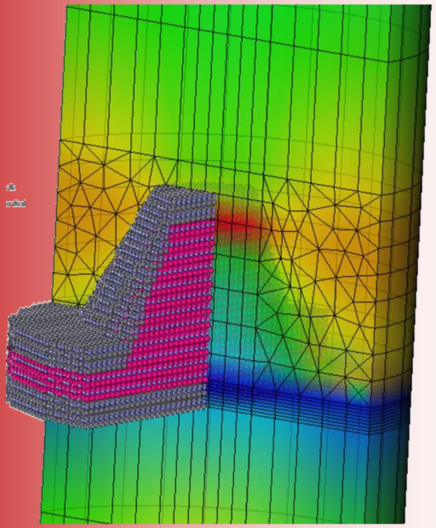
An overview of the TiberCAD capabilities

Alessandro Pecchia



CNR - ISMN ***Institute for Nanostructured Materials***

University of Roma "Tor Vergata"

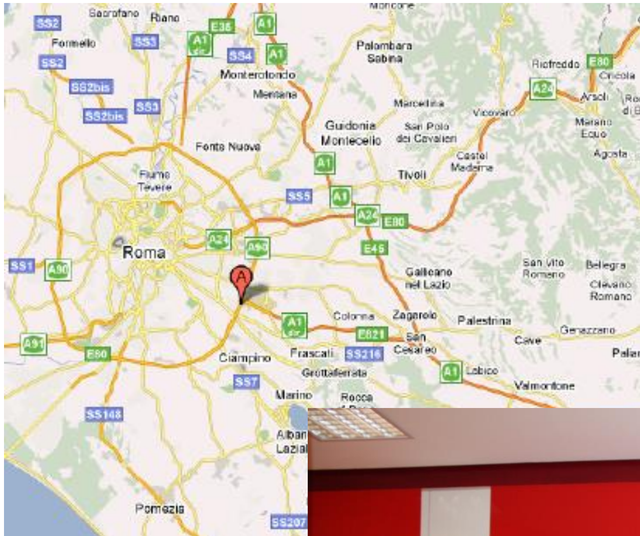
M. Auf der Maur, G. Penazzi, F. Sacconi, G. Romano

