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Full Length Research Paper

Equispaced level conduction band design in the Cd Zn Se/Cd Se quantum well

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A derivation for equispaced conduction band in the $Cd_xZn_{1-x}Se$ quantum well is presented using the coordinate transform (CT) based procedure. The procedure starts with the effective mass Schrödinger equation, with potential tailored along the one dimensional harmonic oscillator (IDHO). The electron effective mass in the well is space dependent and varies proportionally with the potential, taking as the local conduction band edge. A value of 720 meV the conduction band edge according to Dingle's proposal of 85.15 of conduction-valence band partition (Basu, 1997) is adopted in this article. Two Hamiltonians were derived, one exhibits a confining potential (for $\varepsilon = 0$) that may be realized by appropriate grading of x. The second Hamiltonian has a non-confining potential (for $\varepsilon \neq 0$) with the electron effective mass $m(z \to \pm\infty) \to 0$. This is not realizable. Equaispaced level quantum well are scare in the interest of pursuing this work.

Key words: Quantum well, effective mass, Schodinger equation, confinement.

INTRODUCTION

Semiconductor quantum well have been given much attention both theoretically and experimentally for their potential utilization in electronics and photonics. The interesting physics involves the realization and understanding of Qw systems with controllable structural features permitting the assessment of their applications (Hartmann et al., 1999).

Quantization of electron motion due to confining potential at heterojunction of semiconductor Qw are ideal two-dimensional structures to study. The electrons in a Qw displays, quantum phenomena due to the barrier to barrier width (preferred in the z-direction) being of the order of the De Broglie wave length of electron. Our focus is on the conduction band and we seek to calculate the electron effective mass function $m(z)$, potential function $V(z)$, grading function $x(z)$ and the electron wave function $U_i(z)$ for Cd Zn Se/Cd Se Qw. It is very important to have reliable methods for solving the many-electron problem showing the characteristic electronic tendencies. Considered here, is the coordinate transform based procedure (Milanovic and Ikonic, 1996) adopting the electron effective mass theory (Burt, 1999) of a single electron in a periodic potential. An equispaced level in the conduction band of the semiconductor CdZn Se/Cd Se is developed and Dingle's proposal of 85:15 conduction-valence band partition is adopted (Basu, 1997).

CdZn Se/Cd Se belongs to the ternary II – VI alloys with a wide range of band gaps covering the visible region of the electromagnetic spectrum. Recently room temperature LED and laser operation have been observed in Cd Zn Se Qw and intense studies have been carried out on it in terms of their usefulness of blue-green laser diode (Shieo et al., 1996).

Theoretical formalism

Consider a graded Qw structure base upon a Cd Zn Se/Cd Se

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system (Milanovic and Ikonic, 1996) Where

$x = x(z)$ - - - - -(1)

is the grading function

$$V = V(z) \quad (2)$$

is the potential experienced by electrons, also

$$m = m(z) \quad (3)$$

is the effective mass of electrons

$$m(z) = \Delta m\, x(z) + m_{BC} \quad (4a)$$

$$(m_{AC} - m_{BC}) = \Delta m \quad (4b)$$

$$V(z) = \Delta V \quad x(z)$$
$$V(z) = \theta[m(z) - m_{BC}] \quad (5)$$

(I-D time-independent Schrodinger equation)

$$\frac{-\hbar^2}{2}\frac{d}{dz}\left(\frac{I}{m}\frac{d\psi}{dz}\right) + \phi(m - m_{BC})\psi = E\psi \quad (6)$$

We seek the function $m(z)$ and therefore $V(z)$ such that the energy spectrum of Equation (6) has equidistant states same as 1-D Harmonic Oscillator (1-DHO) (Powell and Crasemann, 1962; Milanovic and Ikonic, 1996; Yariv, 1988). Put $z = g(y)$ (introducing a new coordinate). This implies that $dz = g'dy$

Also $\psi = \psi(z) = \psi[g(y)]$

$$\frac{d\psi}{dz} = \frac{d\psi}{g'dy}$$

$$\frac{d^2\psi}{dy^2} - \frac{I}{mg'}\frac{d\psi}{dy}\frac{dmg'}{dy} + qmg'^2\left[E - \theta(m - m_{BC})\right]\psi = 0 \quad (7)$$

