Multiscale approaches for electronic device simulation

M. Auf der Maur[1], A. Pecchia[2],
G. Penazzi[3], A. Gagliardi[4], F. Santoni[1],
A. Di Carlo[1]

(1) University of Rome "Tor Vergata"
(2) CNR-ISMN, Italy
(3) BCCMS, University of Bremen
(4) TU Munich, Germany

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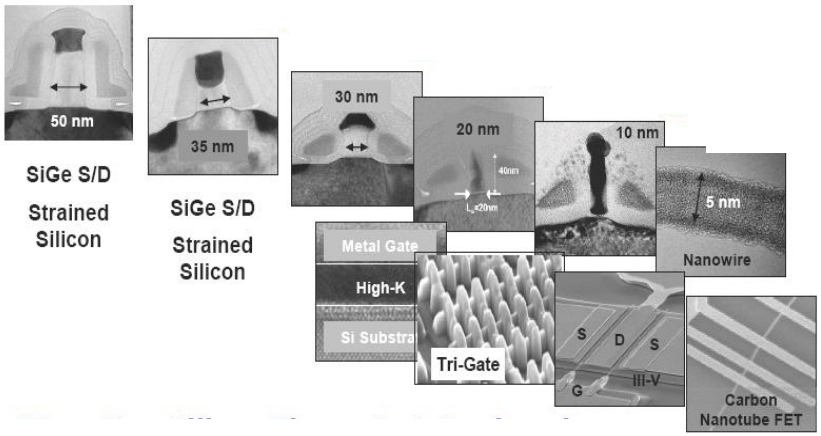
Outline

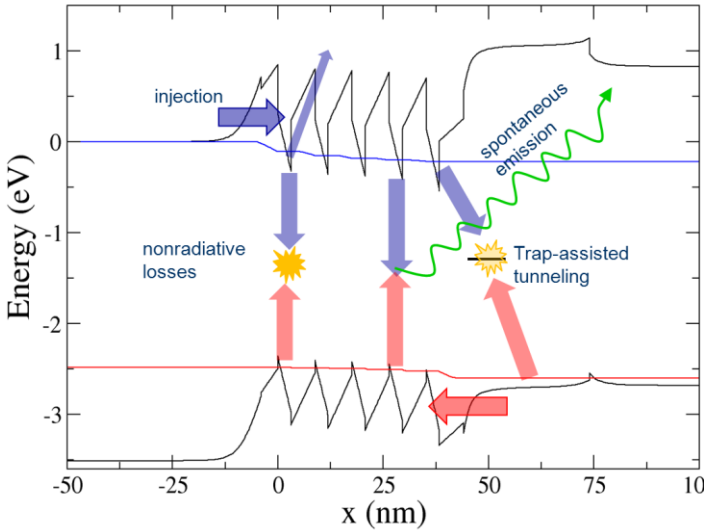
- Why multiscale simulations?
- Multiscale coupling schemes, implementation concepts
- Atomistic/continuous coupling
- Examples
- Outlook

Issues in modern devices

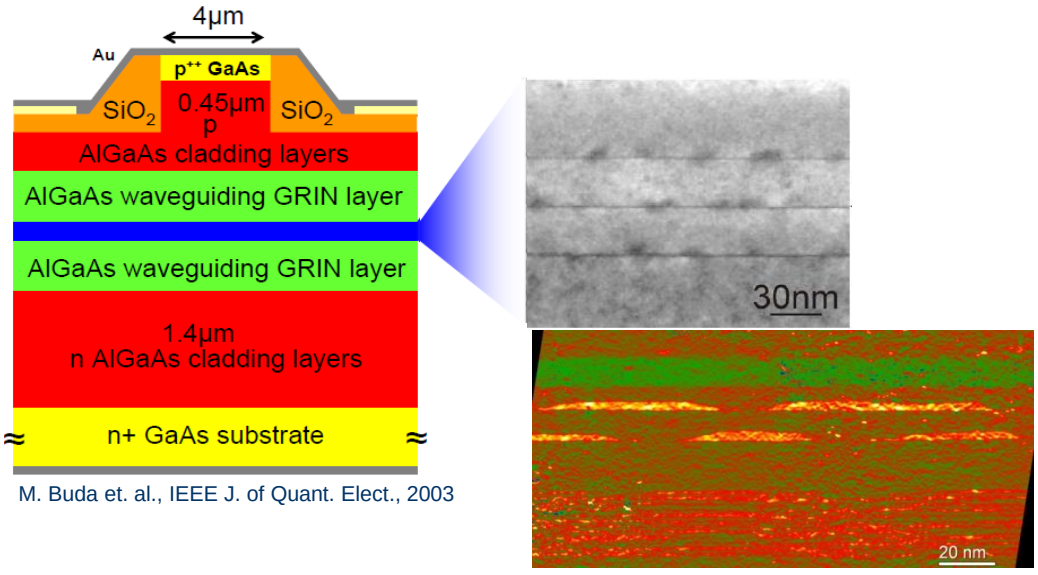
downscaling:



complex interplay of different effects:

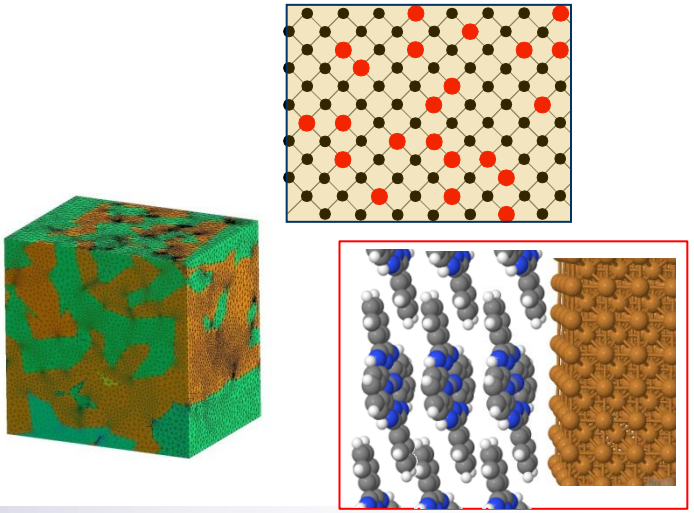


nm scale / low dimensional active regions :



M. Buda et. al., IEEE J. of Quant. Elect., 2003

disordered/complex materials:



Multiscale initiatives

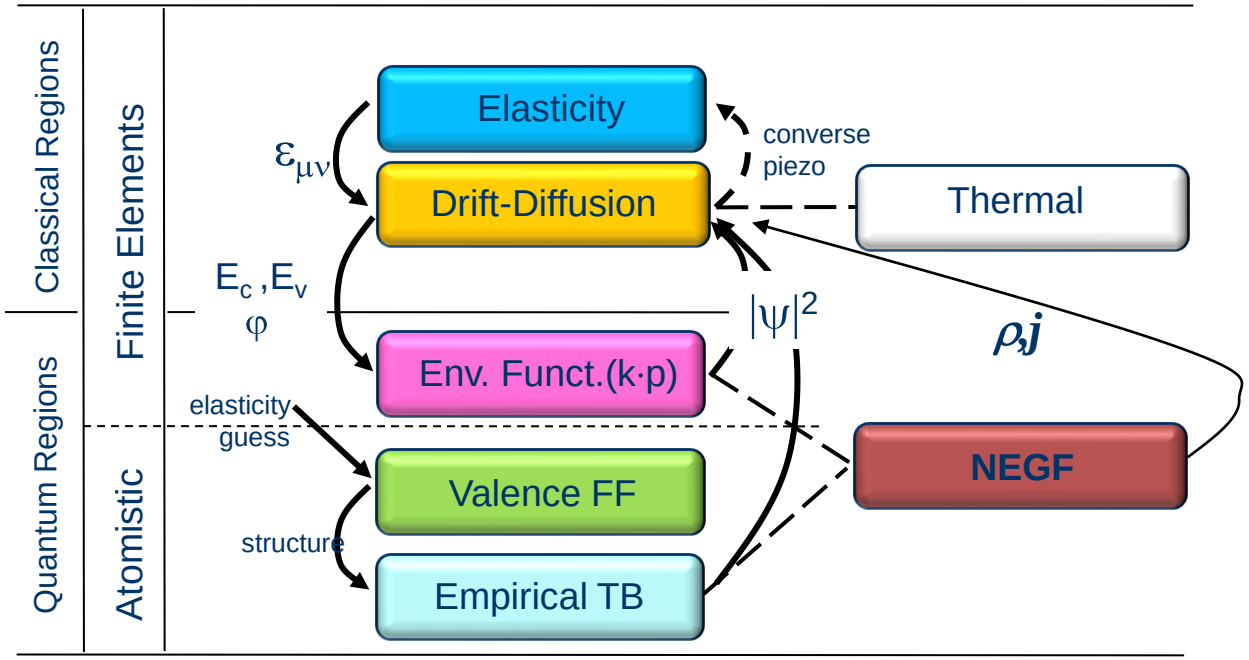
- Increasing number of publications on multiscale simulation of electronic devices

- Several international actions, in US and Europe:
  - Specific calls
  - Since 2012 a ERC bottom up counsil: EMMC
  - Multiscale materials modeling cluster gathering FP7/H2020 projects
  - COST action MultiscaleSolar

Atomistic/discrete + continuum

- Coupling atomistic or discrete models with continuum models is of special interest:
  - ultrascaled devices (few nm dimensions)
  - CNTs, graphene, 2D materials
  - alloy fluctuations (e.g. in InGaN, SiGe)
  - SL, thin layers with sub-ML thickness (e.g. in AlInGaP devices)

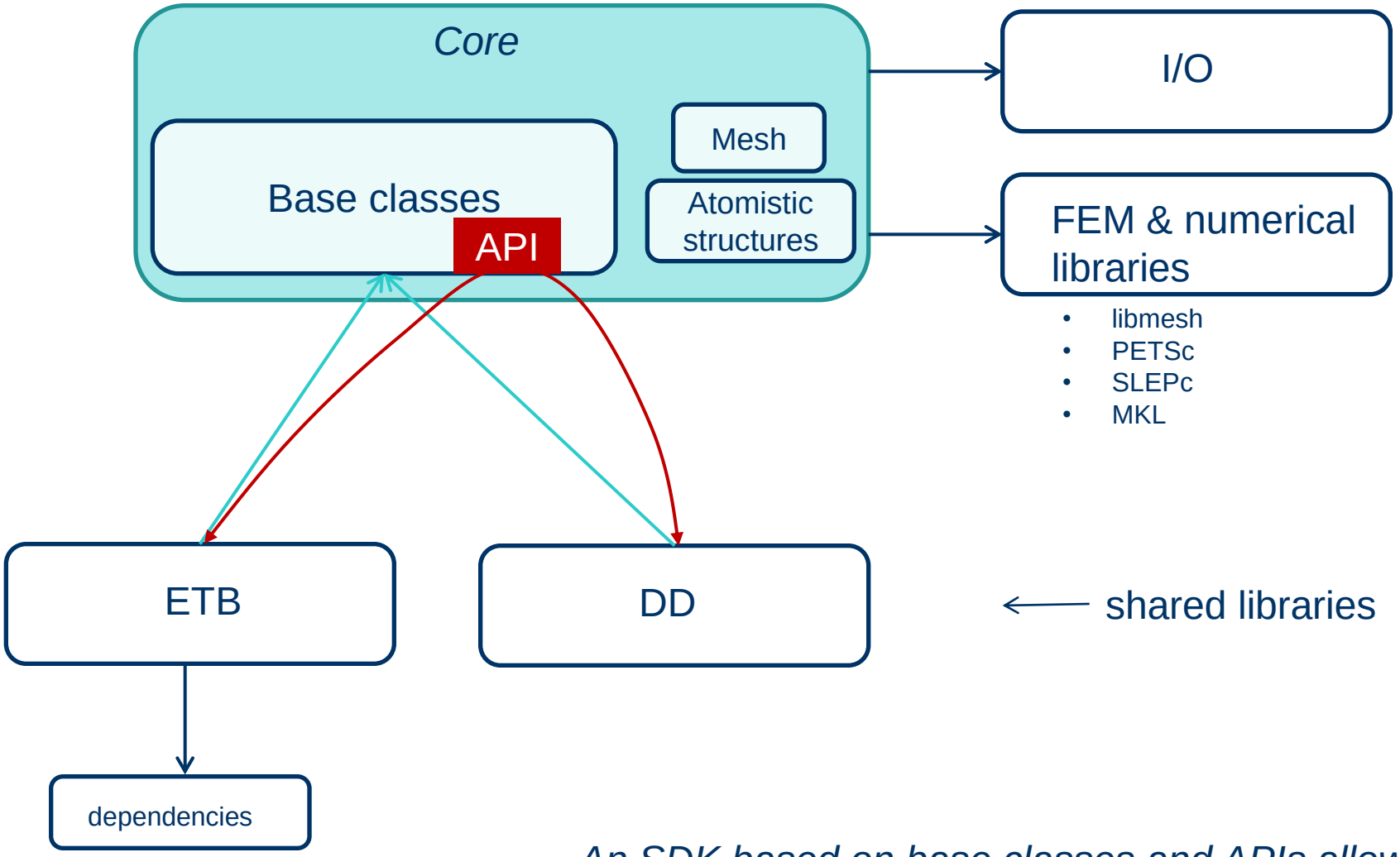
Multiscale/multiphysics components



Implementation: TiberCAD

- Object oriented design
- Implementation is done in modular way, making use of hierarchies of classes
- An API in the base classes provides functionality for interchange of data between modules
- Continuous models are implemented using FEM
- Electronic transport: drift-diffusion, using electrochemical potentials as variables

