Simulation of optical properties of a GaN quantum dot embedded in a AlGaN nanocolumn within mixed Fem/Atomistic method

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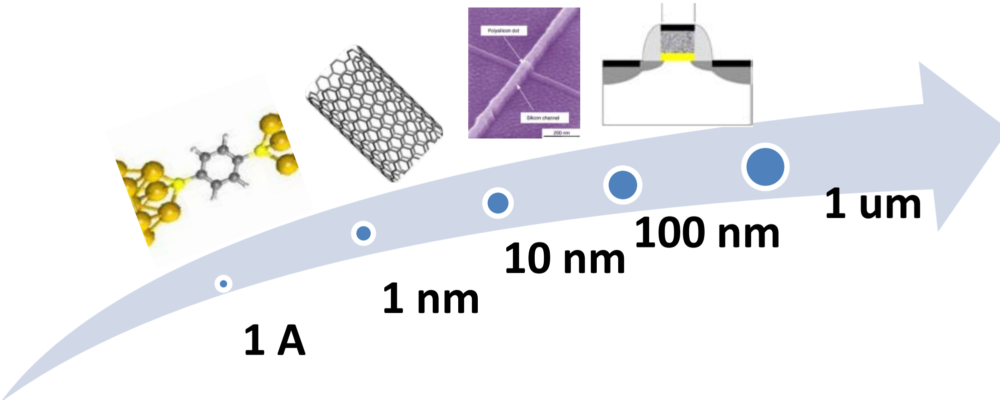
Outline

- Simulation tool
- Device geometry and simulation scheme
- FEM calculation
- Atomistic calculation
- Conclusions

TiberCAD



Modern optoelectronic device industry pushes for reliable numerical models down to nanometer and sub-nanometer scale. A multiscale/multiphysics approach is needed the interaction between small active regions and larger devices.

TIBER CAD

TiberCAD is a TCAD for optoelectronic devices, designed to provide a solution to these needs.

Features:

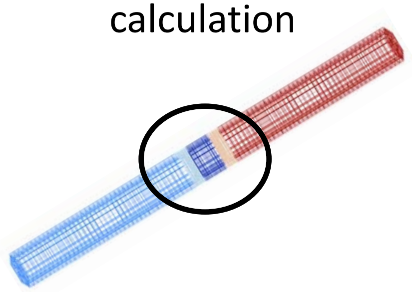
- FEM models: drift diffusion, strain, heating, Shroedinger EFA.
- Atomistic models: empirical tight binding, density functional tight binding.
- DSSC modelling.
- SCC calculations: thermal-drift diffusion, drift-diffusion-quantum charge.

Integration FEM/Atomistic

FEM and atomistic calculations run in the same environment.

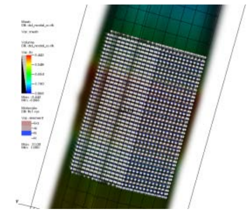
Tools to automatize crystal atomistic structure description and project quantities between atomistic and continuum domain have been developed.

Design geometry and mesh and select region of interest for atomistic calculation



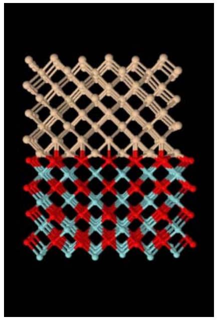
Atomistic structure is innerly generated according to device materials

Continuum media and atomistic calculations information exchange within the same environment



Atomistic generator features:

- Manage most useful Bravais lattices (cubic, hexagonal, fcc, bcc)
- Provide any basis
- Manage pseudomorphic heterostructure and commensurable interfaces
- Provides hydrogen passivation model suitable for any crystal
- Generates minimal periodical structure for bulk, 1D and 2D calculations



FEM/Atomistic interaction

Strain: calculate relative displacement u(x,y,z) and apply displacement to atoms, stretching bond lenght from d_0 to d.

Tight Binding parameters calculated according to Harrison scaling rule:

$$V_{\alpha\beta} = V_{\alpha\beta} \cdot \left(\frac{d_0}{d} \right)^{n_{\alpha\beta}}$$

Potential:

Use FEM potential solution to provide Hamiltonian shifts.

