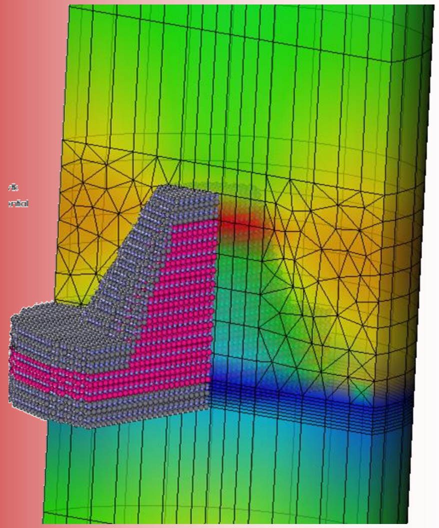
TiberCAD: a tool for multiscale simulation of nanostructured devices

Fabio Sacconi
Matthias Auf der Maur, Giuseppe Romano,
Gabriele Penazzi, Alessandro Pecchia, Aldo Di Carlo

Tiberlab Srl
www.tiberlab.com



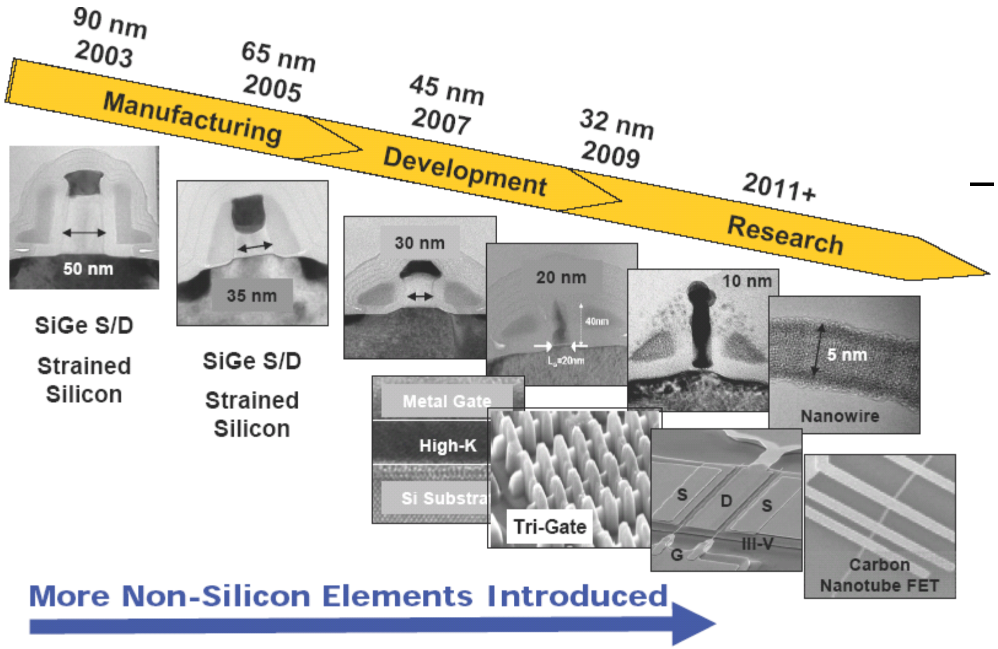
Origin: Spin-off of University of Rome Tor Vergata

Mission: To develop up-to-date innovative software solutions to design and to simulate advanced electronic and optoelectronic devices, based on a ***multiscale*** approach.

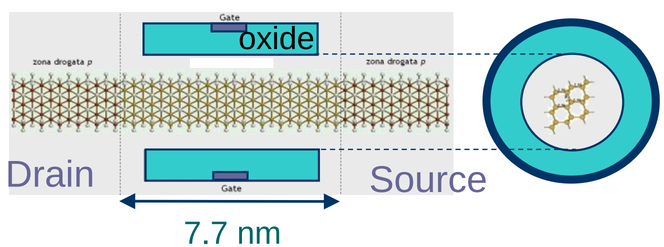
Applications:

- Nanostructured devices and nanoelectronics: nanowire FETs, HEMT, sensors
- Solid State lighting: Qdot and Qwell-based LEDs
- Photovoltaic cells
  - Organic/hybrid PV technologies
  - Dye-sensitized solar cells (DSC) / Perowskite Solid state DSC

Miniaturization Trend



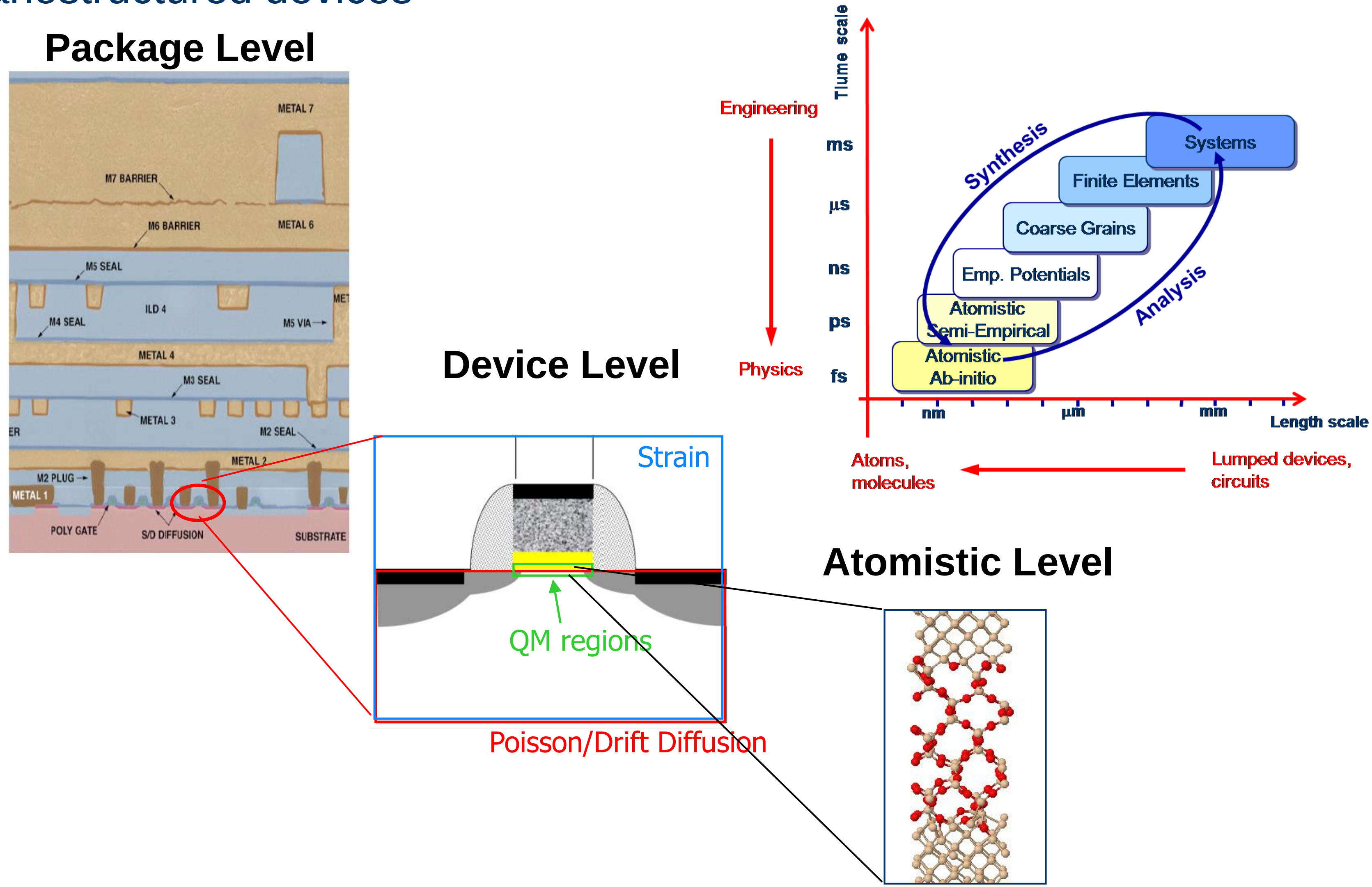
(Source: Intel)

