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Effects of geometry, applied hydrostatic pressure and magnetic field on the electron–hole transition energy in a GaAs–$Ga_{1-x}Al_xAs$ pillbox immersed in a system of $Ga_{1-y}Al_yAs$

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Abstract

In this work, we study the behavior of the electron–hole transition energy in a GaAs–$Ga_{1-x}Al_xAs$ pillbox immersed in a system of $Ga_{1-y}Al_yAs$ as a function of thickness of the ladder barrier potential for a fixed length of the pillbox, length of the pillbox, thickness of the ladder barriers and pillbox position in the host of $Ga_{1-y}Al_yAs$. The behavior of the electron–hole transition energy as a function of an applied hydrostatic pressure and an applied magnetic field is also studied. For both electron and hole we found that in the strong confinement regime ($L \leqslant 10$ Å) energy of the ground state as function of the position of the pillbox relative to the ladder barrier potential presents a behavior similar to the binding energy of a hydrogenic impurity in quantum wells, quantum wires and quantum dots [L. Esaki, R. Tsu, IBM J. Res. Dev. 14 (1970) 61; G. Bastard, Phys. Rev. B 24 (1981) 4714; N. Porras-Montenegro, J. López-Gondar, L.E. Oliveira, Phys. Rev. B 43 (1991) 1824]. Electron–heavy hole transition energies increase with the applied magnetic field. Also, we have found that these transition energies, as a function of the applied hydrostatic pressure, present an excellent agreement with experimental reports by Venkateswaran et al. [phys. Rev. B 33 (1986) 8416].

Keywords: Pillbox; Hydrostatic pressure

1. Introduction

Due to the development of experimental techniques such as the molecular beam epitaxy (MBE) and metal-organic chemical-vapor deposition (MOCVD), there has appeared a great interest in semiconductor heterostructures of low dimensionality such as quantum wells (QWs), quantum well wires (QWWs), and quantum dots (QDs), in which the charge carriers are, respectively, free to move in one and two dimensions completely confined.

Bastard [2] calculated the binding energy of the ground state of a hydrogenic impurity in a QW finding a strong dependence of the energy on the impurity position when it moves along the growth axis of the system. Porras-Montenegro et al. [3] calculated the ground state energy, the binding energy, and the density of states for shallow hydrogenic impurities in cylindrical, infinite-length, GaAs–GaAlAs quantum well wires. Perez-Merchancano and Porras Montenegro [4] calculated the ground state energy and binding energy of shallow hydrogenic impurities in spherical GaAs–GaAlAs quantum dot as a functions of the dot radius. Shu-Shen et al. [5] studied the electronic structures in the hierarchical self-assembly of GaAs/$Ga_{1-x}Al_xAs$ quantum dots. In this work, we are concerned with the study of electron and hole states in a GaAs pillbox determined by a confinement potential due to a layer of $Ga_{0.7}Al_{0.3}As$ surrounded by $Ga_{1-y}Al_yAs$ with $y > 0.3$. In Section 2, we propose the theoretical model. In Section 3, we present our results and, finally, in Section 4, we remark our conclusions.

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2. Theoretical framework

In Fig. 1, we display the diagram for the pillbox showing both, the layers of the different materials in the growth direction and the energy scheme.

The Hamiltonian of an electron (hole) in GaAs pillbox determined by a confinement potential due to a layer of $Ga_{0.7}Al_{0.3}As$ surrounded by $Ga_{1-y}Al_yAs$ may be written as

$$H = \frac{p_{e,h}^2}{2m_{e,h}^*} + V_{e,h}(z,\rho), \tag{1}$$

where the first term is the kinetic energy for the electron (hole), $m_e^*(m_h^*)$ is the corresponding effective mass, and the second term is the confinement potential given as

$$V(z) = \begin{cases} 0 & \text{for } -L/2 \leqslant z \leqslant L/2, \\ V_1 & \text{for } z < -a - L/2, \quad z > L/2 + b, \\ V_2 & \text{for } -L/2 > z \geqslant -a - L/2, \\ & \quad L/2 < z \leqslant L/2 + b, \end{cases} \tag{2}$$

$$V(\rho) = \begin{cases} 0 & \text{for } \rho < R, \\ V_2 & \text{for } \rho \geqslant R. \end{cases} \tag{3}$$