- If no SCC calculation is needed, slow varying potential is projected simply as point potential on atom position.
- If SCC is needed, a projection over an *s*-type orbital with exponential decay is used.

$$V_i = V(r_i)$$

$$V_i = \frac{\tau_i^3}{8\pi} \int V(r_i) e^{-\tau |r - r_i|} dr$$

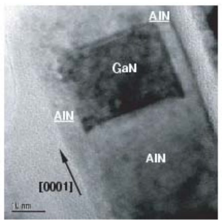
Charge:

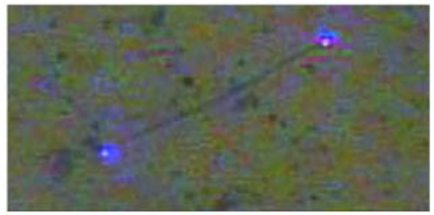
Quantum charge is projected back to FEM grid. An s-type projection with exponential decay is used.

$$n(r) = \sum_i \frac{\tau_i^3}{8\pi} \int \Delta q_i e^{-\tau |r - r_i|} dr$$

Application: Qdot / Nanocolumn

Novel optoelectronic devices based on III-V nanocolumns and quantum dots have been widely proposed



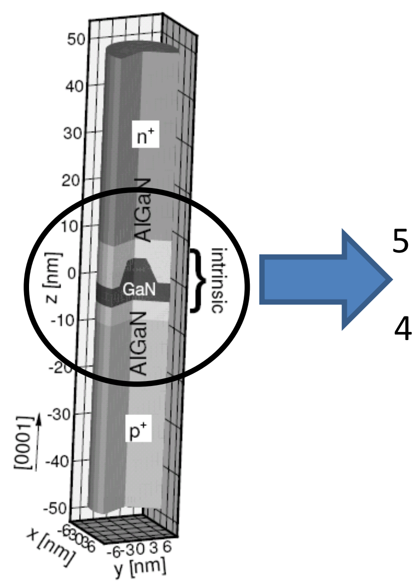


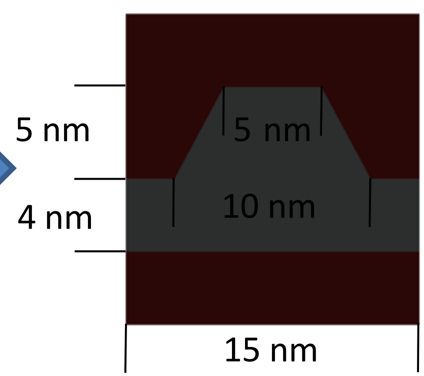
Ristic et al. phys. stat. sol. 202, 367 (2005)

Johnson et al. Nature materials 1, 106 (2002)

Sarusi et al. Phys. Rev. B, 75 (2007)

Examinated structure: GaN Quantum Dot embedded in AlGaN nanocolumn





- GaN/$Al_{0.3}Ga_{0.7}N$ heterostructure
- n-i-p doping profile (1e19÷1e17 cm^{-3})

Goal:

- Optical and electronic behaviour for (0001) and (000-1) growth direction
- Role of piezoelectric field on confined states
- Variation on wettin layer dimension (4÷1 nm)

Simulation scheme

Strain and piezoelectric polarization → Elasticity theory (FEM)

$$E = \frac{1}{2}\int_{\Omega_0} C_{ijkl}(\mathbf{r})\varepsilon_{ij}(\mathbf{r})\varepsilon_{kl}(\mathbf{r})d^3\mathbf{r}$$

M. Povolotskyi et al. Journ. of Appl. Phys. (2006)

IV characteristics → Drift diffusion (FEM)

$$-\nabla(\varepsilon\nabla\varphi - \mathbf{P}) = -\varepsilon(n - p - N_d^+ + N_a^-)$$
$$-\mu_n n(\nabla\phi_n + P_n\nabla T) = R$$
$$-\mu_p n(\nabla\phi_p + P_p\nabla T) = R$$

M. Auf Der Mauer, Ph.D. Thesis (2007)

Quantum states → EFA **k·p** (FEM) / Empirical Tight Binding (Atomistic)

