Multi-scale methods in electronic device simulation

Aldo Di Carlo







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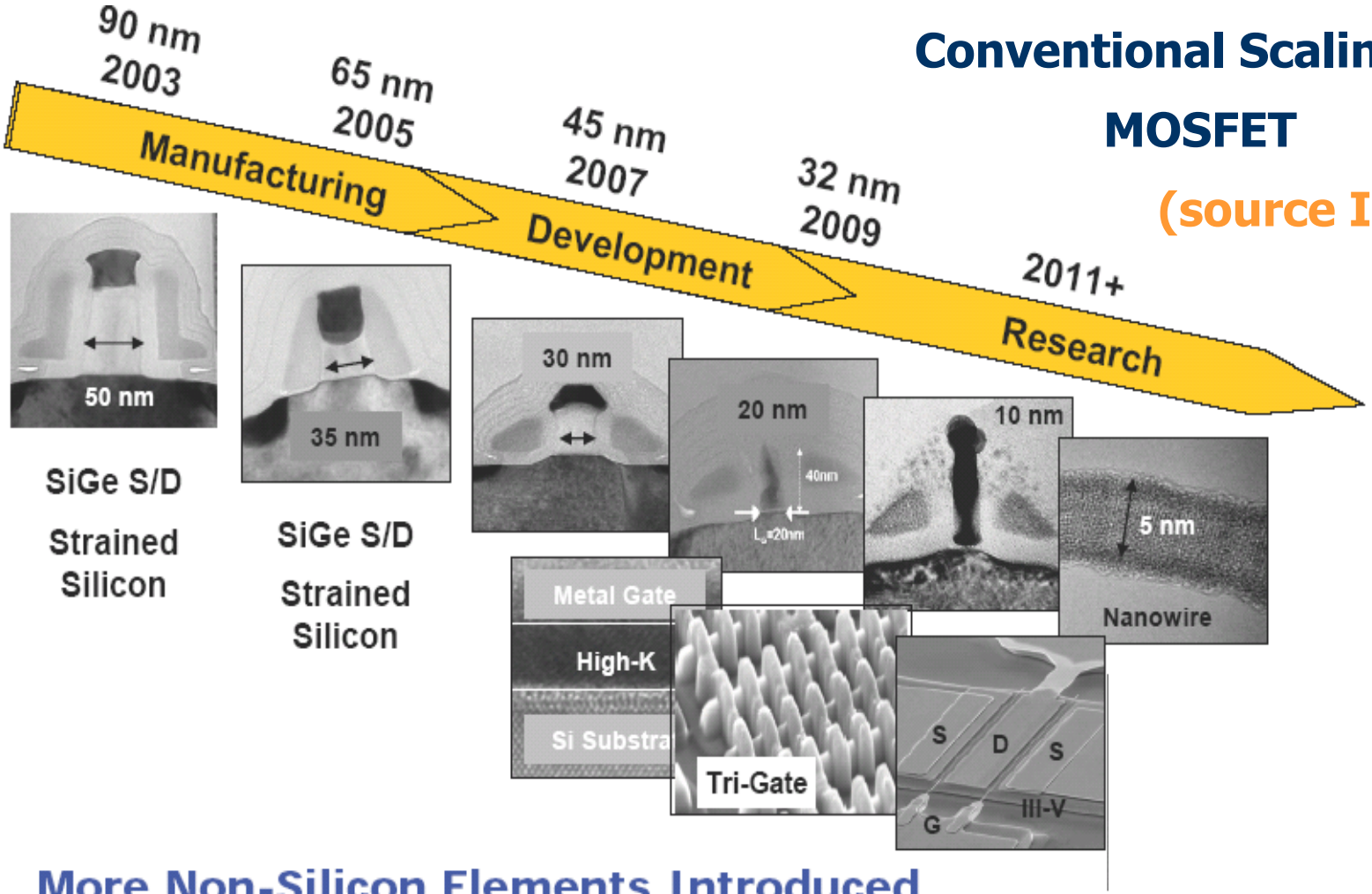
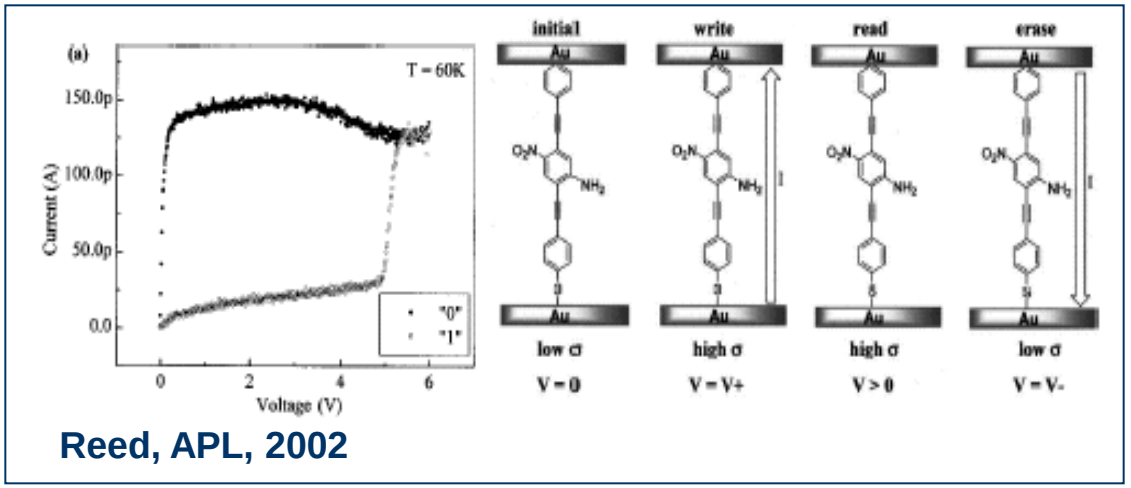
Acknowledgments:
-EU FP7 Projects (SMASH, Clermont 4, Opther, HYMEC) - Lazio Region (Italy)

Top-Down Downscaling



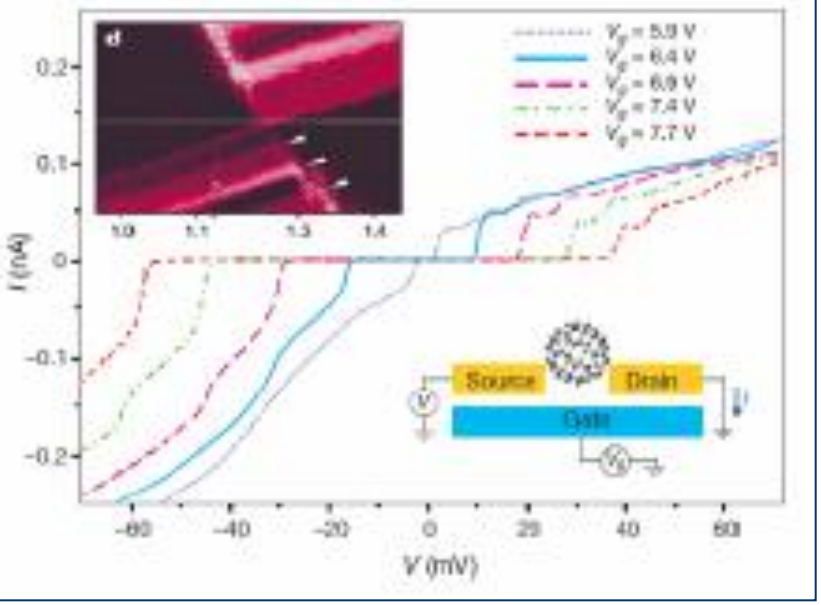
Beyond MOS: molecular electronics

- *Electron transport across molecules*
- *Structural modification*
- *Coulomb blockade*

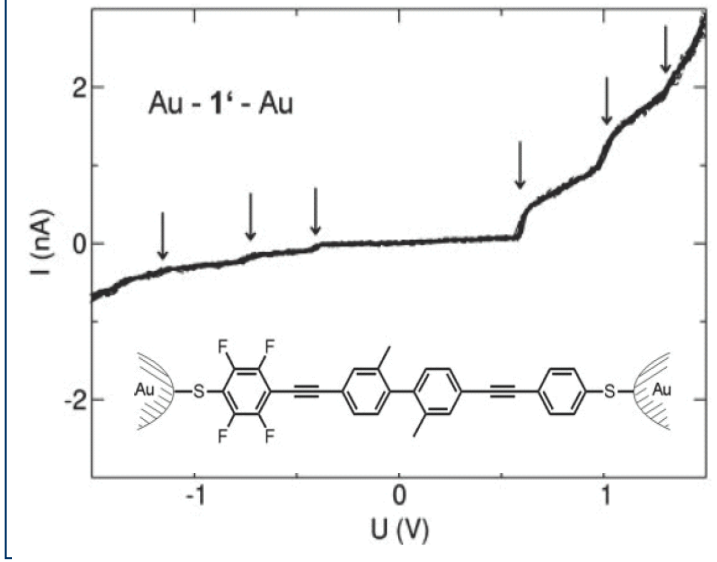


Reed, APL, 2002

H. Park, Science, 2003



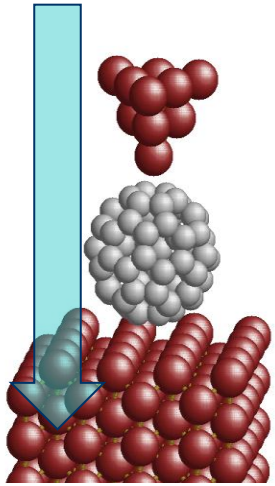
Heiko, PNAS, 2005



Atomistic methods

A. Pecchia, A. Di Carlo, Rep. Prog. Phys. 67 (2004) 1497

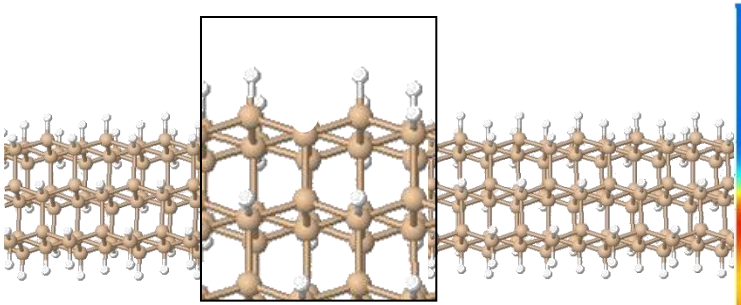
At the nanoscale "every atom matters!"



Density Functional TB + NEGF + scattering
[PRL 100, 136801 (2008)]

Power dissipated in the C60 molecule is 10 nW

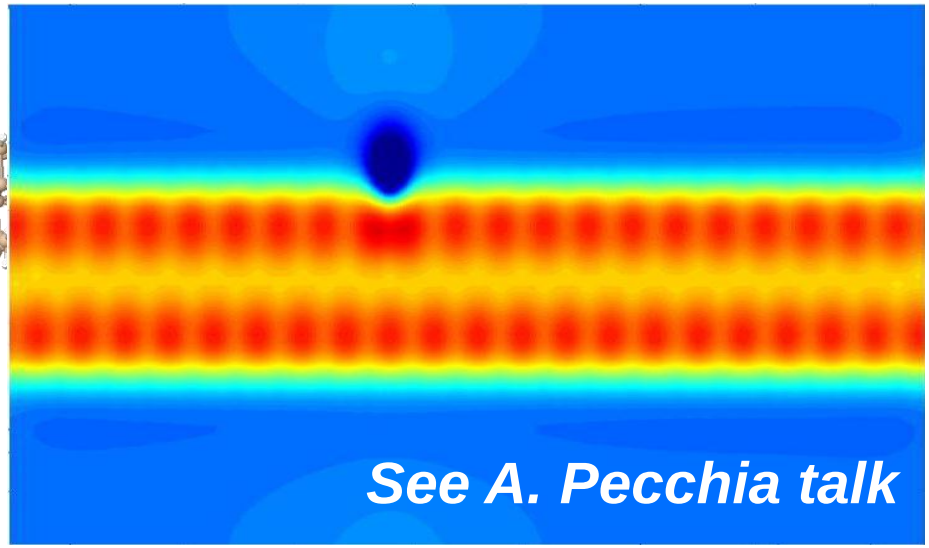
Power calculated as I x V = 10 μW !!!!