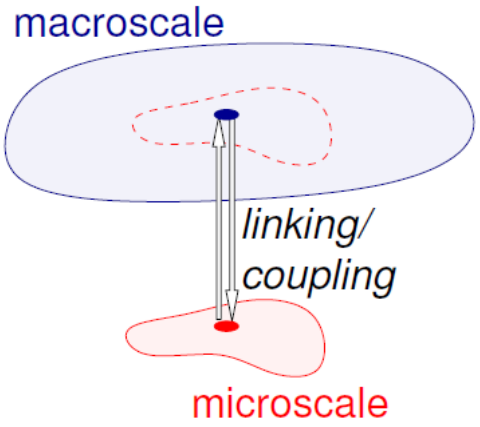
Implementation



An SDK based on base classes and APIs allow to add new modules

Multiscale/multiphysics schemes

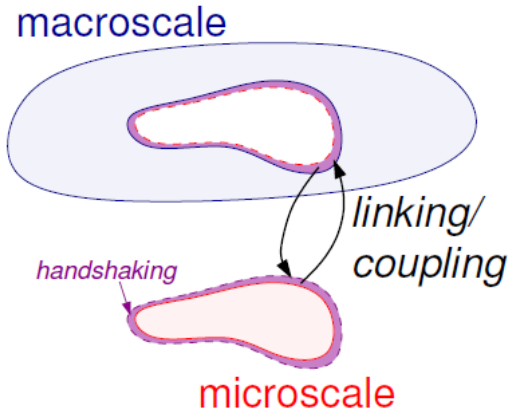
OVERLAP METHOD



- the domains are overlapping
- each model computes physical quantities that act as parameters to the other models.

Schrödinger/Poisson
Material parameters from DFT

BRIDGE METHOD

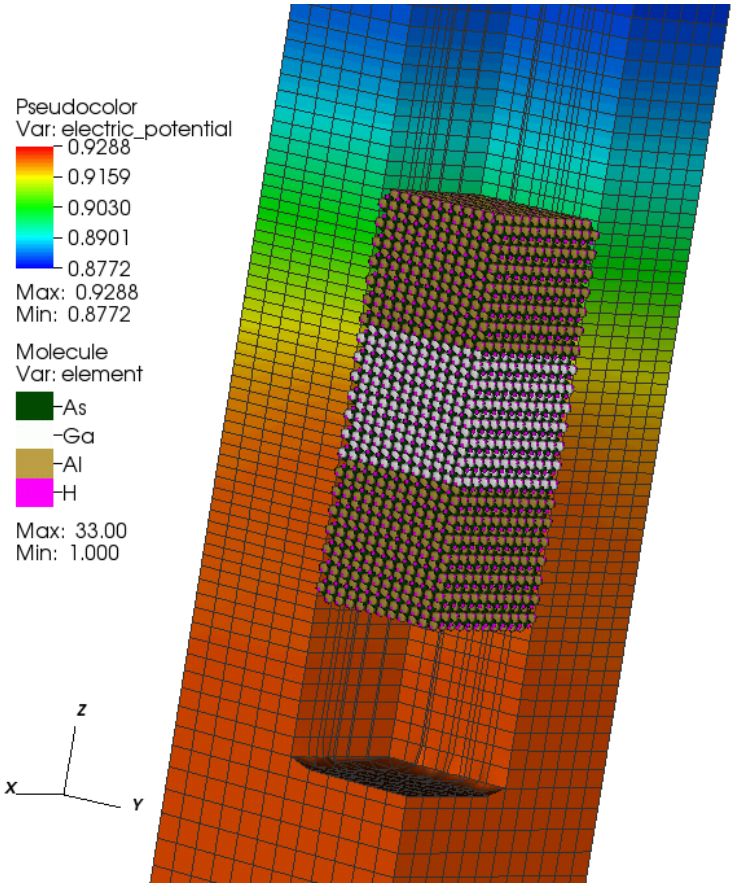


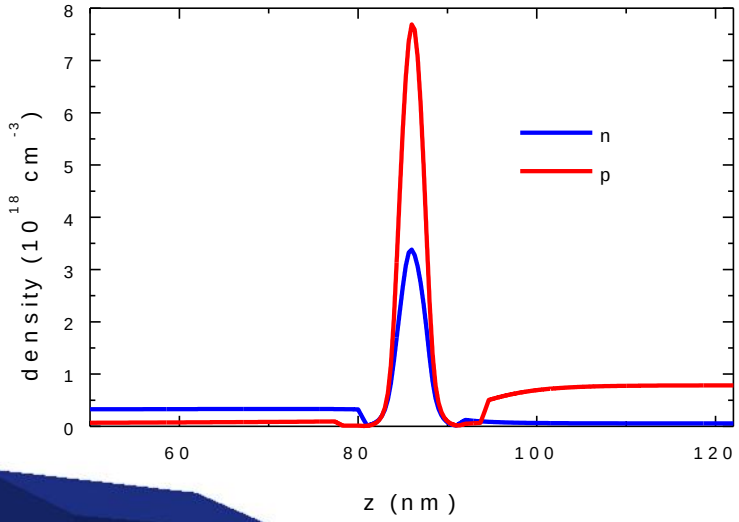
- the domains are contiguous and linked through n-1 dimensional regions.
- each domain provides boundary conditions to adjacent domains.

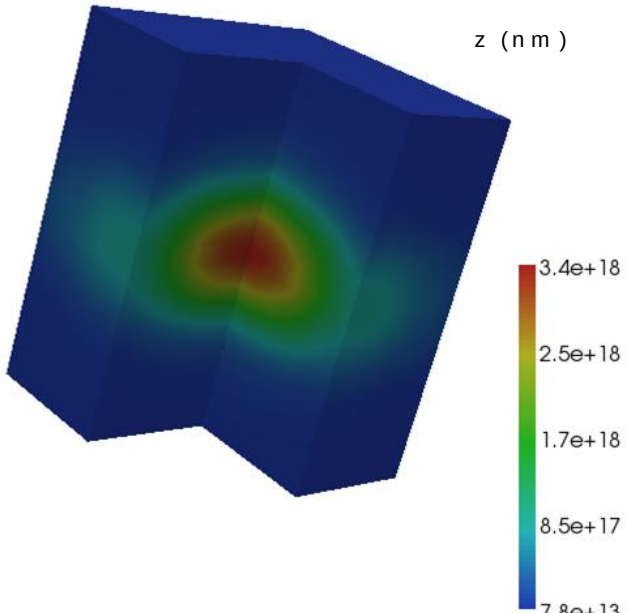
NEGF/drift-diffusion
VFF/continuous elasticity

Overlap scheme

- Schrödinger/drift-diffusion of AlGaAs/Gas nanocolumn

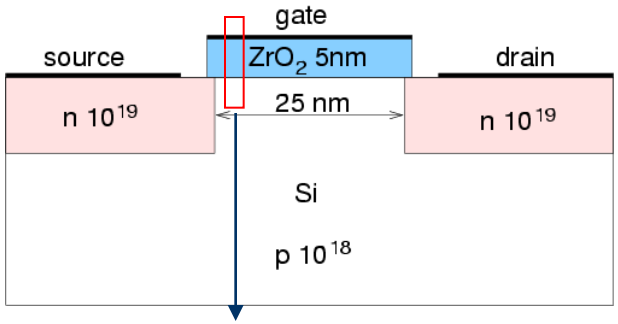


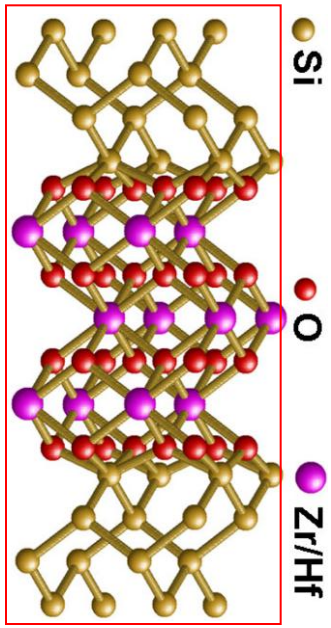




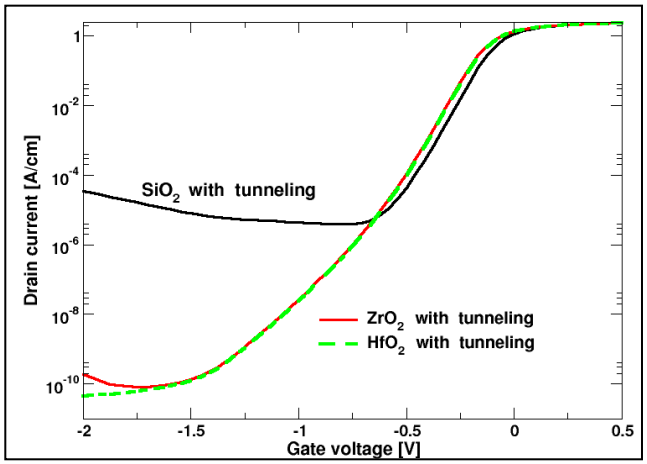
Bridge scheme

Drift-diffusion simulation of a 25 nm MOSFET with SiO_2 and high-κ oxide, including gate-tunneling



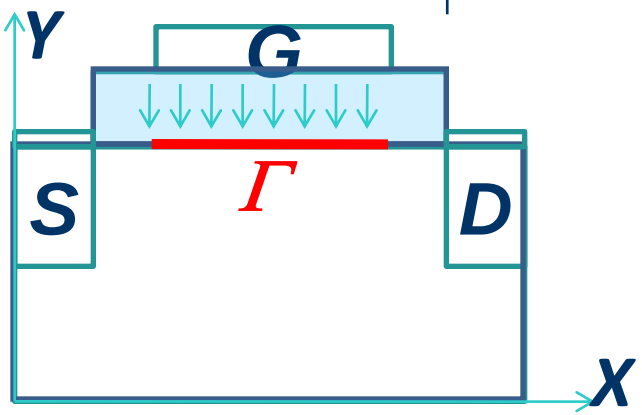


Tunneling current calculation based on a atomistic semi-empirical tight-binding description.