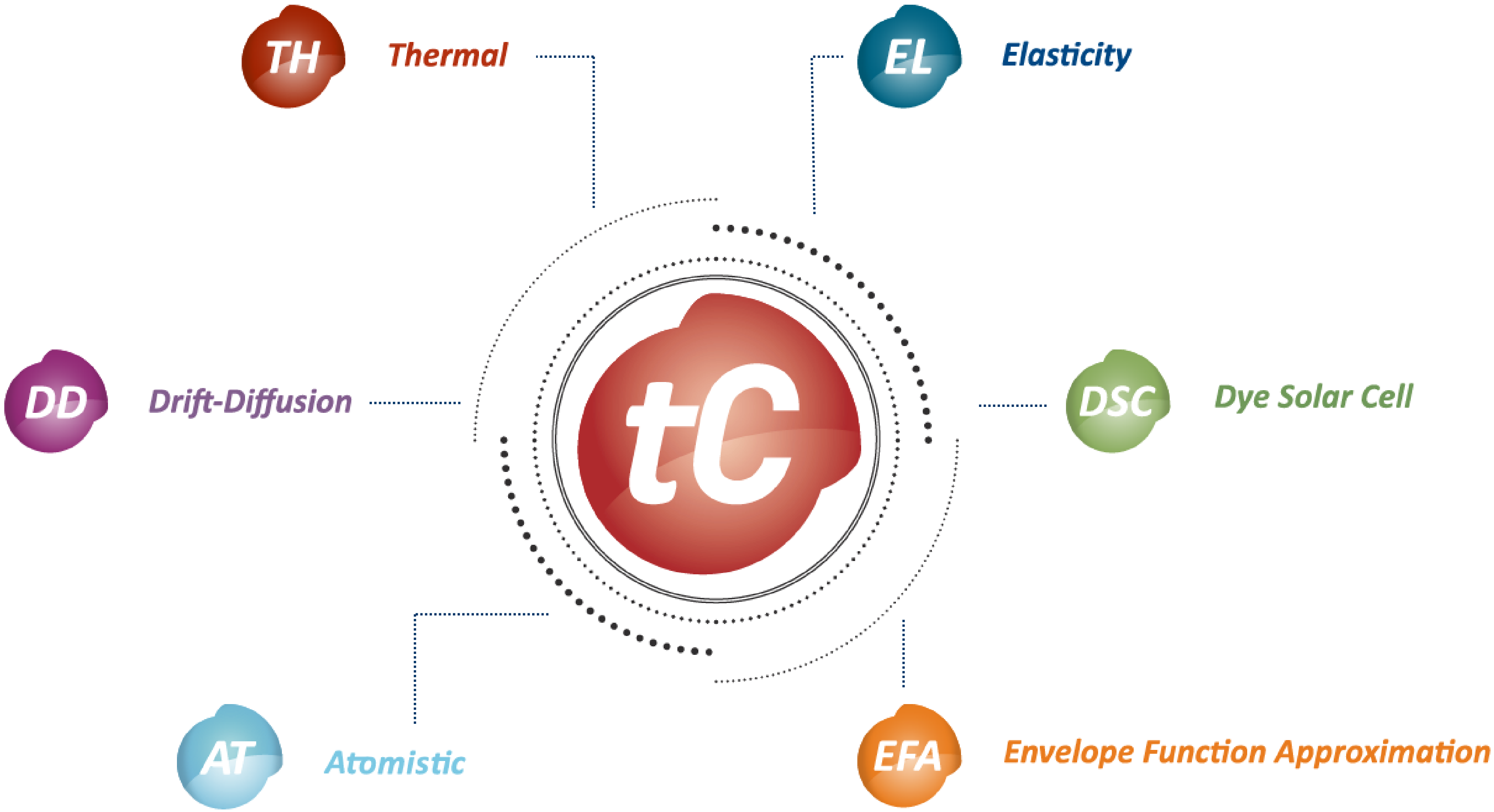


- Downscaling of conventional devices
  - Ballistic transport
  - Tunneling (gate, source/drain)
- New devices based on nanostructures (eg. wires, dots, CNTs)
  - New physics (QM)
  - Atomic details important (surface/interface)

Motivation: Multiscale/Multiphysics modeling

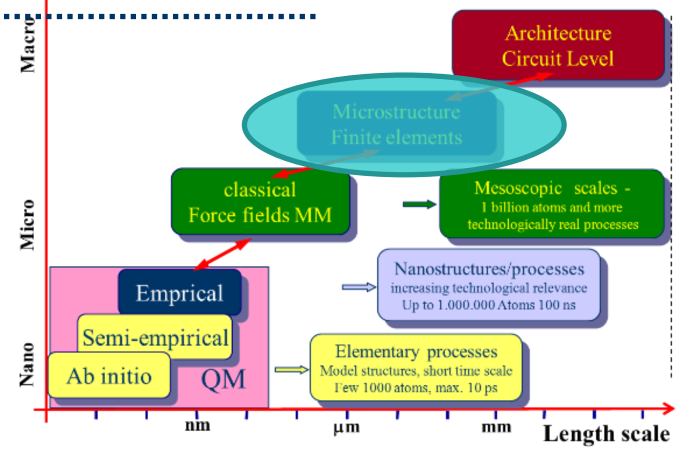
Different physical models on different scales are needed to describe nanostructured devices

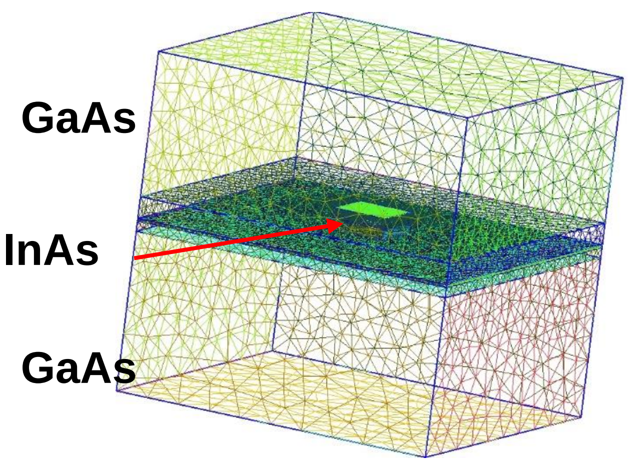




Product Suite

The multiscale approach

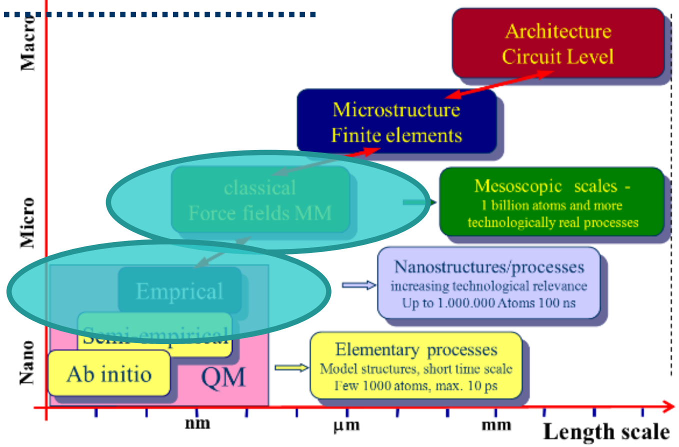




- **Drift-diffusion for transport**
- **Elasticity for heterostructure strain and polarizations**
- **EFA k·p for quantum properties**

Models: PDE solved on FEM grid

The multiscale approach

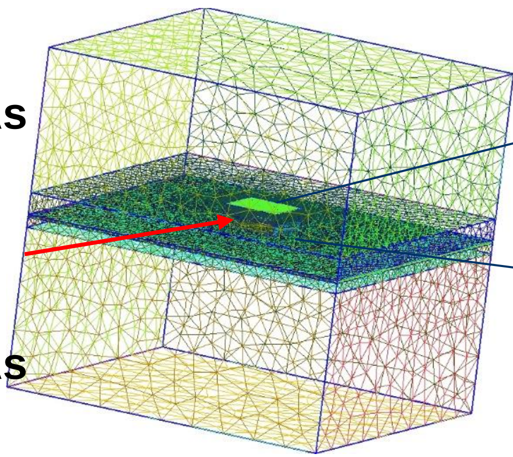


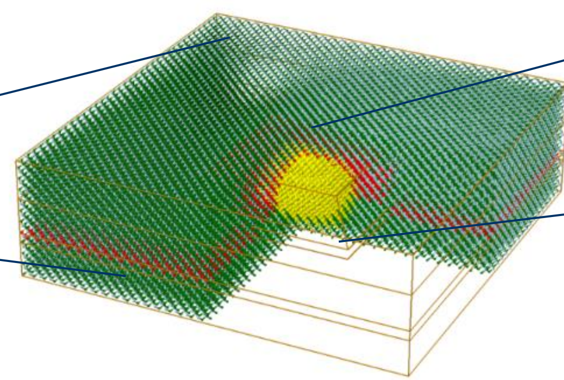
InAs
Quantum Dot

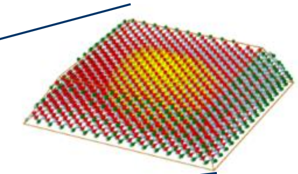
GaAs

InAs

GaAs





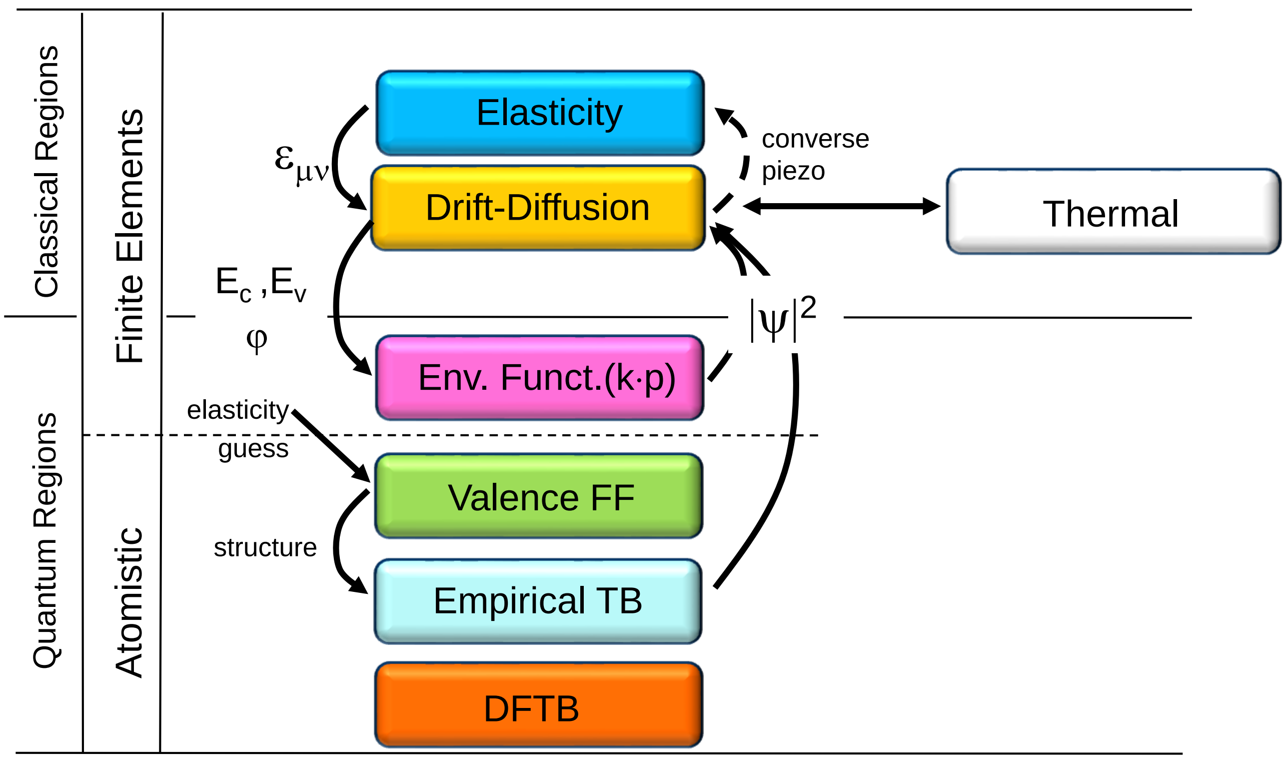


ETB: 140000 atoms

Force Field (VFF)