H-passivated SiNW with one

- Si dangling bond

- OH passivated dangling bond



Micro/macro scale

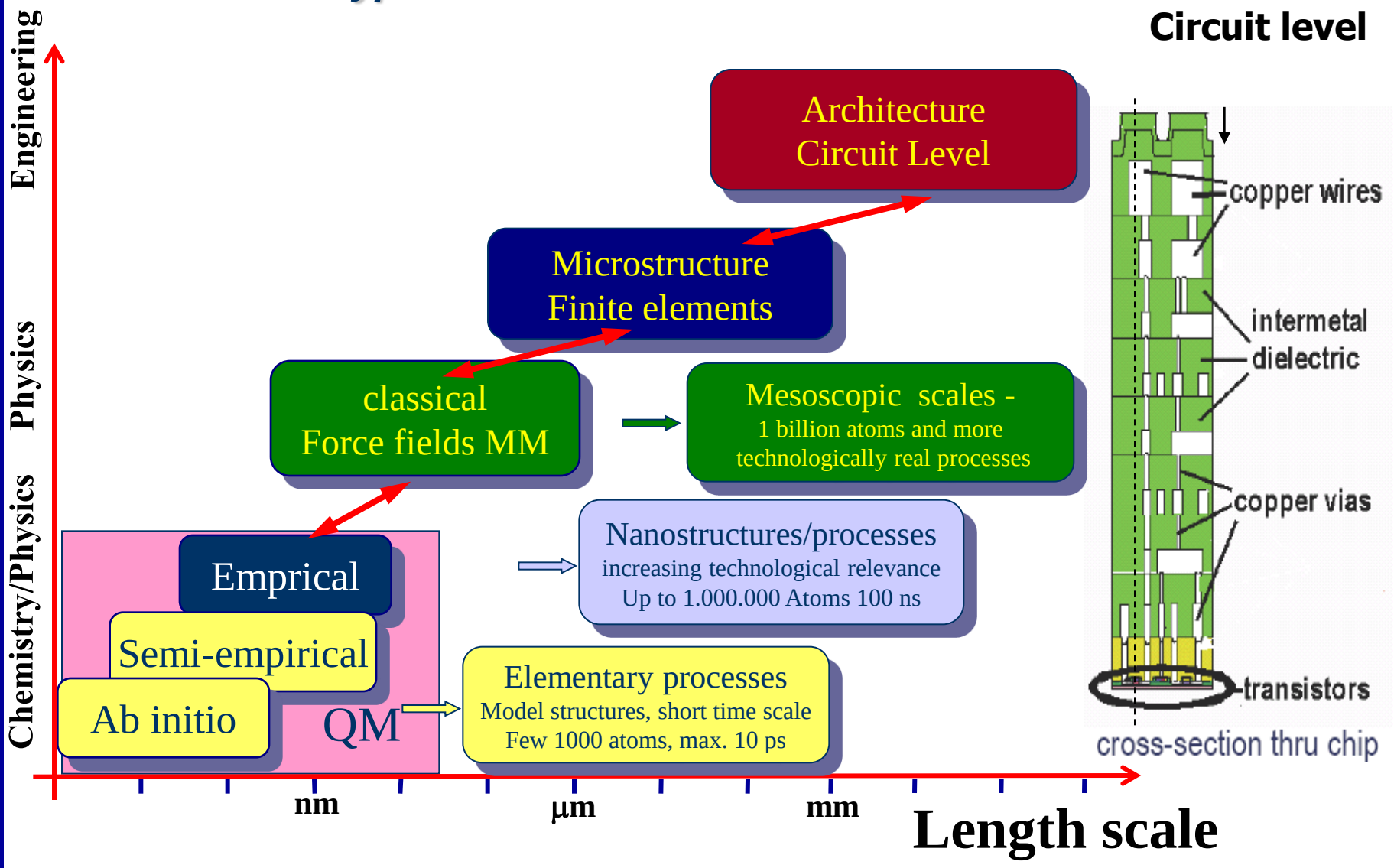
In a real device also micro and macro scale should be considered

- ***Devices should be accessible from a macro scale***
- ***micro/macro scale details are as important as nanoscale features (temperature distribution, electrostatics, strain, air gap, etc.)***
- ***Number of atoms cannot grow to much in simulations***
- ***20 years of experience with Drift-diffusion matters !***

Nano, micro and macro scale should be combined in a multiscale approach

The multiscale problem

Typical Pentium 4 MOSFET section

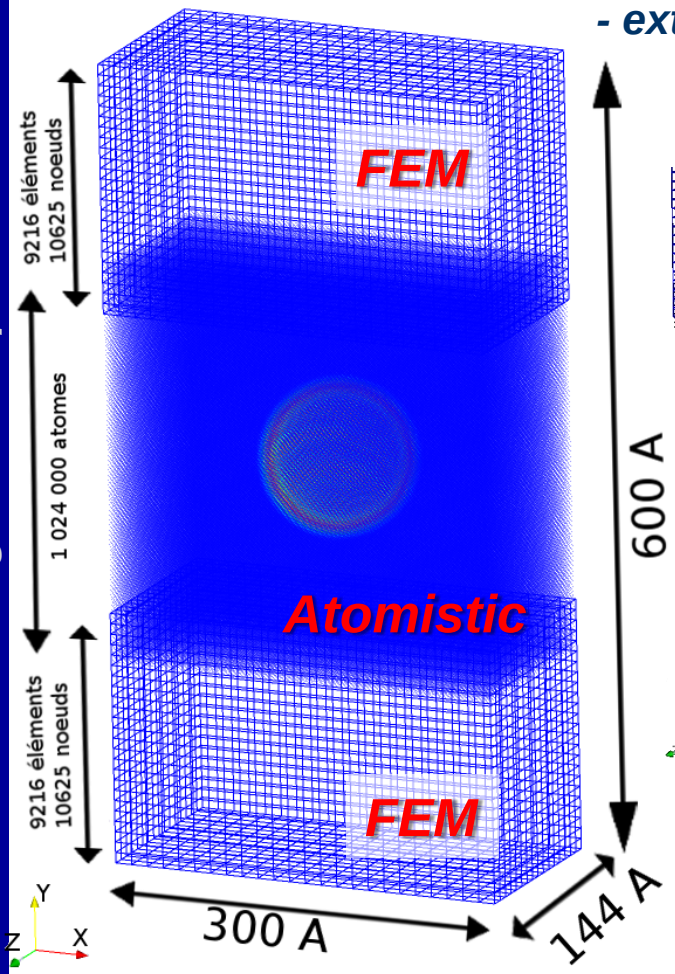


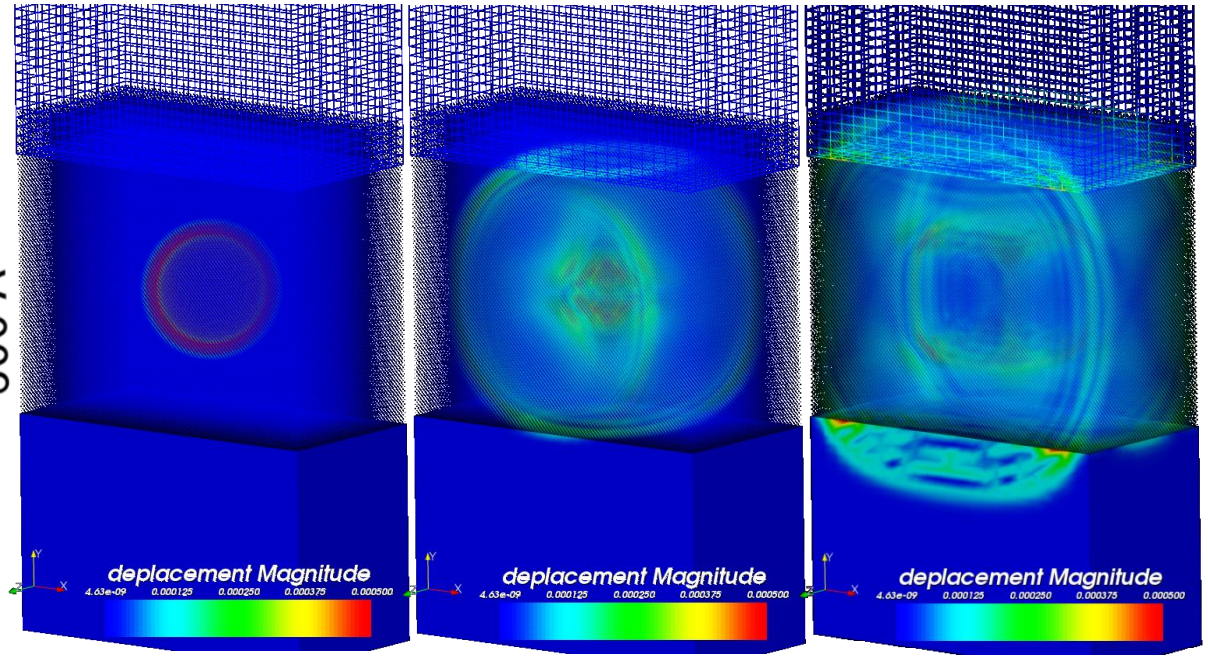
Multiscale methods in material science

Propagation of a shock wave in a crystal

- central region is treated at the atomistic level (MM)

- external part are treated in the continuous approx. (FEM)





Time

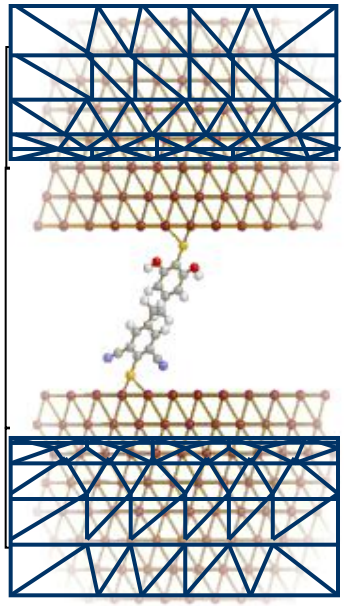
Courtesy of G. Anciaux

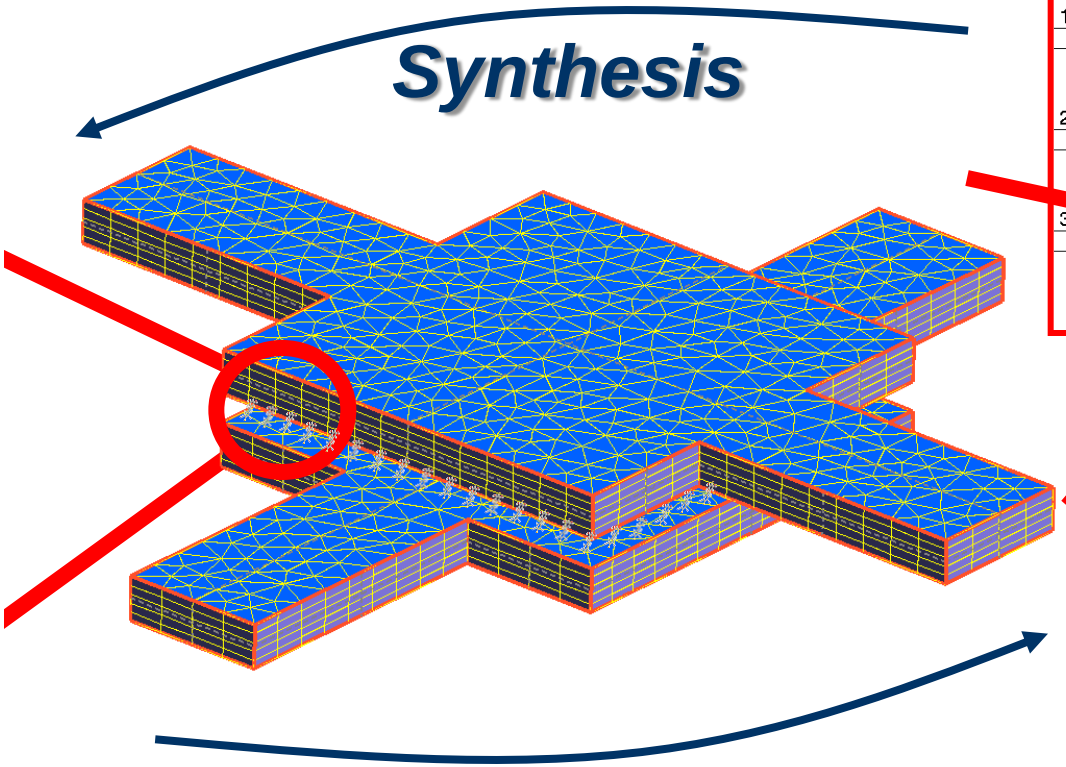
Multiscale simulations: TiberCAD

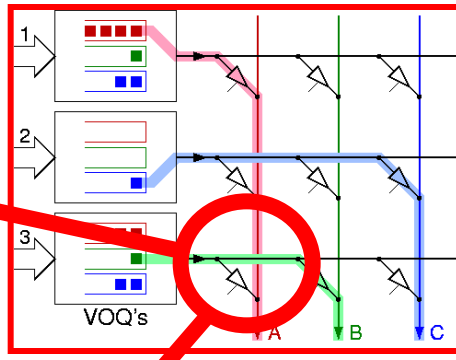
Nanoscale description

Macro-Microscopic description (Strain, Drift-Diffusion , Heat, etc)