Coupled simulations

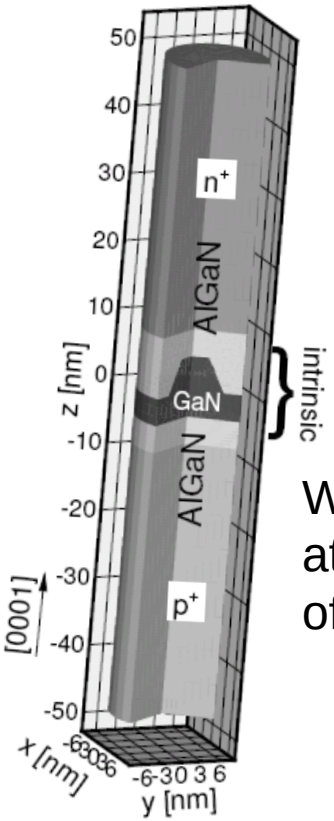
Tunneling current as boundary condition at Si/SiO_2 interface Γ



M. Auf der Maur et al., J. Comput. Electron., (2007)

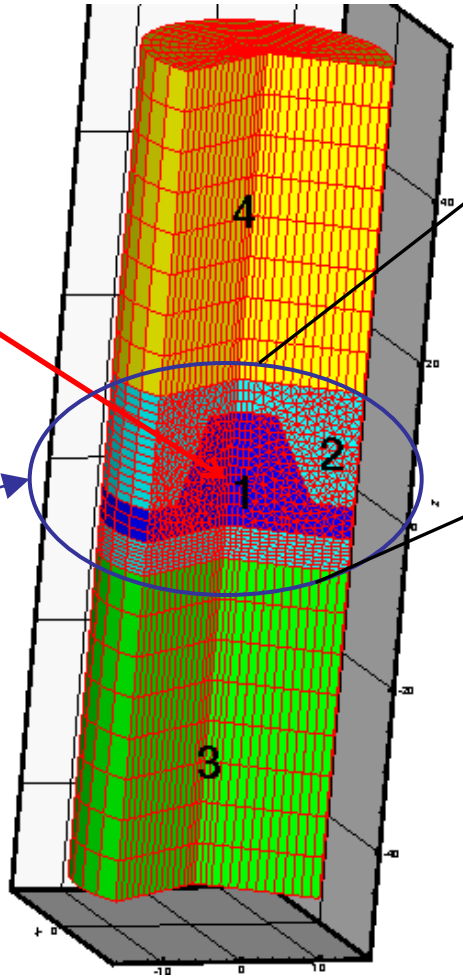
The atomistic structure

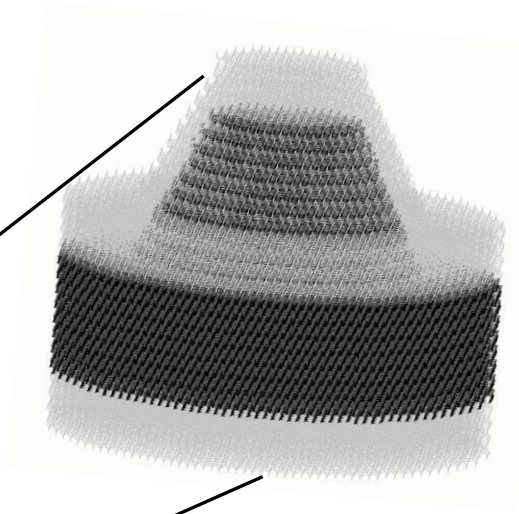
Top-down approach for definition of atomistic structure

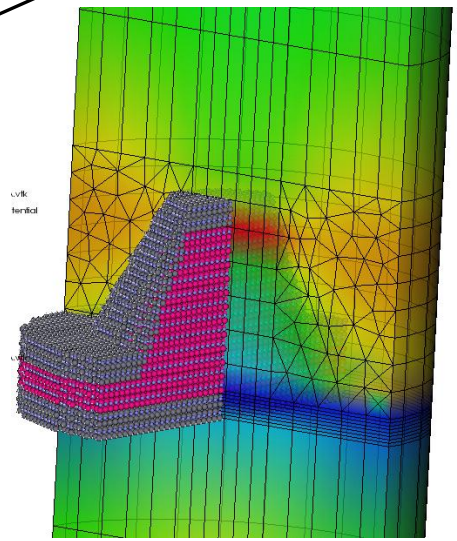


GaN quantum dot

Want to have atomistic model of active region

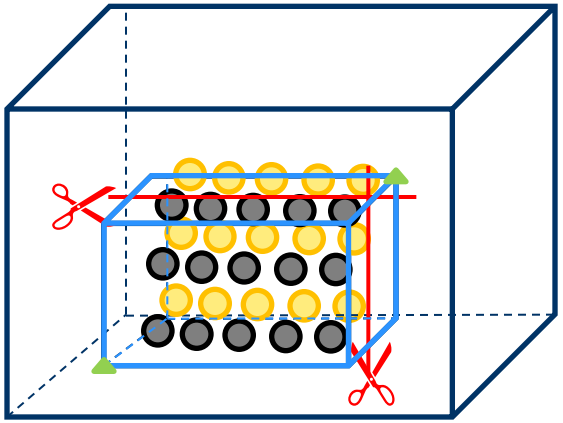






Atomistic structure generation

- We can assure a consistent atomistic structure using a top down approach:



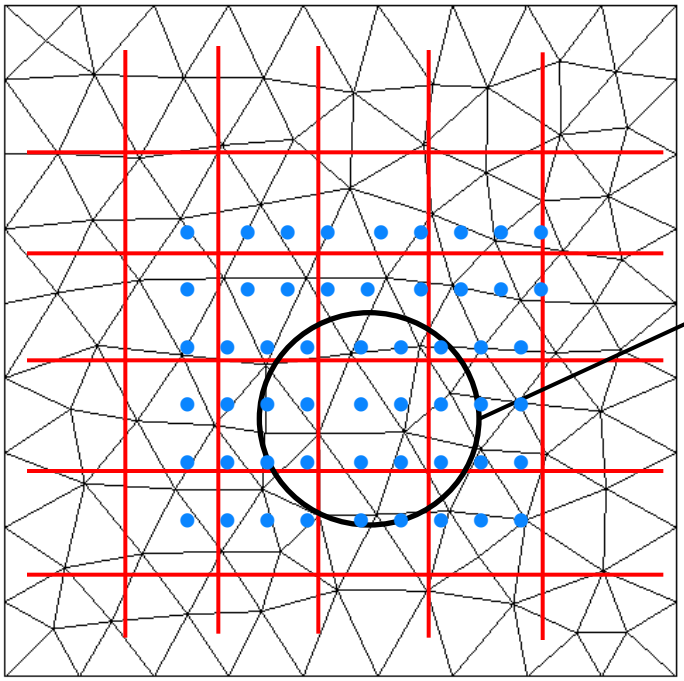
1. Identify relevant volume
2. Fill up with atoms using the crystal basis
3. Cut / fold atoms outside of the structure

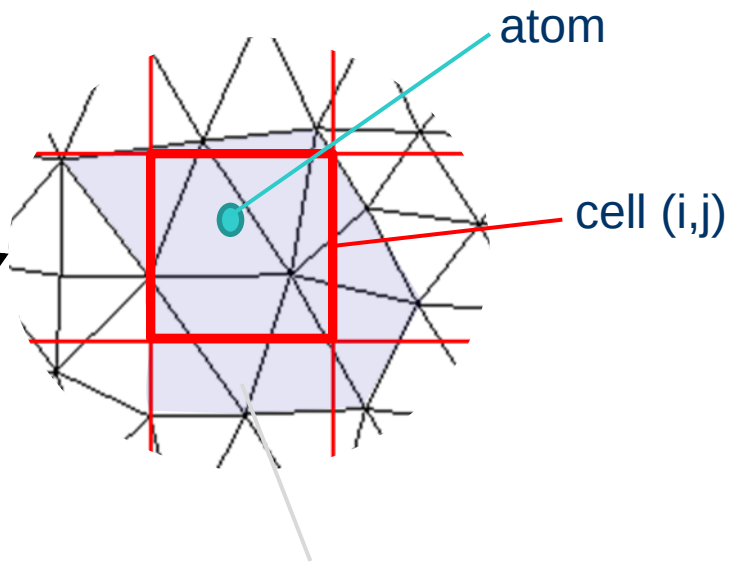
It is important that all atoms are lying **inside** *the simulation domain*

- The approach works for pseudomorphic structures with commensurate interfaces
- Structure is strained to the reference material
- Every atom is associated to a mesh element
- Can produce random alloys (uniform and non-uniform)

Atom to element association

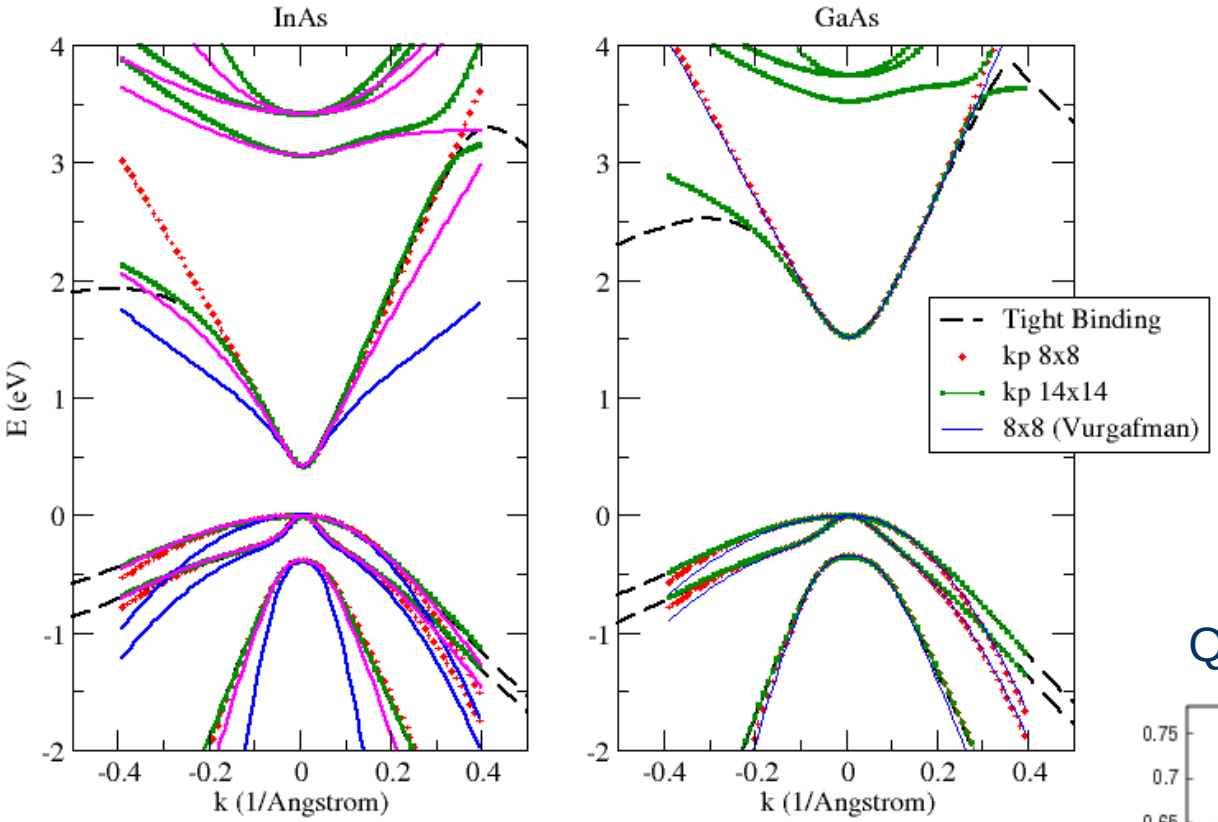
- Bond map calculation and atom to element association are the most time consuming operations in structure generation
- Association is efficiently done with the help of a regular tensor grid

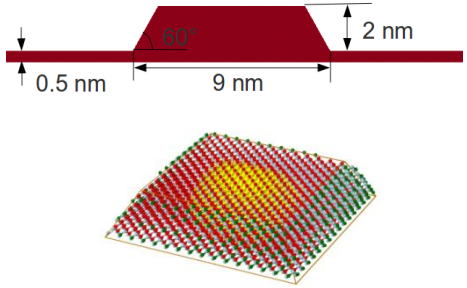




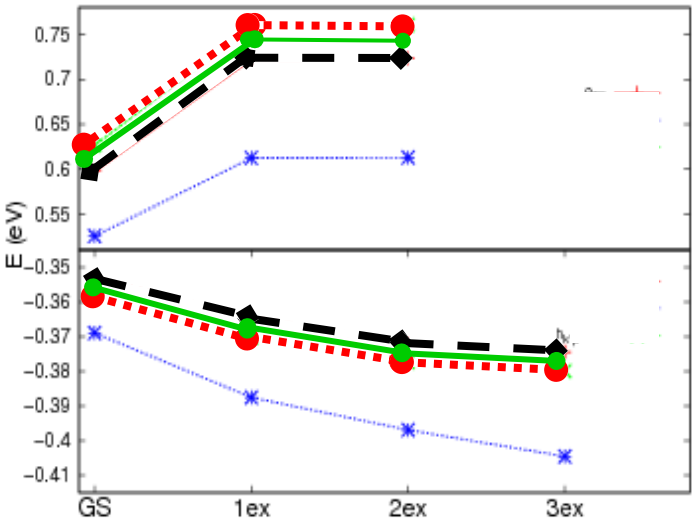
⇒ For each cell (i,j) we build a list of elements touching it

Consistency: e.g. k·p vs. ETB





QDot energy states:



For a **consistent** framework, need to fit parameters consistently!

