Competition between the pseudomorphic strain mechanism with the piano-keyboard effect on the effective potential profile for coupled holes in layered heterostructures

A. Mendoza-Álvarez[1] (*alejandro.mendoza@ibero.mx*), J.J. Flores-Godoy[1] (*job.flores@ibero.mx*),

G. Fernández-Anaya[1] (*guillermo.fernandez@uia.mx)*), L. Diago-Cisneros (*ldiago@fisica.uh.cu*)[2].

[1]*Dep. de Física y Matemáticas, Universidad Iberoamericana, C.P. 01219, México D.F.*

[2]*Facultad de Física, Universidad de la Habana, C.P. 10400, la Habana, Cuba*

Formulation of the Problem

Several new features in the metamorphosis of the standardized fixed-height V_{eff} profile for holes, in the presence of gradually increasing valence-band mixing and biaxial pseudomorphic strain, are presented. In some $III - V$ unstrained semiconducting layered heterostructures a fixed-height potential, is not longer valid for *lh*. Indeed, we found –as predicted for electrons, permutations of the V_{eff} character for *lh*, that resemble a "*keyboard*", together with band offset changes, whenever the valence-band mixing varies from low to large intensity. Meanwhile for strained heterostructures, the former behavior, had been also detected for *hh*. Strain is able to diminish the *keyboard* effect on V_{eff}, and also makes it emerge or vanish occasionally. We found that multiband-mixing effects and stress induced events, are competitors mechanisms that can not be universally neglected by assuming a fixed-height rectangular spatial distribution for fixed-character potential energy, as a reliable test-run input for heterostructures.

Sinopsis of Fundamentals and Motivation

The problem of quantum transport of charge carriers (electrons and holes) is narrowly linked to the study of spectral properties in heavy and light hole tunneling in semiconductor quantum heterostructures, as the appreciation of the fundamental transport properties of these materials can be directly applied to the analysis, design and functioning of practically all device structures that are currently technologically important. For many actual practical solutions and technological applications, due to the impressive development of low-dimensional electronic and optoelectronic devices, it is drastically important to include the valence-band mixing,[1] *i.e.* the degree of freedom transverse to the main transport direction, whenever the holes are involved. This phenomenology, early quoted by Wessel and Altarelli in resonant tunneling [2], has been lately pointed up for real-life technological devices.[1] If the electronic transport through these systems, engage both electrons and holes, the low-dimensional device response depends on the slower-heavier charge-carrier's motion through specific potential regions.[3] It is unavoidable to recognize that in the specialized literature there is plenty of reports studying several physical phenomena derived from hole mixing effects, *via* standard existing methods.

However, just a few reports are available, concerning the evolution of the effective potential, as a central topic of investigation. Earliest striking elucidations due to Milanović and Tjapkin for electrons,[4] and recalled much later by Pérez-Álvarez and García-Moliner for a fully unspecific multiband theoretical case,[5] are fundamental cornerstones in this concern. The metamorphosis of the effective *band offset* potential V_{eff}, "felt" by charge carriers depending on the transverse momentum value, is so far, the better way to graphically mimic, the phenomenon of the in-plane dependence of the effective mass, also refereed as the valence-band mixing for holes. This is essentially the case of the carriers' transverse motion connection with the V_{eff} they interact with and is the main porpoise under investigation here. We assume the last widely understood as crucial, for charge and spin carriers' quantum transport calculations through standard quantum barrier (QB) – quantum well(QW) layered systems.