Circuit simulation



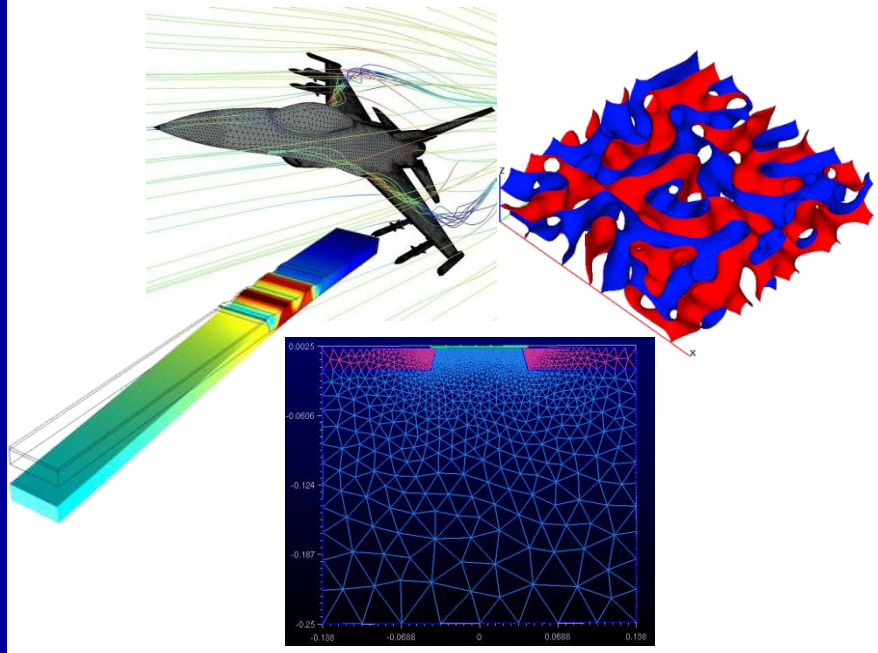




TIBER CAD

www.tibercad.org

Multiscale components



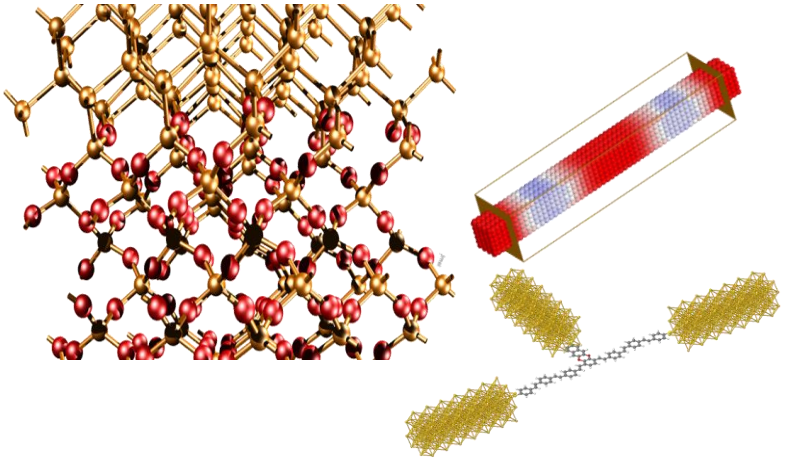
Finite Element Method

- FEM is the method in engineering problems (deformation/strain, heat, Maxwell, etc. etc.)

-Drift-diffusion (DD) like schemes have been solved with box integration methods.

- DD-FEM have been heavily developed in the last 20 years in the Math community (***Hecht, Marrocco, Brezzi, Sacco, Chen)***

- many FEM library in GPL



Atomistic local basis

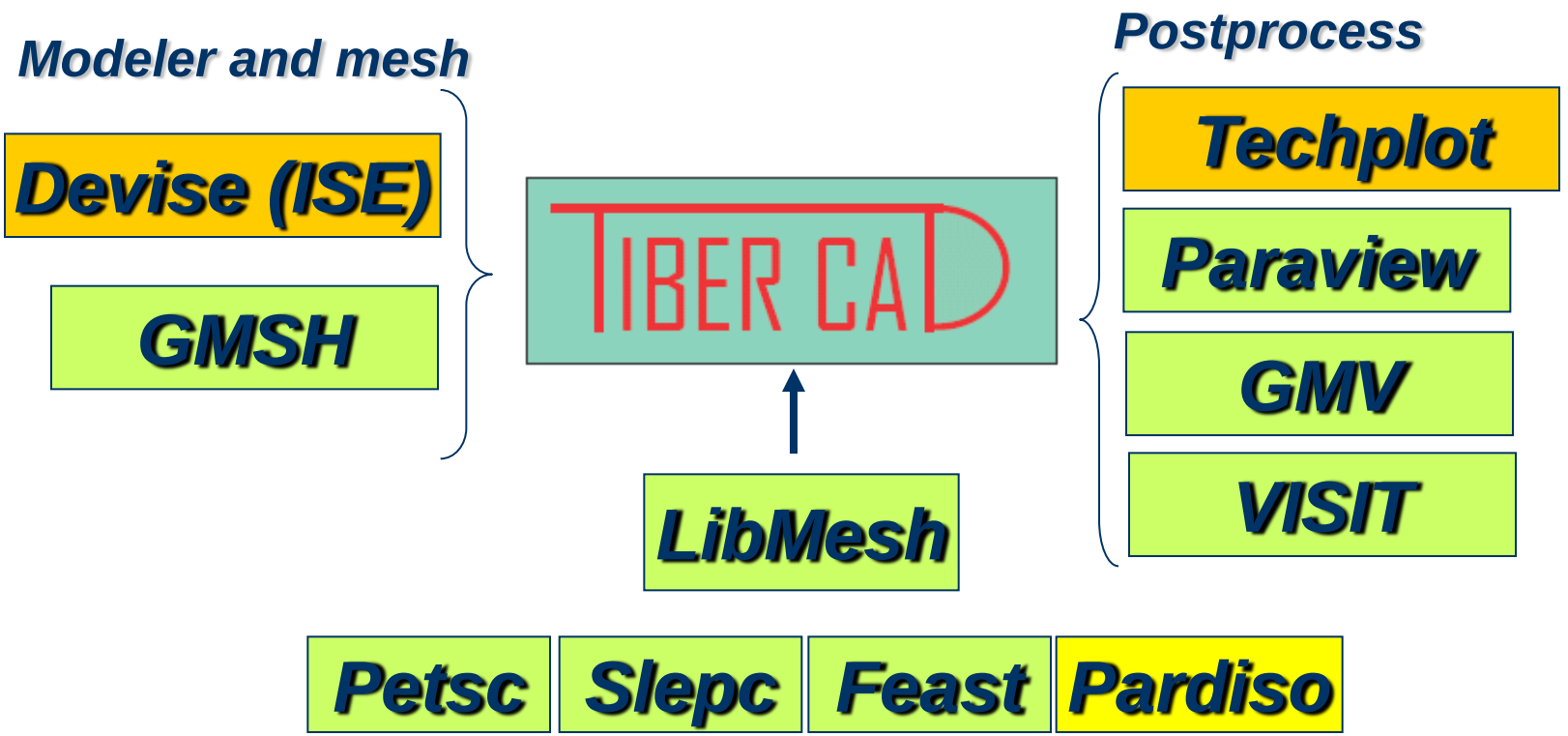
- Localized basis approach are very well suited for device simulations

- Empirical approaches (ETB)

- Aproximate DFT (DFTB)

- Full DFT (Siesta, DMOL, etc.)

TiberCAD structure



Development is done in C++ / C / Fortran in Linux, porting to other UNIX-like environments and Windows has been achieved

TiberCAD is freely downloadable at www.tibercad.org

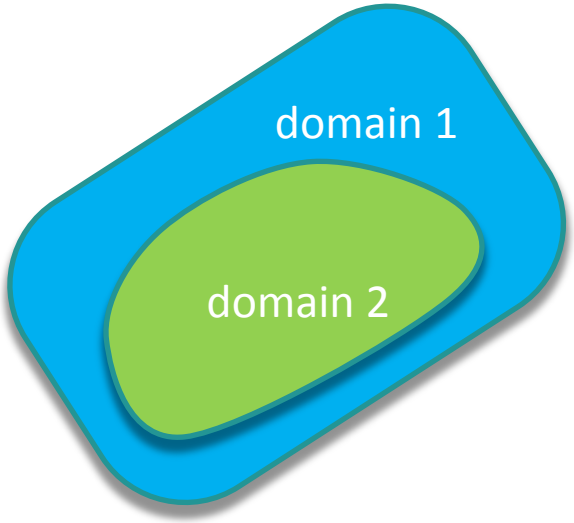
TiberCAD models

- Mechanical deformation with any kind of constrain
- Semiconductor Strain including piezoelectric effect
- Drift-Diffusion transport of electrons / holes / excitons / Ions (+ Poisson)
- Heat transport (Fourier and Boltzmann related methods)
- Quantum mechanics based with **k·p** envelope function approximation
- Empirical Tight-Binding (sp3d5s*, or any other basis)

- Classical molecular mechanics
- Atomistic description via Density Functional TB (Fraunheim/Aradi)
- *NEGF library*
- *Maxwell solver*

Multiscale methods

OVERLAP METHOD



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

BRIDGE METHOD

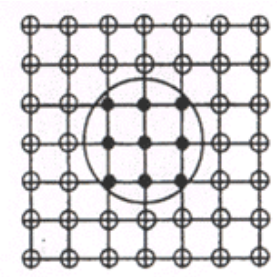
- the domains are contiguous and linked through n-1 dimensional regions.
- each domain provides boundary conditions to adjacent domains.

Multiscale simulations: BRIDGE method

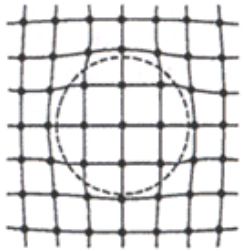
1) Strain: Continuum elasticity model and Valence force field

Continuum Elasticity model (CE)

Whenever we deal with device composed by crystals with different lattice constant, we have to deal with strain.



Lattice match



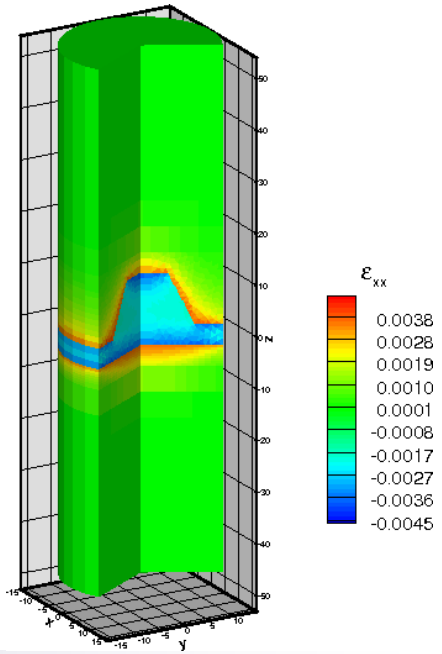
Lattice mismatch

$$\varepsilon_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)$$

$$\varepsilon_{ij}(\boldsymbol{r}) = \tilde{\varepsilon}_{ij}(\boldsymbol{r}) + \varepsilon^0_{ij}(\boldsymbol{r})$$

$$\frac{\partial}{\partial x_k}\left(C_{iklm}\varepsilon_{lm}\right) = \frac{1}{2}\frac{\partial}{\partial x_k}\left[C_{iklm}\left(\frac{\partial u_l}{\partial x_m} + \frac{\partial u_m}{\partial x_l}\right)\right] = f_i$$

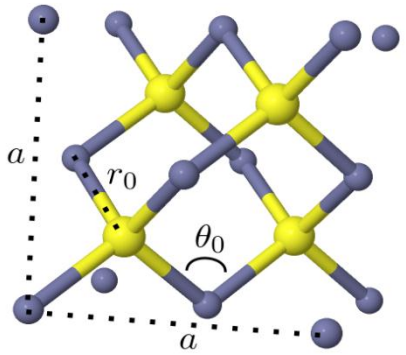
This PDE is solved with FEM technique



GaN dot in a/AlGaN nanocolumns

Valence Force Field (VFF)

We included a Keating model to calculate strain at an atomistic level



$$U = \sum_i U_{i\alpha} + U_{i\beta}$$

$$U_{i\alpha} = \sum_j \frac{3\alpha_{ij}}{16 r_{0ij}^2} \left(|\boldsymbol{r}_{ij}|^2 - r_{0ij}^2 \right)^2$$

$$U_{i\beta} = \sum_j \sum_{k \neq j} \frac{3\beta_{ijk}}{8 r_{0ij} r_{0ik}} \left(\boldsymbol{r}_{ij} \cdot \boldsymbol{r}_{ik} - r_{0ij} r_{0ik} \cos\theta_{0ijk} \right)^2$$

The equilibrium position is that one which minimizes *U*.
We use a nonlinear conjugate gradient minimization technique.