According to the method of separation of variables, we can write for the wave function of the electron (hole) as

$$\psi(\rho, z, \varphi) = \phi(\rho)\chi(z)\zeta(\varphi), \tag{4}$$

where $\varsigma(\varphi) = e^{im\varphi} = 1$ with $m = 0$ for the ground state,

$$\chi(z) = \begin{cases} Ae^{ik_1 z} + Be^{-ik_1 z} & \text{for } -L/2 < z < L/2, \\ Ce^{k_2 z} + De^{-k_2 z} & \text{for } -a - L/2 \leqslant z \leqslant -L/2, \\ Fe^{k_2 z} + Ge^{-k_2 z} & \text{for } L/2 \leqslant z \leqslant L/2 + b \\ He^{k_3 z} & \text{for } z \leqslant -a - L/2, \\ Me^{-k_3 z} & \text{for } z \geqslant L/2 + b, \end{cases} \tag{5}$$

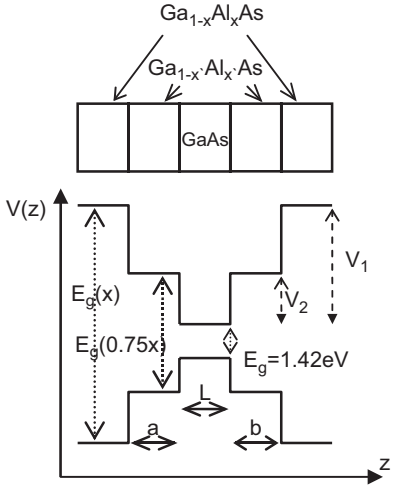

Fig. 1. Scheme of the system.

and

$$\phi(\rho) = \begin{cases} CJ_0(k'\rho) & \text{for } \rho < R, \\ C\frac{J_0(k'R)}{K_0(kR)}K_0(k\rho) & \text{for } \rho \geqslant R, \end{cases} \tag{6}$$

with

$$k' = \sqrt{\frac{2m_{eh}^*}{\hbar^2}E_\rho} \quad \text{and} \quad k = \sqrt{\frac{2m_{eh}^*}{\hbar^2}(E_\rho - V_{2)}}.$$

Here, ρ, z and φ are the cylindrical coordinates, $J_0(k'\rho)$, $K_0(k\rho)$ are the well-known Bessel functions of first and second order, respectively.

$\chi(z)$ and $\phi(\rho)$ and their derivates must satisfy the boundary conditions for the different regions in Fig. 1, in order to obtain the transcendental equation. This equation allows us to find the energy of the ground state for the electron (hole) in this system.

In order to take into account pressure and temperature effects on the carrier states, the Hamiltonian in Eq. (1) for any kind of carrier must be written as

$$H = -\frac{\hbar^2}{2m_{w,b}^*(P,T)}\nabla^2 + V(z,P,T), \tag{7}$$

where the subscripts w and b stand for the quantum well and the barrier layer materials, respectively. $m_{w\,c}^*(P,T)$ and $m_{b\,c}^*(P,T)$ are the well and barrier materials parabolic conduction effective masses as functions of P and T [6]:

$$m_{wc}(P,T) = \left[1 + 7.51\left(\frac{2}{E_g(P,T)} + \frac{1}{E_g(P,T) + 0.341}\right)\right]^{-1} m_0, \tag{8}$$

where $E_g(P, T)$ is the stress-dependent band gap for the GaAs semiconductor at the Γ point and low temperatures [7].

The barrier-effective mass depends on the aluminum concentration (x or y) as

$$m_{bc} = m_{wc} + 0.083xm_0. \tag{9}$$

It is well known that for single QWs larger than 50 Å in width, the non-parabolic effective mass effects are less than 5% [8].

In order to take into account the magnetic field effects on the carrier states, the Hamiltonian in Eq. (1) for any kind of carrier must be written as

$$\hat{H} = \frac{1}{2m^*}\left(\hat{p} + \frac{e}{c}\hat{A}\right)^2 + V(\rho, z), \tag{10}$$

where $\hat{A} = (1/2)\vec{B} \times \vec{r}$ and $\vec{r} = \sqrt{\rho^2 + z^2}$. In our case, the magnetic field is applied in z direction.