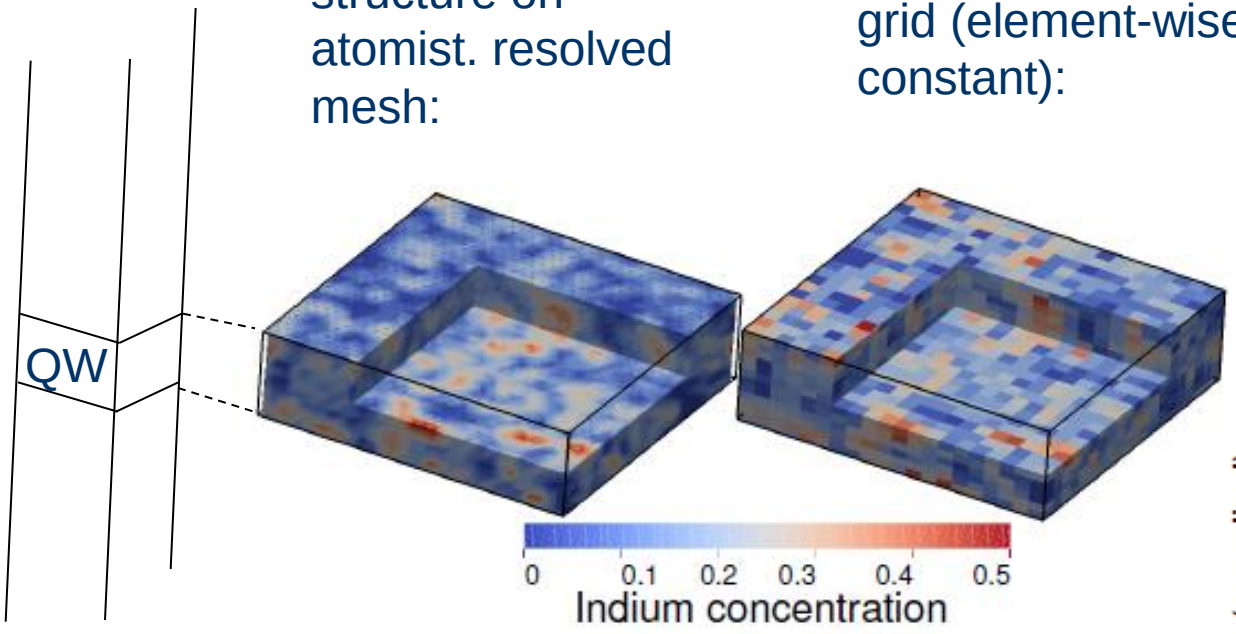
ETB
8x8 orig.
8x8 fit
14x14

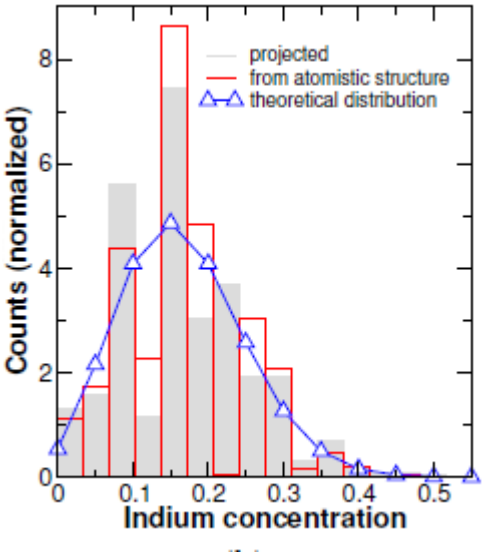
Structural consistency

- Map atomistic random alloy structure on FE grid

From atomistic structure on atomist. resolved mesh:

Projection on FE grid (element-wise constant):

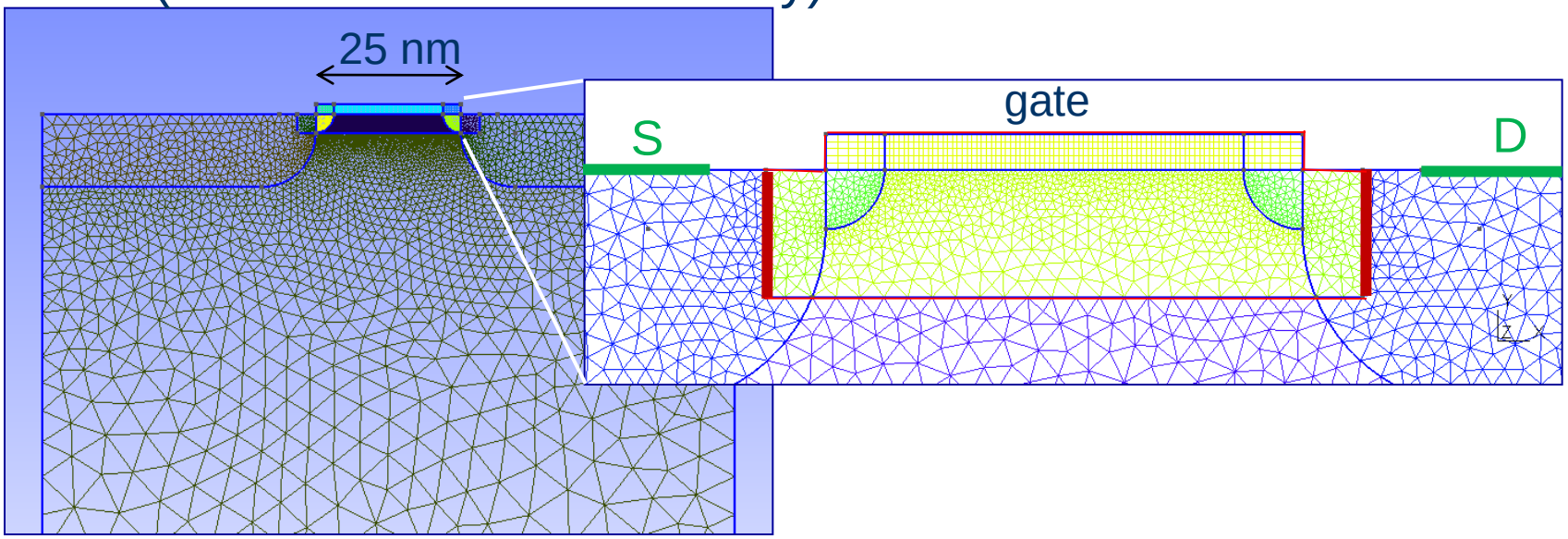


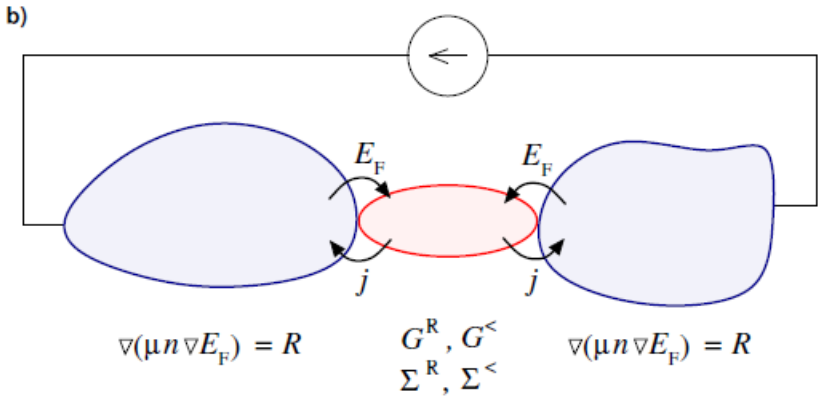


Mean conc.: 15%
Control volume: sphere, 0.5 nm radius

Example: MOS with NEGF/DD

- Mix between overlap (Schrödinger/Poisson) and bridge (current at NEGF boundary) schemes



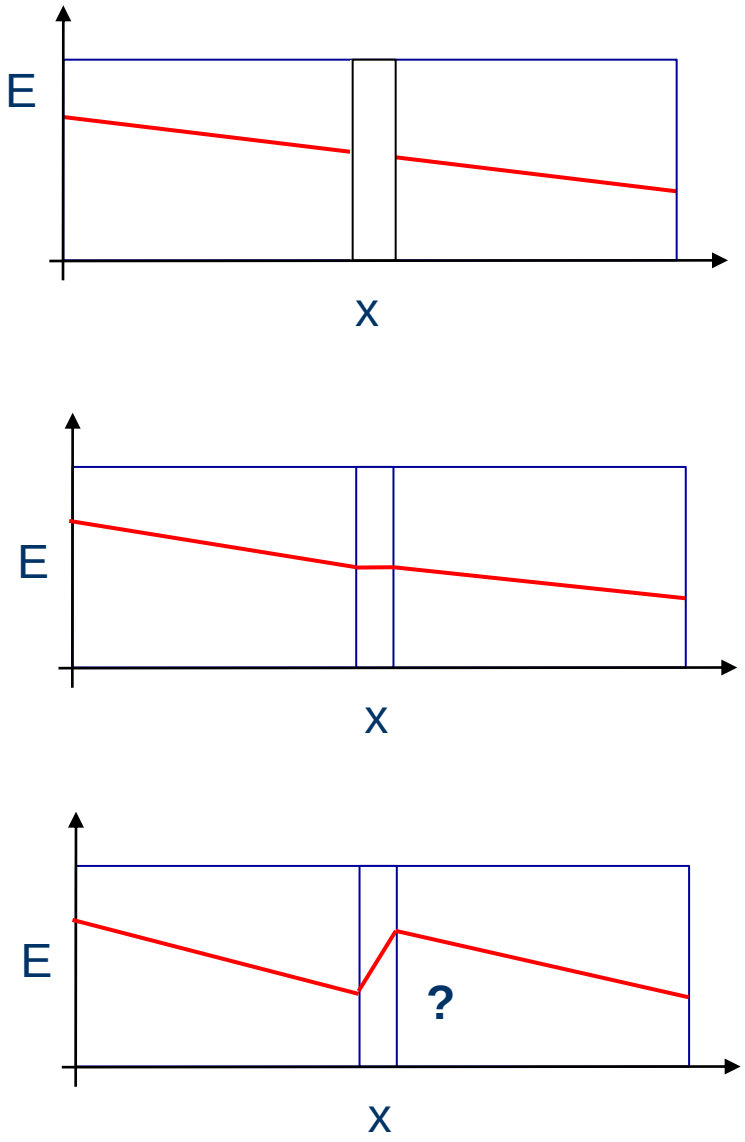


drift-diffusion

Fully self-consistent

NEGF (ballistic)