Sinopsis of Fundamentals and Motivation

On general grounds, V_{eff} is given by the difference for $3D$ band edge levels as long as the transverse momentum (κ_{T}) values are negligible.[5] For finite κ_{T}, this assertion is no longer valid and the mixing effects reveal. The mechanism responsible for this behavior, is the increment of the κ_{T}-quadratic proportional term, yielding even to invert the roles of QW and QB. [4,5] Some authors had declared ashift upward in energy, of the bound states in the effective potential well as the transverse wave vector increases.[7] By letting grow κ_{T}, were found the valence-band mixing effects to arise and V_{eff} to change.[8] They conclude a larger reduction for V_{eff} as a function of κ_{T}, for light holes (*lh*) respect to that for heavy holes (*hh*).[8] Recently, a valence-band mixing first-principle theory within the envelope function approximation (EFA) was proposed, which had approximated the superlattice potential energy by considering only the linear and quadratic responses to the heterostructure perturbation.[6] These former works,[4,5,7,8,6] were motivating enough and put us on an effort to try a more comprehensive vision, of how V_{eff} evolves spatially with κ_{T} for *hh* and *lh*. This section is devoted to demonstrate, the feasibility of a V_{eff} profile evolution, as a reliable follow-up tool for finding the response of a layered semiconductor system —with spatial-dependent effective mass—, on travelling holes throughout it, by tuning the valence-band mixing and including strain effects.

The outline for this work is the following: We presents briefly the theoretical framework to quote valence-band V_{eff} for both unstressed and stressed systems. Graphical simulations on V_{eff} evolution, are exposed [9]. We exercise and discuss highly specialized $III - V$ semiconductor binary(ternary)-compound cases, that support the main contribution of the present study and suggest possible applications.

Basic theoretical formulation

The movement equation of multiband systems, invariant in the presence of plane shifts *[x, y]*, has the following form [10]:

$$\frac{d}{dz}\left[B(z)\frac{dF(z)}{dz} + P(z)F(z)\right] + Y(z)\frac{dF(z)}{dz} + W(z)F(z) = O_N, \qquad (1)$$

where $B(z)$ and $W(z)$ are, in general, $(N \times N)$ Hermitian matrices and is fulfilled $Y(z) = -P^\dagger(z)$.

Cuadratic Eigenvalue Problem (QEP) [7, 11,12] :

$$Q(k_z)\Gamma = \{k_z^2 \mathcal{M} + k_z \mathcal{C} + \mathcal{K}\}\Gamma = O_N, \qquad (2)$$

$$\mathcal{M} = \begin{pmatrix} -m_{hh}^* & 0 & 0 & 0 \\ 0 & -m_{lh}^* & 0 & 0 \\ 0 & 0 & -m_h^* & 0 \\ 0 & 0 & 0 & -m_{hh}^* \end{pmatrix} \qquad (3)$$

where $\qquad \mathcal{M} = -B, \quad \mathcal{C} = 2iP \quad \text{and} \quad \mathcal{K} = W.$ $\qquad (4)$

$$\det[Q(k_z)] = q_0 k_z^8 + q_1 k_z^6 + q_2 k_z^4 + q_3 k_z^2 + q_4, \qquad (5)$$

The operator $\widehat{W}_{\text{eff}}$ for the effective *band offset* potential [8, 12]:

$$\widehat{W}_{\text{eff}} = \begin{pmatrix} W_{11} & W_{12} & 0 & 0 \\ W_{12}^* & W_{22} & 0 & 0 \\ 0 & 0 & W_{22} & W_{12} \\ 0 & 0 & W_{12}^* & W_{11} \end{pmatrix} \tag{6}$$

$$\left[\widehat{W}_{\text{eff}} - V_{\text{eff}} I_4\right] \Psi(z) = O_4, \tag{7}$$

At zero valence-band mixing, one has:

$$V(z) = \begin{cases} 0 & ; & z < z_l \, (10) \\ V_b - V_a = V_{\text{eff}} & ; & z_l < z < z_r \, (11) \\ 0 & ; & z > z_r \end{cases} = \Theta V_{\text{eff}}, \tag{8}$$

The effective potential operator $\widehat{W}_{\text{eff}}$ in the presence of biaxial strain [14]:

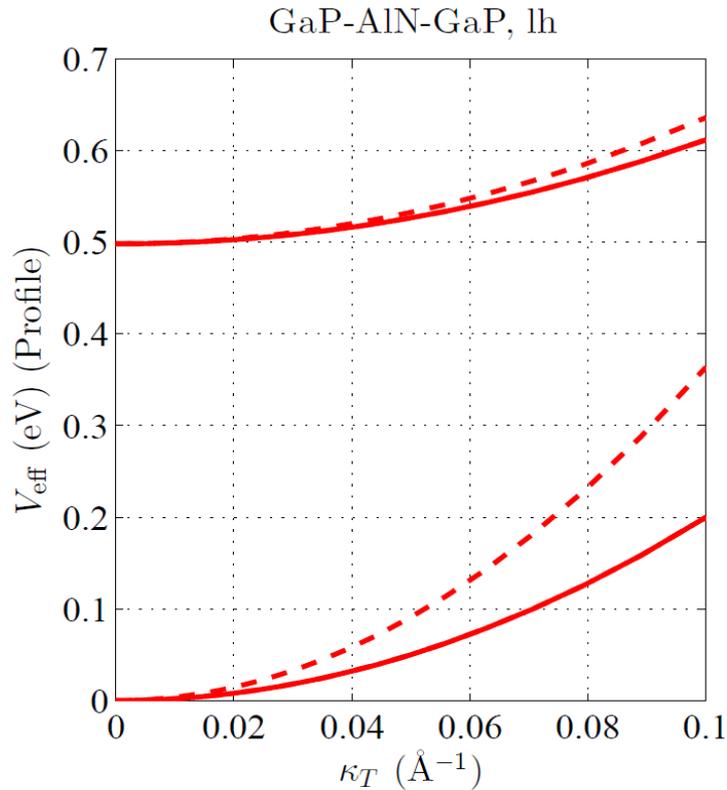$$\widehat{\widetilde{W}}_{\text{eff}} = \widehat{W}_{\text{eff}} + U_s I_4, \tag{9}$$
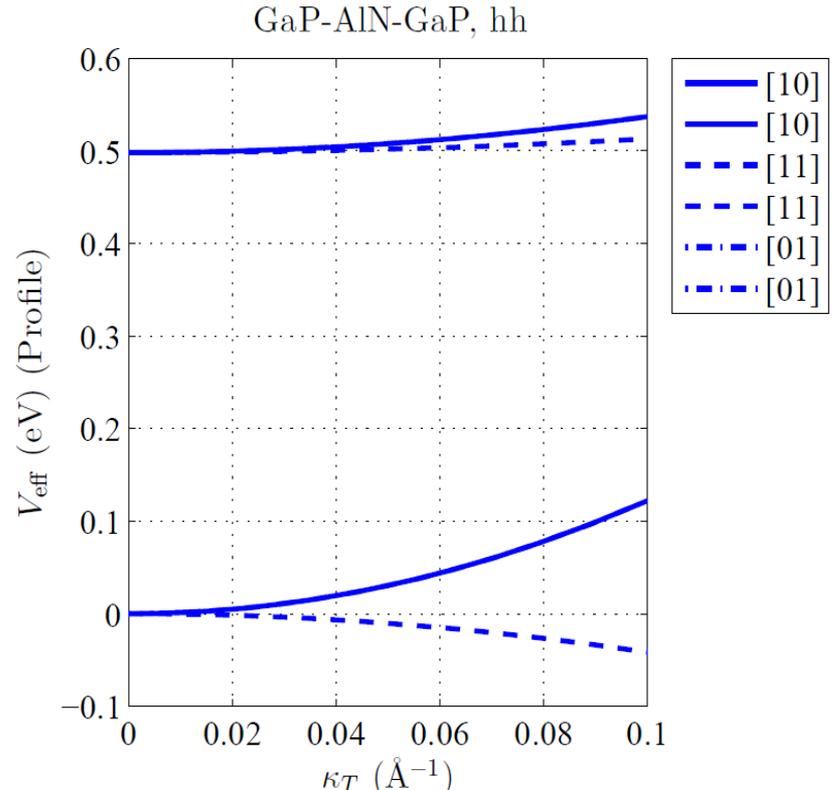
Where the accumulated strain energy resulting:

$$U_s = -\{a_v(2\varepsilon_1 + \varepsilon_3) + b(\varepsilon_1 - \varepsilon_3)\}, \tag{10}$$

Numerical Results and Discussion

To gain some insight into the rather complicated influence of the band mixing parameter κ_T, on the effective *band offset*, we display several graphics in the present section. The central point here, is a reliable numerical simulation for the spatial distribution of V_eff while the valence-band mixing increases from $\kappa_\mathrm{T} \approx 0$ (uncoupled holes) to $\kappa_\mathrm{T} = 0.1\mathring{\mathrm{A}}^{-1}$ (strong hole band mixing).