3. Results

In our results, we first explore the role of the width of the first barrier confining potential on the electron and hole energy in the pillbox structure. Second, we look at the hydrostatic pressure effects on the carrier first energy level.

In our calculations, without applied hydrostatic pressure and in the regime of low temperature, we have used $m_e^* = 0.0665m_0$, $m_h^* = 0.3m_0$, and for the dielectric constant $\varepsilon = 12.58$. We assumed that the band gap discontinuity in a GaAs–$Ga_{1-x}Al_xAs$ QD pillbox heterostructure is distributed about 40% on the valence band and 60% on the conduction band with the total band gap difference ΔE_g between GaAs and $Ga_{1-x}Al_xAs$ given as a function of the Al concentration $x<0.45$ as $\Delta E_g(\text{eV}) = 1.247x$ [10].

In Fig. 2, we present the energy of the electron ground state in a pillbox of GaAs with radius of 100 Å as function of the length of the pillbox for different thicknesses of the barriers. We observe that the energy of the electron diminishes as the length of the pillbox is increased. As observed, the energy for the total confinement is greater than when only the 1D confinement (z-direction) is considered. Another fact is related to the presence of the potential barrier. It can be noted that this influence is greater for lower values of the width of the barriers with V_2 confinement potential.

Also, it can be seen that variation of width of the barrier with V_2 confinement potential, practically does not change the carrier energy as width of the structure increase. This situation is similar for both electron and hole energies. Our results indicate that the role of width of barrier with V_2 confinement potential in the heterostructure modifies by a small amount the electron light-hole transition energy, when L is greater than 50 Å.

In Fig. 3, we display the energy for the heavy-hole ground state as a function of thickness of V_2 potential barrier for different lengths of the pillbox. As expected, energy for larger widths of the well is less than for narrower wells and changes more appreciably for lower values of the barrier width. Obviously, total energy is higher than 1D energy, due to 3D confinement when the radial potential is considered.

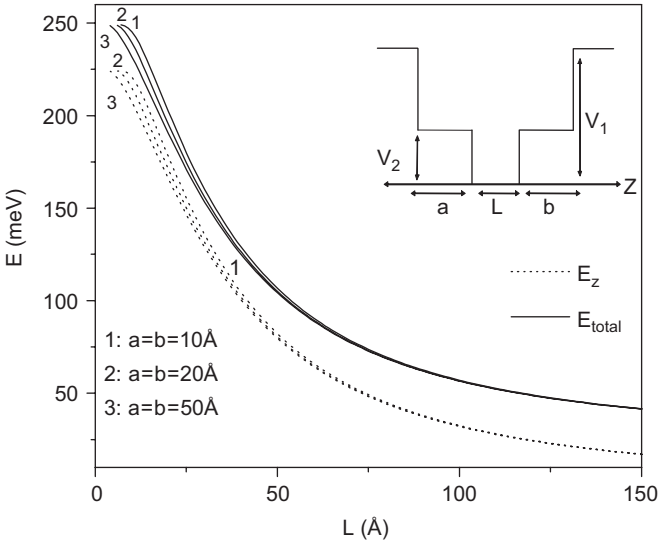

Fig. 2. Energy of the electron ground state in a GaAs–$Ga_{0.7}Al_{0.3}As$ pillbox immersed in a system of $Ga_{0.6}Al_{0.4}As$ as a function of the length of the pillbox for different thicknesses of the barriers: for $a = b = 10$, 20, 50 Å. Solid line is for the total energy while the dot line is for the energy in the z-direction (E_z). The inset depicts the energy diagram for the pillbox immersed in a system of $Ga_{0.6}Al_{0.4}As$.