6x6 EFA **k·p** (valence), EFA single band (conduction)
$sp^3d^5s^*$ VCA

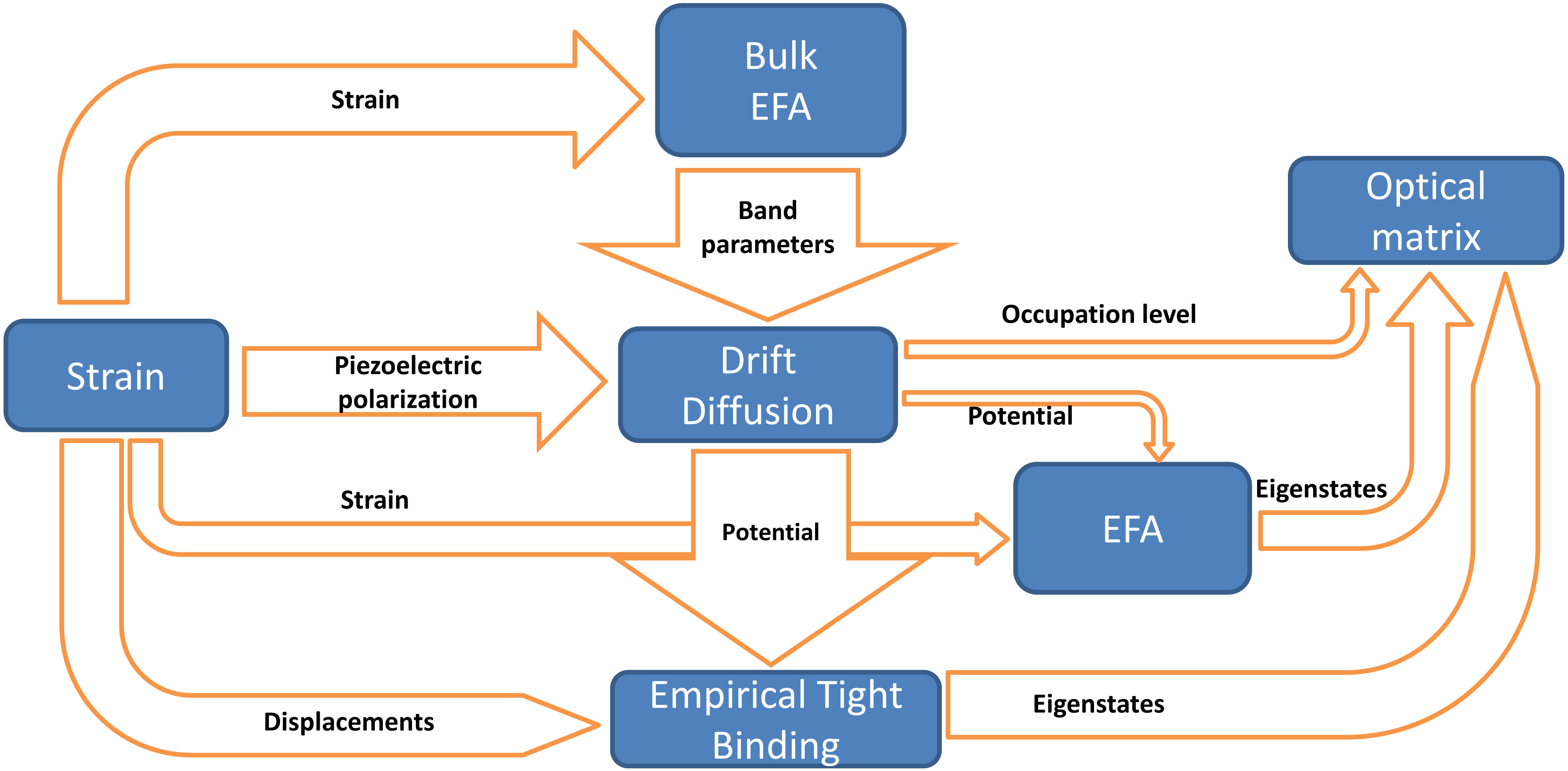
S. L. Chuang and C. Chang, Phys. Rev. B **54 (1996)**
Jancu et al. Phys. Rev. B 57, 6493 (1998)

Optical properties (spontaneous emission) → Optical matrix elements (EFA **k·p** (FEM), ETB)