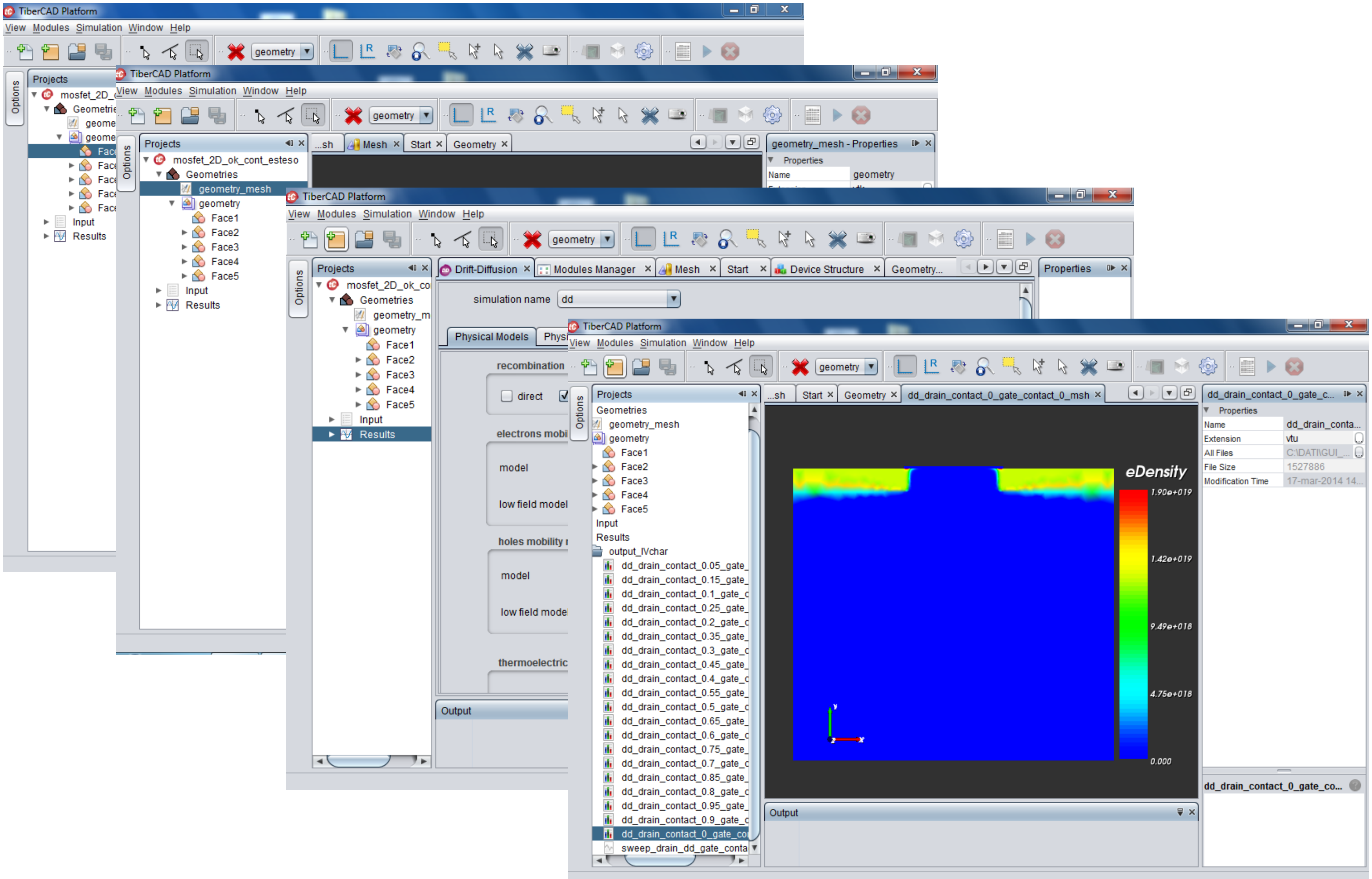
Models: Atomistic solvers

Physical models overview



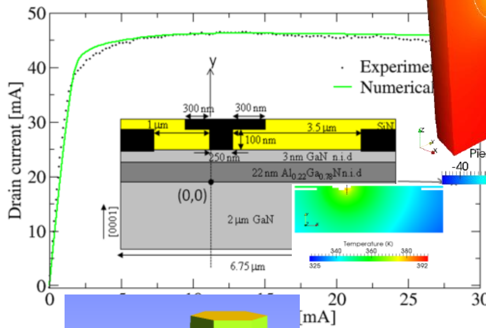
Physical models even from different scale can be **linked or self-consistently coupled** for a correct description of nanostructured electronic devices

Graphical User Interface

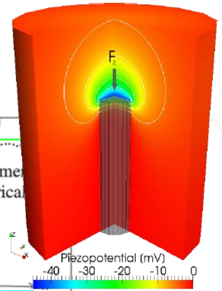


Applications

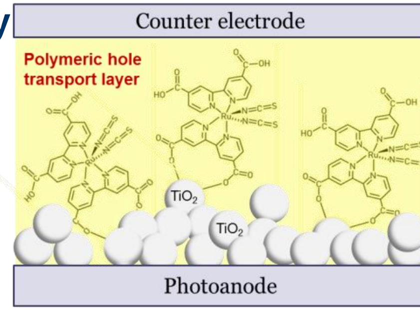
Heat dissipation



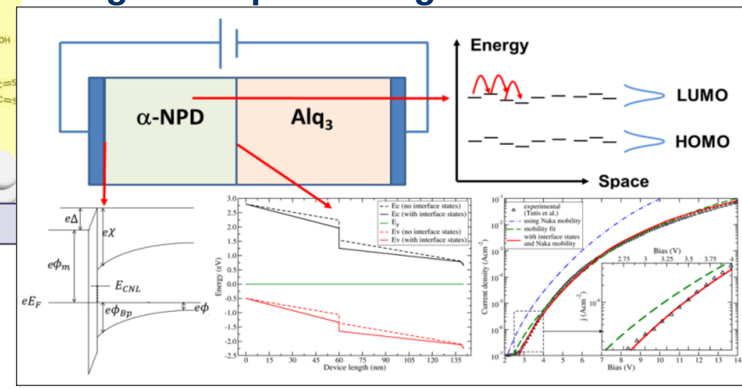
Piezoelectricity

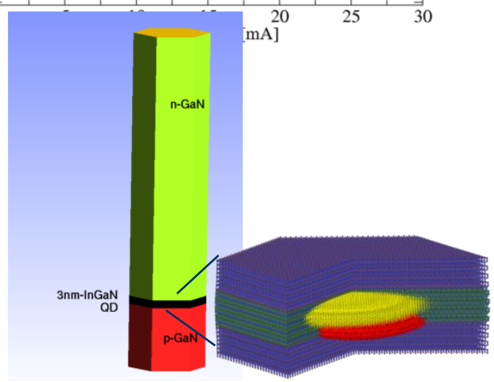


DSSC/OPV module

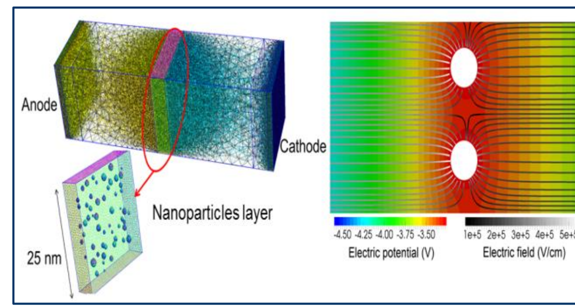


Charge transport in organic semiconductors

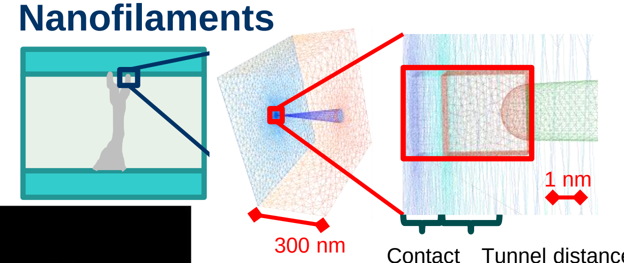




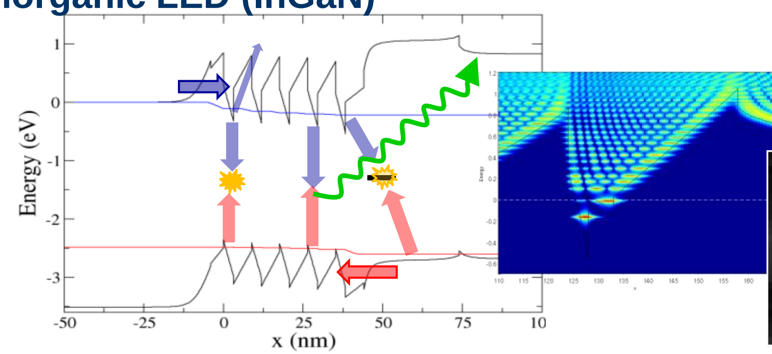
Memristors



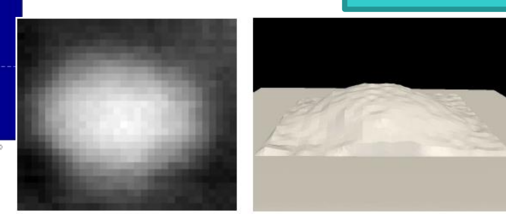
Nanofilaments



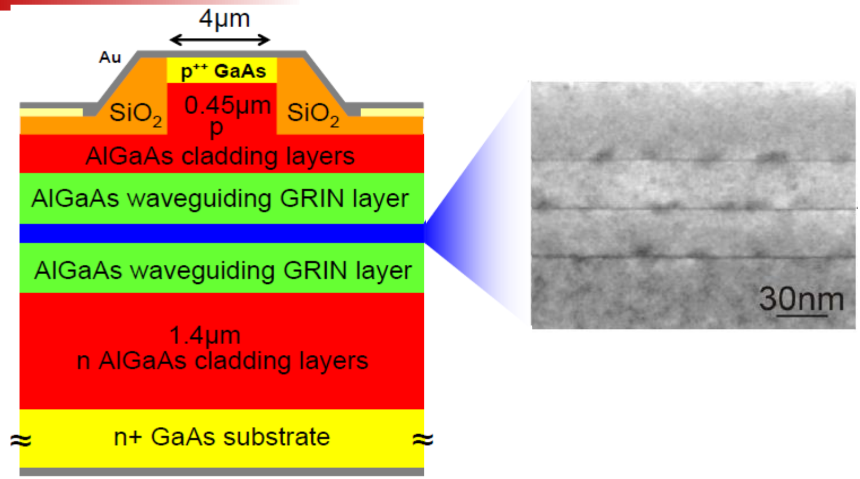
Inorganic LED (InGaN)