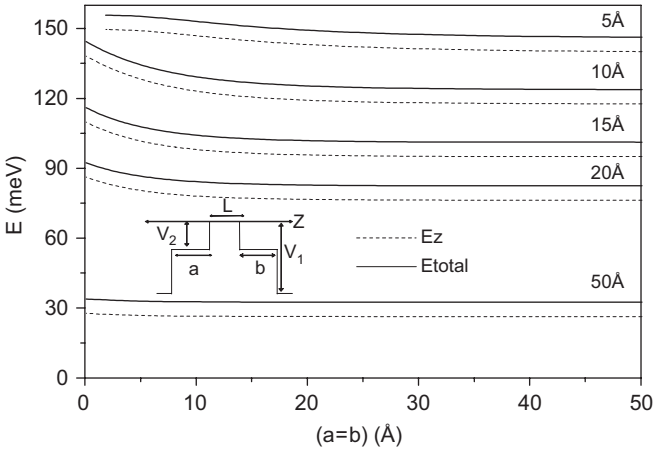

Fig. 3. Energy for the heavy-hole ground state in a pillbox of GaAs–$Ga_{0.7}Al_{0.3}As$ immersed in a system of $Ga_{0.6}Al_{0.4}As$ as a function of the width of the V_2 barrier potential for different lengths of the pillbox.

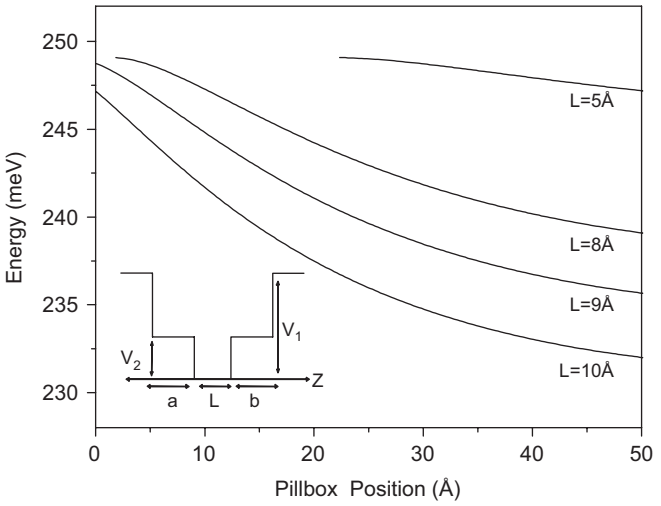

Fig. 4. Energy of the electron in a pillbox of GaAs–$Ga_{0.7}Al_{0.3}As$ with $R = 100$ Å immersed in a system of $Ga_{0.6}Al_{0.4}As$ as a function of the pillbox position inside the host of $Ga_{0.6}Al_{0.4}As$, for different lengths of the pillbox. The inset depicts the energy diagram for the pillbox immersed in host of $Ga_{0.6}Al_{0.4}As$.

Energy for the electron in a pillbox of GaAs–$Ga_{0.7}Al_{0.3}As$ with radius 100 Å as a function of pillbox position inside the host of $Ga_{0.6}Al_{0.4}As$ is presented in Fig. 4. We observe that energy diminishes as the pillbox approaches the V_1 potential barrier. It is important to stress that for small lengths of the pillbox ($L \leqslant 10$ Å), the energy of the ground state presents a behavior similar to the binding energy of a hydrogenic impurity in quantum wells, wires and dots [1–3]. As the pillbox is a quantum dot, note that there is a small size of the pillbox for which there are no bound states.

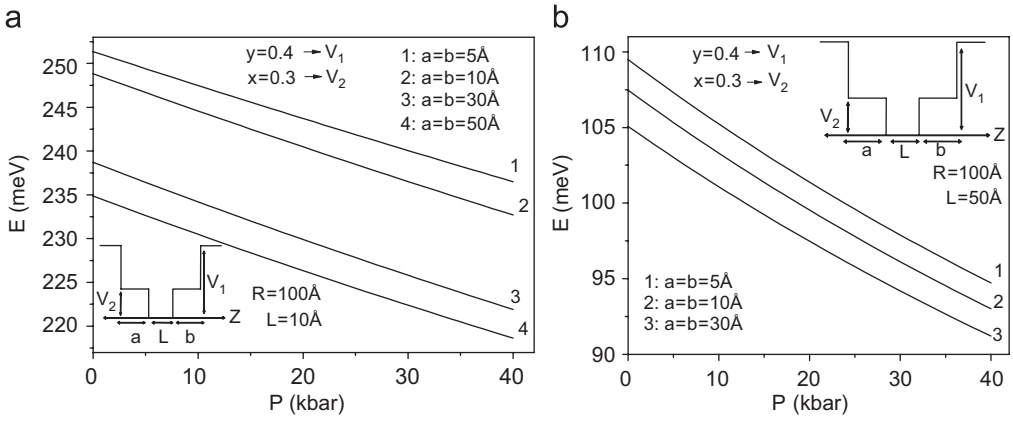

Fig. 5. Electron energy as a function of the hydrostatic pressure applied on a pillbox box of GaAs–GaAs–$Ga_{1-x}Al_xAs$ immersed in a system of Ga_yAl_yAs with $x = 0.3$ (V_2) and $y = 0.4$ (V_1), for two lengths of the pillbox (a) $L = 10$ Å and (b) $L = 50$ Å.