S. L. Chuang and C. Chang, Physics of optoelectronic devices (1995)

L. C. Lew Yan Voon, Phys. Rev. B, 47 (1993)

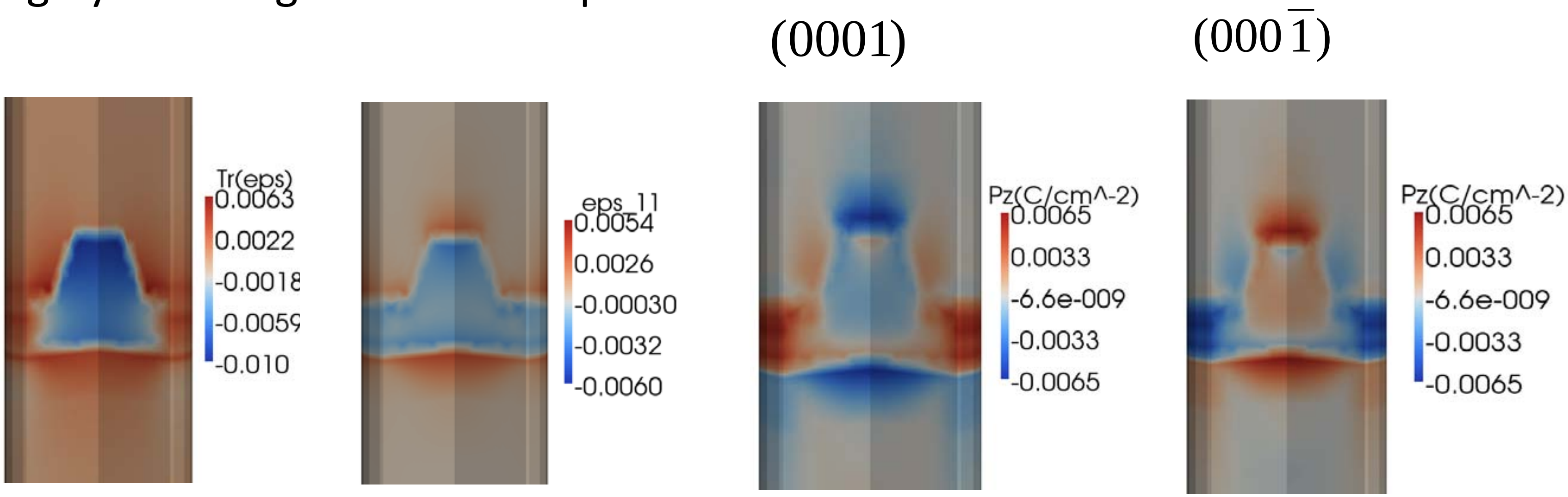
Simulation scheme



Results – strain profile

4 nm wetting layer structure

Highly inhomogeneous strain profile.

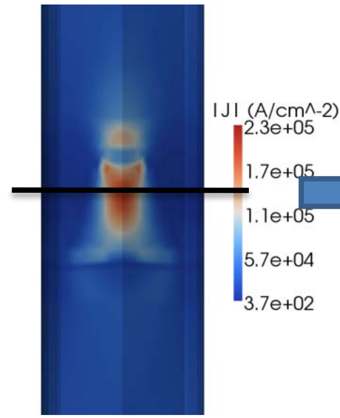


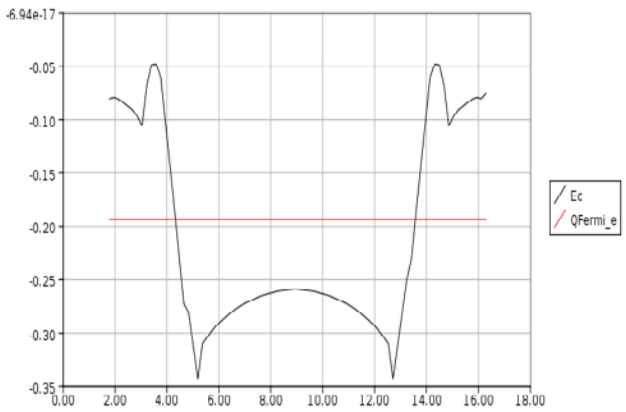
Piezoelectric field along z direction is inverted.

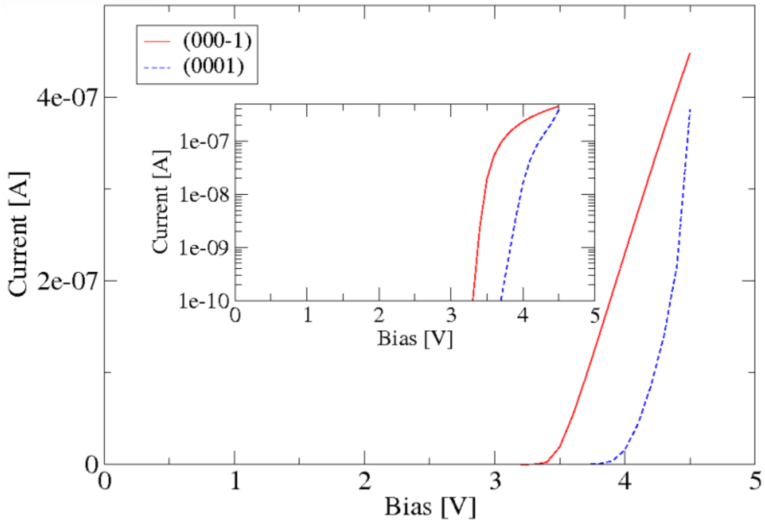
As the device is asymmetric respect to z-axis inversion, it has strong effects on both electrical and optical properties.