A Gagliardi, F. Santoni, A. Di Carlo

Tiber…

Optolab group

University of 'Tor Vergata'
is the second University in Rome



OptoLab group

TiberCAD people

Prof. Aldo Di Carlo

Dr. A. Pecchia

Dr. M. Auf der Maur

tiberCAD

Multiscale Device Simulator

http://www.tiberlab.com

Dr. A. Gagliardi

Dr. F. Sacconi

Mr. F. Santoni

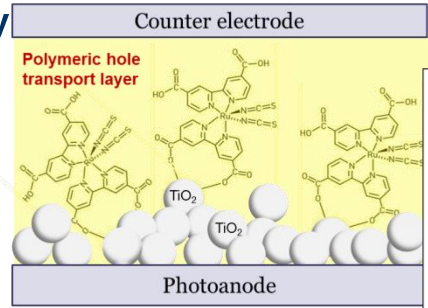
Dr. G. Romano

Dr. G. Penazzi

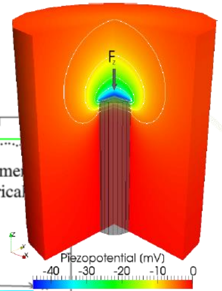
Mr. W. Rodrigues

Applications

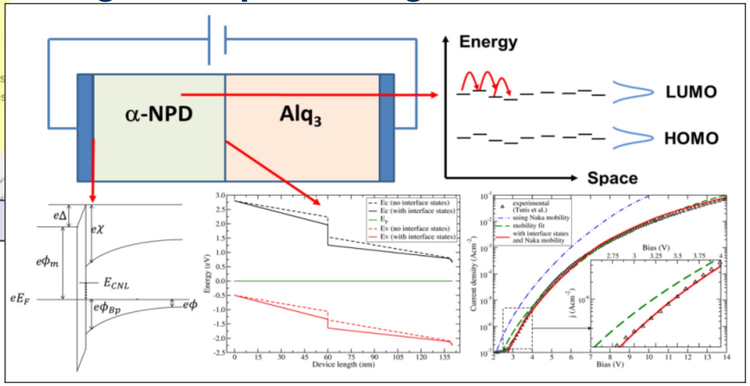
DSSC/OPV module



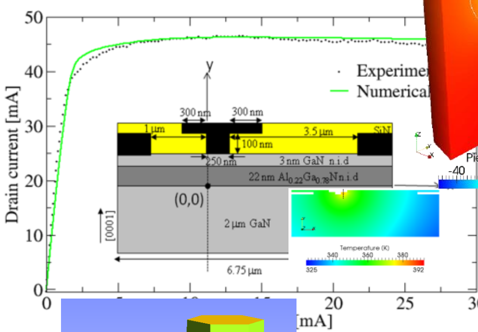
Piezoelectricity

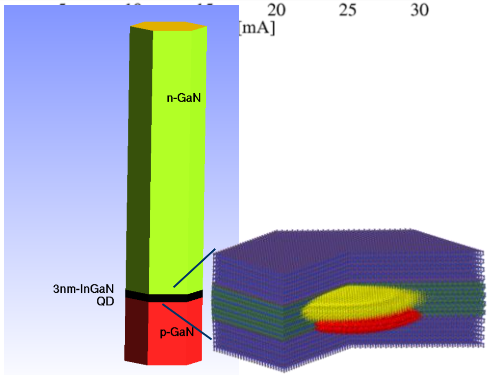


Charge transport in organic semiconductors

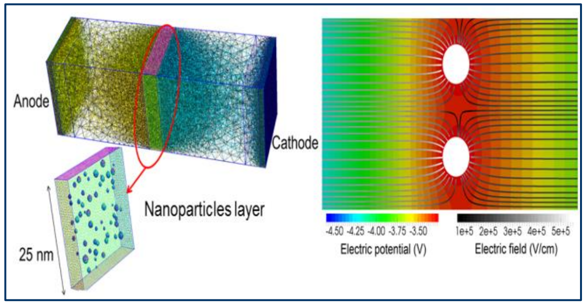


Heat dissipation

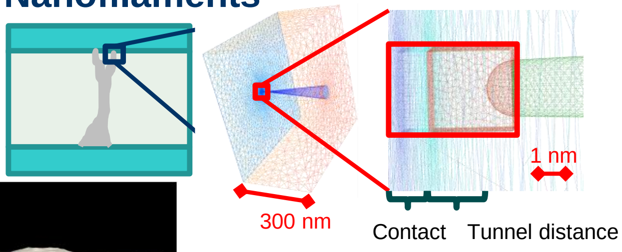




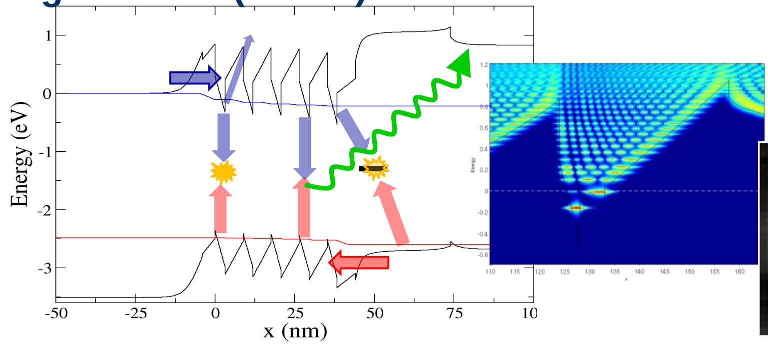
Memristors



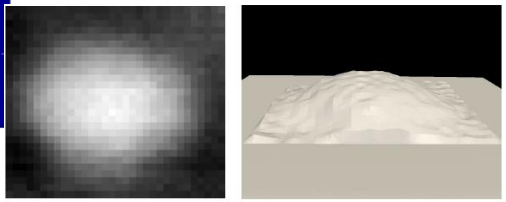
Nanofilaments



Inorganic LED (InGaN)

