and intense laser field can be used as a tuning parameter for the electronic structure of donor impurities in GQWWs. We see that the variation of the binding energy under a negative electric field is quite different from the positive field values. The negative electric field affects the binding energy more than the field in the opposite direction. The graded quantum well becomes sharper or flatter depending on whether the electric field is applied in the  $+z$  or  $-z$  direction. The electron moves towards the right side of the structure under a  $-F$  field. Thus the electron and impurity ion become close to each other



**Figure 2.** Binding energy of a donor impurity localized at the centre of a GQWW as a function of the laser-field amplitude  $\alpha_0$  for wire dimensions  $L_x = L_z = L = 250 \text{ \AA}$  according to different values of electric field  $F$  applied in the  $\pm z$ -directions. The inset show the potential profile of the graded quantum wells in the  $z$ -direction for a negative electric field value ( $F = -30 \text{ kV cm}^{-1}$  and  $\alpha_0 = 50 \text{ \AA}$ ).

and Coulombic interaction between the electron and impurity increases, so this behaviour gives an increment in the binding energy. Also in contrast to the behaviour for  $+F$  field values, we found that as the  $-F$  field value increases, the position of the maximum moves towards smaller value of  $\alpha_0$ . As a result, the probability of tunnelling of the donor electron can be increased or decreased depending on the direction of the external electric field. This control over tunnelling could be desirable for some device applications. Furthermore, in contrast to the previous case ( $L = 50 \text{ \AA}$ ) for  $L = 250 \text{ \AA}$ , the impurity binding energy increases with increasing  $\alpha_0$ , since, in the presence of a laser field, electrons mostly localize in the lower part of the ‘dressed’ well and on increasing the laser field electrons begin to localize in the upper part of the ‘dressed’ well with large well width. Due to this behaviour in the range of small well widths, the impurity binding energy decreases on increasing  $\alpha_0$ . On the other hand for large well dimensions, first the localization of the electrons and then also the binding energy increases with  $\alpha_0$ . But for further laser field values, electrons begin to localize in the upper part of the ‘dressed’ well with large well widths. Thus the Coulombic interaction between the electron and impurity ion becomes weak, and consequently the impurity binding energy begins to decrease with  $\alpha_0$ .

In figures 3(a) and (b), we present results for the photoionization cross-section as a function of the normalized photon energy of a donor impurity placed at the centre of a graded quantum-well wire for several laser-field amplitude  $\alpha_0$  values and wire dimensions  $L = L_x = L_z = 50 \text{ \AA}$  and  $L = L_x = L_z = 250 \text{ \AA}$ , respectively. As the laser-field amplitude  $\alpha_0$  increases, the magnitude of the photoionization cross-section increases, but it decreases for higher photon energies. An intense laser field leads to a decrement of the binding energy and this case leads to the increment of the photoionization cross-section. The photoionization cross-section increases since the binding energy decreases with the electric field effect. As is seen in figure 3(a), for



**Figure 3.** (a) The photoionization cross-section as a function of the normalized photon energy of a donor impurity placed at the centre of a graded quantum-well wire for several laser-field amplitude  $\alpha_0$  values for wire dimensions  $L = L_x = L_z = 50 \text{ \AA}$ . The solid line corresponds to  $F > 0$  (the electric field is applied in the  $+z$  direction), the dashed line corresponds to  $F < 0$ , and the dashed circle corresponds to  $F = 0$ . (b) The photoionization cross-section as a function of the normalized photon energy of donor impurity placed at the centre of graded quantum-well wire for several laser-field amplitude  $\alpha_0$  values for wire dimensions  $L = L_x = L_z = 250 \text{ \AA}$ . The solid line corresponds to  $F > 0$  (the electric field is applied in the  $+z$  direction), the dashed line corresponds to  $F < 0$ , and the dashed circle corresponds to  $F = 0$ .



$\alpha_0 = 0$ , the photoionization cross-section is independent of both the electric field strength and the applied electric field direction. However, as  $\alpha_0$  increases it becomes sensitive to the strength and the direction of the external electric field just as the binding energy does. As is seen in figure 3(b), for the wider wire dimensions, this behaviour of the photoionization cross-section is reversed.

#### 4. Conclusions

In this study, the intense laser-field dependence of the impurity binding energy and donor-related photoionization cross-section in a graded quantum-well wire under an external static electric field is calculated in the effective mass approximation by using a variational method. We have found that for the GQWW an intense laser-field amplitude  $\alpha_0$  provides an important effect on the electronic and optical properties. For example, the binding energy in narrow wire dimensions becomes sensitive to the electric field, while the binding energy for the wider wire dimensions becomes independent of the electric field strength with the effect of an intense laser field. The electric field, when applied in different directions ( $-z$  or  $+z$  direction) to the GQW, leads to the distortion in different directions of the graded well potential, and so the impurity binding energy increases or decreases, depending on the Coulombic interaction between the electron and the impurity. This control over tunnelling could be desirable for some device applications.

The measurement of photoionization in low-dimensional systems would be of great interest for understanding the optical properties of carriers in QWWs for which the photoionization can give information about the impurity position and the distribution inside the heterostructure.

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