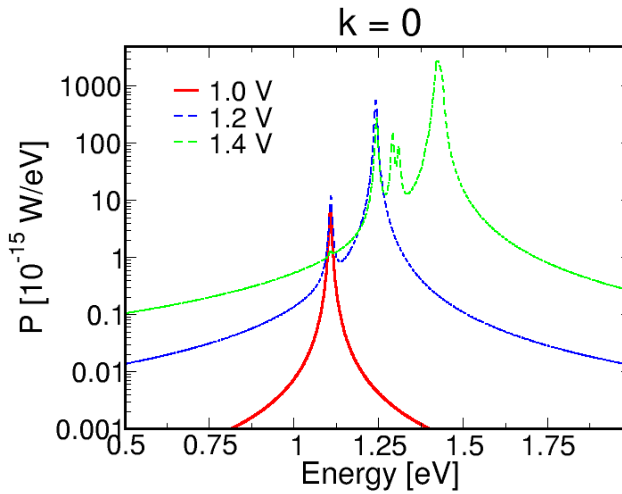
Quantum DOTs

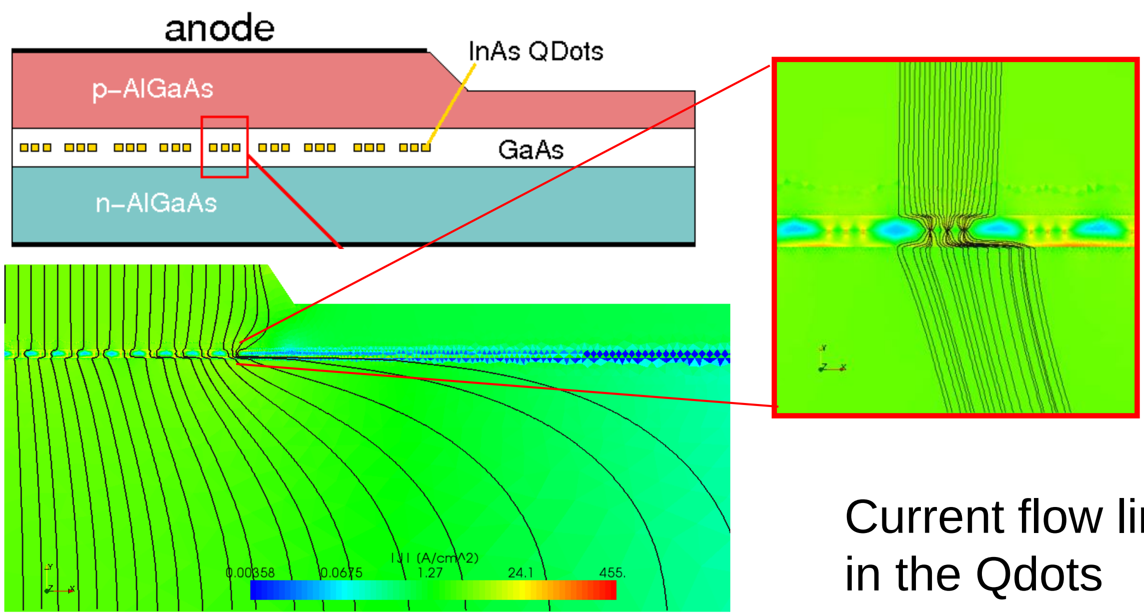


InAs Qdots LEDs



M. Buda et. al., IEEE Journal of Quantum Electronics, 2003





LED Optical spectra

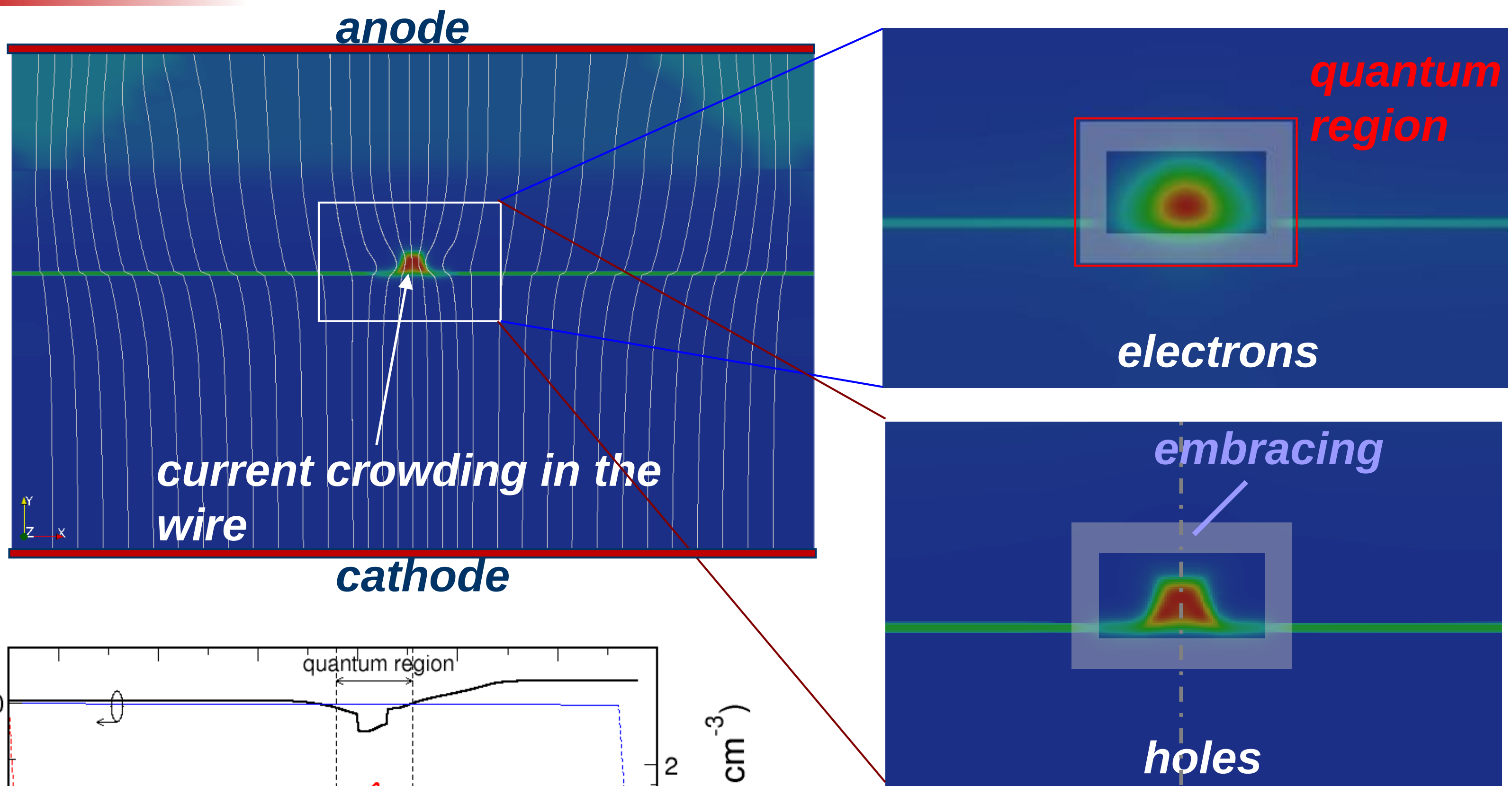
Strain: ***Elasticity***

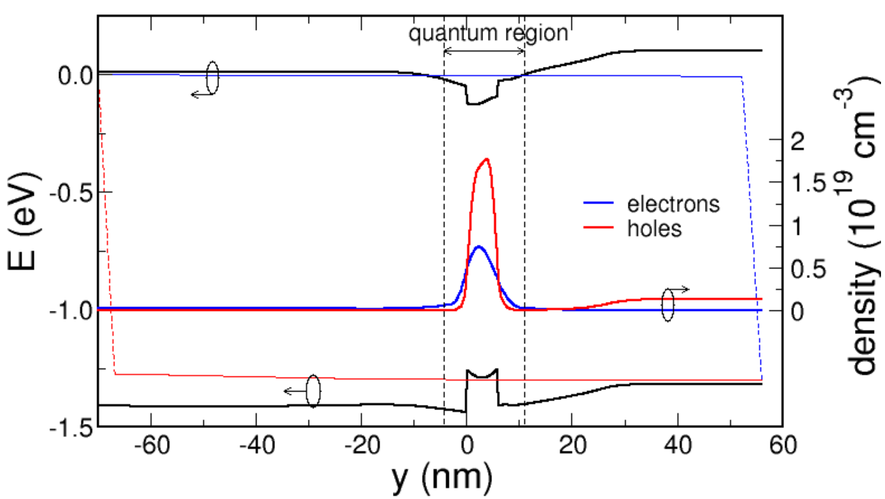
Transport: ***Drift-diffusion***

Quantum: ***k·p***

Current flow lines in the Qdots

InGaAs Quantum wire





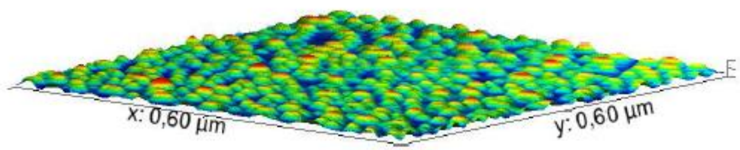
Self-consistent

k·p quantum model/ **Drift-diffusion**

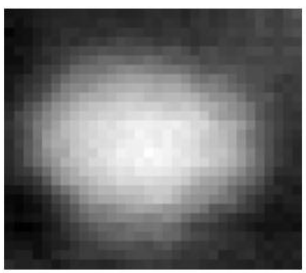
Particle densities and band profiles

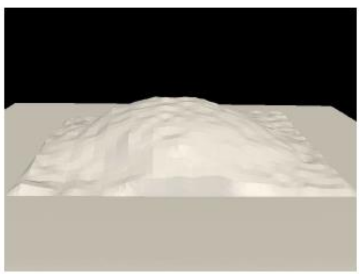
From exp. to simulation model: InP surface Qdots

AFM image:

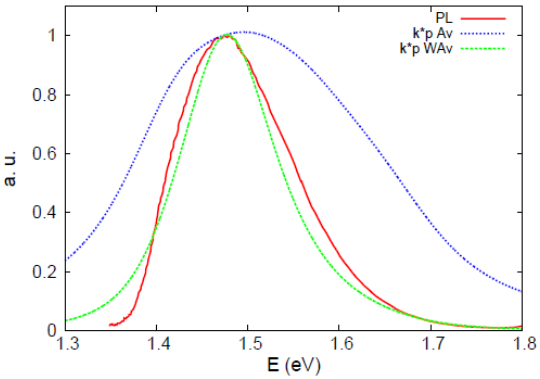


Exp. sample



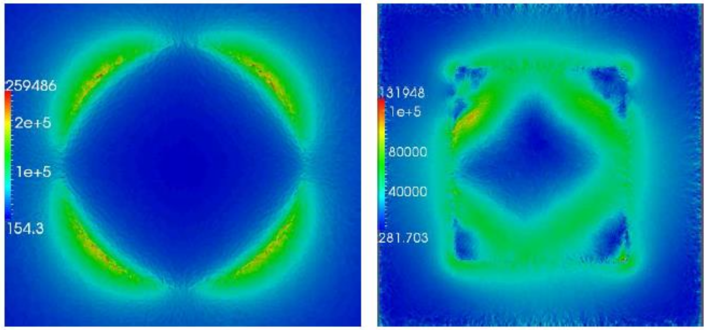


2D AFM micrography
-> Extrapolated 3D QD structure

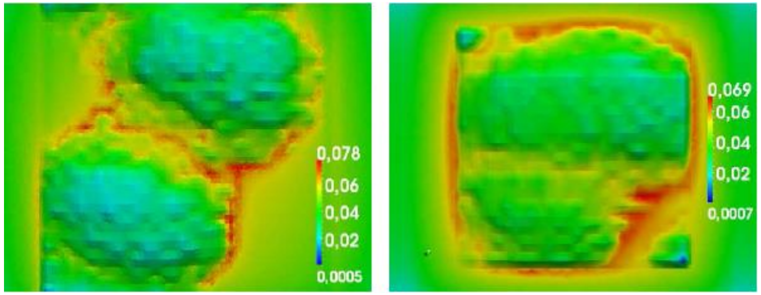


Idealized dot

Realistic dot



Strain field maps



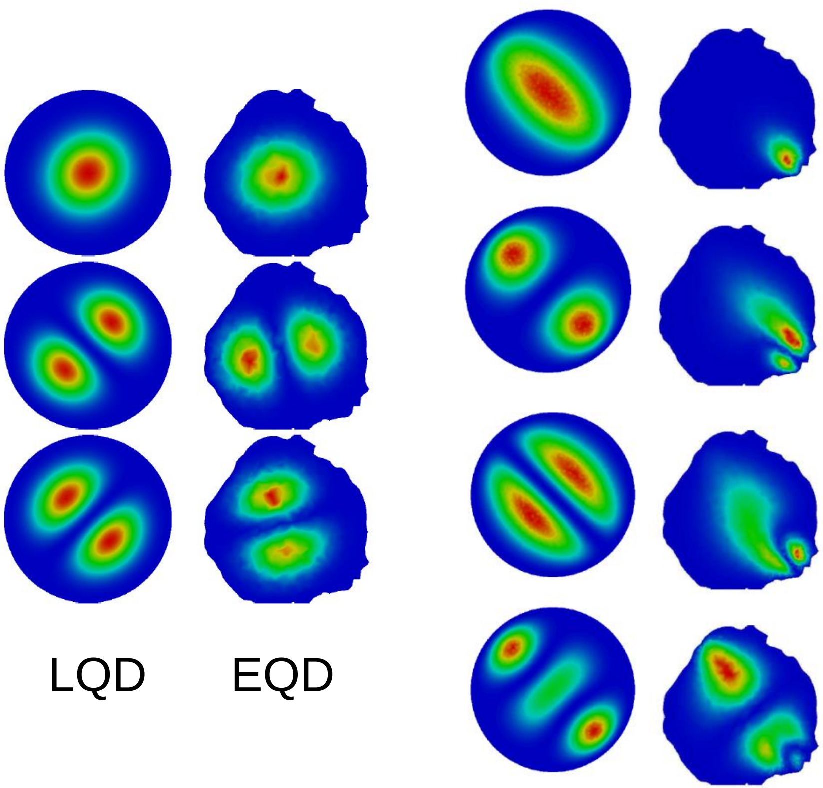
Closely coupled dots

D. Barettin et al. Nanotechnology, 25, 195201, (2014)

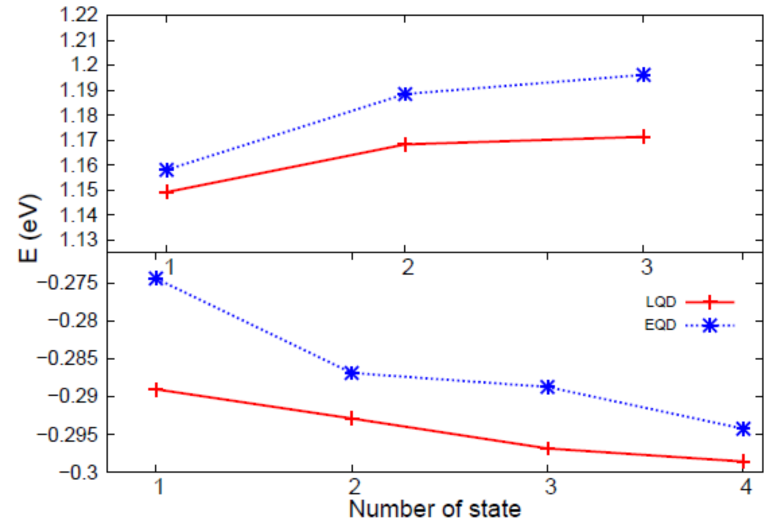
D. Barettin et al. J. Appl Phys. 117, 094306, (2015)

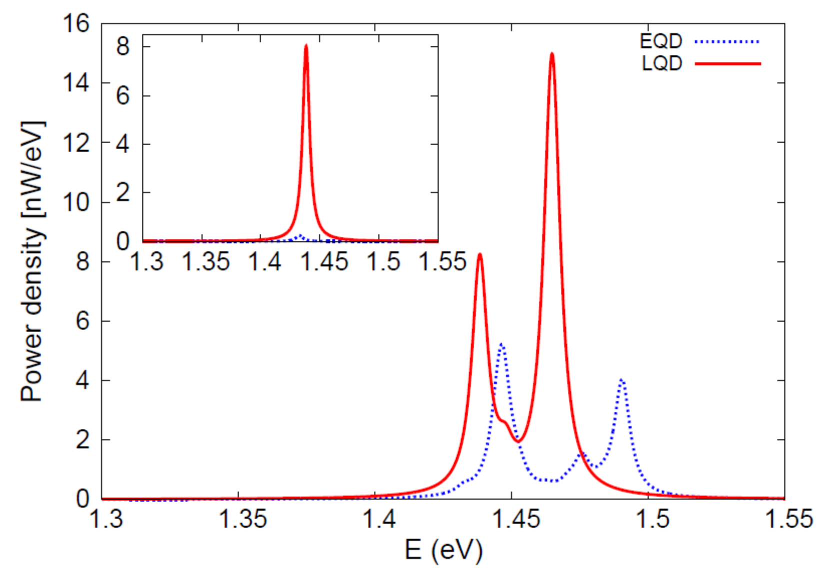
InP surface Qdots: Electronic properties