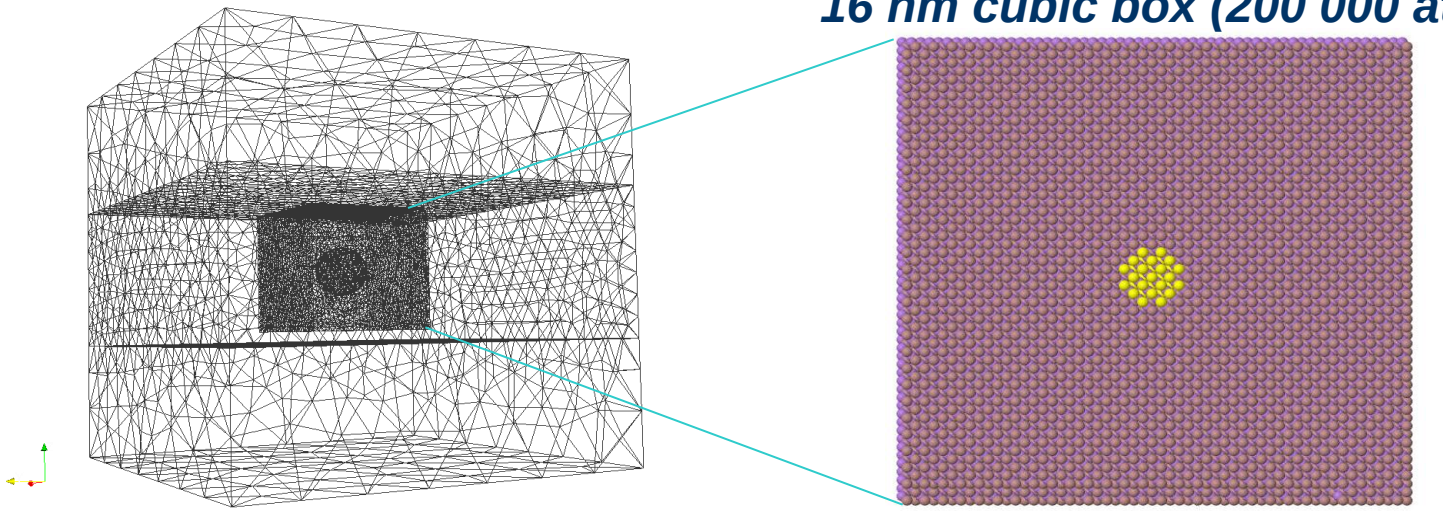
Advantages:

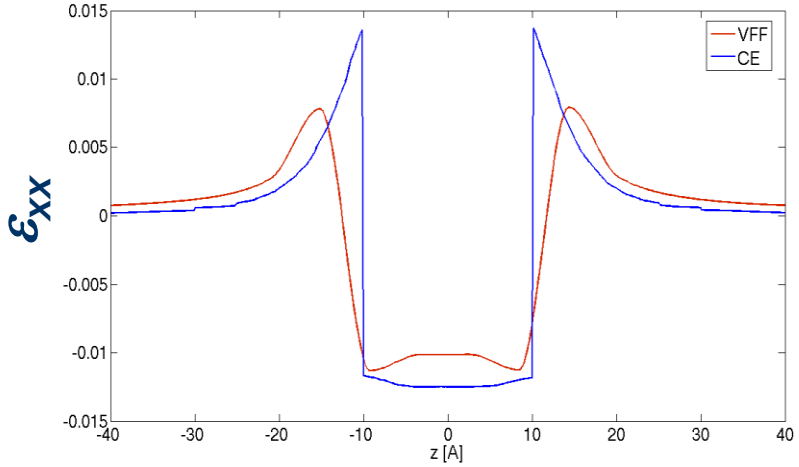
- **Most efficient atomistic technique.**
- **Description beyond effective medium (random alloy)**
- **Include internal strain**
- **More accurate for some classes of nanostructures**

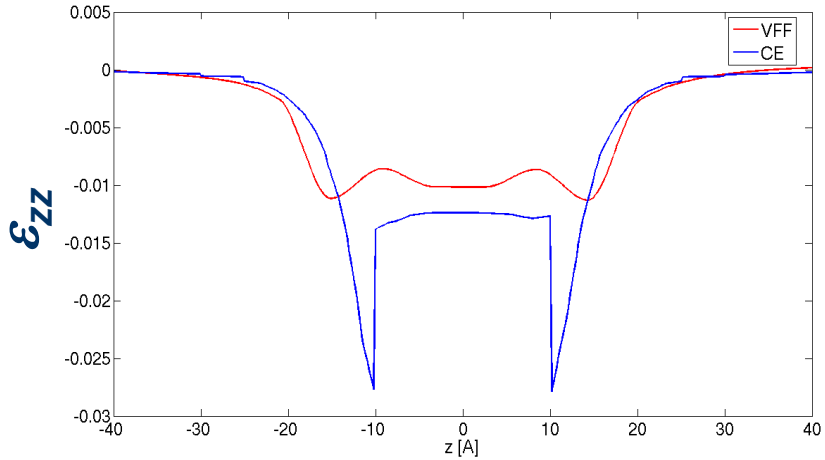
Multiscale strain: Mixing VFF and CE

Spherical InAs quantum dot in GaAs box

16 nm cubic box (200 000 atoms).

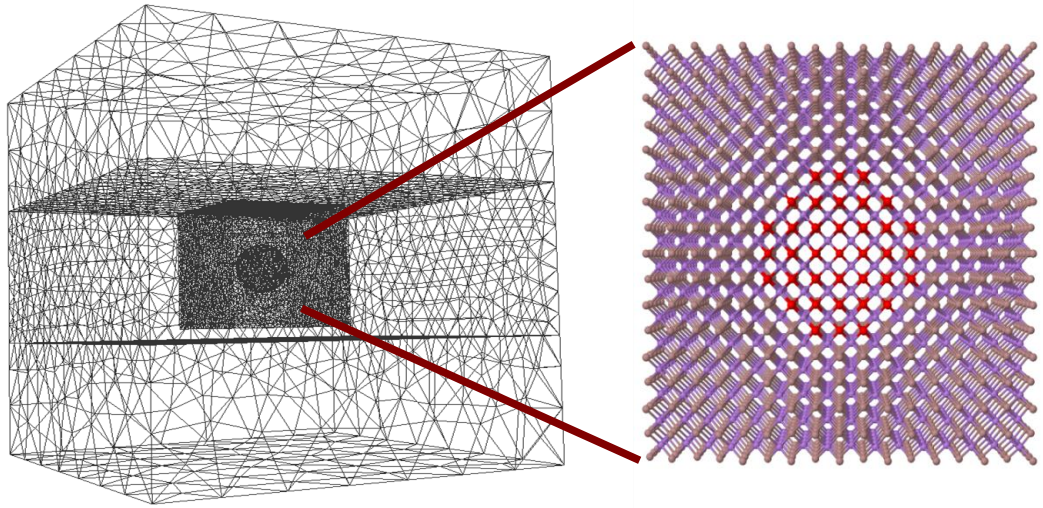






Good agreement a few nanometers outside the dot but CE fails in the Dot region. VFF is CPU demanding

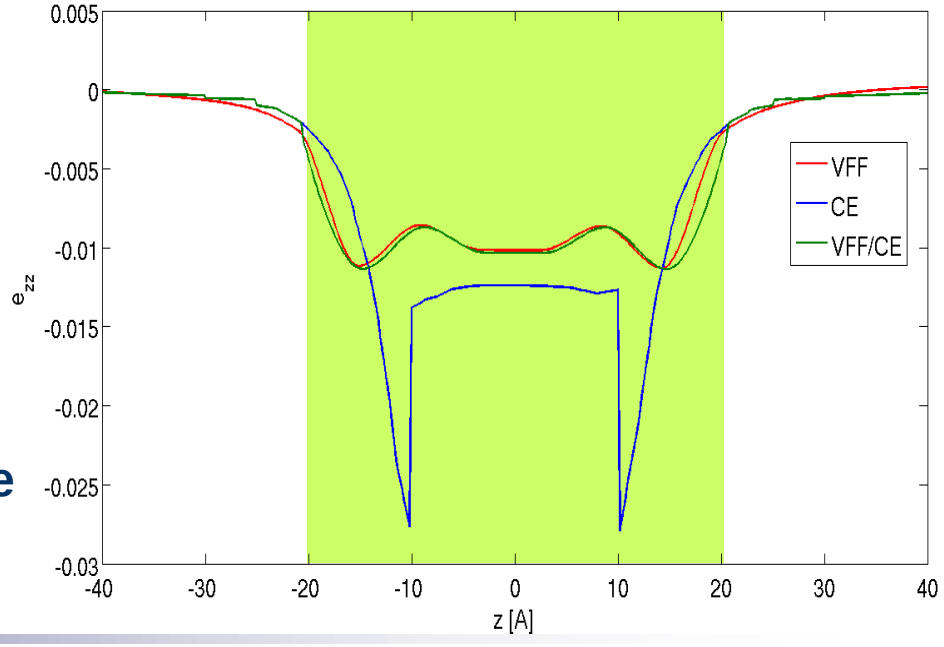
Multiscale strain



Now atomistic structure is only defined in a smaller box (4nm) with 4000 atoms

CE/VFF approach

1) **Solve CE everywhere with lattice match boundary condition at the substrate**
2) **Apply displacement to atoms**
3) **Fix external atoms as a boundary condition for VFF(bridge method)**
4) **Solve VFF in the smaller structure**
5) **Join results**



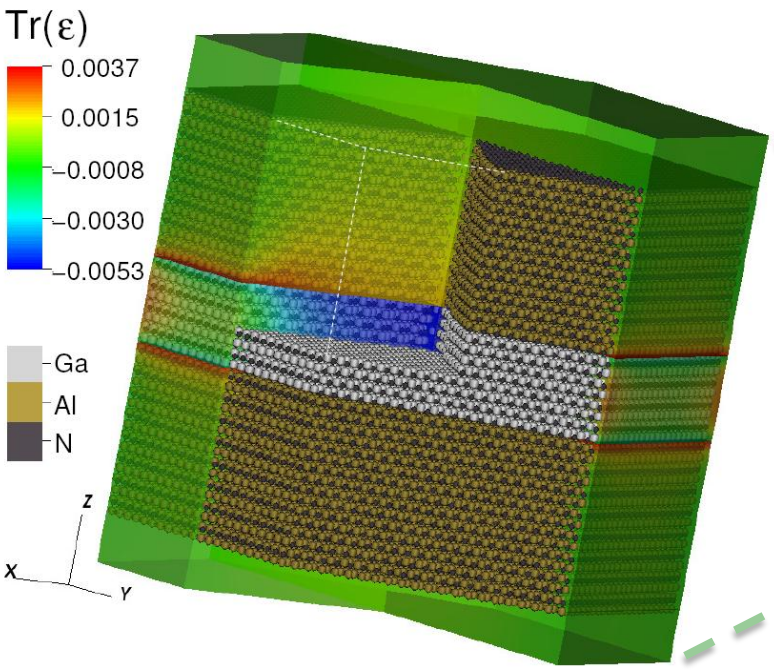
Multiscale simulations: OVERLAP method

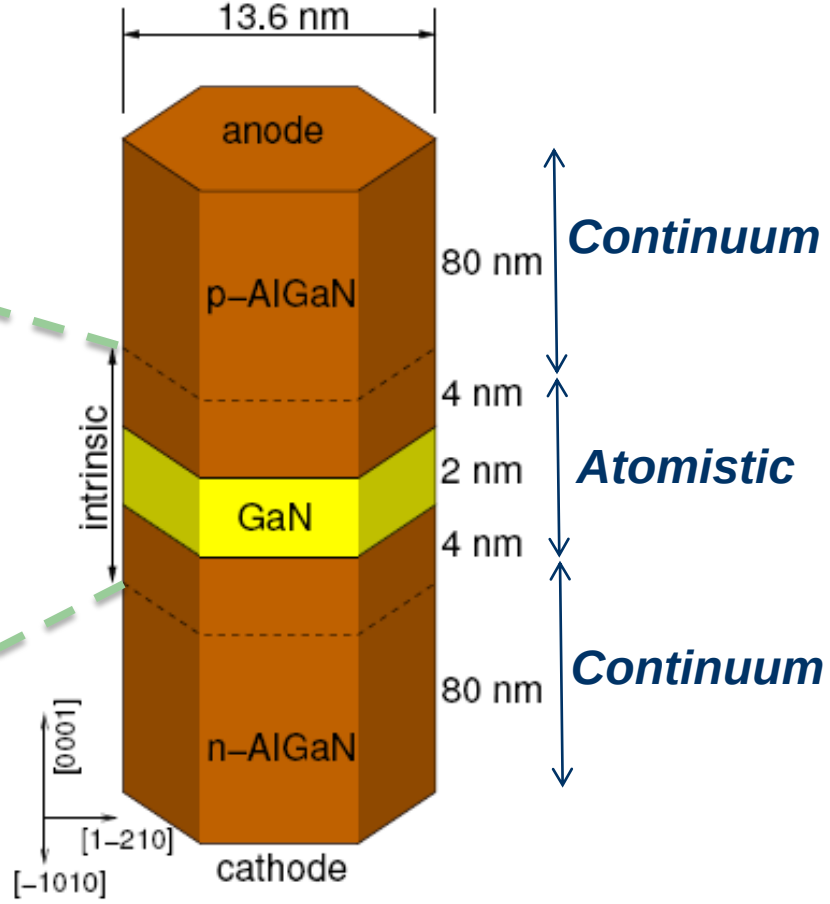
2) Nitride-based Nanorod : Drift-Diffusion, ETB and k.p

Simulation of GaN/alGaN nanowire LED

FP7-EU project SMASH

Multiscale CE/VFF Strain calculation





M. Auf der Maur IEEE TED 58, 1425 (2011)

FEM/Atomistic interaction

Strain:

Tight Binding parameters calculated according to extended 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.