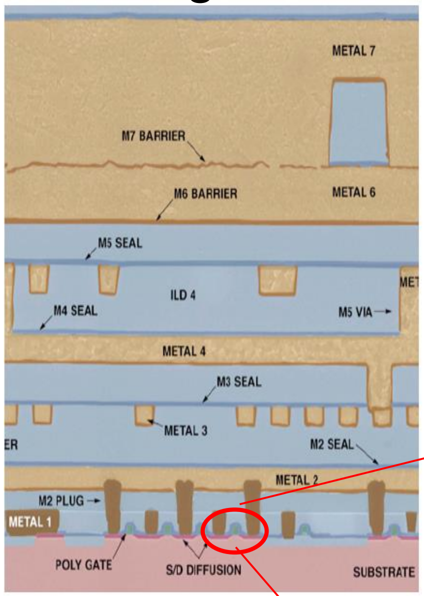


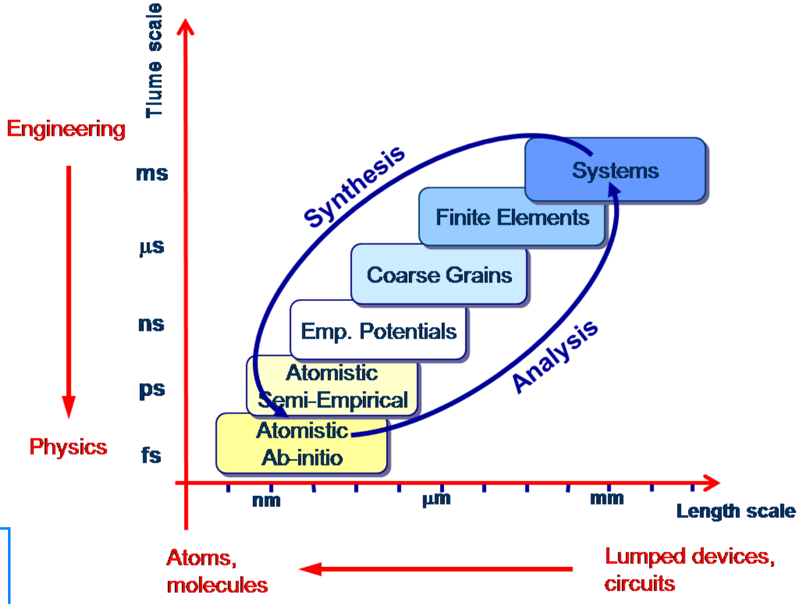
Quantum DOTs



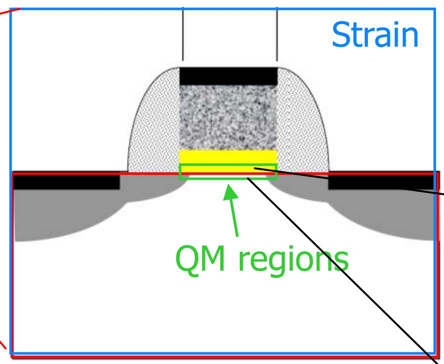
Different physical models on different scales are needed to describe electronic devices