Put $\underline{\psi} = \underline{\psi}(y) = \psi[g(y)] = \psi(z)$

$\underline{m} = \underline{m}(y) = m[g(y)] = m(z)$

$$\frac{d^2\underline{\psi}}{dy^2} - \frac{I}{\underline{m}g'}\frac{d\underline{m}g'}{dy}\frac{d\underline{\psi}}{dy} + q\underline{m}g'^2\left[E - \theta(\underline{m} - m_{BC})\right]\underline{\psi} = 0 \quad (8)$$

The term with the first derivative $\frac{d\underline{\psi}}{dy}$ in Eq.(8) may be eliminated by introducing a new function u(y)

$$u(y) = \underline{\psi}(y)\exp\left[-\frac{1}{2}\int_{y_o}^{y}\frac{1}{\underline{m}g'}\frac{d\underline{m}g'}{dy}dy\right]$$

$$\psi(y) = \frac{1}{k}\sqrt{\underline{m}g'}\,U(y) \quad (9)$$

Equation (8) becomes

$$\frac{d^2u}{dy^2} + \left[A(y) + qmg'^2\left\{E - \theta(m - m_{BC})\right\}\right]U = 0 \quad (10)$$

Where

$$A(y) = \frac{1}{2}\frac{d}{dy}\left[\frac{1}{mg'}\frac{dmg'}{dy}\right] - \frac{1}{4}\left[\frac{1}{mg'}\frac{dmg'}{dy}\right]^2 \quad (11)$$

Potential for 1-DHO denoting equispaced level is used

$$V = \frac{1}{2}m_{LHO}\left(\frac{\Delta E}{\hbar}\right)^2 y^2 + V_o \quad (12)$$

Substituting for V in the Schrödinger equation

$$\frac{d^2u}{dy^2} - q\left[E - V_o - \frac{q}{4}\; m_{LHO}(\Delta E)^2 y^2\right]m_{LHO}\,u = 0 \quad (13)$$

Comparing Equations (8) and (13) we get

$$\underline{m}g'^2 = m_{LHO} \quad (14)$$

Comparing Equations (11) and (13) we get

$$A(y) - q\underline{m}g'^2\,\theta(m - m_{BC}) = -q\left(V_o + \frac{q}{4}m_{LHO}(\Delta E)^2 y^2\right)m_{LHO} \quad (15)$$

Substituting A(y) into Equation (15) we have

$$\overline{m}\frac{d^2\overline{m}}{dt^2} - \frac{5}{4}\left(\frac{d\overline{m}}{dt}\right)^2 - \frac{4\overline{m}^2}{\Delta E}\left\{\theta(\overline{m} - m_{BC}) - V_o\right\}\overline{m}^2 + t^2 = 0 \quad (16)$$

Introducing new variables

$$t = y\sqrt{qm_{LHO}\Delta E} \Rightarrow \frac{dt}{dy} = \sqrt{qm_{LHO}\Delta E}$$

$$\frac{dz}{dt}\cdot\sqrt{qm_{LHO}\Delta E} = \sqrt{\frac{m_{LHO}}{\underline{m}}}$$

$$z(t) = \frac{1}{\sqrt{q\Delta E}}\int_{t_o}^{t}\frac{dt}{\sqrt{\overline{m}(t)}} \quad (17)$$

And

$$V^2(t) = \Delta E / [4\theta\overline{m}(t)]$$

gives

Substitute for $\frac{d\overline{m}}{dt}$ *and* $\frac{d^2\overline{m}}{dt^2}$ in Equation (16)

$$2V\frac{d^2V}{dt^2}+\left(\frac{dV}{dt}\right)^2-1\left[\frac{4(\theta m_{BC}+V_o)}{\Delta E}+t^2\right]V^2+1=0 \qquad (18)$$

Put $V = S_1(t)S_2(t)$ into Equation (18) Wronskian squared equals unity.
Equation (18) becomes

$$\frac{d^2S}{dt^2}-\left[\frac{t^2}{4}+\frac{\theta m_{BC}+V_o}{\Delta E}\right]S=0 \qquad (19)$$