$$V_i = V(r_i)$$

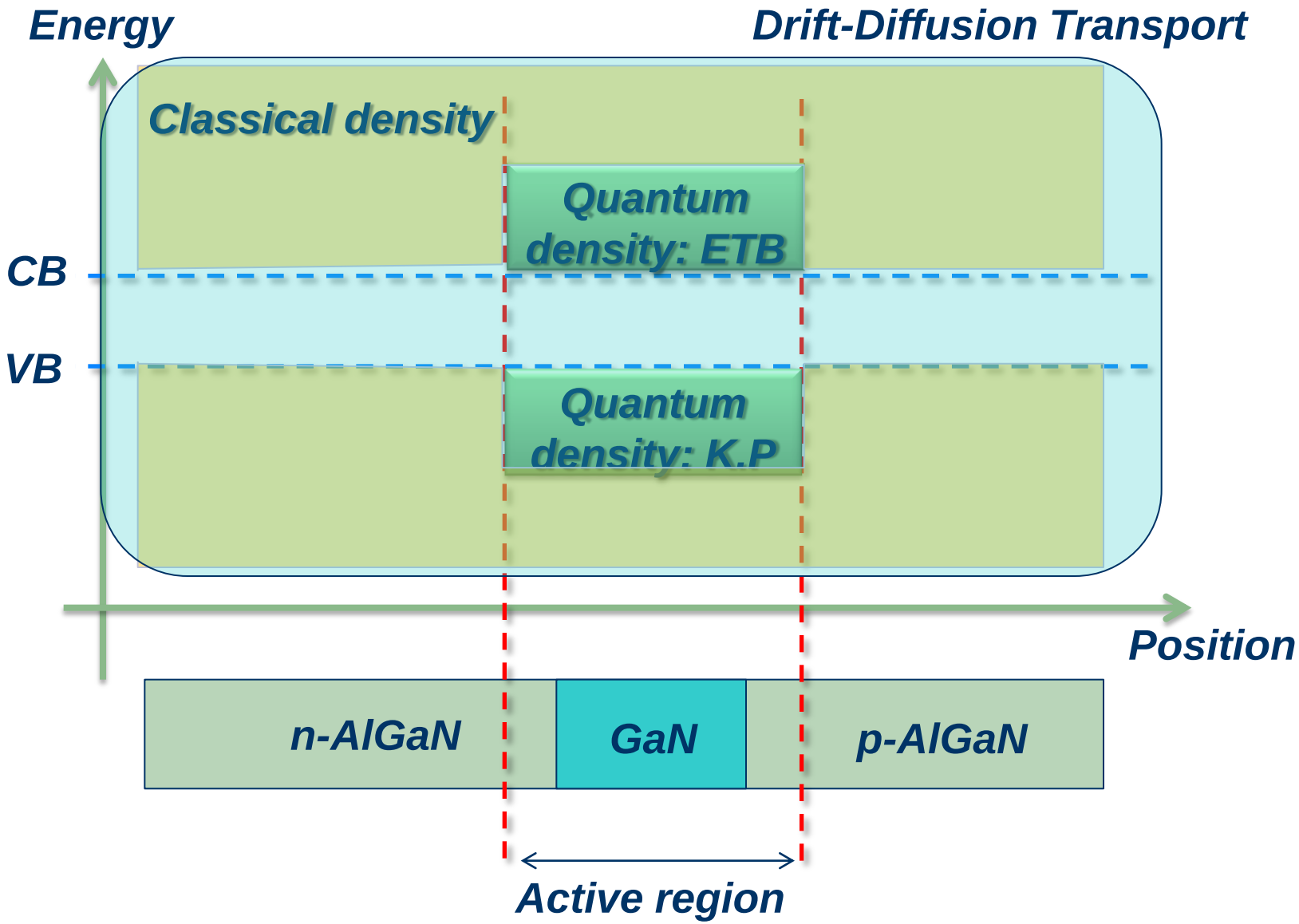
$$V_i = \frac{\tau_i^3}{8\pi} \int V(r_i) e^{-\tau |r - r_i|} dr$$

Charge:

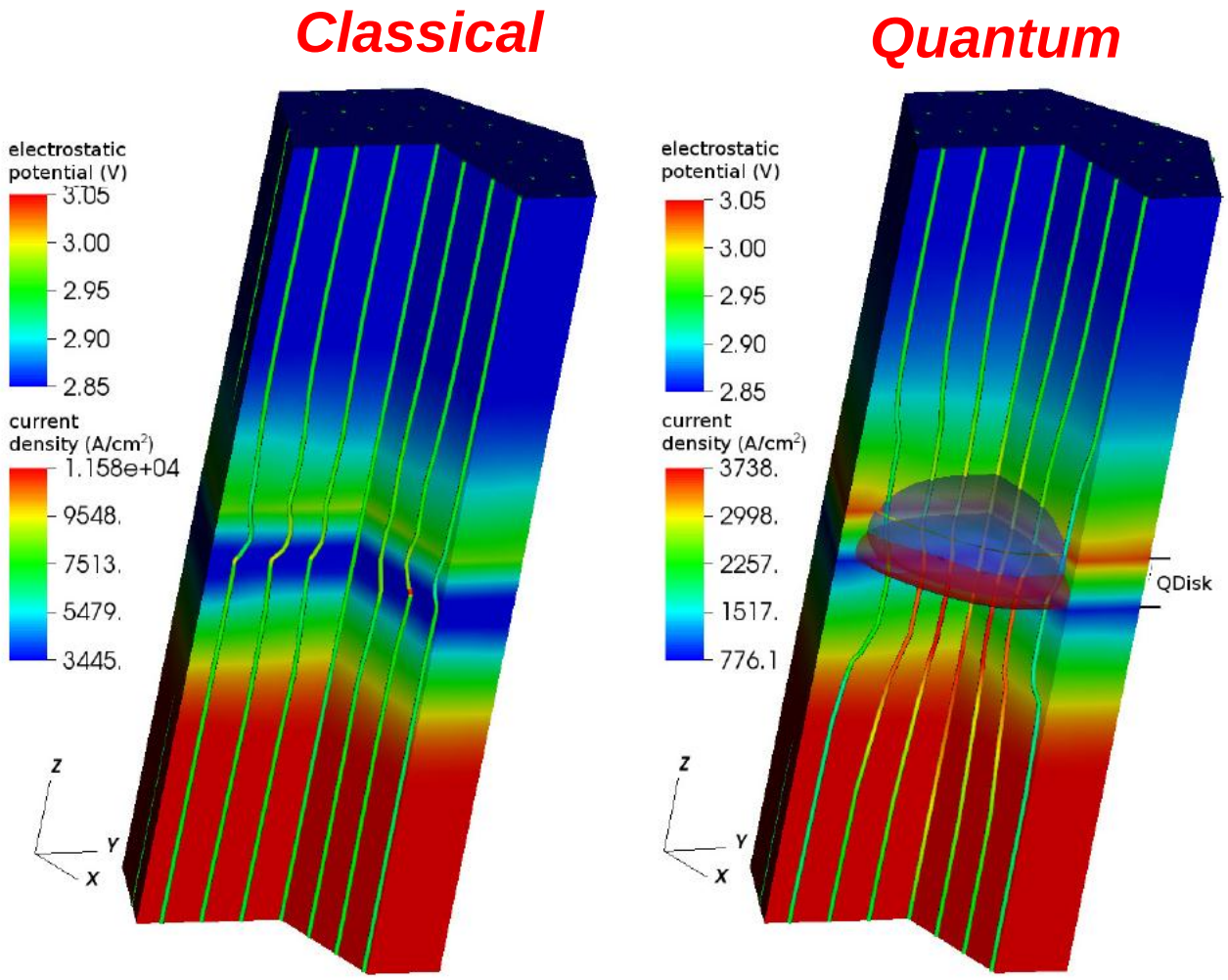
Quantum charge is projected back to FEM grid. An s-type projection with exponential decay is used.

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

Phase space and overlap Multiscale

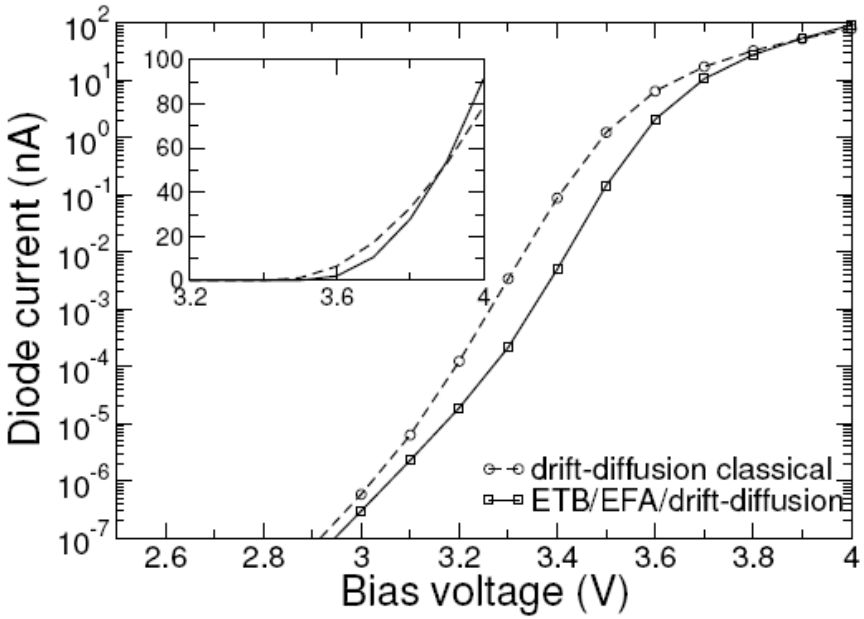


ETB/k.p/Poisson/Drift-Diffusion



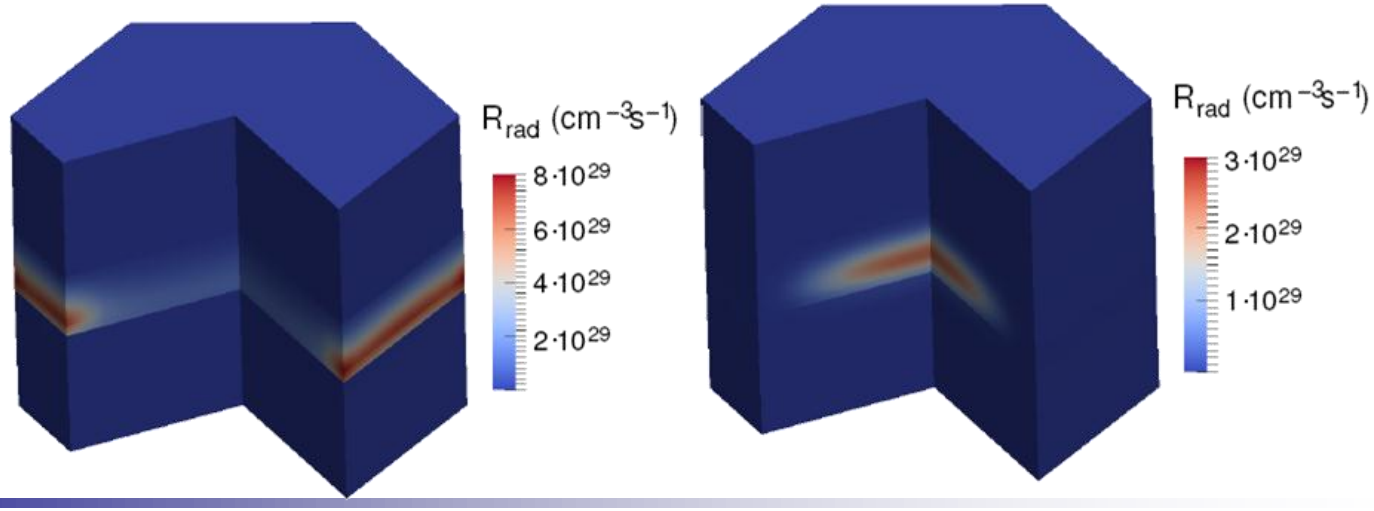
The electrostatic potential and current flow lines around the intrinsic part of the column. Classical and quantum results. The selfconsistent EFA/ETB/drift-diff. results shows also the contours of the electron and hole densities at half of the mean density inside the intrinsic region.

Current and radiative recombinations



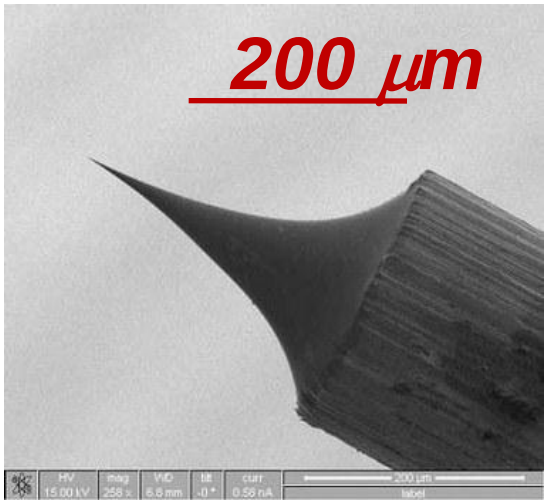
Comparisons between classical and quantum simulations shows that in classical simulations radiative recombinations originates from a region very close to the surface of the column, while using the quantum mechanical particle densities, the bulk radiative recombination rate results to be mainly concentrated at the center of the quantum disk due to the spatial confinement of the carriers.