Electron states Hole states



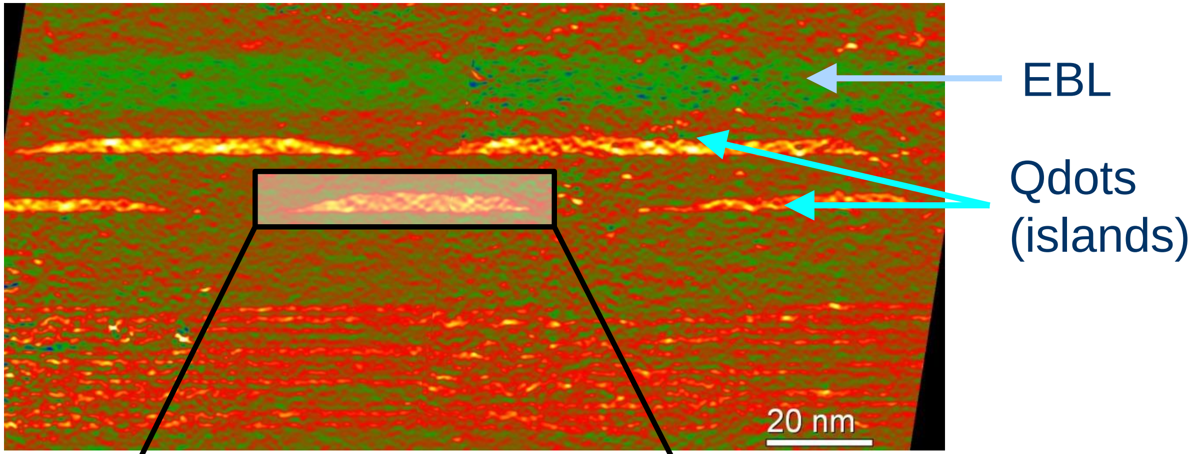
LQD EQD

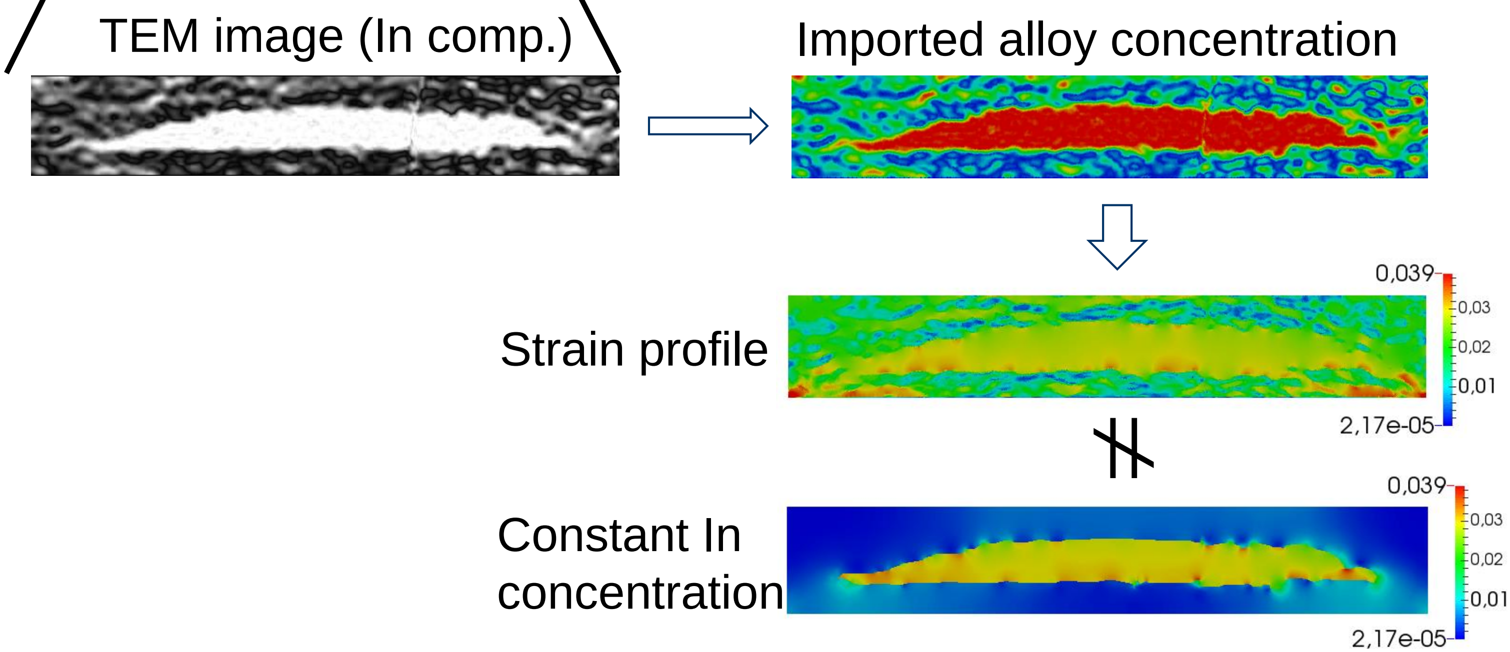




Quantum states, optical spectra for extrapolated (EQD) and idealized (LQD) Qdots

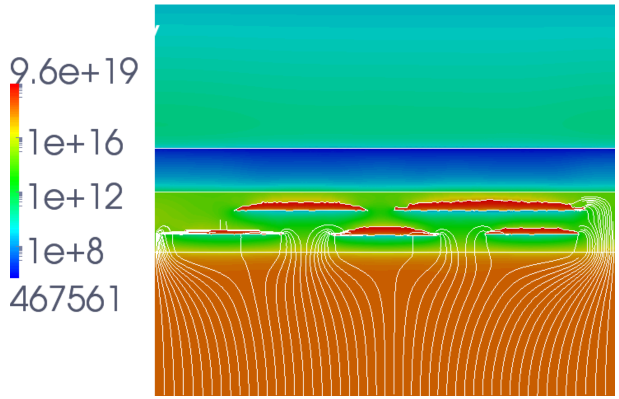
From exp. to simulation model : Shape and alloy effects in Qdot system



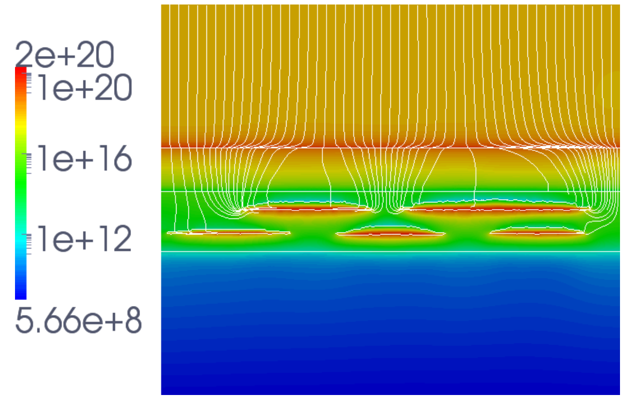


Shape and alloy effects in Qdot system: Current densities

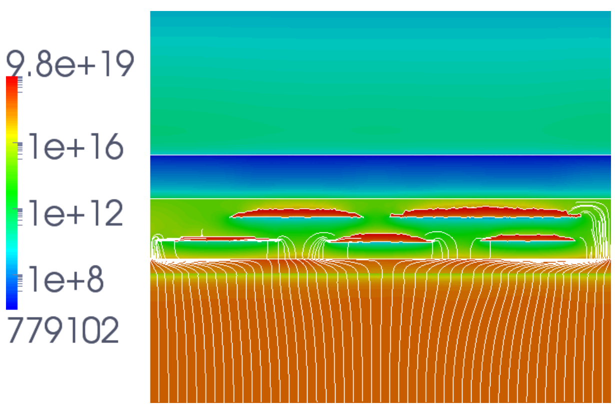
electron current density

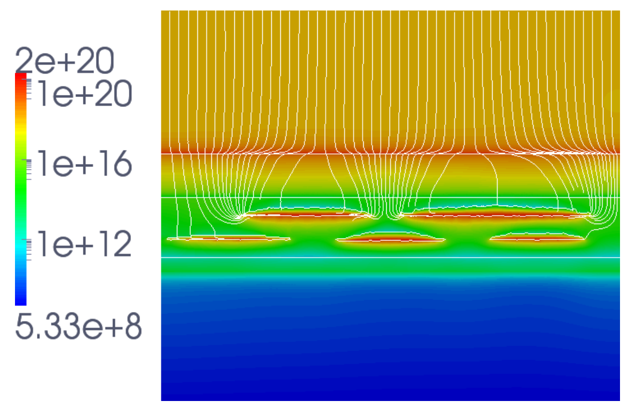


Hole current density

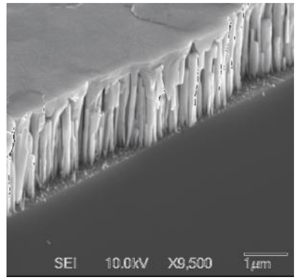


Increasing electron current density with electron-rich layer

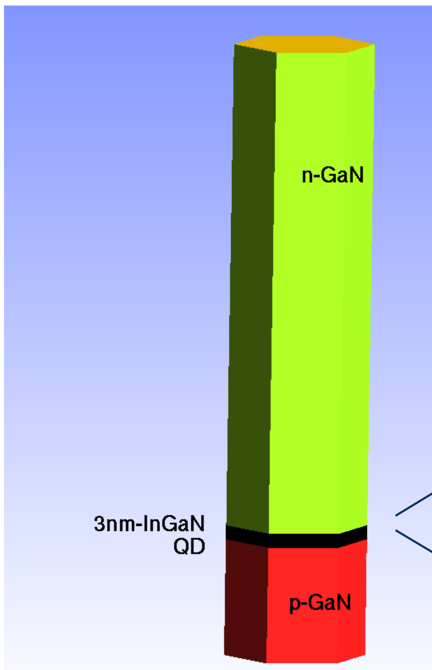




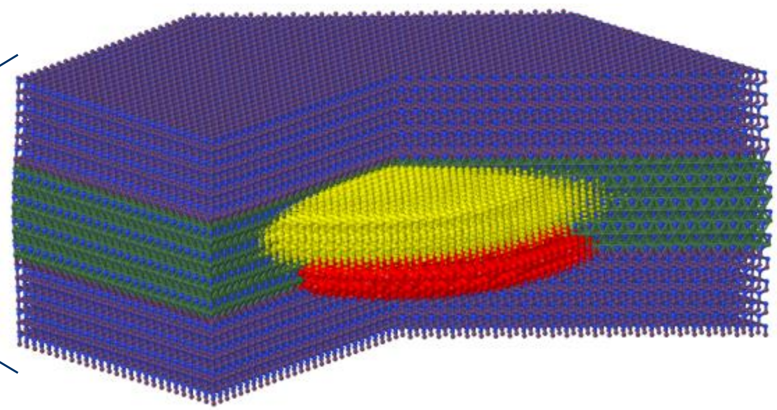
Modelling nanopillars InGaN/GaN LEDs



- small footprint on the substrate, allows:
- **defect-free** material
- growth on various substrates (Silicon)
- growth on large area substrates without lattice strain



Empirical Tight Binding model $sp^3d^5s^*$+SO applied to InGaN active region

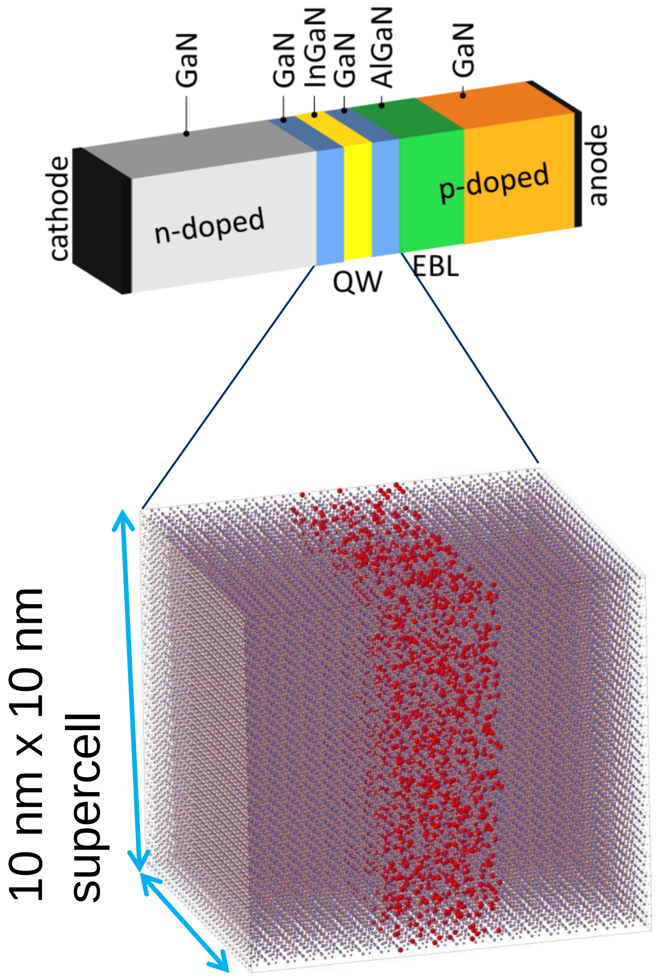


-> GS electron and hole states wawefunctions

F. Sacconi et al., IEEE Trans. Electr. Dev. (2012)

InGaN/GaN QW LED Simulation: 1D + atomistic

Model system: 3 nm single quantum well, 15/20/25/30/35% In, p-i-n structure:

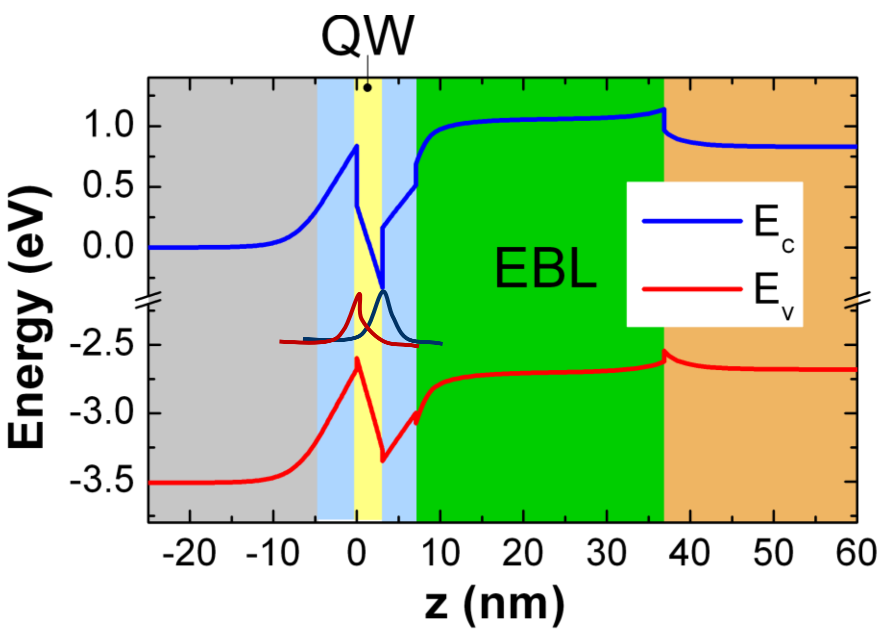


Atomistic models: VFF, ETB

Continuous models are solved in 1D

⇒ No in-plane potential fluctuations

Typical band profile near maximum efficiency:

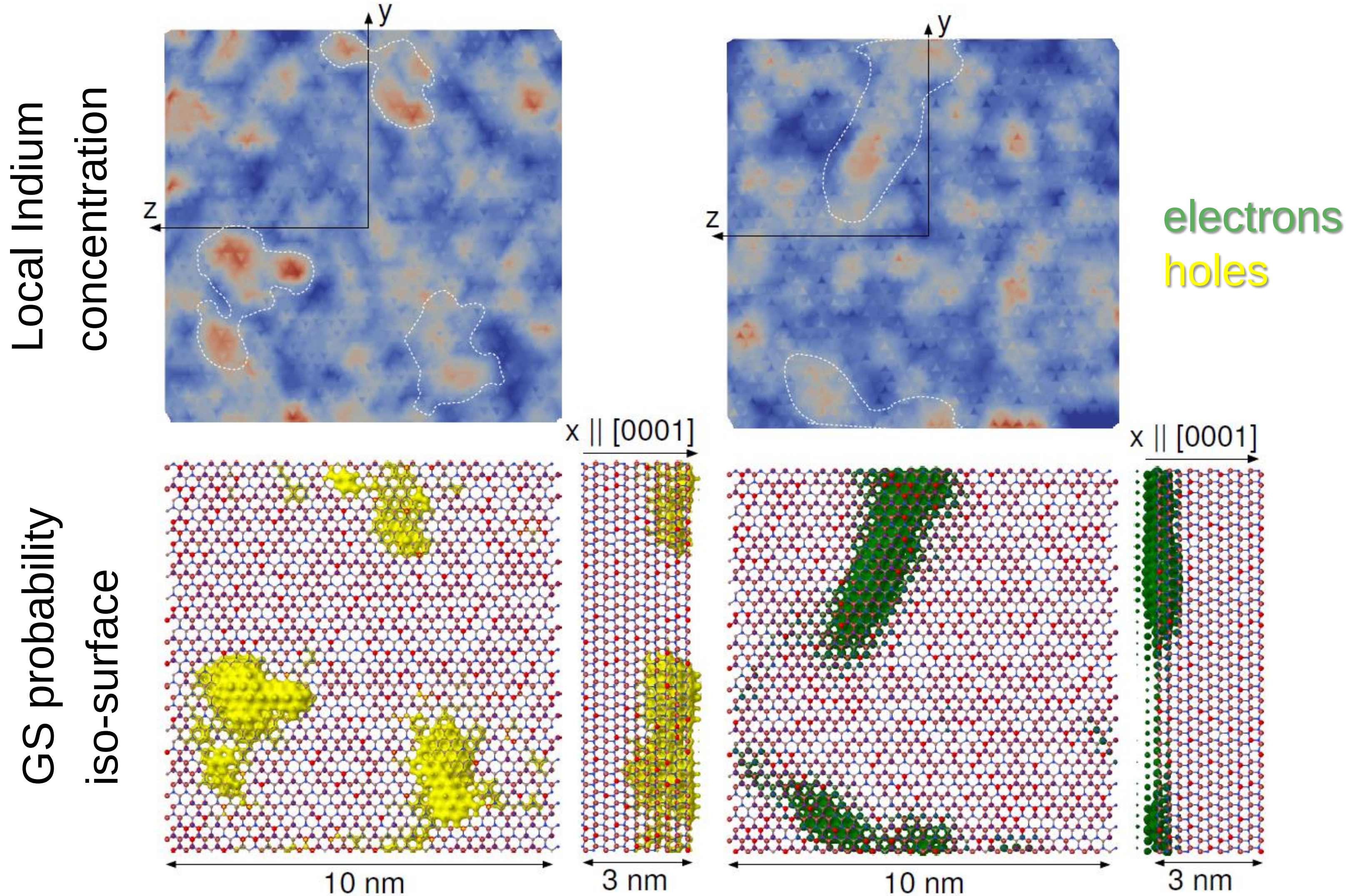


el-hl overlap is reduced due to QCSE

M. Auf der Maur et al. PRL 116, 027401 (2016)

InGaN/GaN QW LED: Localization behavior

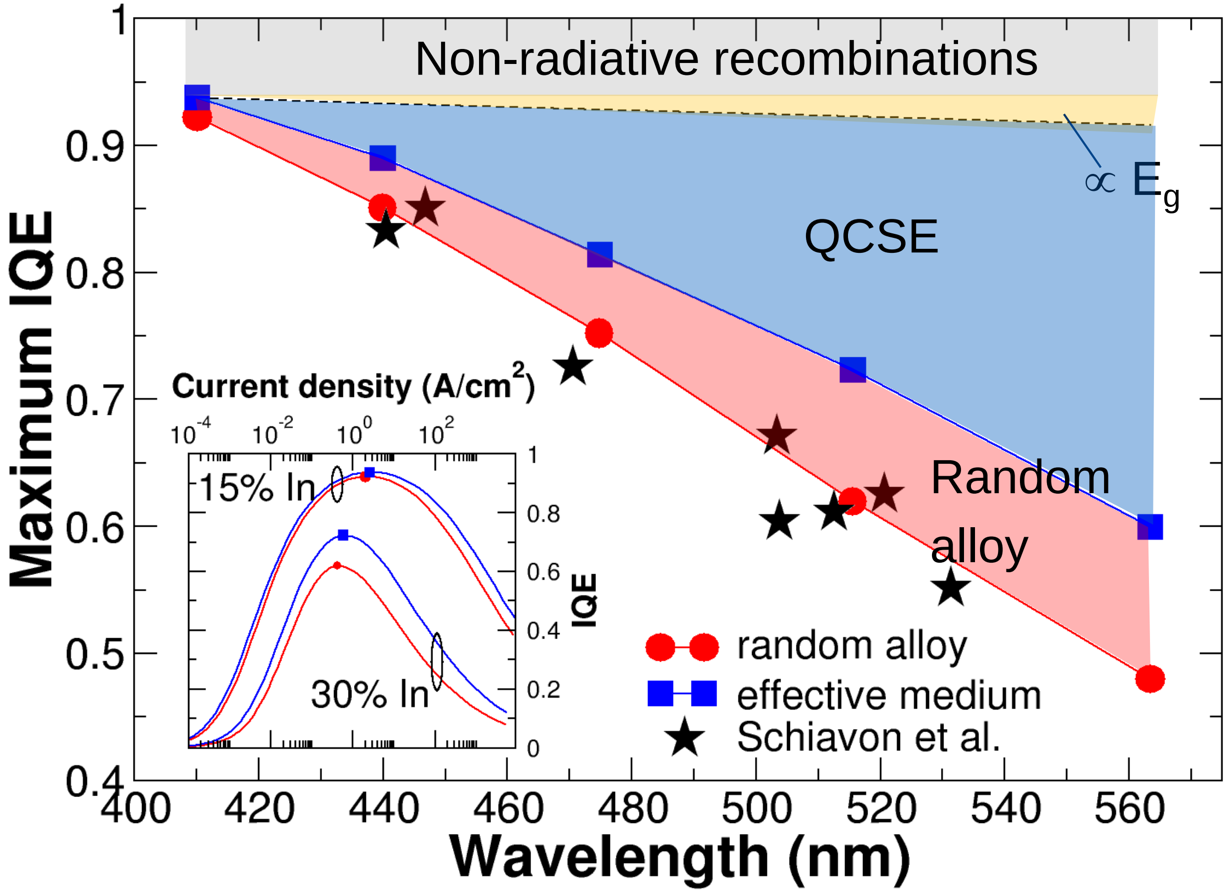
Correlation of local In concentration with wave function localization



M. Auf der Maur et al. PRL 116, 027401 (2016)

InGaN/GaN QW LED: Simulation vs. experiment

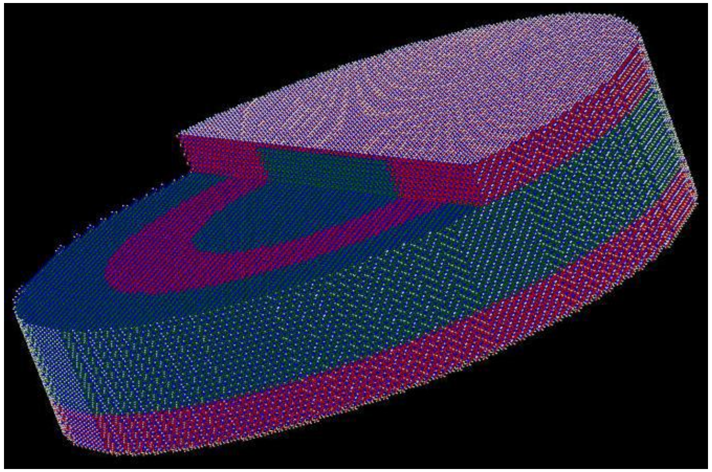
Assume optimistic case: constant *A* and *C* (measured values) ⇨ how does the peak IQE vary with wavelength?