Equation (19) is the well-known parabolic cylinder equation (Weber differential equation) (Abramowitz and Stegun, 1972). A choice of linearly independent solutions of Equation (19) is the even $S_e(t)$ and the odd $S_o(t)$ solutions, generated from the fundamental boundary conditions (Powell and Crasemann, 1962):

$$S_e(o)=1\ ;\ S_e^1(o)=0 \qquad (20)$$

$$S_o(o)=0\ ;\ S_o^1(o)=1$$

Suitable linear combinations of these two solutions are,

$$S_1(t)=C_1S_e(t)+C_2S_o(t) \qquad (21)$$

$$S_2(t)=C_3S_e(t)+C_4S_o(t) \qquad (22)$$

C_1, C_2, C_3 *and* C_4 are arbitrary constants and are solution of Equation (19)

From the requirement that the Wronskian squared $\left(S_1S_2^1-S_1^1S_2\right)^2=1$

Using the identity

$$4(C_1C_3)(C_2C_4)=(C_1C_4+C_2C_3)^2-(C_1C_4-C_2C_3)^2$$

and introducing new constants

$$C_e=C_1C_3$$
$$C_o=C_2C_4$$
$$V(t)=S_1(t)S_2(t)$$
$$V(t)=(C_1S_e+C_2S_o)(C_3S_e+C_4S_o)$$

The general solution of Equation (18) reads

$$V(t)=C_eS_e^2(t)\pm\left[\sqrt{1+4C_eC_o}\right]S_e(t)S_o(t)+C_oS_o^2(t) \qquad (23)$$

and the general solution of Equation (16) for $\overline{m}(t)$ is as follows

$$\Rightarrow\overline{m}(t)=\frac{\Delta E}{4\theta V^2(t)}$$

$$\overline{m}(t)=\frac{\Delta E/4\theta}{\left\{C_eS_e^2(t)\pm\left[\sqrt{1+4C_eC_o}\right]S_e(t)S_o(t)+C_oS_o^2(t)\right\}^2} \qquad (24)$$

From Equation (17)

$$z(t)=\frac{2}{\Delta E}\sqrt{\frac{\theta}{q}}\int_{t_o}^{t}\left[C_eS_e^2(t)\pm\sqrt{1+4C_eC_o}\,S_e(t)S_o(t)+C_oS_o^2(t)\right]dt \qquad (25)$$

Equations (24) and (25) thus give the required $m(z)$ dependence to get equidistant levels, with some prescribed values of parameters $\theta, m_{BC}, \Delta E,$ *and* V_o. The even and odd solutions of the parabolic cylinder of Equation (19) can be written as

$$S_e(t)=\frac{1}{2U(o)}\left[U(t)+U(-t)\right] \qquad (26)$$

$$S_o(t)=\frac{1}{2U'(o)}\left[U(t)-U(-t)\right] \qquad (27)$$

where various properties of the functions $U(t)$ *and* $U(-t)$ are given in Abramowitz and Stegun (1972).

$$U(a,\pm t)=\frac{\left(2\pi^{1/4}\right)}{\sqrt{\Gamma^2\left(\frac{1}{2}+a\right)T}}\exp\{\mp\sigma-v(a,\pm t)\} \qquad (28)$$

$$Where \quad T=\sqrt{t^2+4a}$$

Put $1+4C_eC_o=0$. Here we have $C_o=-\frac{1}{4C_e}$. It is convenient to use a new constant $\in$ defined from $4C_e^2U_0^2=U_0^2(1+\in),\ where\ U_o=U(o)$ and $U_o^1=d\,U(t)/dt\ at\ t=0$. The solution $\overline{m}(t)$ may then be written as

$$\overline{m}(t)=\frac{\Delta E}{\theta}\frac{U_o^2U_o'^2(1+\in)}{[U(t)U(-t)]^2\left[1+\frac{\in}{4}\left(\sqrt{\frac{U(t)}{U(-t)}}+\sqrt{\frac{U(-t)}{U(t)}}\right)^2\right]^2} \qquad (29)$$

Simplifying equation (29),

$$\overline{m}(t)=\frac{\Delta E}{4\theta}.\frac{\left(t^2+4a\right)\exp\left(-4V_e(t)\right)(1+\in)}{\left[1+\in Cosh^2\left(\sigma(t)-V_o(t)\right)\right]^2}. \qquad (30)$$