Classical radiative recombinations ***Quantum radiative recombinations***

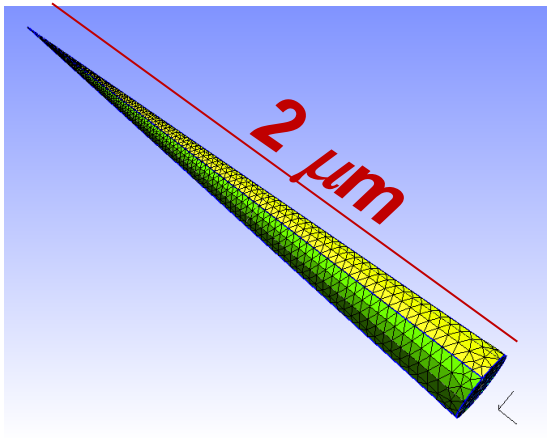


Continuum/Atomistic Modeling of STM

Tungsten STM tip

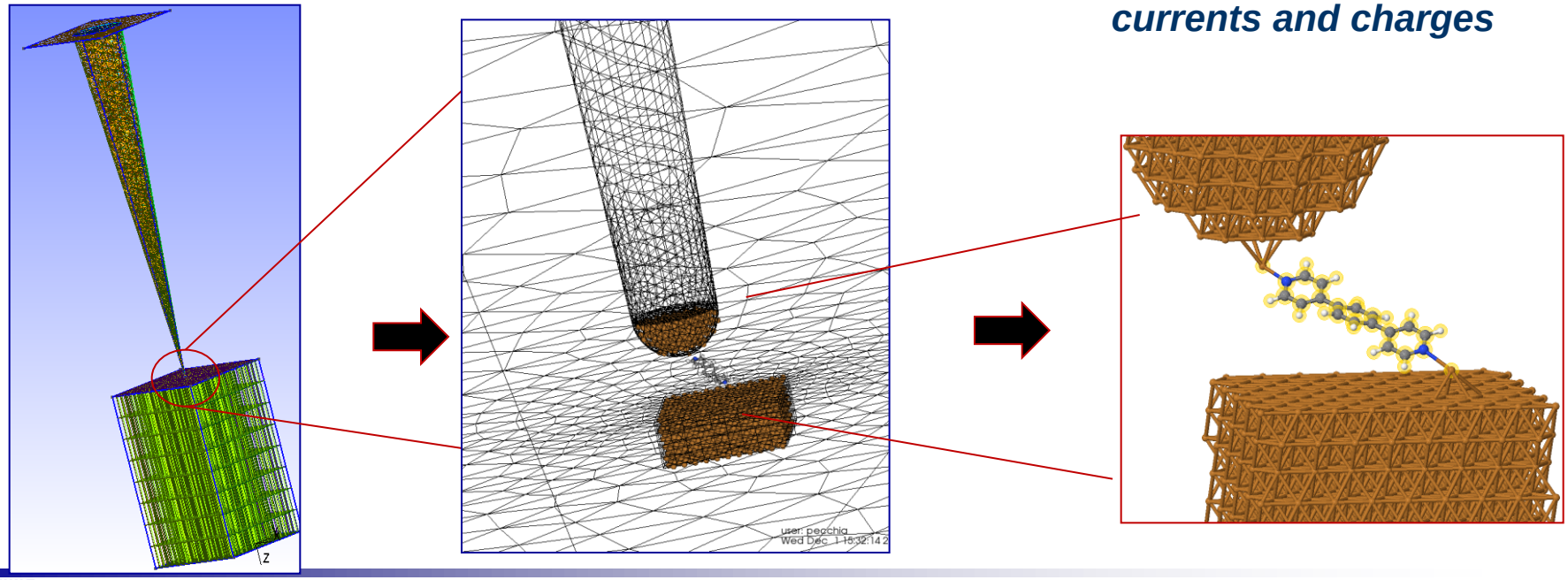


Idealized model of the tip



Here the STM tip and the probed molecule and substrated is modelled by using a multiscale FEM/atomistic approach

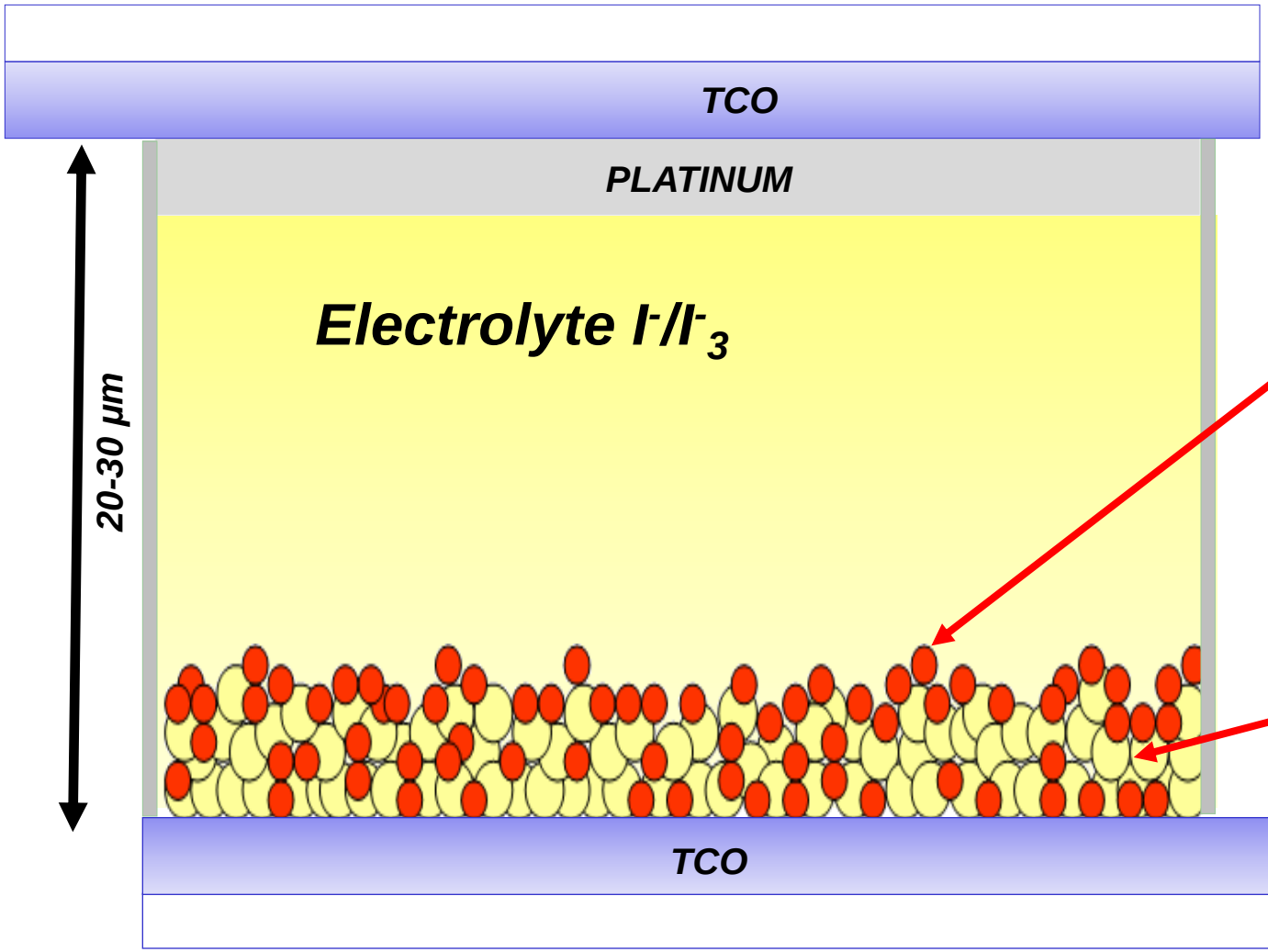
FEM domain is used to calculate potential and Fermi levels while the atomistic approach uses NEGF to obtain tunneling currents and charges

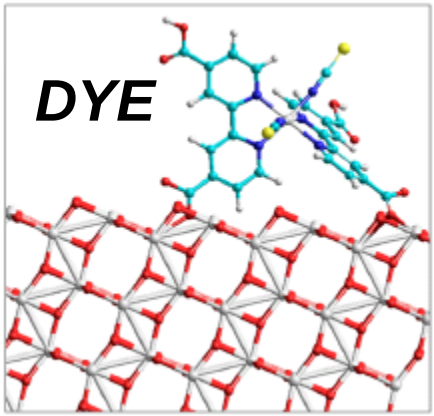


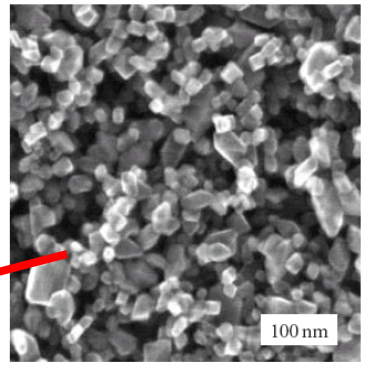
Multiphysics/Multiscale

Dye Sensitized Solar Cells (Graetzel Cells)

Scheme of a DSC

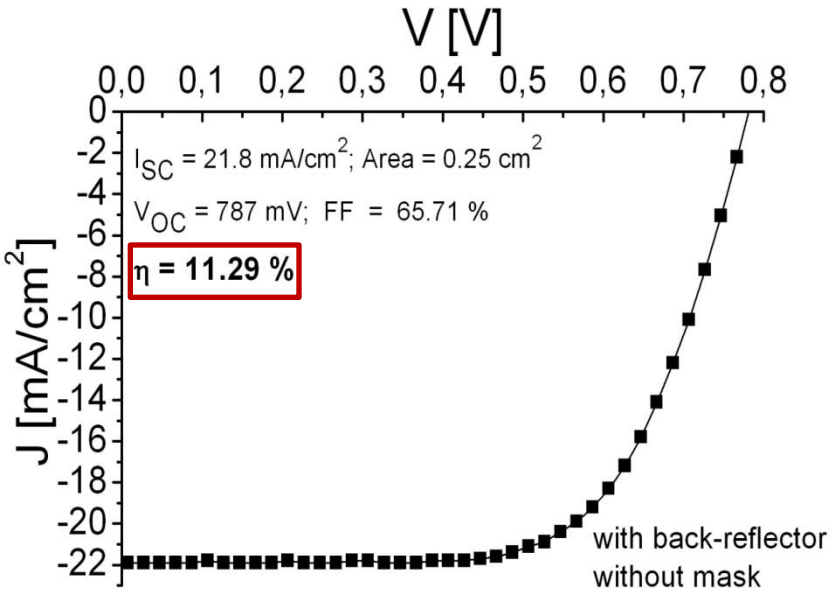


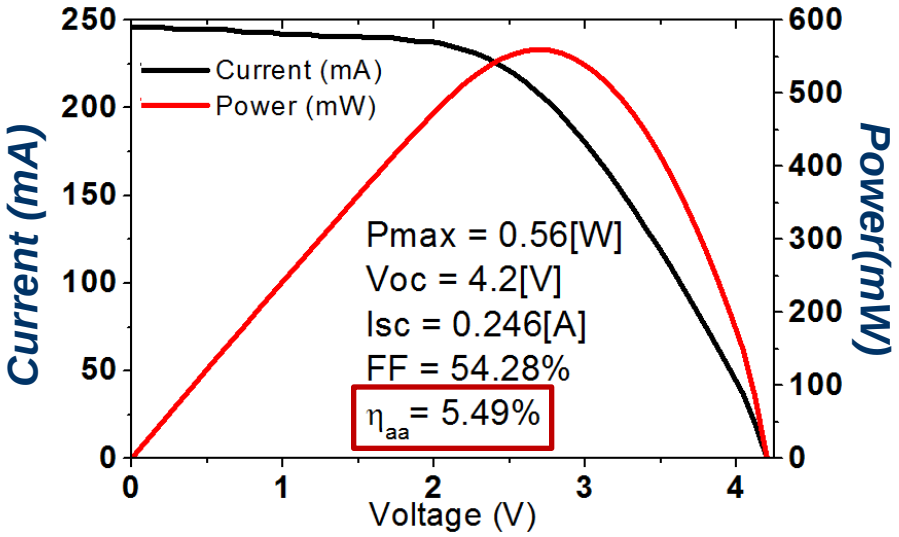


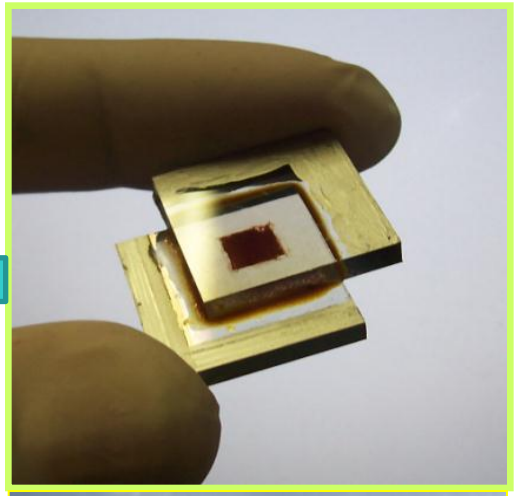


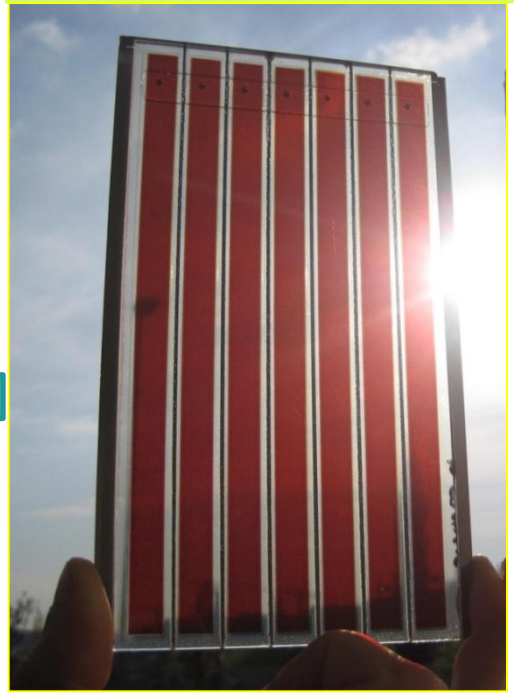
TiO2

DSC cells and modules (our exp. results)