⇒ Random alloy fluctuations explain the missing contribution to the green gap

M. Auf der Maur et al. PRL 116, 027401 (2016)

GPU/CUDA developments



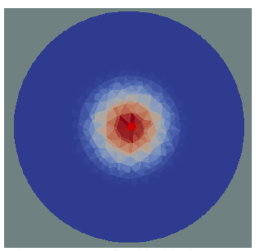


Fig 3:State 1 confined inside the Dot

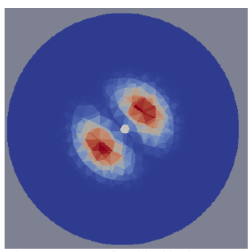


Fig 4:State 3 confined inside the Dot

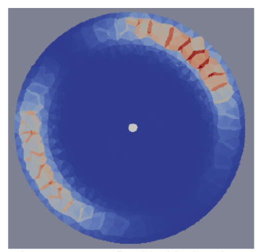
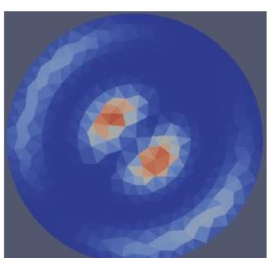
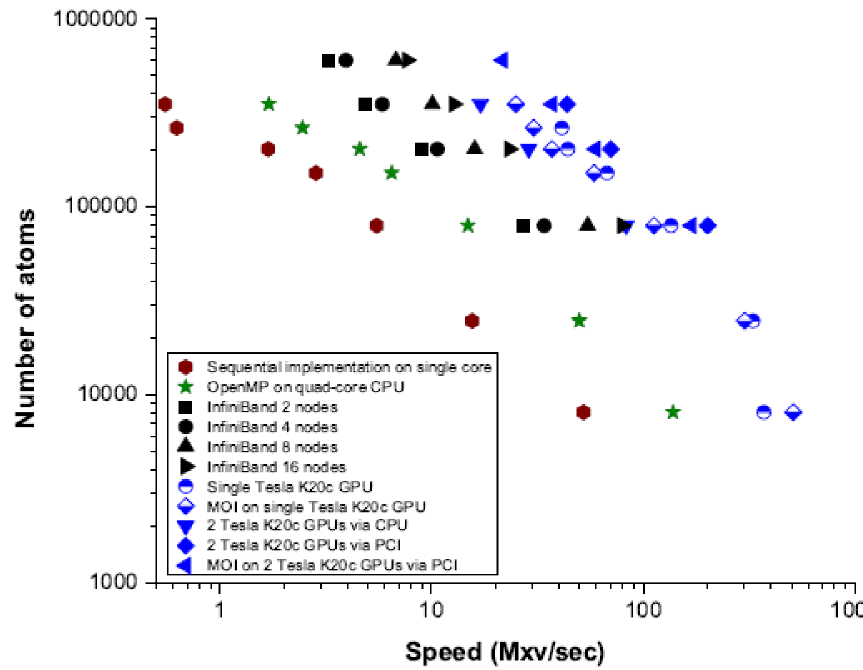


Fig 5:State 8 confined inside the Ring



1,000,000 atoms on a WS!



W. Rodrigues, A. Pecchia, A Di Carlo, Comp. Phys. Comm. (2014)

Selected publications

- **Efficiency Drop in Green InGaN/GaN Light Emitting Diodes: The Role of Random Alloy Fluctuations**
  Matthias Auf der Maur, Alessandro Pecchia, Gabriele Penazzi, Walter Rodrigues, and Aldo Di Carlo
  Phys. Rev. Lett. 116, 027401 (2016)

- **Broadband light sources based on InAs/InGaAs metamorphic quantum dots**
  L. Seravalli, M. Gioannini, F. Cappelluti, F. Sacconi, G. Trevisi, and P. Frigeri
  Journal of Applied Physics 119, 143102 (2016)

- **Inter-dot strain field effect on the optoelectronic properties of realistic InP lateral quantum-dot molecules**
  Daniele Barettin, Matthias Auf der Maur, Roberta De Angelis, Paolo Prosposito, Mauro Casalboni, and Alessandro Pecchia
  Journal of Applied Physics 117, 094306 (2015)

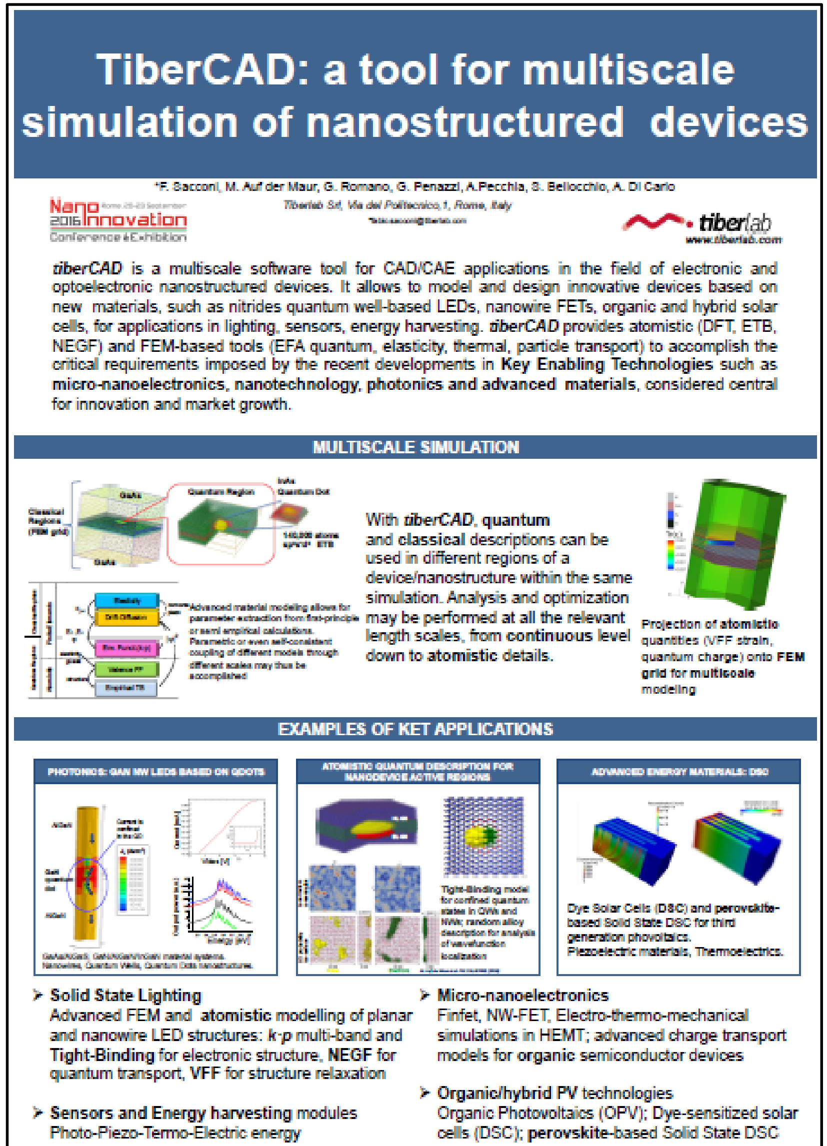
- **Multiscale approaches for the simulation of InGaN/GaN LEDs**
  Matthias Auf der Maur
  Journal of Computational Electronics, Volume 14, Issue 2, pp 398-408 (June 2015)

- **Model of a realistic InP surface quantum dot extrapolated from atomic force microscopy results**
  Daniele Barettin, Roberta De Angelis, Paolo Prosposito, Matthias Auf der Maur, Mauro Casalboni and Alessandro Pecchia
  Nanotechnology 25 (2014) 195201 (9pp)

- **AlGaN/GaN HEMT degradation: An Electro-Thermo-Mechanical Simulation**
  M. Auf der Maur, A. Di Carlo
  IEEE Transactions on Electron Devices, Vol. 60, Issue 10 (2013), pages 3142-3148

- **Optoelectronic Properties of Nanocolumn InGaN/GaN LEDs**
  Fabio Sacconi, Matthias Auf der Maur, Aldo Di Carlo
  IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 59, NO. 11, NOVEMBER 2012

- **The Multiscale Paradigm in Electronic Device Simulation**
  Matthias Auf der Maur, Gabriele Penazzi, Giuseppe Romano, Fabio Sacconi, Alessandro Pecchia, and Aldo Di Carlo
  IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 58, NO. 5, MAY 2011


TiberCAD: a tool for multiscale simulation of nanostructured devices

*F. Sacconi, M. Auf der Maur, G. Romano, G. Penazzi, A.Pecchia, S. Bellocchio, A. Di Carlo
Tiberlab Srl, Via del Politecnico,1, Rome, Italy

tiberCAD is a multiscale software tool for CAD/CAE applications in the field of electronic and optoelectronic nanostructured devices. It allows to model and design innovative devices based on new materials, such as nitrides quantum well-based LEDs, nanowire FETs, organic and hybrid solar cells, for applications in lighting, sensors, energy harvesting. *tiberCAD* provides atomistic (DFT, ETB, NEGF) and FEM-based tools (EFA quantum, elasticity, thermal, particle transport) to accomplish the critical requirements imposed by the recent developments in **Key Enabling Technologies** such as **micro-nanoelectronics, nanotechnology, photonics and advanced materials**, considered central for innovation and market growth.

MULTISCALE SIMULATION

With *tiberCAD*, **quantum** and **classical** descriptions can be used in different regions of a device/nanostructure within the same simulation. Analysis and optimization may be performed at all the relevant length scales, from **continuous** level down to **atomistic** details.

Advanced material modeling allows for parameter extraction from first-principle or semi empirical calculations. Parametric or even self-consistent coupling of different models through different scales may thus be accomplished

Projection of **atomistic** quantities (VFF strain, quantum charge) onto **FEM grid** for **multiscale** modeling

EXAMPLES OF KET APPLICATIONS

PHOTONICS: GAN NW LEDS BASED ON QDOTS

ATOMISTIC QUANTUM DESCRIPTION FOR NANODEVICE ACTIVE REGIONS

ADVANCED ENERGY MATERIALS: DSC

Dye Solar Cells (DSC) and perovskite-based Solid State DSC for third generation phovoltaics. Piezoelectric materials, Thermoelectrics.

- **Solid State Lighting**
  Advanced FEM and **atomistic** modelling of planar and nanowire LED structures: *k·p* multi-band and **Tight-Binding** for electronic structure, **NEGF** for quantum transport, **VFF** for structure relaxation
- **Sensors and Energy harvesting** modules
  Photo-Piezo-Termo-Electric energy
- **Micro-nanoelectronics**
  Finfet, NW-FET, Electro-thermo-mechanical simulations in HEMT; advanced charge transport models for **organic** semiconductor devices
- **Organic/hybrid PV** technologies
  Organic Photovoltaics (OPV); Dye-sensitized solar cells (DSC); **perovskite**-based Solid State DSC

Thank you

*Additional info about **TiberCAD**:*
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