Let us analyse the case $\in=0$ *and* $\in\neq0$ separately

The case $\in=0$

$$m(t)=\frac{\Delta E}{4\theta}.\frac{\left(t^2+4a\right)\exp\left(-4V_e(t)\right)}{\left[1+\in Cosh^2\left(\sigma(t)-V_o(t)\right)\right]^2}$$

It is reasonable here to take the minimum mass, at the origin, to be $m(o) = m_{BC} = 0.13$ (corresponding to CdSe). The parameter V_o, and hence a, are found by setting $\in = 0$ and $t = 0$ in Equation (30)

$$\overline{m}(t) = \frac{\Delta E}{4\theta}\left(t^2 + 4a\right)$$ Putting

$\in = 0$ and $V_e(t) \to 0$ for $a >> 1$

$$\overline{m}(t) = \frac{\Delta E}{4\theta}\left(t^2 + 4a\right) \text{ and } z(t) = \frac{2}{\Delta E}\sqrt{\frac{\theta}{q}}\, Sin\,h^{-1}\frac{t}{2\sqrt{a}} \quad - \quad (31)$$

$\overline{m}(z)$ may now be written explicitly from Equation (31)

$$\therefore\ \overline{m}(z) = m_{BC}\ Cosh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\, z\right) \quad - \quad - \quad (32a)$$

Using Equations (5) and (32a)

$$V(z) = \theta\, m_{BC}\ Sinh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\, z\right) \quad - \quad - \quad (32b)$$

Using Equations (4) and (32a)

$$x = \frac{m_{BC}}{\Delta m}\ Sinh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\, z\right) \quad - \quad - \quad (32c)$$

We now briefly analyse the wave function $U_{i(z)}$ corresponding to eigenstates E_i from Equation (13). Introducing new coordinate

$$\frac{d^2u}{dt^2} + \left(\frac{E - V_o}{\Delta E} - \frac{t^2}{4}\right) u = 0 \quad - \quad - \quad (33)$$

The eigenfunctions $\underline{U(t)}$ are the well-known Hermite functions.

$$\psi_i(t) = \left(q\Delta Em\ (t)\right)^{1/4}\ U_i(t)\ (i = o) \quad - \quad (34)$$

This is the ground state wave function - - 35)

$$Ui\ (z) = \psi_i(z) = \left(\frac{1}{i!2^i}\right)^{1/2}\ \left[q\ \Delta Em\ (z)\right]^{1/4}\ H_i(z) e^{-\frac{1}{2}(z)^2}$$

For $i = 0,1,2$

$$H_o(z) = 1,\ H_1(z) = 2z \ \text{ and } \ H_2(z) = 4z^2 - 2 \quad - \quad (36)$$

Substituting values for $H_i(s)$ (Powell and Crasemann 1962; Russel 1998), we have

$$U0(z) = \psi_0(z) = \left(q\,\Delta Em_{BC}\right)^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ z\right).e^{-\frac{1}{2}(z)^2}$$

$$U1(z) = \psi_1(z) = 2\left(\frac{1}{4}q\,\Delta Em_{BC}\right)^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ z\right).\,z\,e^{-\frac{1}{2}(z)^2}$$

$$U2(z) = \psi_2(z) = \frac{2}{2}\left(\frac{1}{4}q\Delta Em_{BC}\right)^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\,z\right).\left(2z^2 - 1\right)e^{-\frac{1}{2}(z)^2} \quad - \quad (37)$$

For the case of $\in \neq 0$

From Equations (30) and (31)

$$m(t) \to m(z) = m_{AC}\,.\,\frac{Cosh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}z\right)\exp\left(-4V_e(t)\right)}{\left[1 + \in Cosh^2\ \left(\sigma(t) - V_o(t)\right)\right]^2}\,. \quad - \quad (38)$$

$$a = a\left(m_{AC}\right) = \frac{\Delta V}{\Delta m}.\frac{m_{AC}}{\Delta m}$$

From Equations (4) and (38)

$$x(z) = \frac{1}{\Delta m}\left[m(z) - m_{BC}\right]$$

And from Equations (5) and (38)

$$V(z) = \theta\left[m(z) - m_{BC}\right]$$

For the purpose of numerical illustration of the above theory, we consider the ternary alloy $Cd_xZn_{1-x}Se$ and graded quantum-well structures based upon it. The electron effective masses in the conduction-band Γ- valley are taken as 0.13 and 0.17 (in free electron mass units) for CdSe and ZnSe, respectively, and the Γ-valley conduction-band offset at the CdSe/ZnSe interface is taken to be 720 meV.