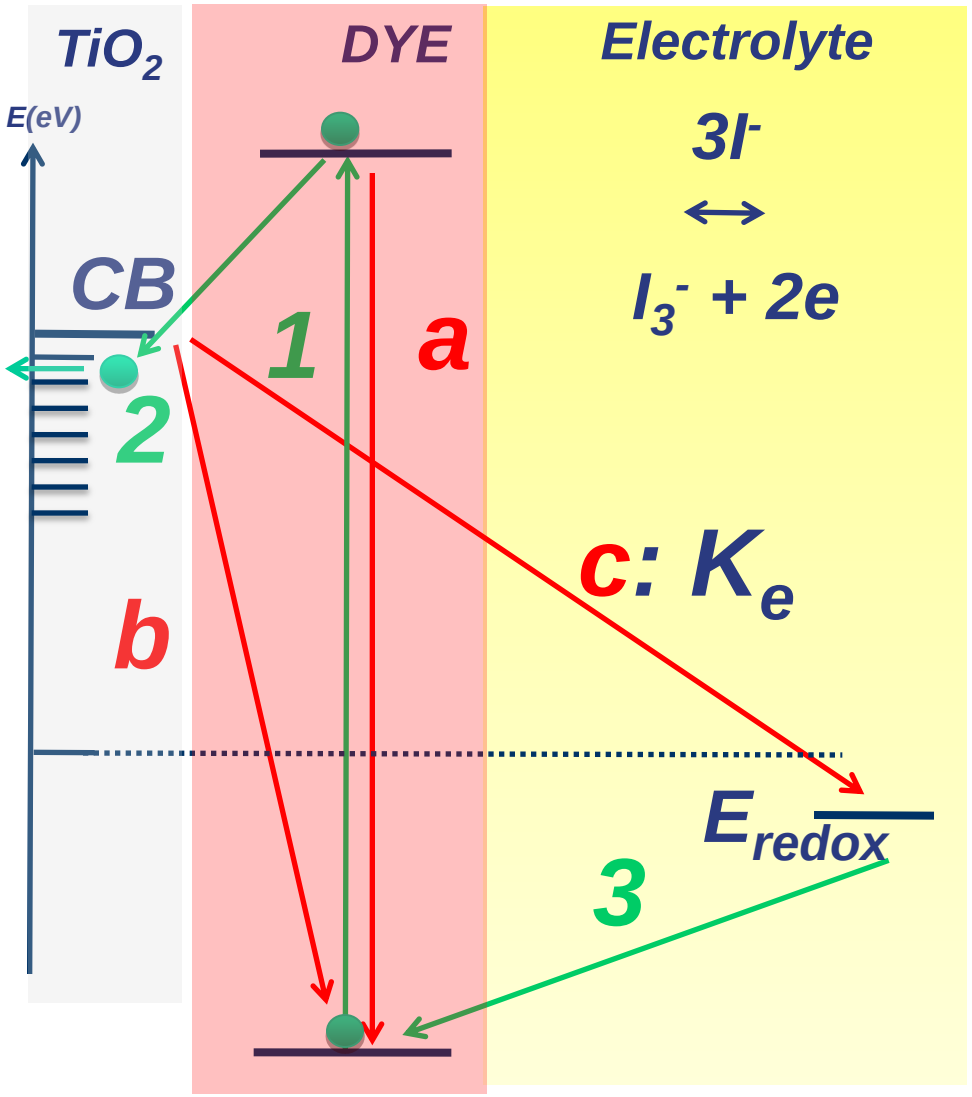




Small area

Large area

DSC Kinetic: Important rate constants

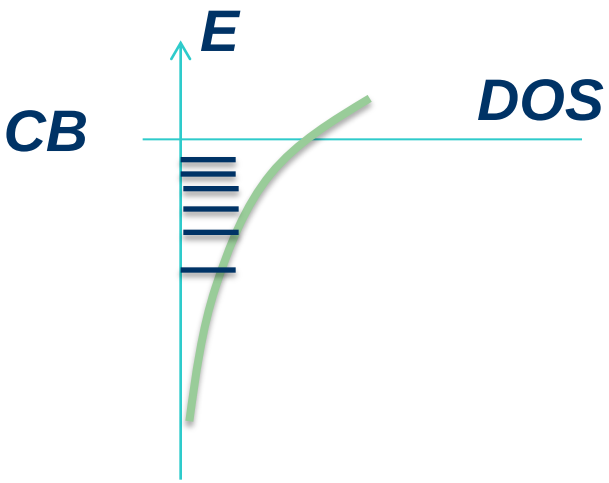


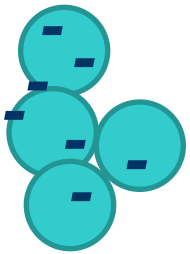
1. Dye Excitation
2. Electron Injection into TiO_2 Conduction Band
3. Oxidation of the electrolyte

a. Dye relaxes into its ground state
b. Dye regenerated by TiO_2
c. Electrolyte Reduces at TiO_2 surface

Assumptions

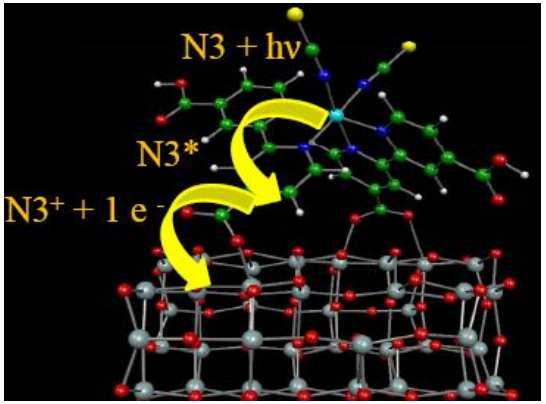
1) We assume a exponential tail of trap states in TiO2





Request (1): trap state calculation in the nanoparticle and in the cluster

2) Electro injection from Dye to TiO2 is ideal



Request (2): Simulation of the transfer dynamics also in presence of the electrolyte

Theoretical model

Cathode:

$$-e\mu_{I^-} n_{I^-} \nabla\phi_{I^-} = \frac{3}{2}\frac{V}{R_L}$$

$$-e\mu_{I_3^-} n_{I_3^-} \nabla\phi_{I_3^-} = -\frac{1}{2}\frac{V}{R_L}$$

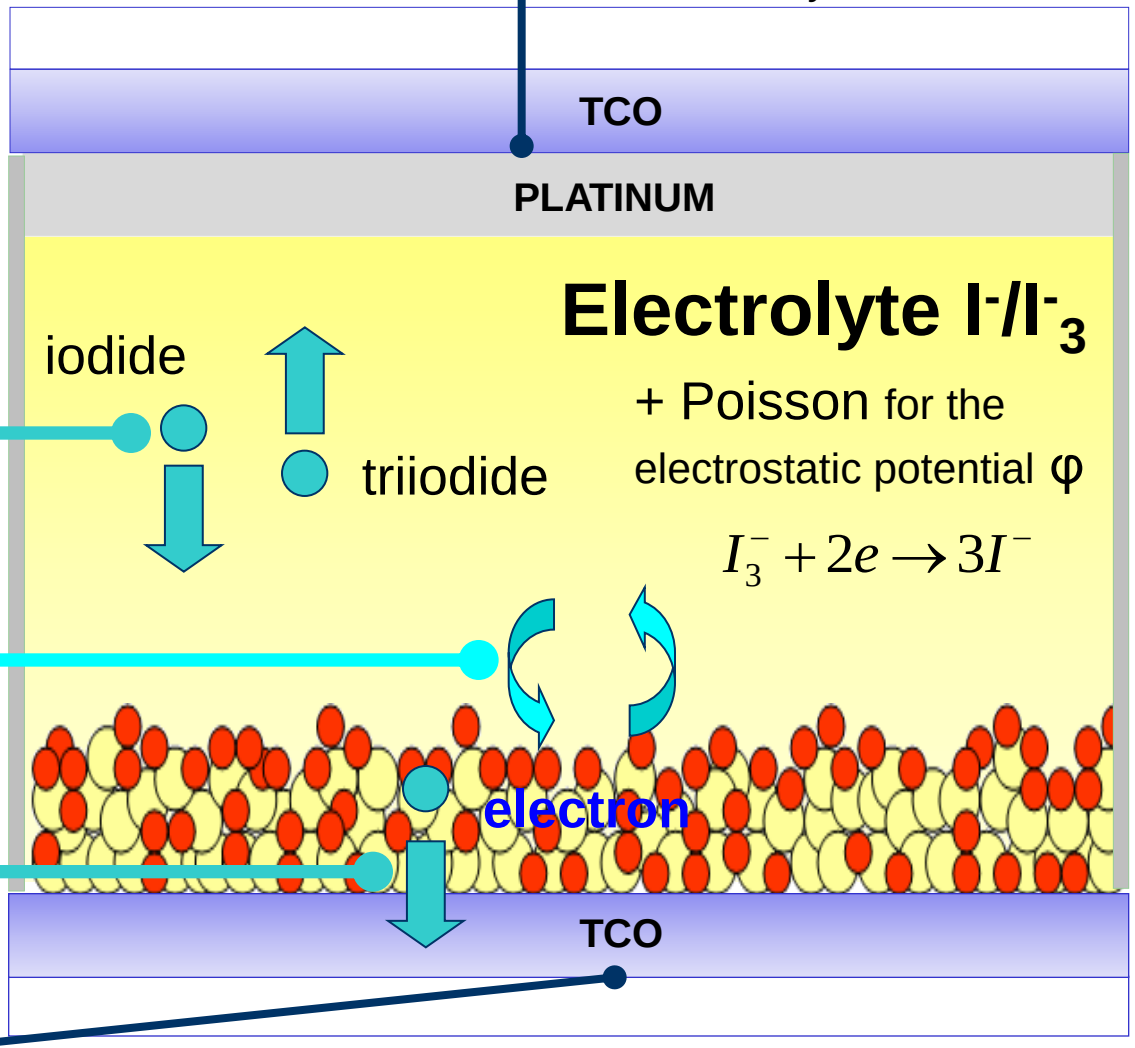
Local boundary conditions

$$\nabla\cdot\left(\mu_{I_3^-} n_{I_3^-} \nabla\phi_{I_3^-}\right) = \frac{1}{2}(R-G)$$

$$\nabla\cdot\left(\mu_{I^-} n_{I^-} \nabla\phi_{I^-}\right) = -\frac{3}{2}(R-G)$$

$$R = k_e\left[n_e^{\beta}\sqrt{\frac{n_{I_3^-}}{n_{I^-}}} - \bar{n}_e^{\beta}\sqrt{\frac{\bar{n}_{I_3^-}}{(\bar{n}_{I^-})^3}}\, n_{I^-}\right]$$