Package Level

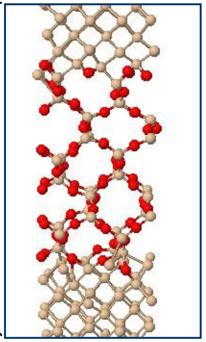




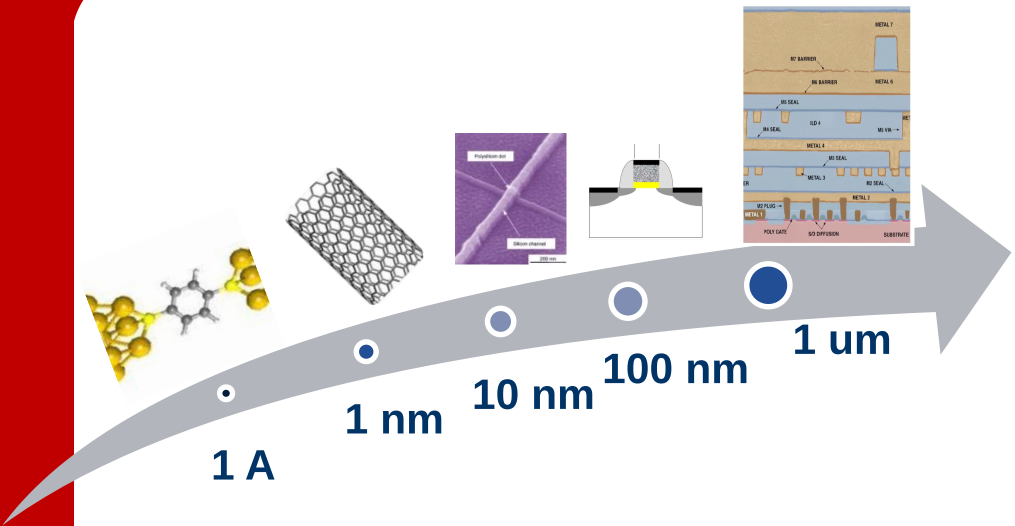
Device Level

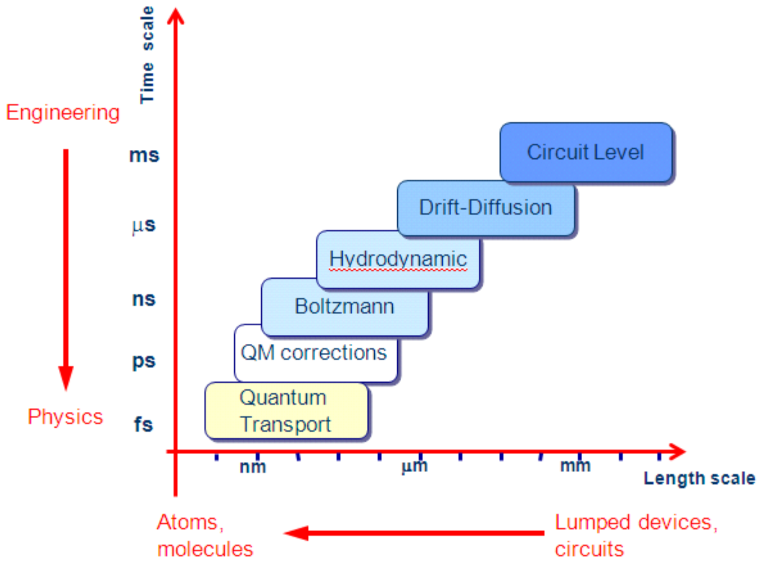


Atomistic Level



Introduction: TiberCAD



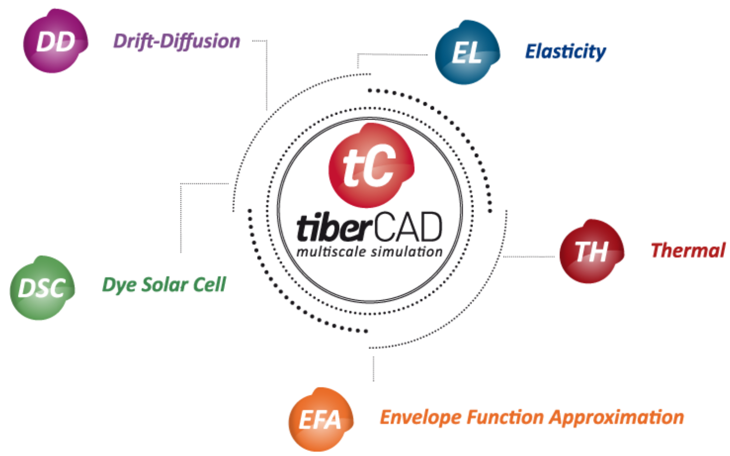


Features:

drift diffusion, strain, thermal, EFA

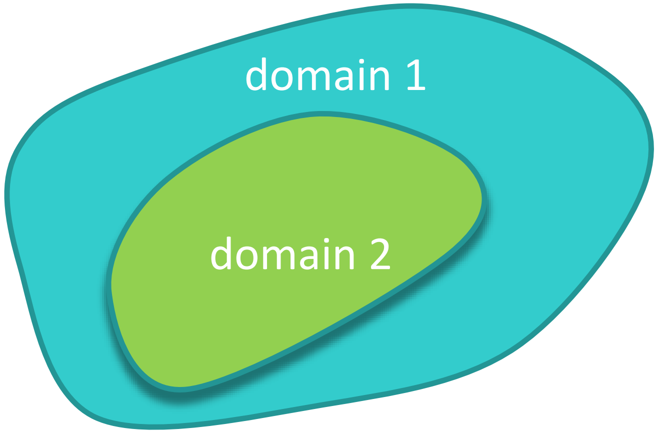
VFF, ETB, DFTB

Organics, DSSC modelling.