Results – electrical properties

Current is confined in the QDOT region

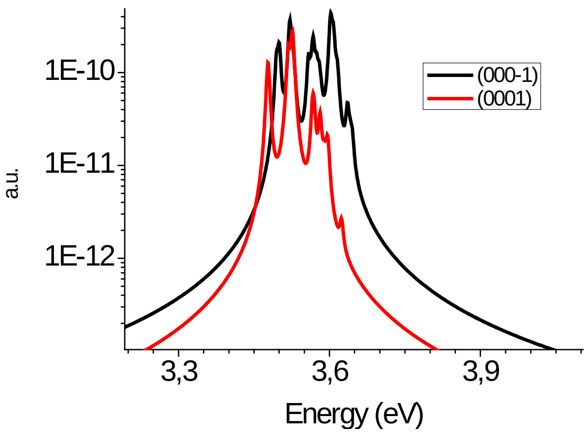




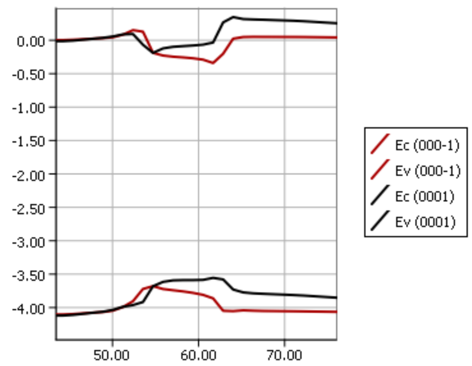


(000-1) growth direction exhibits lower threshold voltage, meaning higher electrical efficiency

Optical spectra



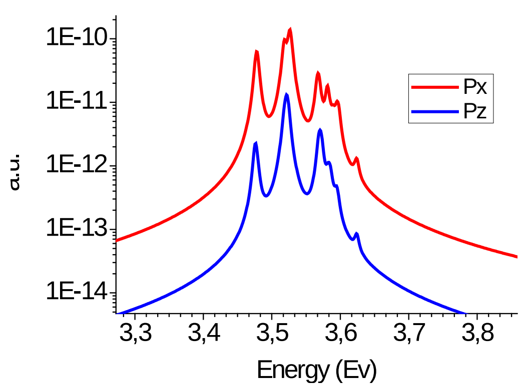
Spontaneous emission spectra differs for different growth direction. A shift is due to different band bending.



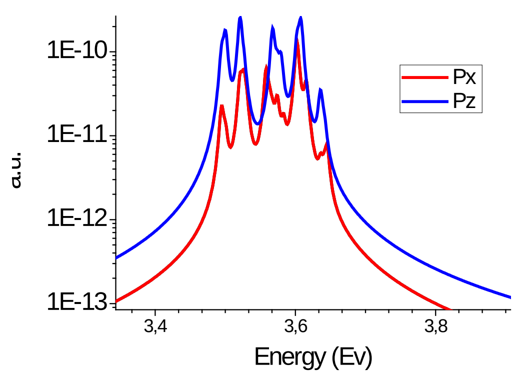
$$\frac{\eta_{000\bar{1}}}{\eta_{0001}} = \frac{P^{opt}_{000\bar{1}}}{P^{opt}_{0001}} \frac{I_{000\bar{1}}}{I_{000\bar{1}}} = 16\%$$

An increase of efficiency is calculated for (000-1) direction

(0001)



$(000\bar{1})$



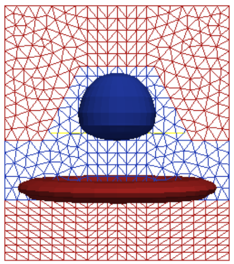
Growth direction induces deep changes in emitted light polarization direction.

Effect of strain on states simmetry.

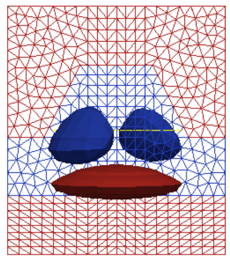
Eigenstates

Position and simmetry of electron and hole states are modified by the external field. States are confined both in the QDOT and in the wetting layer.