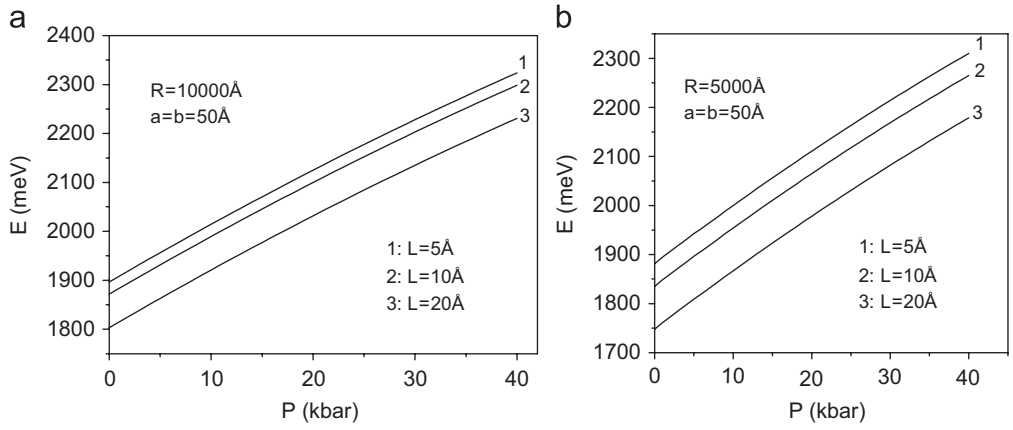

Fig. 6. e–lh (a) and e–hh (b) transition energy as a function of the hydrostatic pressure applied on a pillbox of $GaAGa_{1-x}Al_xAs$ immersed in a system of Ga_yAl_yAs, for different lengths of the pillbox and Al concentrations $x = 0.3$ (V_2) and $y = 0.4$ (V_1) in the limit of large R of the pillbox (that is in the QW limit).

The electron energy as a function of the applied pressure is presented in Fig. 5 for two widths of the well of the structure, $L = 10$ Å (a) and $L = 50$ Å (b). These energies decrease with hydrostatic pressure, mainly due to the diminishing of barrier height with pressure. According to these results, an important fact is that the width of the barrier with height V_2 modifies by a small amount the energy of the carrier in strong and low confinement regimes.

In Fig. 6, we display the electron–light hole (e–lh) and the electron–heavy hole (e–hh) transition energies as a function of the applied hydrostatic pressure on a pillbox box of $Ga_{1-x}Al_xAs$, in the limit of large R for different lengths of the pillbox. The results show, as expected, that the transition energy increases with the hydrostatic pressure and diminishes with the width of the barrier with V_2 potential confinement, and is lower for e–hh than for e–lh transition energy taking into account that radius is larger in e–lh than in e–hh case.

In comparing our results with transition energies reported by Venkateswaran et al. [11], for electron–light hole and electron–heavy hole transition energy, we prepared our pillbox in order to look like a quantum well with the well width of 150 Å, that is the width of the wells of the super-lattice in sample 3 of Ref. [11]. As shown in Fig. 7, we found an excellent agreement between reports in Ref. [11] and our results for direct transition energies, up to approximately 40 kbar. Effectively, as it was shown in Figs. 2 and 3 for well widths of 150 Å, the width of the barriers does not matter for the value of the carrier energy. Clearly, our results for the e–lh and e–hh transition energies are higher than the experimental reports due to the fact that our system is not exactly a QW since in our results the radius of the pillbox is equal to 5000 Å.

In Fig. 8, we show that e–hh transition energy increases not only with hydrostatic pressure applied on a pillbox of GaAs–$Ga_{1-x}Al_xAs$ but also with applied magnetic field on the structure. Also we found that for the same structure described in Fig. 1, these variations in the e–lh transition energies are less than in the e–hh case.