a)

b)

Figure 1. (Color online) Panel (a)/(c) displays a cut of the V_{eff} profile for *lh*/*hh* (red/blue lines), at the interface plane between left and middle layers, as a function of κ_T. Panel (b)/(d)shows the progression of the *band offset* at the same interface for *lh*/*hh* (red/blue lines), *i.e.* the difference between the upper-edge and lower-edge of the V_{eff} profile. We have considered a *GaP*/lAlN/*GaP* stress-free layered heterostructure.

In Figure 2, the V_{eff} valence-band mixing dependence, exhibits a neatly permutation of the V_{eff} character as the one predicted for electrons [12]. This permutation pattern is what we call as "*keyboard*" effect, and was detected for *lh* only in stress-free systems. This strike interchange of roles for QB-like and QW-like layers, whenever the in-plane kinetic energy, varies from low to large intensity, represents the most striking contribution of the present study.
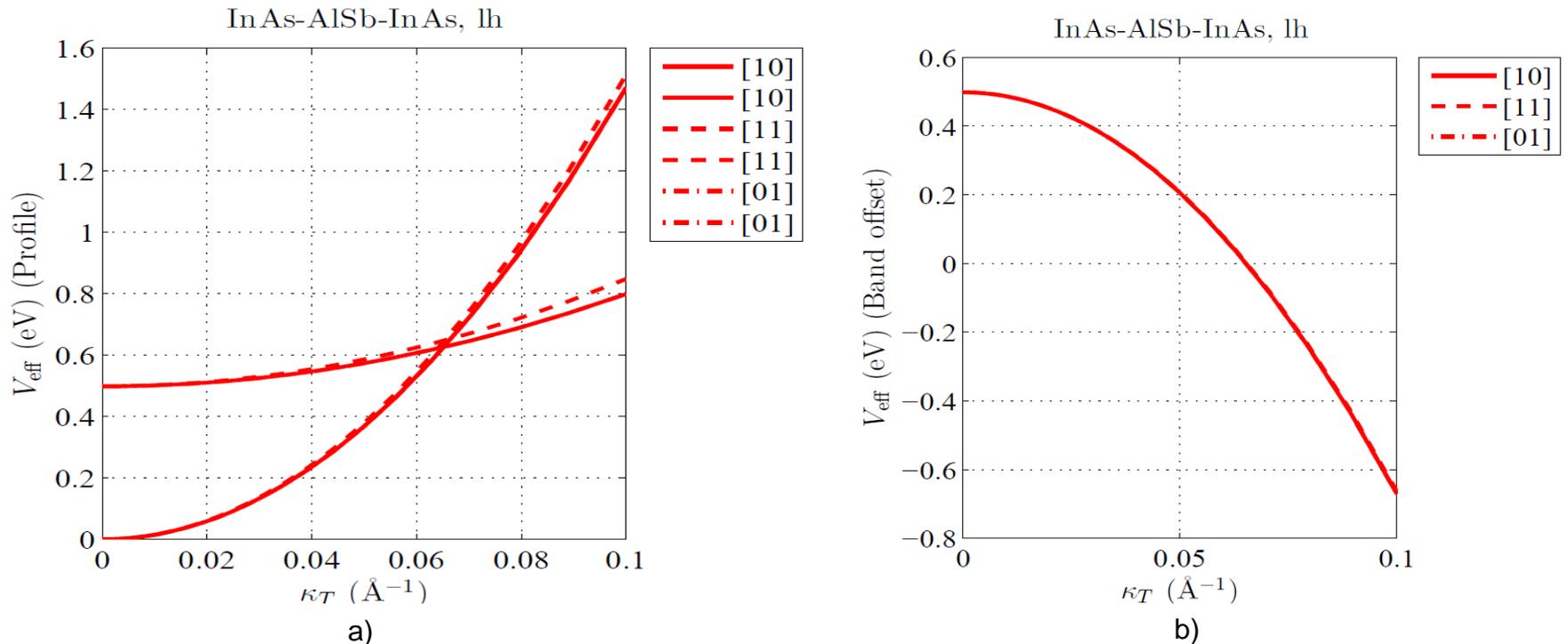
Figure 2. Panel (a) displays a cut of the V_{eff} profile for *lh* (red line), at the interface plane between left and middle layers, as a function of κ_T. Panel (b) shows the progression of the *band offset*, at the same interface for *lh*, ti.e. the difference between the upper-edge and lower-edge of the V_{eff} profile. We have considered a *InAs/AlSb/InAs* stress-free layered heterostructure.