Multiscale/multiphysics schemes

OVERLAP METHOD



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

Schrödinger/Poisson

Transport parameters from DFT

BRIDGE METHOD

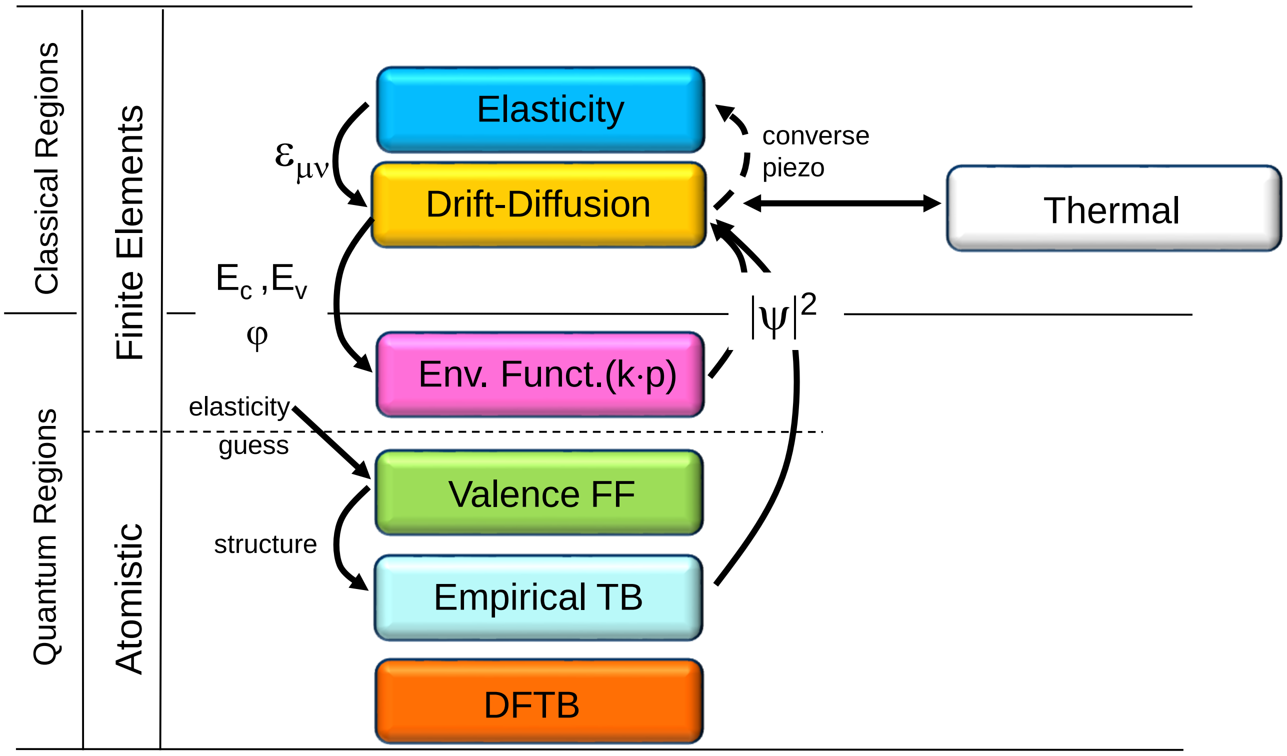
- each domain provides boundary conditions to adjacent domains.

NEGF/drift-diffusion

VFF/continuous elasticity

M. Auf der Maur, G. Penazzi , G. Romano, F. Sacconi, , A. Pecchia , A. Di Carlo
IEEE Trans. Electron Devices, 58, 1425 (2011)