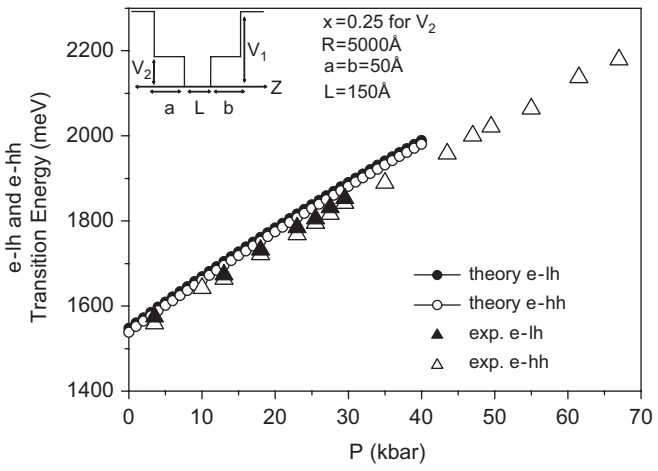

Fig. 7. Electron–light hole (e–lh) and electron–heavy hole (e–hh) transition energies as functions of the hydrostatic pressure applied on a pillbox of GaAs–$Ga_{1-x}Al_xAs$ 100 Å immersed in a system of Ga_yAl_yAs with chosen dimensions to simulate those of the quantum wells in sample 3 in Ref. [11], that is with $R = 5000$ Å, $L = 150$ Å, and $a = b = 50$ Å and Al concentrations $x = 0.25$ (V_2) and $y = 0.4$ (V_1). (●) and (▲) are for e–lh theoretical and experimental results, respectively. (○) and (Δ) are for e–hh theoretical and experimental results, respectively. Experimental reports are taken from Ref. [11], sample 3, in Fig. 9.

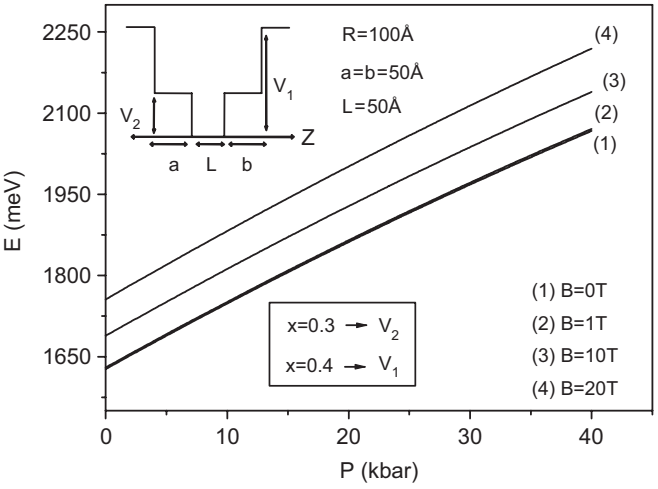

Fig. 8. Electron–heavy hole transition energy as a function of the hydrostatic pressure applied on a pillbox of GaAs–$Ga_{1-x}Al_xAs$ immersed in a system of Ga_yAl_yAs for different applied magnetic fields on the structure. $x = 0.3$ (V_2) and $y = 0.4$ (V_1).

4. Conclusions

In this work using the effective mass approximation, we have calculated the ground state energy for the electron and hole in a $Ga_{1-x}Al_xAs$ pillbox immersed in a host of $Ga_{1-y}Al_yAs$ as a function of the thickness of the barrier potential for a fixed length of the pillbox, as a function of the length of the pillbox when the thickness of the barriers remained constant, and as a function of the pillbox position in the host of $Ga_{1-y}Al_yAs$. We have examined the behavior of the energy of the ground state in this system for different Al concentrations. As an important fact, we found that for small lengths of the pillbox ($L \leqslant 10$ Å) the energy of the ground state as function of the relative position to the barrier potential presents a behavior similar to the binding energy of a hydrogenic impurity in quantum wells, wires and dots. We also found that there are critical values of the pillbox length for which there are no bound states. On the other hand, we found that the ground state energy decreases with the applied hydrostatic pressure and with the applied magnetic field. Also, we have found for the electron–light and electron–heavy hole transition energy an excellent agreement between our work and experimental results.

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