In this example we find the variation of the effective mass and of the potential and eventually the grading function x(z), required to obtain equispaced levels with ΔE= 30 meV. Plots of m(z), V(z), x(z) and Ui(z), with z are obtain using Equation (32). For the case of $Cd_xZn_{1-x}Se$

m_{AC} = 0.17 emu in CdSe
m_{BC} = 0.13 emu in ZnSe
ΔE = 30 meV
ΔV = 720 meV conduction-band offset at interface of CdSe/ZnSe

$$a_o = \frac{720\ \ meV}{\left(0.17\ - 0.13\ \right)emu}\ .\ \frac{0.13\ emu}{30\ \ meV}$$

$$a_o\left(m_{BC}\right) = \frac{24}{0.04}\ 0.13 = 78.00$$

The value of a_o is associated with m_{BC}. That $a_o\left(m_{BC}\right)$. This implies that $a_o\left(m_{AC}\right) = \dfrac{720\ \ meV}{\left(0.17\ - 0.13\right)}\,.\,\dfrac{0.17\ emu}{30\ meV}$

$$a_o\left(m_{AC}\right) = \frac{24}{0.04}.0.17 = 102\ .00$$

In the early work on GaAs/AlGaAs quantum wells Dingle in 1975 (Basu, 1997), proposed that the band gap ΔE_g should be partitioned in the ratio 85:15. This proposal was widely accepted and in most subsequent work the band offset was calculated according to this proposal. That is $\Delta E_C : \Delta E_V$ partitioned in the ratio 85:15 of ΔE_g.

$$85\ \%\ \ of\ \ \Delta E_g \approx 0.720\ \ eV\ \ = 720\ \ meV$$

720meV is taken as ΔE_c, the conduction band offset for CdSe/CdZnSe system:
Where ΔE_g *is* $0.84eV$ (David, 1991).

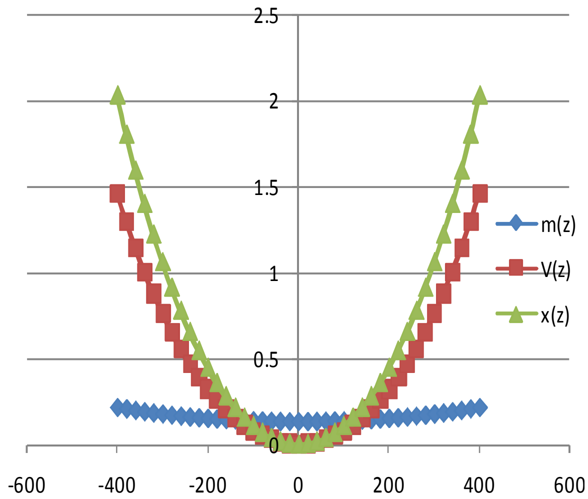

Figure 1. The effective mass m (z), the potential v(z) and the mole fraction x(z) for $Cd_xZn_{1-x}Se$.

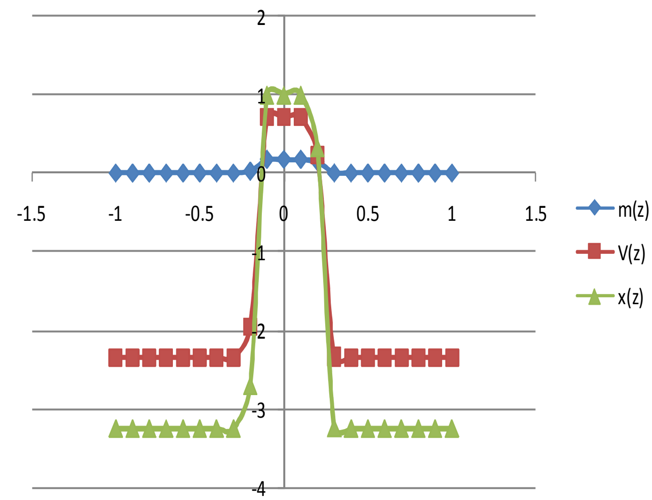

Figure 3. The effective mass m (z), the potential v(z) and the mole fraction x(z) for $Cd_xZn_{1-x}Se$.