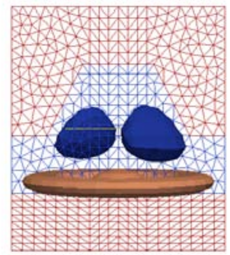
(0001)



Hole 0 (red)
Electron 0 (blue)

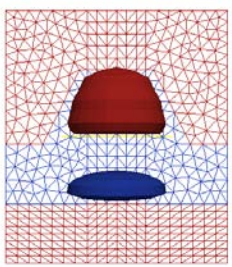


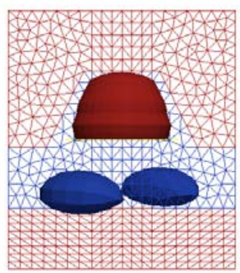
Hole 1
Electron 1

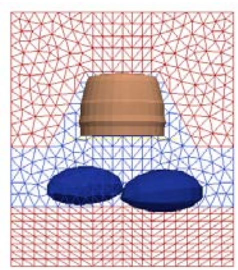


Hole 2
Electron 2

$(000\bar{1})$



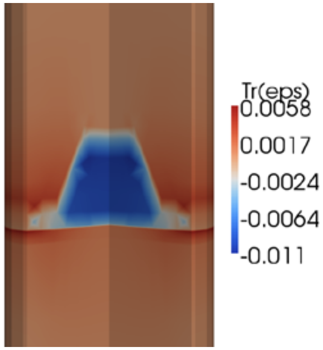


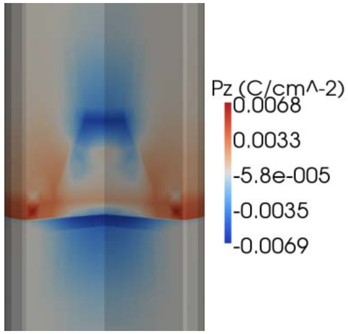


Electron (eV)	Hole (eV)	**0-0**	**3.4761 eV**
-0.23103	-3.70712	0-1	3.4779 eV
-0.18878	-3.70890	0-2	3.4797 eV
-0.18878	-3.71074	1-0	3.5183 eV
-0.18278	-3.71278	1-1	3.5201 eV
-0.14380	-3.71557	1-2	3.5220 eV

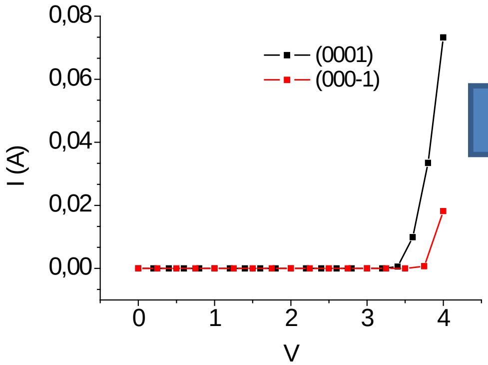
Electron (eV)	Hole (eV)	**0-0**	**3.4946 eV**
-0.09765	-3.59229	0-1	3.4951eV
-0.07132	-3.59273	0-2	3.5002 eV
-0.07132	-3.59784	1-0	3.5210 eV
-0.03409	-3.60160	1-1	3.5214 eV
-0.03408	-3.60176	1-2	3.5265 eV

Results – smaller wetting layer



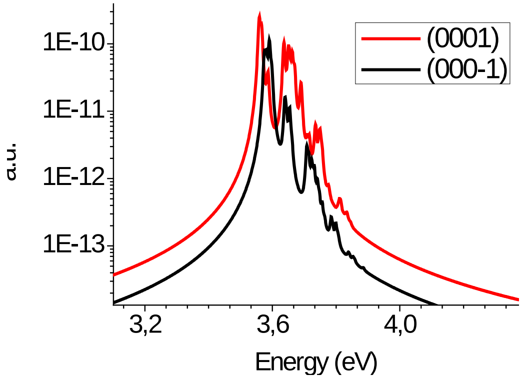


Strain magnitudo is almost unaffected: variation range is the same between the 4 nm wetting layer and 1 nm wetting layer devices.



Opposite IV behaviour:
(0001) Direction shows smaller threshold voltage.