$$\nabla\cdot\left(\mu_e n_e \nabla\phi_e\right) = (R-G)$$

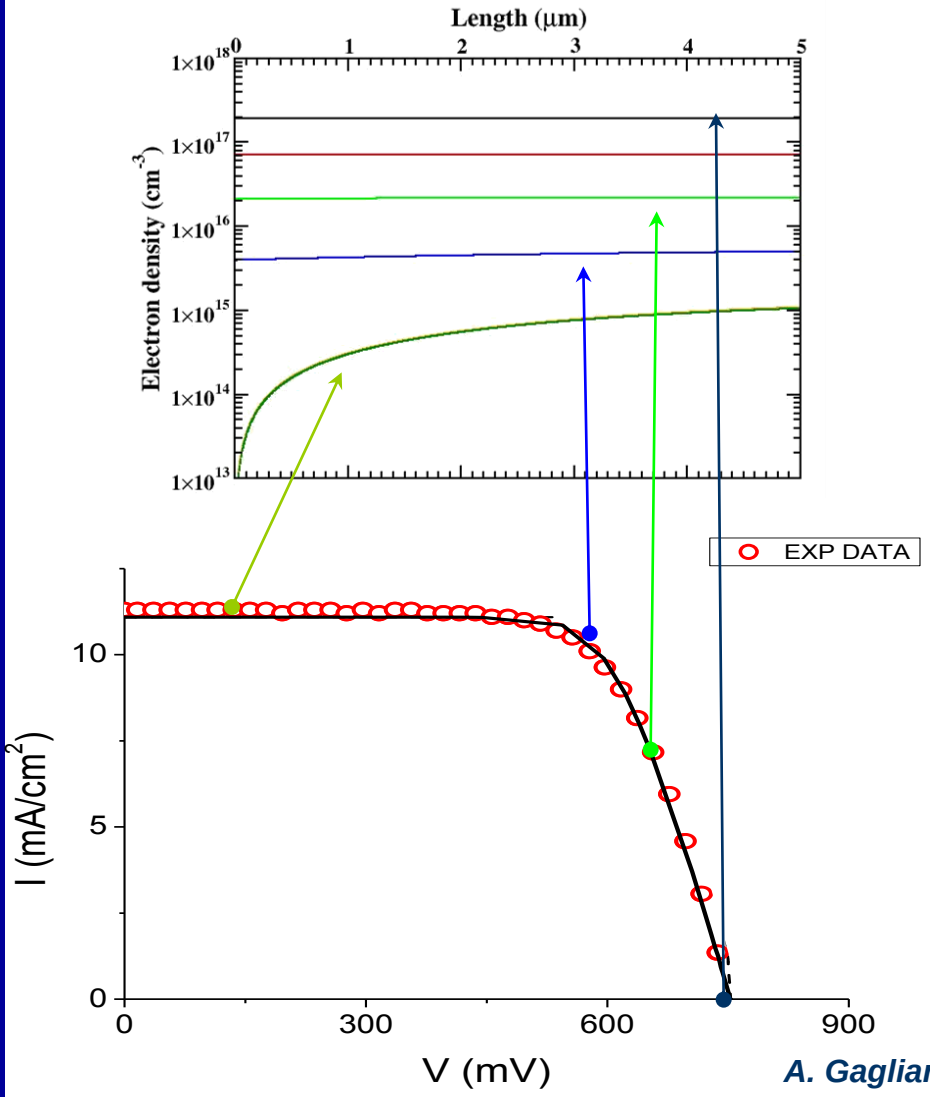


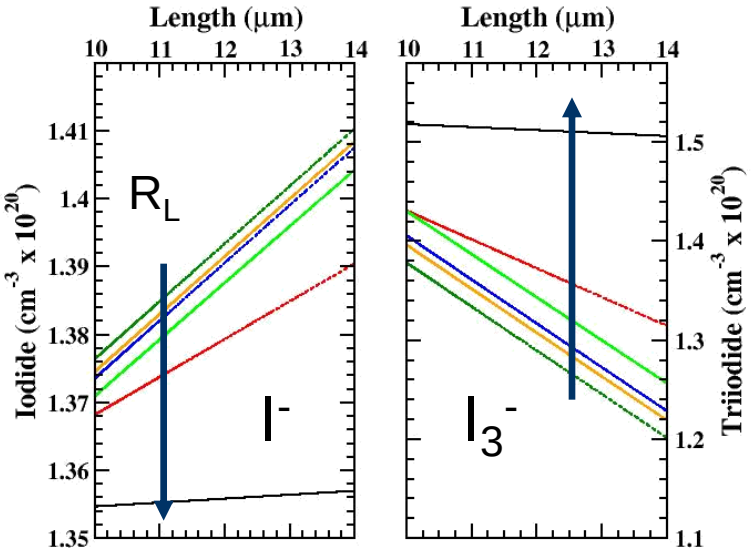
Anode:

No ionic current: $\nabla\phi_{I_3^-} = \nabla\phi_{I^-} = 0$ Ohmic contact: $\nabla\varphi = 0$

1D simulations

❖ The DSC is driven by a concentration unbalance between electrons and redox pair induced by the illumination. The drift component is negligible.





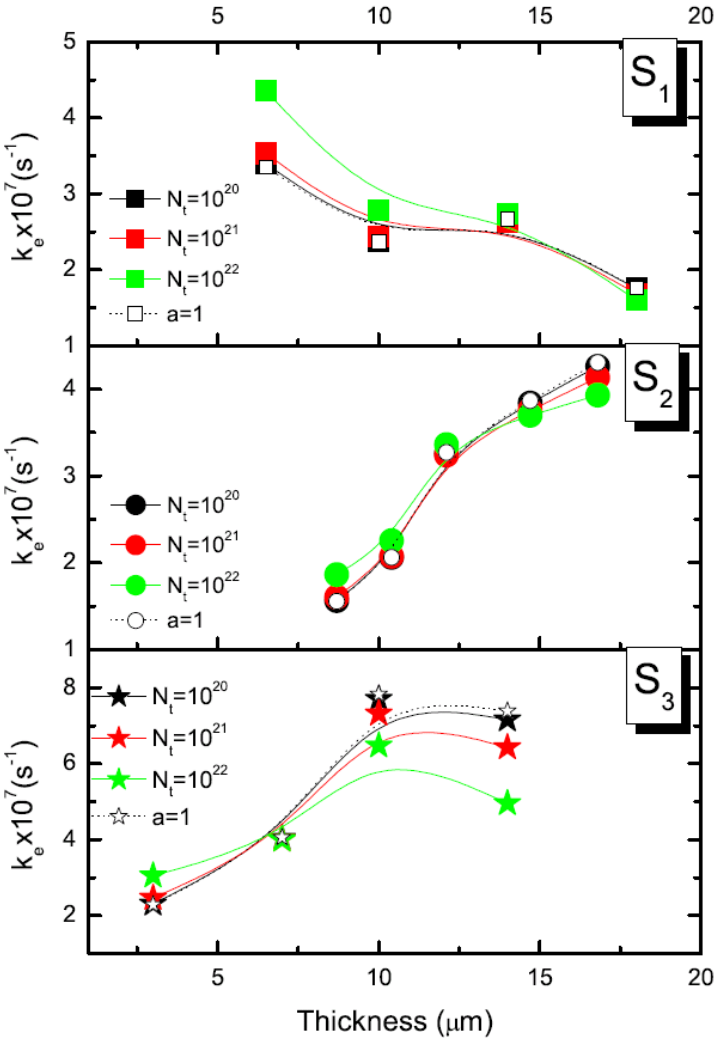
Concentration profile in the electrolyte region close to the cathode

However, μ and K_e lump to many physical process and their value is still system dependent.

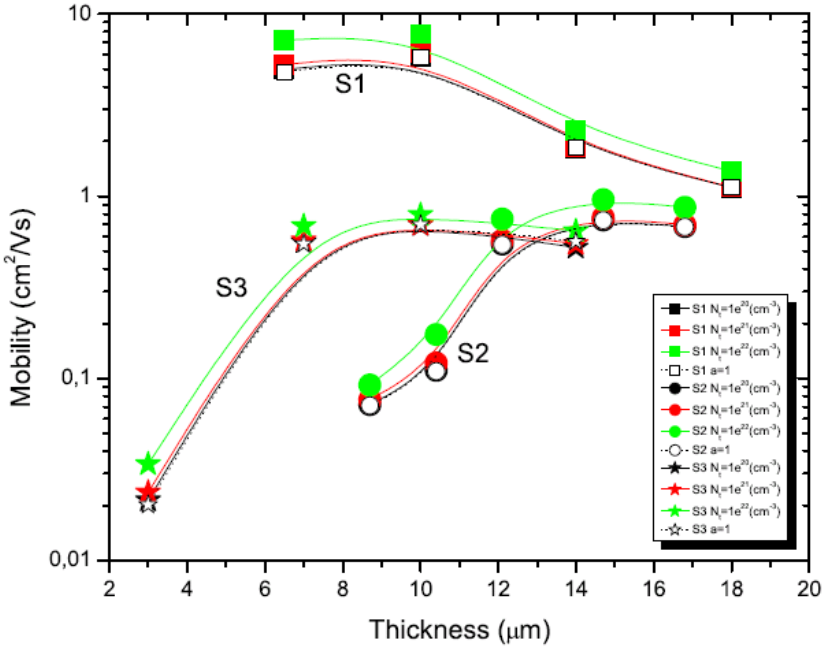
A. Gagliardi et al, IEEE J. Sel. Top. Quantum Electr. 16, 1611, 2010

Macroscopic parameters

Recombination costant



Mobility



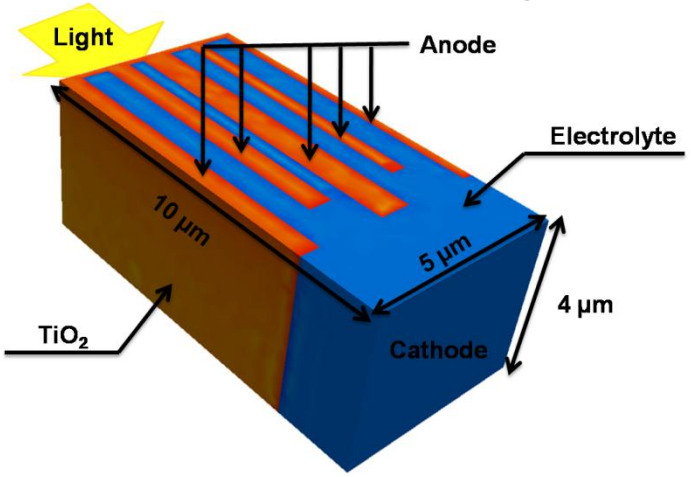
Macroscopic parameters are still device dependent:

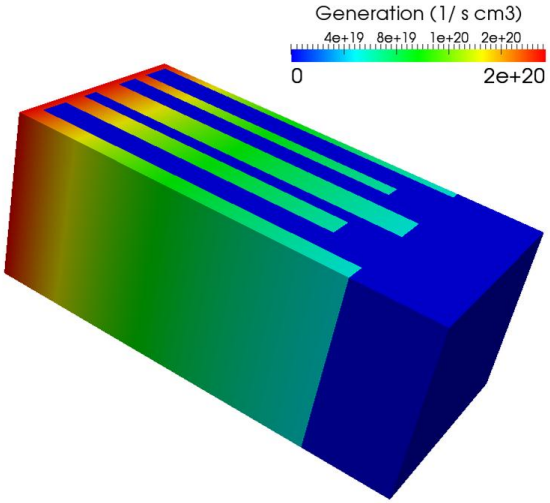
a microscopic description is required.

D. Gentilini , submitted to JPC C

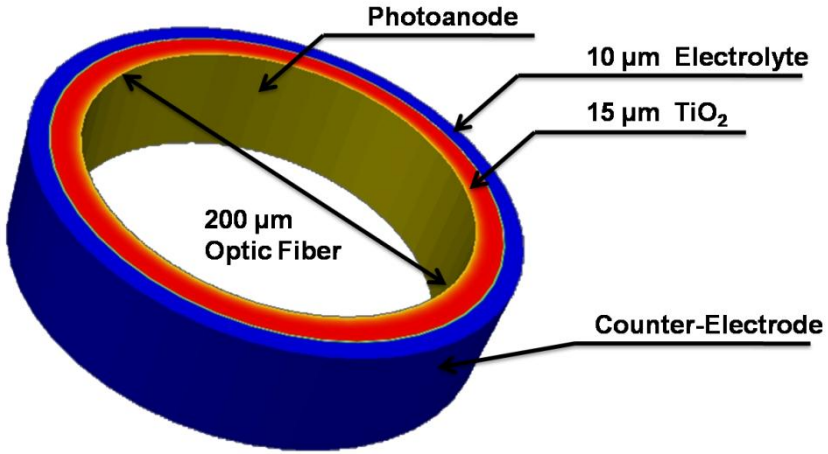
3D simulations of Dye Solar Cell

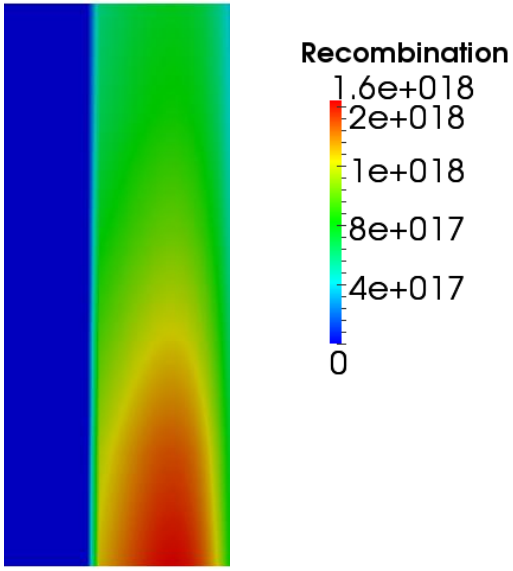
Nano/micro structured Dye Solar Cell





Fiber Dye Solar Cell





A. Gagliardi et al, IEEE Tran. Electr. Dev. 2011

Conclusions

- Multiscale/multiphysics is requested in real modern devices where different length scales models are linked together.
- TiberCAD in one of the first consistent attempt to answer this request.
- The main effort was related to the connection between models. The Multiscale infrastructure has been defined.
- But … we are just at the beginning, much effort is still needed.
- Next: NEGF library to perform nice Drift-Diffusion / NEGF simulations etc. etc.

Additional details at http://www.tibercad.org