Turning now to built-in elastic stressed layered heterostructures, we are interested to answer a simple question: whether or not the existence of a pseudomorphic strain becomes a weak or a strong competitor mechanism, able sometimes just to diminish the *keyboard* effect on V_{eff}, or even make it rises/vanishes occasionally. Figure 3 exhibits an unexpected *keyboard* effect risen for *lh* in a *InP*:*GaP*/*AlSb*/*GaP* layered heterostructure under a pseudomorphic strain, in comparison with a stress-free heterostructure. This evidence encourages to suggest U_s (10), as a trigger mechanism in the presence of valence-band mixing to influence on V_{eff},
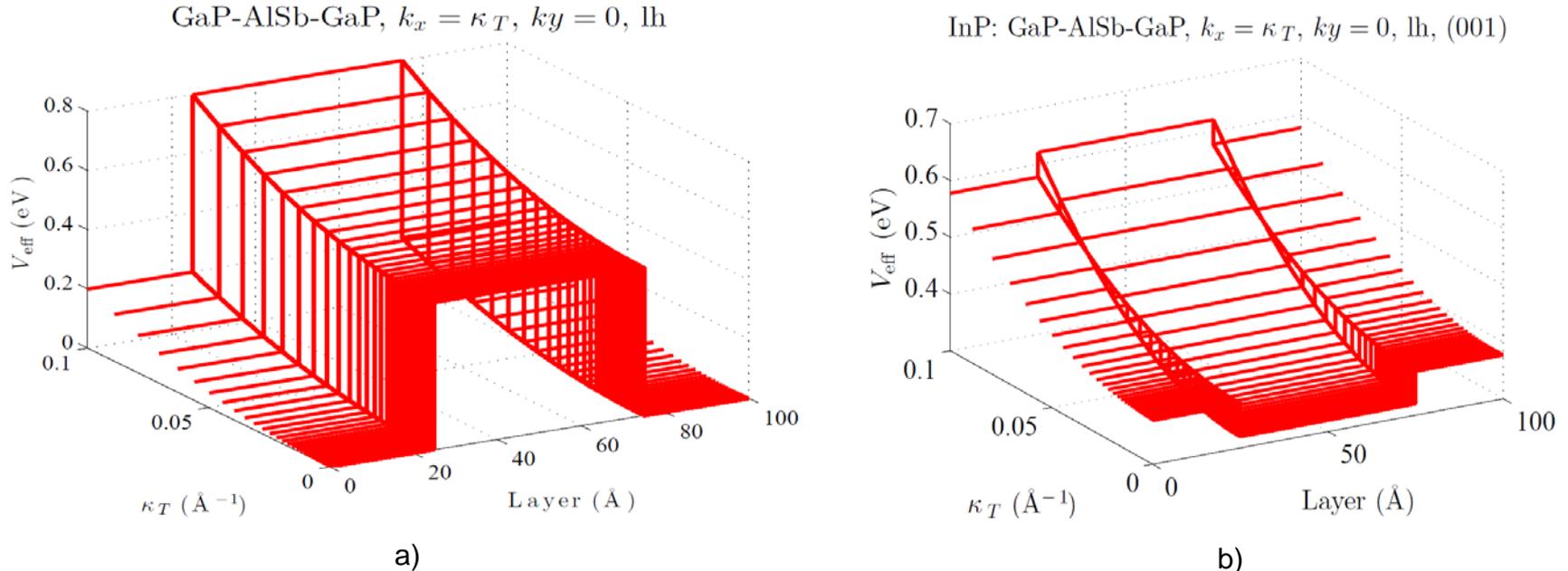
Figure 3. (Color online) Panel (a) displays the $3D$-perspective evolution of the stress-free V_{eff} profile for *lh* as κ_T and layer dimension grow. Panel (b) shows the same for a *InP*:*GaP*/*AlSb*/*GaP* strained layered heterostructure.