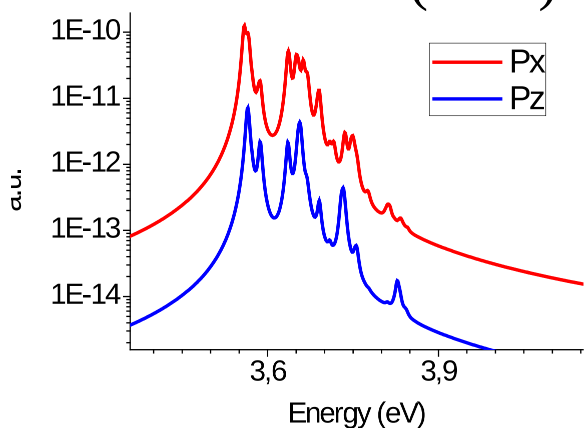
Optical spectra



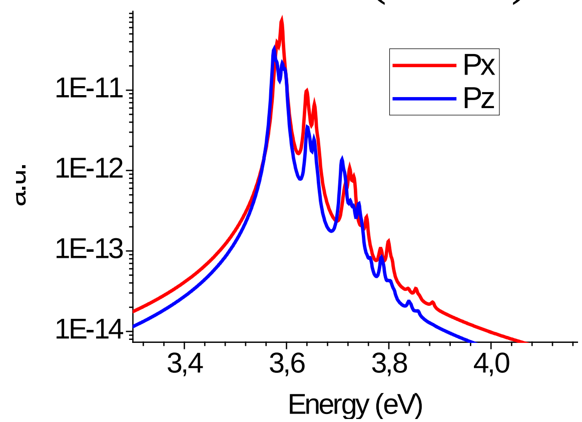
A better confinement in the quantum dot leads to more homogeneous optical emission between (0001) and (000-1) direction

$$\frac{\eta_{000\bar{1}}}{\eta_{0001}} = 4\%$$

(0001)



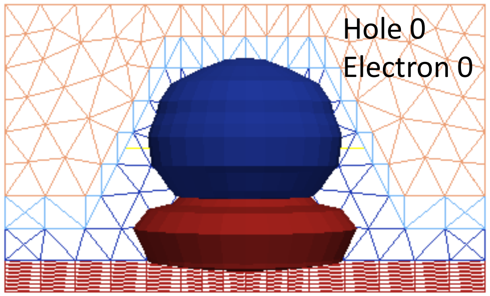
$(000\bar{1})$

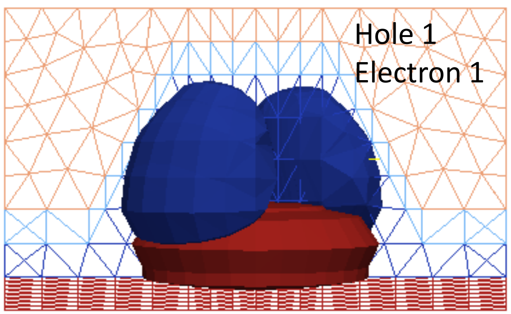


The effect on polarization is reduced

Eigenstates

(0001)



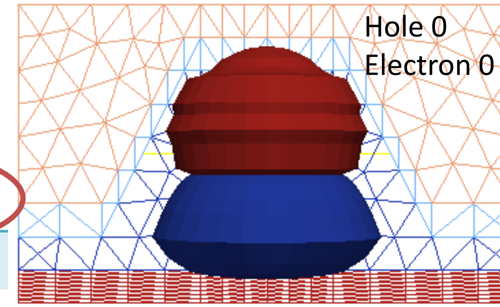


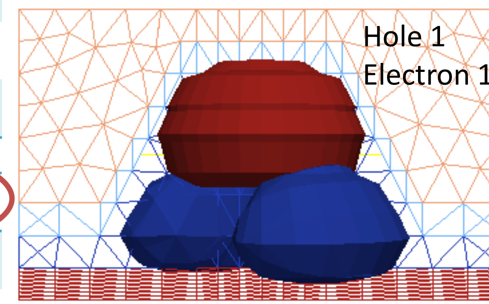
Eigenstates swap their position.
Electron and hole states always confined in the dot region.

Electron (eV)	Hole (eV)	**0-0**	**3.5590 eV**
-0.09029	-3.64933	0-1	3.5650eV
-0.01960	-3.65530	0-2	3.5667 eV
-0.01960	-3.65696	1-0	3.6297 eV
0.01339	-3.66987	1-1	3.6357 eV
0.05965	-3.67320	1-2	3.63736 eV

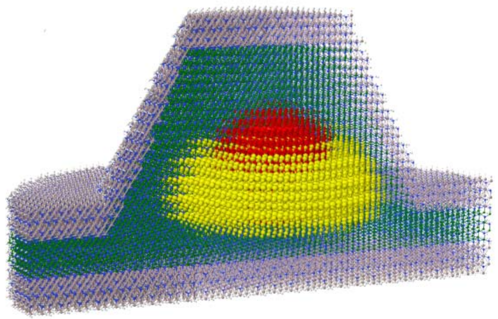
Electron (eV)	Hole (eV)	**0-0**	**3.5749eV**
-0.19790	-3.77279	0-1	3.5771eV
-0.13445	-3.77502	0-2	3.5814 eV
-0.13445	-3.77932	1-0	3.6382 eV
-0.06496	-3.78824	1-1	3.6405 eV
-0.06208	-3.78936	1-2	3.6445 eV