Fully coupled strategy



- Solve DD everywhere as a first guess
- Solve NEGF with potential BC imposed

  compute ρ and j
- In the DD ∩ NEGF regions remove

$$\frac{1}{q}\nabla \cdot \mathbf{J}_n = R - G$$

$$\frac{1}{q}\nabla \cdot \mathbf{J}_p = G - R$$

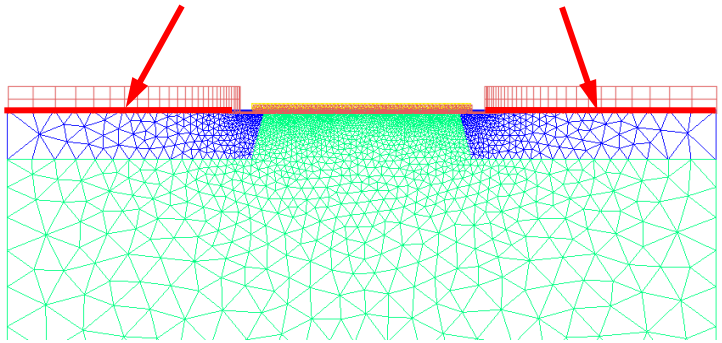
- Solve DD, with j as BC

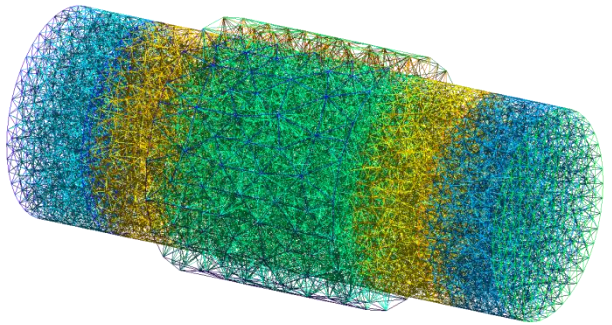
Convergence problems can appear:
Idea: introduce a predictor for the current density in DD

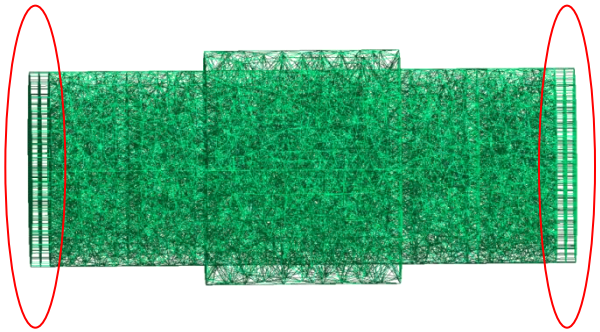
Creation of 'contacts'

- NEGF needs contact layers for definition of contact Green's functions / self-energies

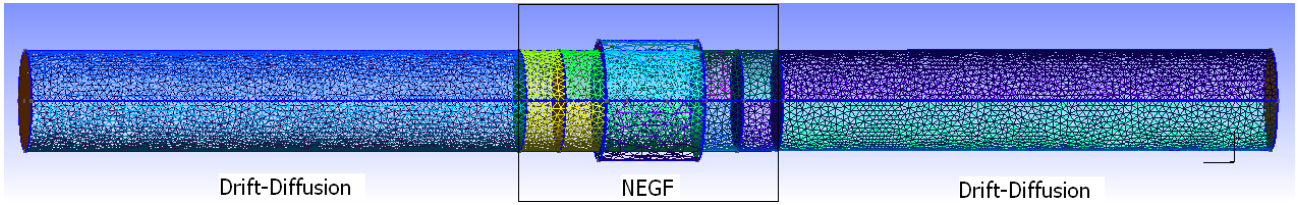
N-1 dimensional Contacts



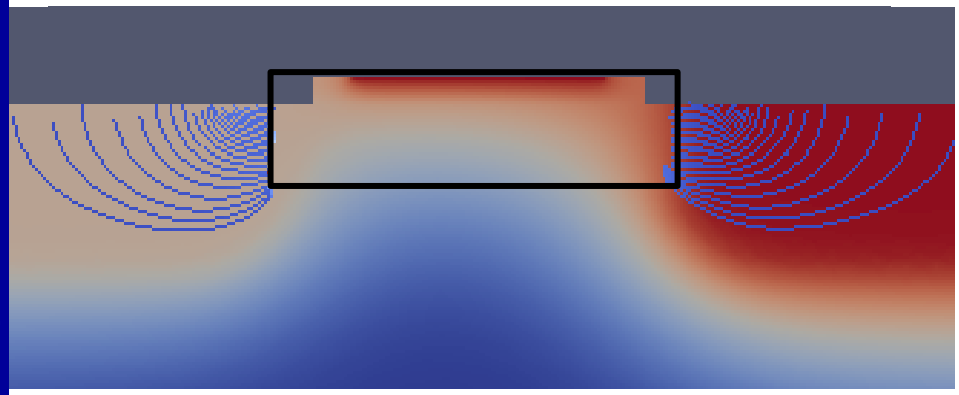


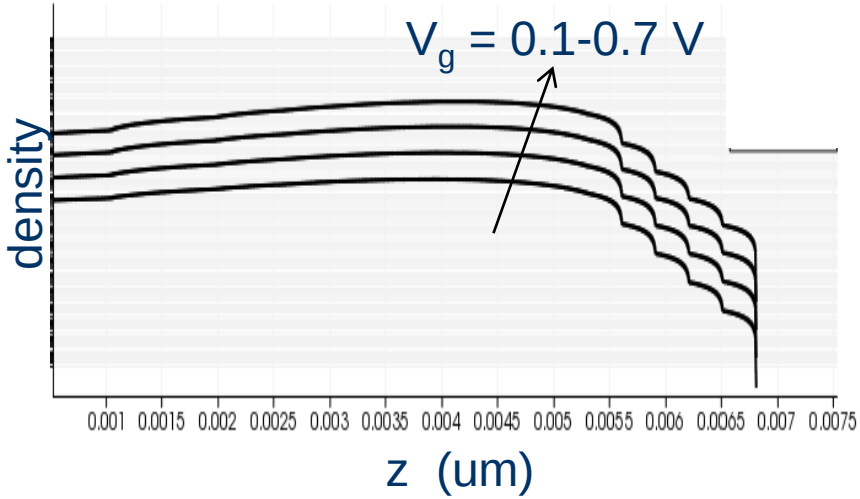


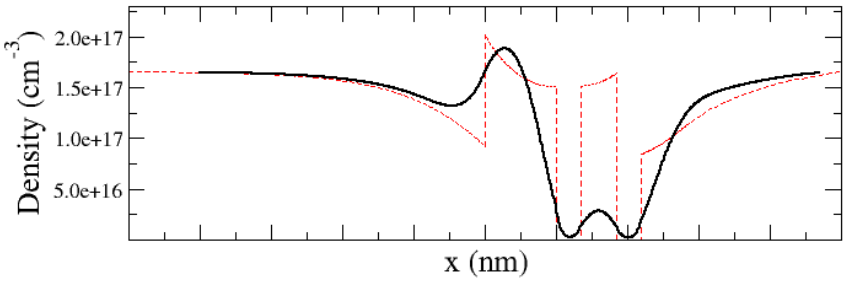
- Automatic mesh creation using *lib*MESH classes
- General extrusion of planar contacts in 1,2,3D