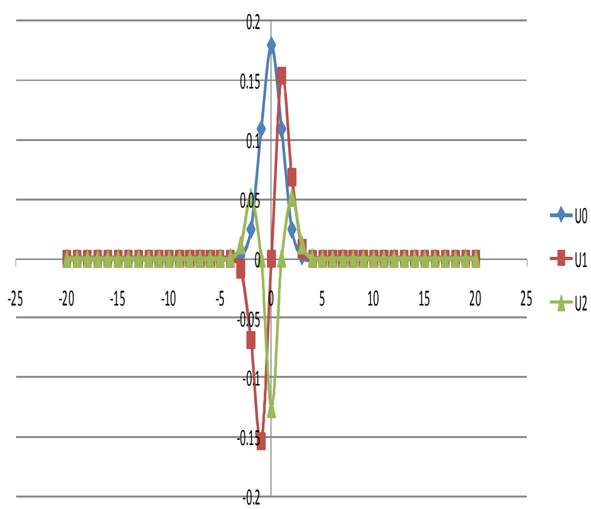

Figure 2. The normalized wave functions $Ui(z)$ of the first three bound state for $Cd_xZn_{1-x}Se$.

RESULTS, DISCUSSION AND CONCLUSION

The results are given in Figures 1 to 3.

The solutions with the "+" sign of the root term in Equations (24) and (25) are considered because $\overline{m}_+(t) = \overline{m}_-(t)$, the "-" sign gives nothing physically different. Equation (32a) is an even function of t. In Equation (38) when we set the arbitrary constant t to zero, $z(t) = -z(-t)$. It therefore suffices to consider half of the domain, $t \geq 0, i.e, z \geq 0$, only because $m(z)$ is an even function.

For $\in \neq 0$ we found $\overline{m}(t)$ asymptotically behave as follows $\overline{m}(t \to +\infty) \to 0$ and thus also $\overline{m}(z \to +\infty) \to 0$ which is a drop below the conduction-band edge of the BC compound.

In the limit $t \to \pm\infty$. This implies that $\overline{m}(t \to \infty) \to 0$, and therefore $m(z \to \infty) \to 0$. The accompanying potential in Equation (32b) will behave in the same manner. On the other hand if $\in = 0$, we found that $\overline{m}(t \to +\infty) \to +\infty$ and $m(z \to +\infty) \to +\infty$, as also does the potential, that is $V(z \to +\infty) \to +\infty$.

The choice $\in = 0$ delivers a classically confining potential (CP) and $\in \neq 0$ a non confining potential (NCP) because it is asymptotically bounded. In both cases the energy spectrum is fully discrete, just as that in 1DHO, with confining wave functions.

In all cases where the potential is not confining, confinement is made possible by $\overline{m}(z \to +\infty) \to 0$. This confinement occurs in very much the same way as does the potential. In effect, just as the electron tends to avoid regions where its potential exceeds the total energy, it also avoids regions where the kinetic energy will be large there by exceeding the total energy.

Certainly if any of the effective mass, potential and grading function are to be realized, there are some restrictions to be observed related to a limited parameters offered by real semiconductors (David, 1991).

The Equations (32a), (32b) and (32c) gives the ideal of a physically realizable QW structure. The deviation of the real structure from the idealized one is due to the accumulation of electrons in the lower gap material (say CdSe) side at the two heterointerfaces, which lead to band bending at the interfaces (Das et al., 1990). This deviation will perturb energies of state below the barrier top, which remain bounded, while those above would dissolve into continuum. Yet only those which are close to the barrier top (Lee et al., 1996) will be seriously affected by truncation therefore the influence of truncation is negligible for all practical purposes (Milanovic and Ikonic, 1996).

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