Conclusions

We present an alternative procedure to simulate graphically, the phenomenon of the transverse degree of freedom influence together with biaxial tensile strain impact on the effective scattering potential.

i) For low-intensity valence-band mixing regime, a fixed-height rectangular distribution of the potential-energy, is a good trial as a standard reference frame, for a theoretical treatment involving both flavors of holes under study. However this assertion is no longer valid, whenever the mixingeffects reveal.

ii) At variance with the opposite for *hh*, the *lh* exclusively, experience the striking *keyboard* effect and permutations of V_{eff} in stress-free systems. Nevertheless, in strained heterostructures, the former behavior, had been also found for *hh*.

iii) Evidences of this sort, mediated by *hh-lh* coupling and strain, foretell their usefulness in experimental applications, valence-band profile tuning, valence-band offset manipulation and in theoretical analysis of hole tunneling.

iv) Pseudomorphic strain is able to diminish the *keyboard* effect on V_{eff}, and also makes it emerge or even vanish eventually.

v) We conclude that the multiband-mixing effects modulated by stress induced events, are competitors mechanisms that can not be universally neglected by assuming a fixed-height rectangular spatial distribution for fixed-character potential energy, as a reliable test-run input for semiconducting heterostructures.

References

[1] G. Klicmeck, R. Ch. Bowen, and T. B. Boykin, Superlattices and Microstructures 29, 187 (2001).

[2] R. Wessel and M. Altarelli, Phys. Rev. B 39, 12802 (1989).

[3] H. Schneider, H. T. Grahn, K. Klitzing, and K. Ploog, Phys. Rev. B 40, 10040 (1989).

[4] V. Milanovic, and D. Tjapkin, Phys. Stat. Sol(b) 85, 685 (1988).

[5] Rolando Pérez-Álvarez and Federico García-Moliner,\Transfer Matrix, Green Function and related techniques:Tools for the study of multilayer heterostructures", (Ed. Universitat Jaume I, Castell_on de la Plana, Espa~na), 2004.

[6] Bradley A. Foreman, Phys. Rev. B **76**, 045327 (2007).

[7] S. Ekbote, M. Cahay and K. Roenker, J. App. Phys. 110, 924 (1999).

[8] L. Diago-Cisneros, H. Rodríguez-Coppola, R. Pérez- Alvarez, and P. Pereyra, Phys. Rev. B **74**, 045308 (2006).

[9] A Mendoza-Álvarez, J J Flores-Godoy, G Fernández-Anaya and L Diago-Cisneros, Generalized Eigenvalue Problem criteria for multiband-coupled systems: Hole mixing phenomenon study, *Phys.Scr.* **84**, 055702 (2011).

[10] Rolando Pérez-Álvarez and Federico García-Moliner,"*Transfer Matrix, Green Function and related techniques:Tools for the study of multilayer heterostructures*", (Ed. Universitat Jaume I, Castellón de la Plana, España), 2004.

[11] A Mendoza-Álvarez, J J Flores-Godoy, G Fernández-Anaya and L Diago-Cisneros, Coupled Spinors Orthonormalization Criteria in Multiband Systems, *Rev. Mex. Fis.* **57** (1) pp: 40-45, (2011).

 [12] J.J. Flores Godoy, A. Mendoza-Alvarez, L. Diago Cisneros and G. Fernández Anaya, "*Valence-Band effective-potential evolution for coupled holes"*, Physica Status Solidi B, 1-6 (2013) **DOI** 10.102/pssb.201248211

[13] V. Milanovic, and D. Tjapkin, *Phys. Stat. Sol(b)* **110**, 687 (1982).

[14]] Joachim Piprek, "*Semiconductor Optoelectronic Devices. Introduction to Physics and simulation*", (Ed. Elesevier, Acadenic Press), 2003.