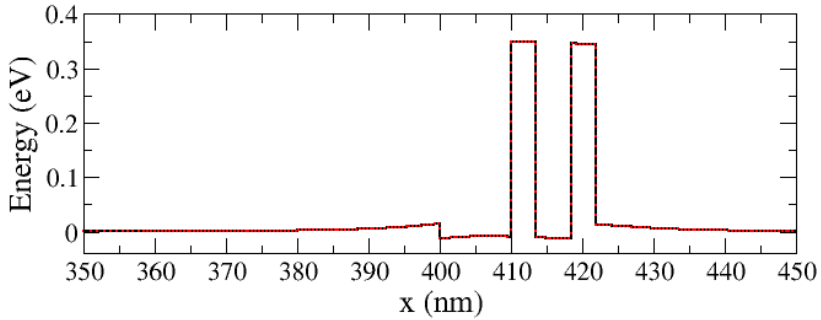


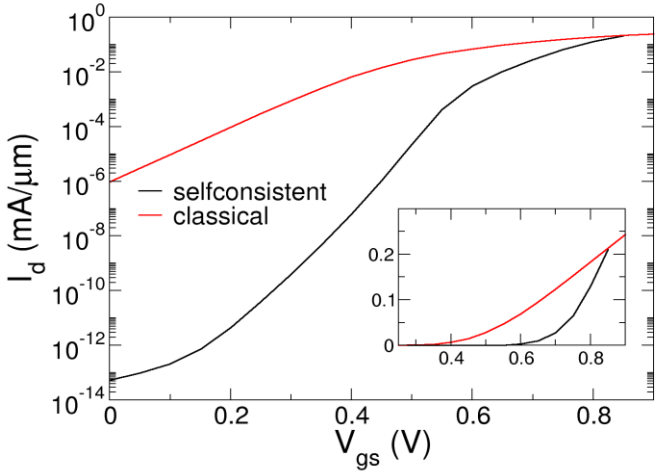
MOS: quantum/classical





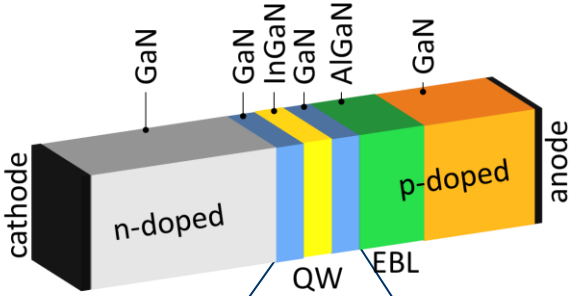


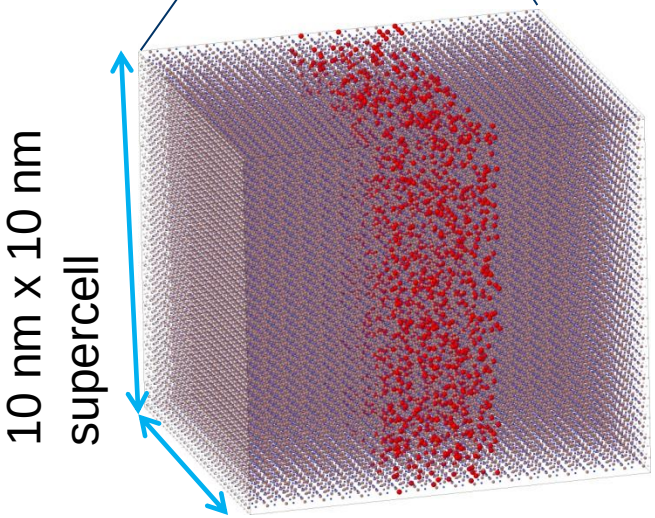




1D continuum + atomistic for QW LED

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



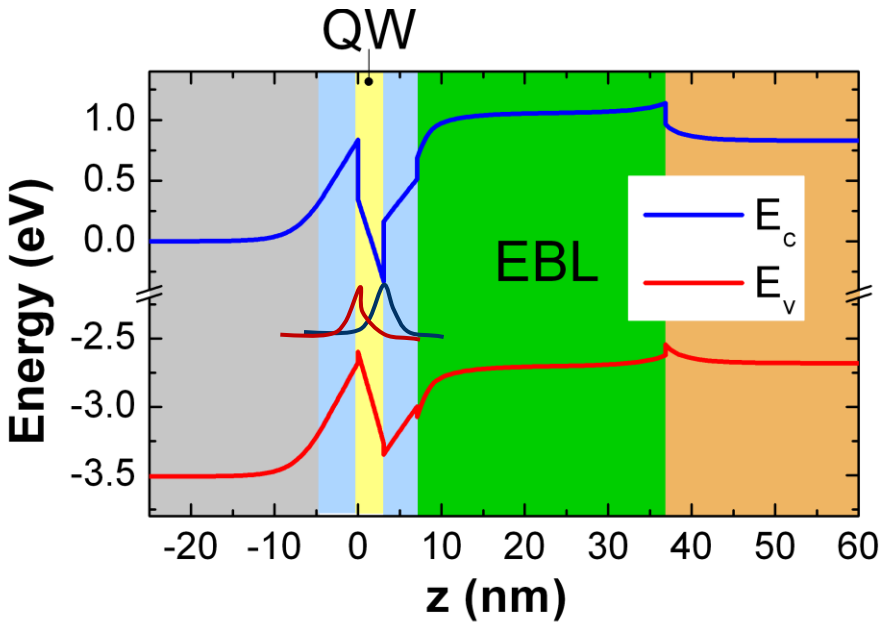


Atomistic models: VFF, ETB

Continuous models are solved in 1D

⇒ No in-plane potential fluctuations

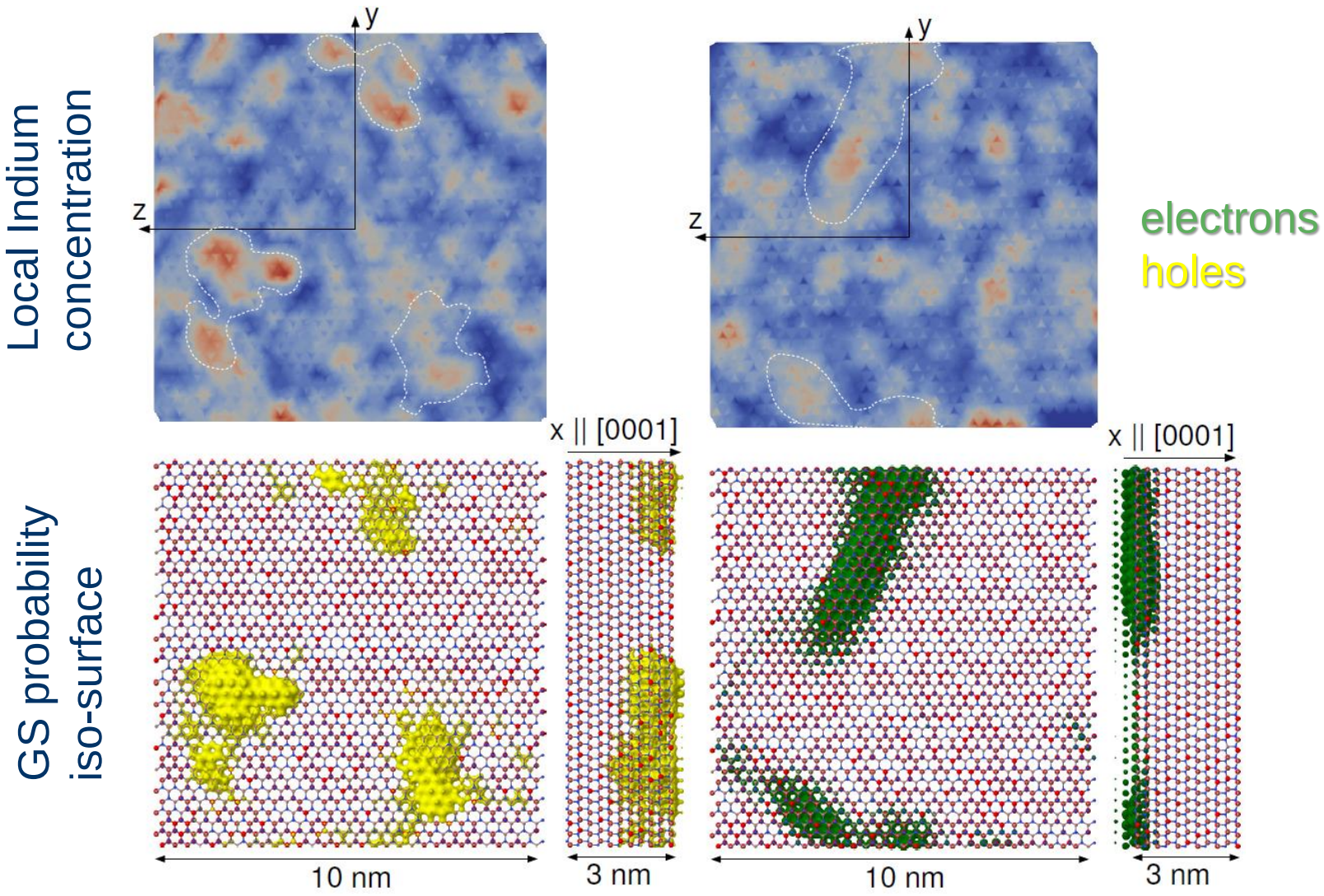
Typical band profile near maximum efficiency:



el-hl overlap is reduced due to QCSE

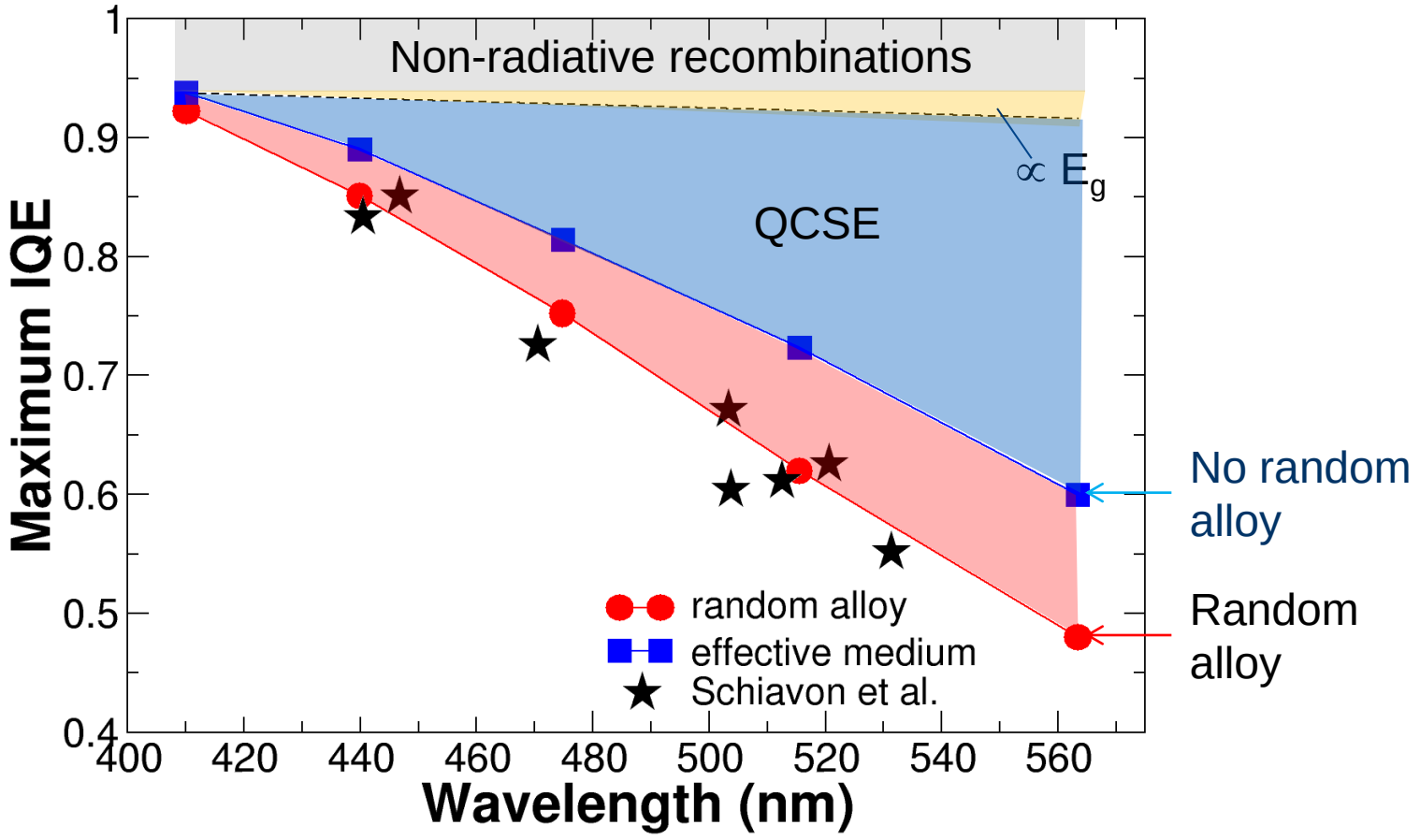
Localization behavior

- Correlation of local In concentration with wave function localization



Simulation results vs. experiment

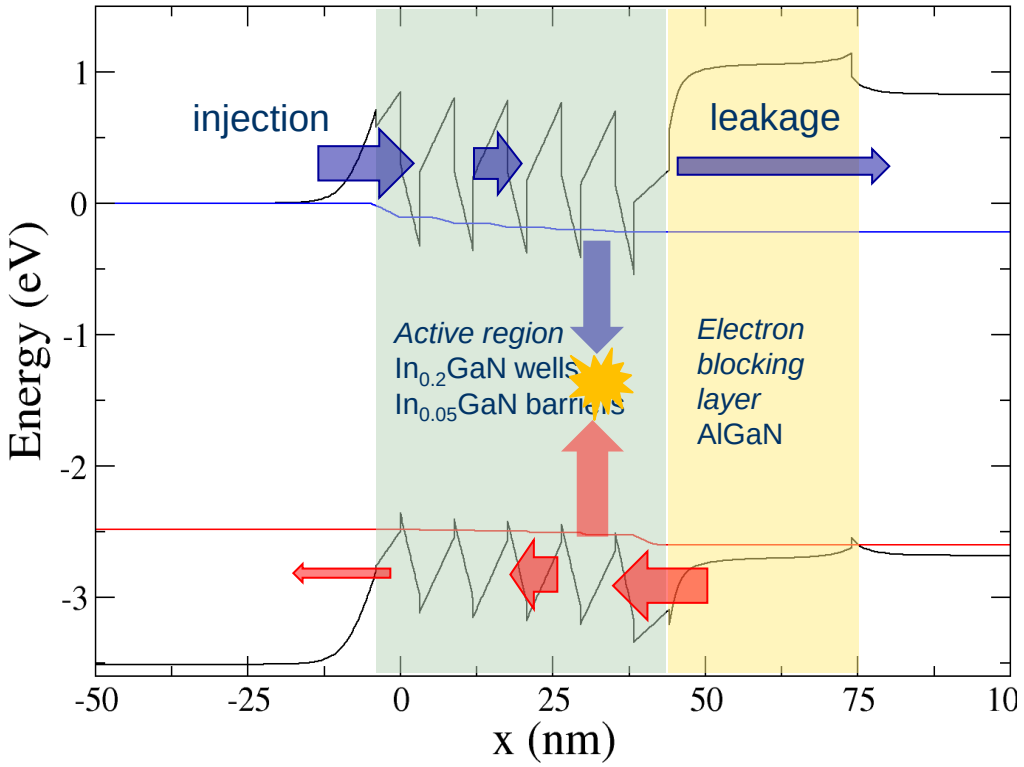
- Wavelength dependency of the quantum efficiency is well reproduced by the calculation:



Schiavon et al., Phys. Status Solidi B 250, No. 2 (2013)
Auf der Maur et al., PRL 2016

DD/NEGF coupling for QW LEDs

- Multiscale approaches using atomistic models are very interesting for III-nitride LED simulations (alloy disorder etc)



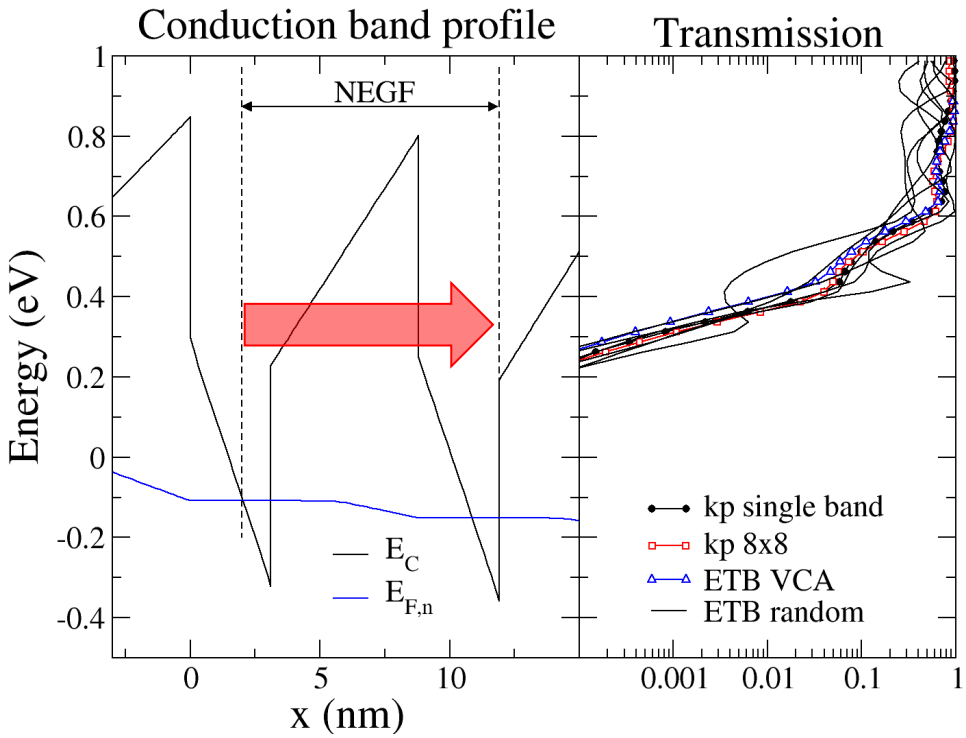
Peculiarities:

- Strong built in field due to spontaneous and piezoelectric polarization (wurtzite crystal)
- Large injection barriers
- Deep acceptor level

NEGF on whole LED? Would need all relevant recombination mechanisms (SRH, Auger).