$(000\bar{1})$

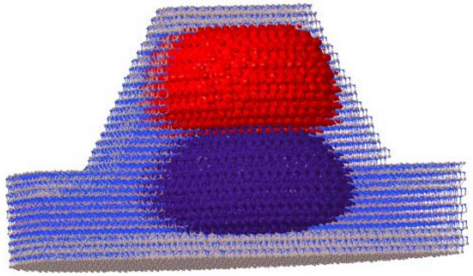




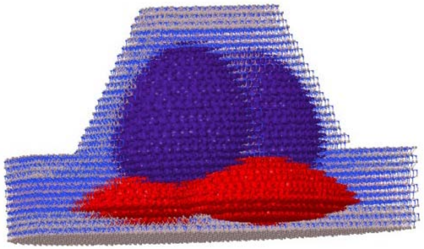
ETB Calculation



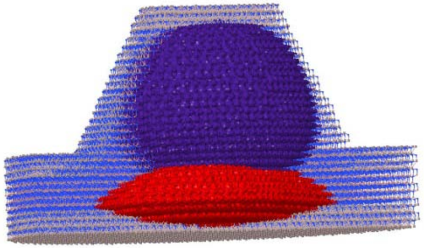
ETB ground states at equilibrium (no potentials and strain projection)



ETB (000-1) ground states



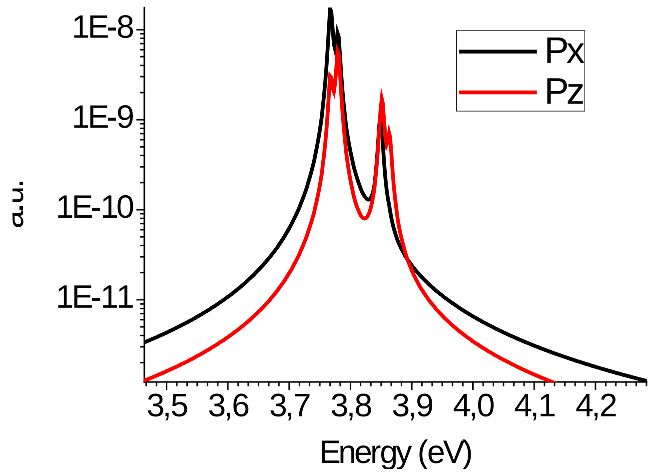
ETB (0001) 2nd states



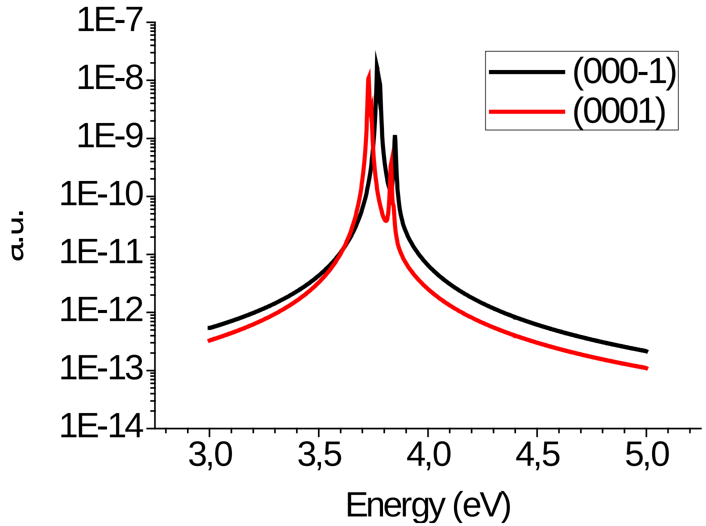
ETB (0001) ground states

- No more exact cylindrical simmetry slightly modify states
- States spatial distribution in z direction is in good agreement between TB and EFA

ETB spectra



Polarization in 000-1 direction



Emission spectra comparison

(0001)

Electron (eV)	Hole(eV)
0.060443	-3.6677
0.16262	-3.68028

$(000\overline{1})$

Electron (eV)	Hole(eV)
-0.07026	-3.83546
0.013448	-3.83795

Conclusions

- ❑ Proposed a novel simulation tool for mixed atomistic / FEM optoelectronic calculations.
- ❑ Application to a Qdot/nanocolumn based device.
- ❑ Large piezoelectric effects on both electrical and optical properties.
- ❑ EFA and TB are in good qualitative agreement, even though energy levels and simmetry are quite different.

Thank you for the attention