Inter-well transport in LED

tunneling across $In_{0.05}Ga_{0.95}N$ barrier:

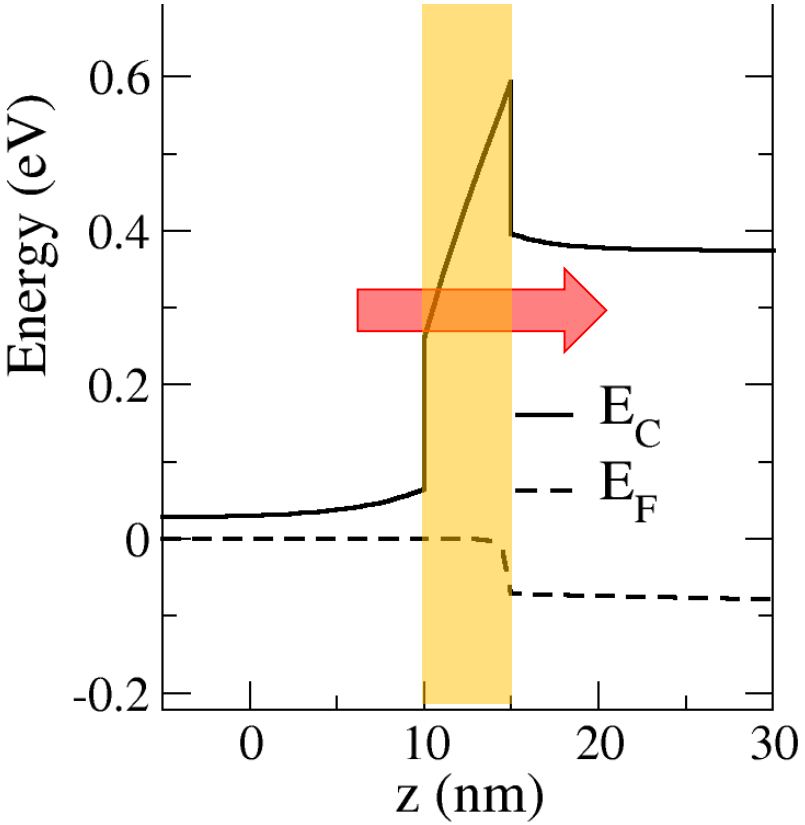


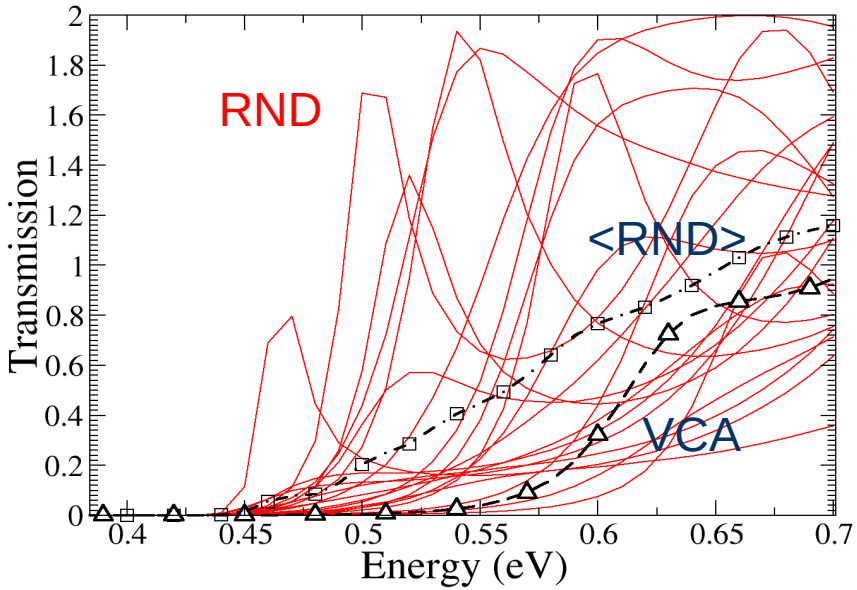
Extracted barrier resistivity:

- Pure drift-diffusion: 15 Ωcm²
- 8 band k·p: 1.33 Ωcm²
- Random alloy ETB: 0.28 – 1.26 Ωcm²

Transport across EBL

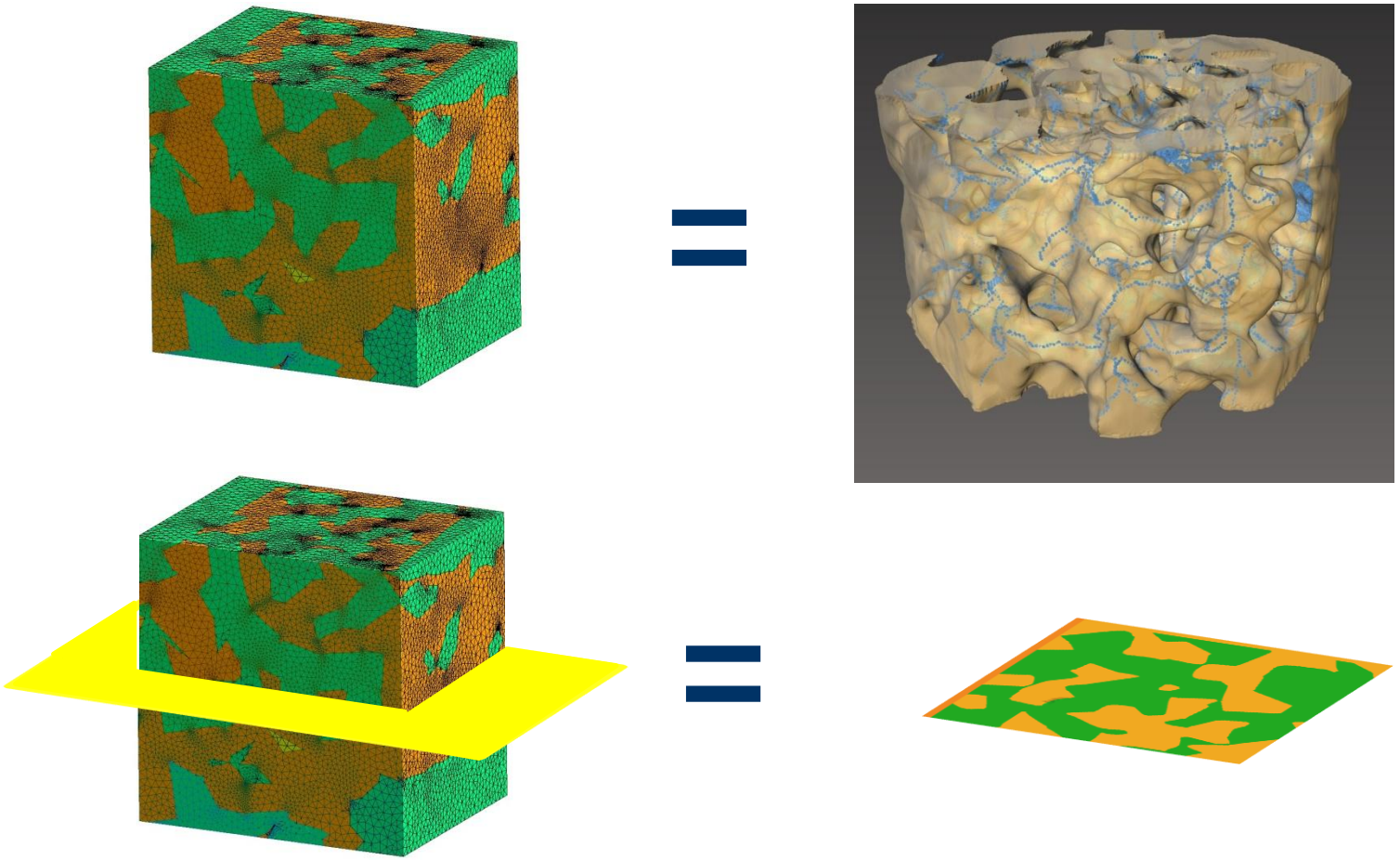
tunneling across $Al_{0.2}Ga_{0.8}N$ EBL:





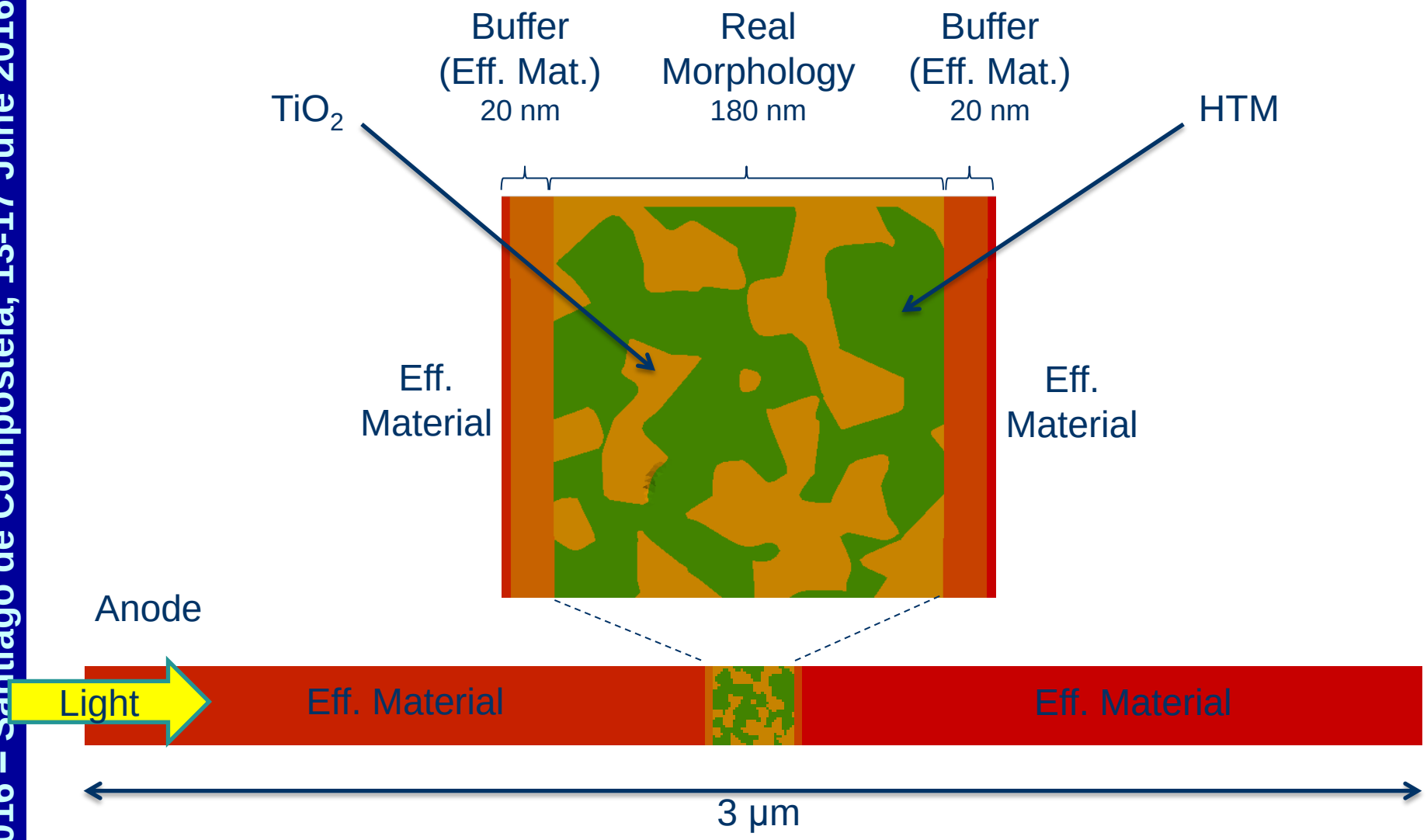
Considerable fluctuations due to random alloy: similar to defect assisted tunneling

P3HT/TiO2 morphology

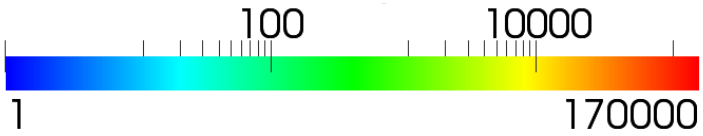


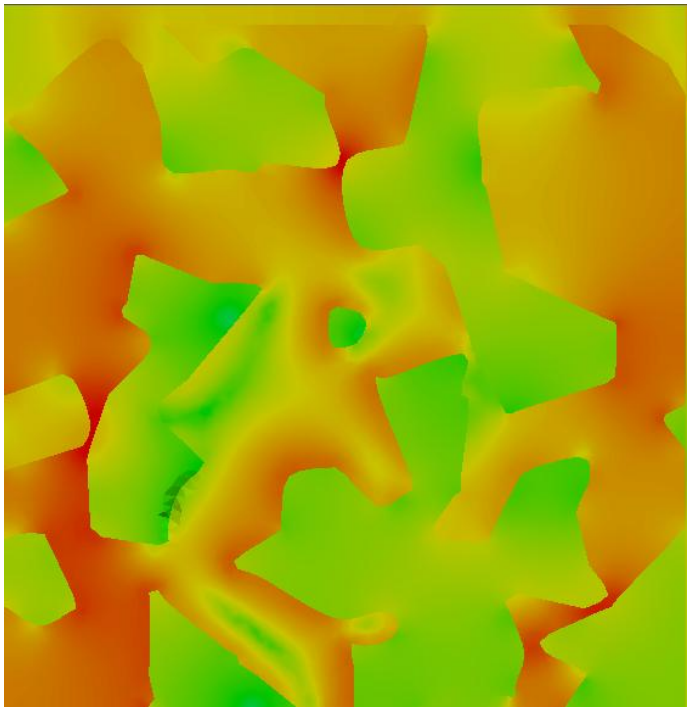
Paul A. Midgley & Rafal E. Dunin-Borkowski , "**Electron tomography and holography in materials science**", Nature Materials 8, 271 - 280 (2009) .

Model of the blend

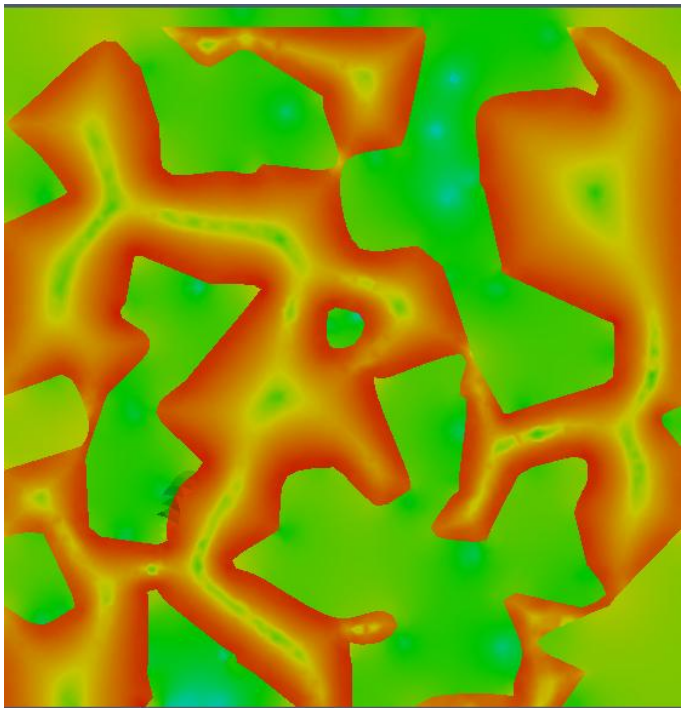


Effect of interface traps



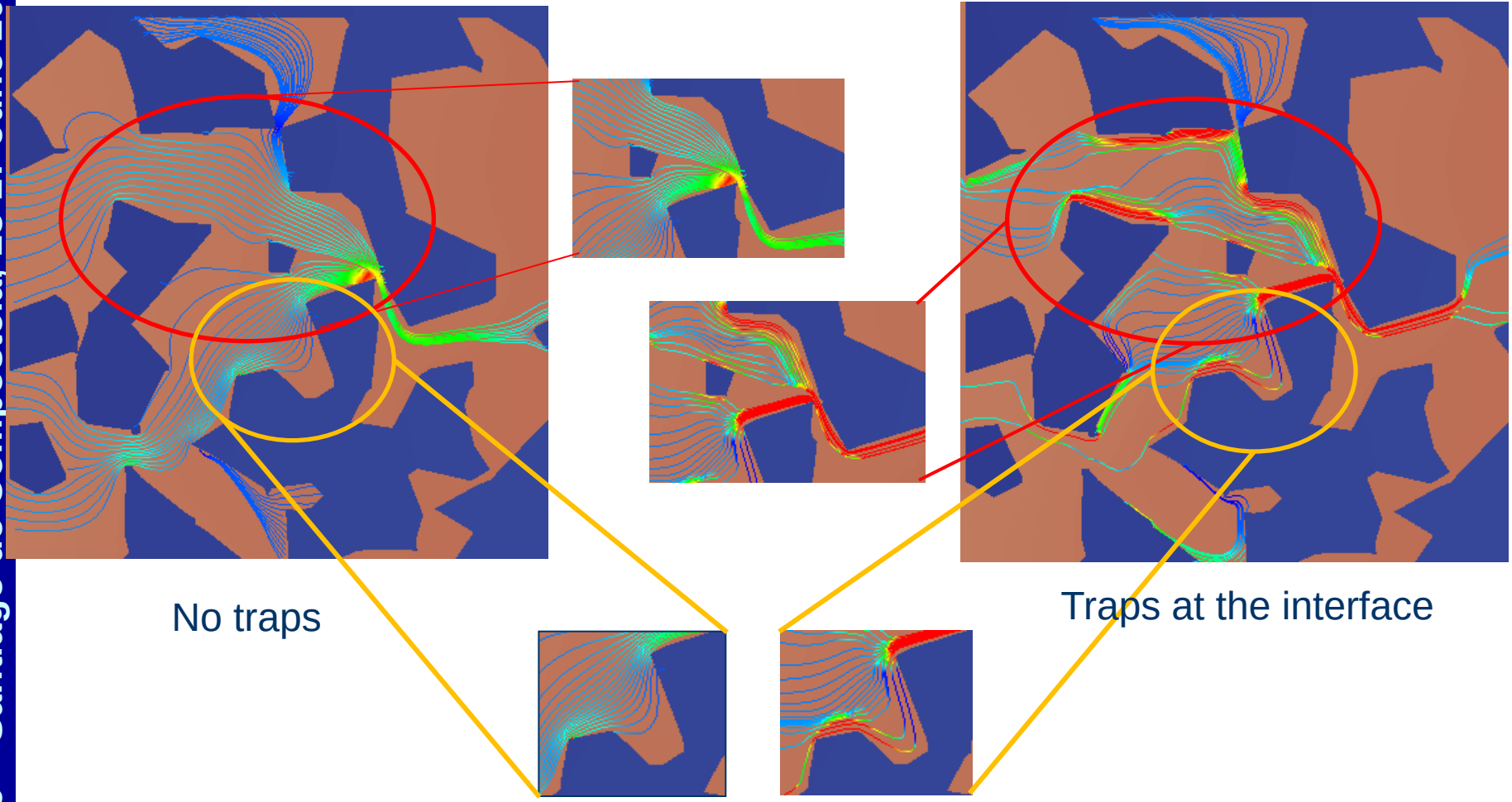


No interface traps



Interface traps

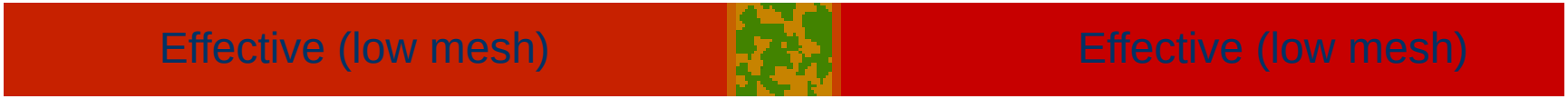
Effect of traps II



Effective model

Photoanode

Cathode



DOS renormalization

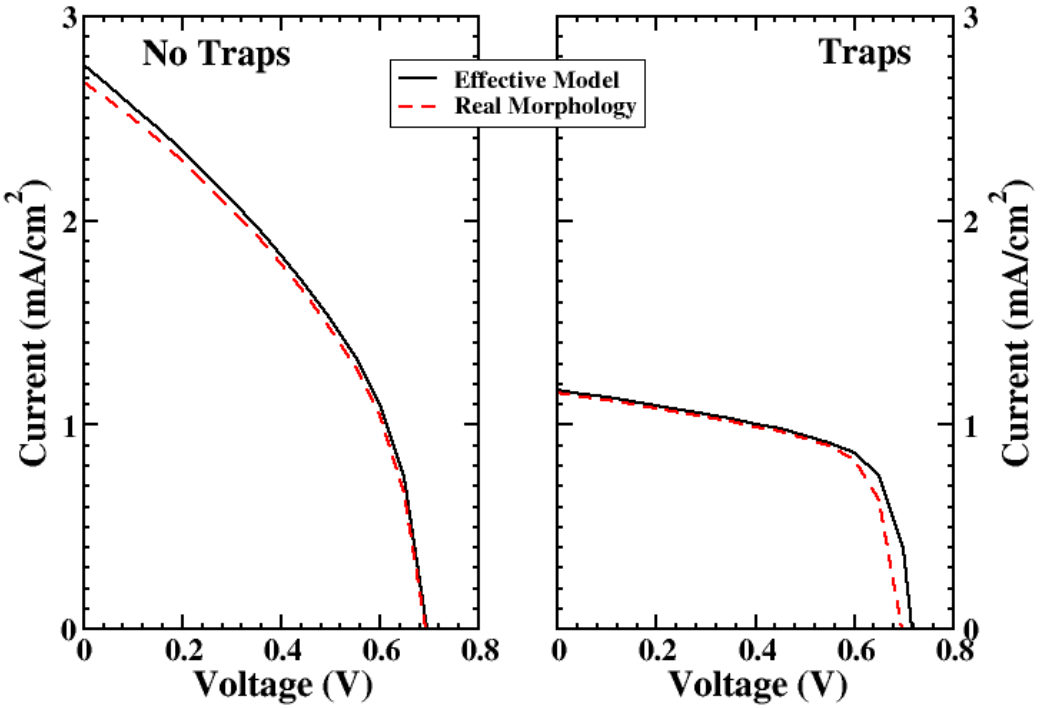
$$N_c^{eff} = (1-\delta) N_c^{TiO_2} + \delta N_c^{HTM}$$

$$N_v^{eff} = (1-\delta) N_v^{TiO_2} + \delta N_v^{HTM}$$

R and G renormalization

$$\int R_{eff}\, dS = \int R_{int}\, dL$$

$$\int G_{eff}\, dS = \int G_{int}\, dL$$



Conclusions/Outlook

- Multiscale approaches are needed in order to embed nanometer-scale active regions into their macroscopic environment
- Top down approach for definition of atomistic structure
- Transparency / extendability
- Efficiency of the microscale models is crucial for concurrent simulations

Current work:

- Generalizations for atomistic structures
- Further work on coupling NEGF/DD
- Coupling of kinetic MC/DD
- Mathematical basis for such couplings?

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