Models overview

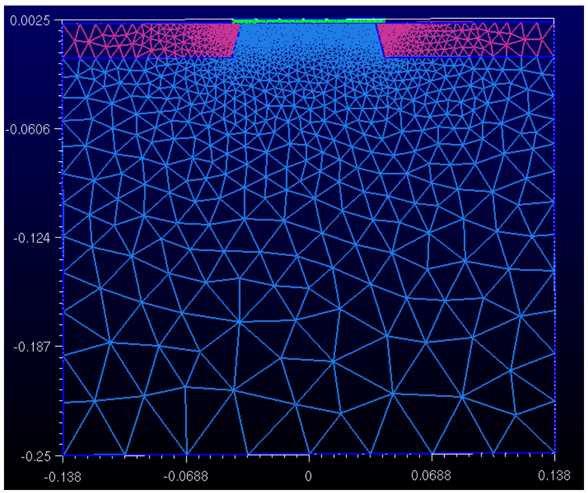


General Structure

GMSH

Device Modelling

Mesh Generation



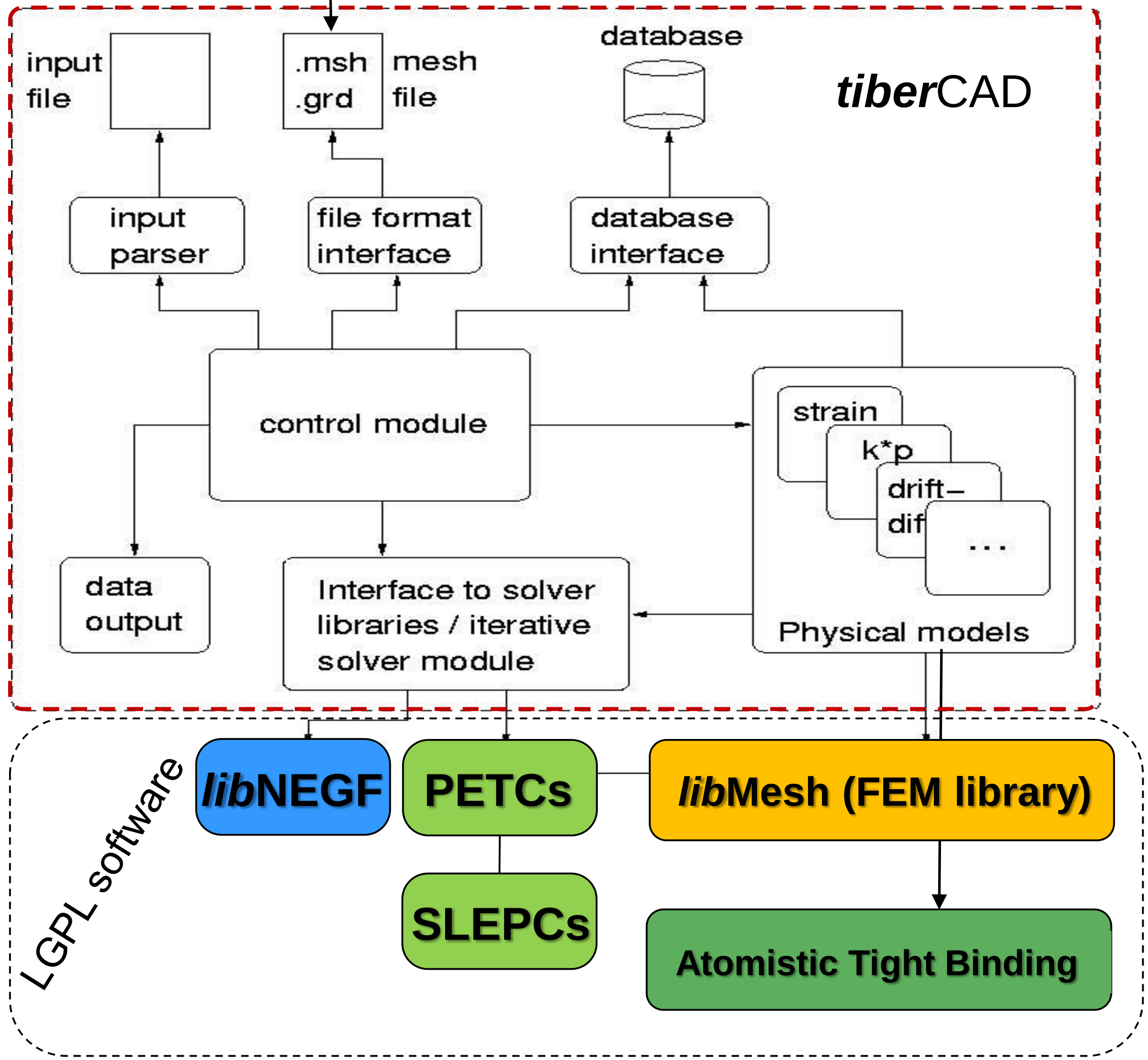
GPL software

Proprietary GUI/CAD/mesher

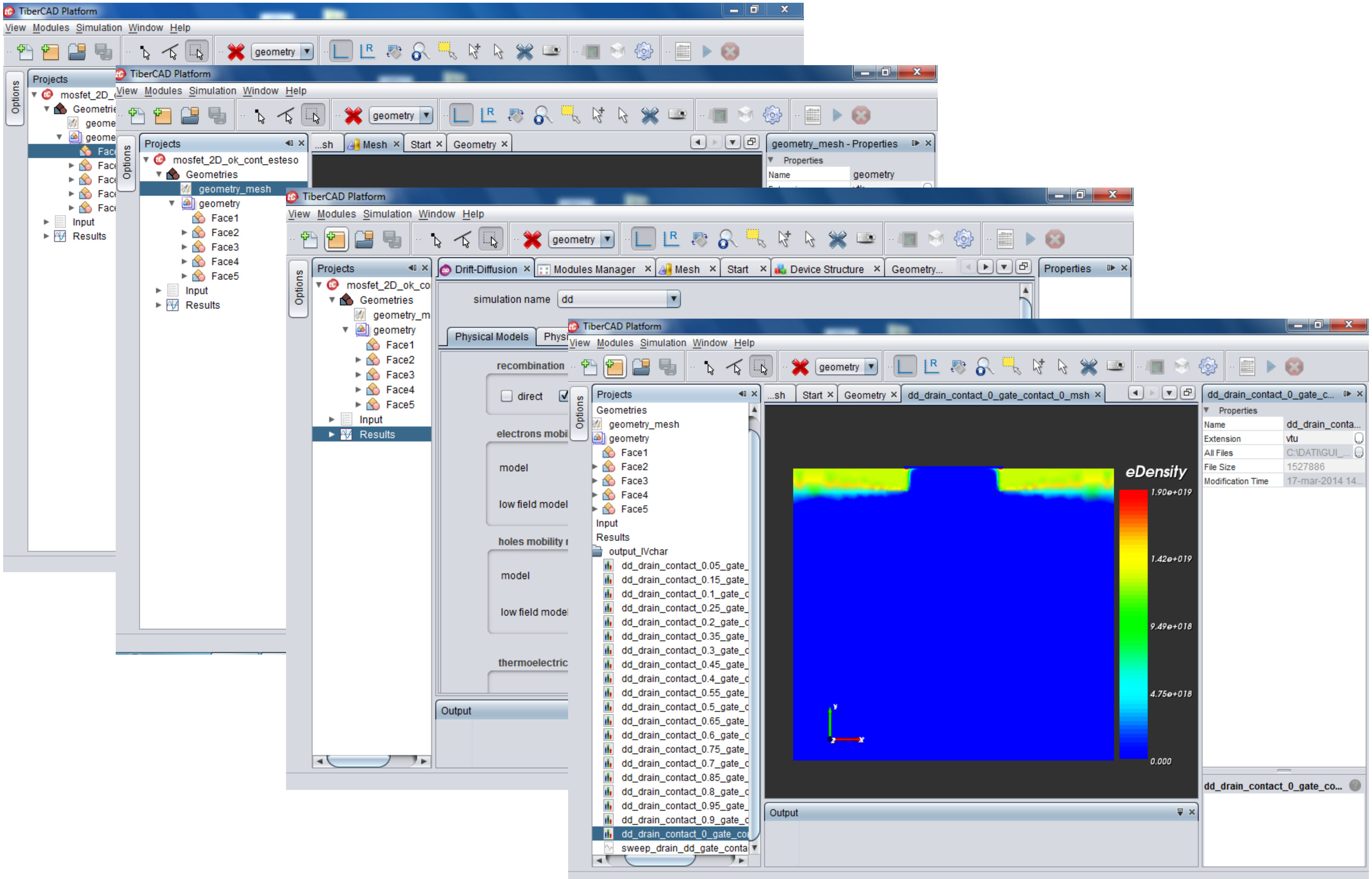
Under developement

Postprocessing

Paraview



GUI development



TiberCAD input file - Modules

```
Module elasticity
{
  name = strain
  regions = all
  plot = (Strain,  Stress, Displacement)

  Solver {
    preconditioner = lu
    method = pconly
  }

  Physics {
    body_force lattice_mismatch {
      reference_material = GaN
    }
  }

  Contact substrate { type = clamp }
}
```

Drift-Diffusion

Drift-Diffusion equations

- Consider only $M^{(0)}$ and $M^{(1)}$, assuming carriers in thermal equilibrium (T_e=T_0)
- Assume term ($\mathbf{u}\nabla\mathbf{u}$) is negligible
- Define mobility and diffusivity: $\mu=q\tau/m^*$ and $D=k_B T_0 \mu/q$

Current equations

$$\mathbf{J}_n = qn\mu_n\mathbf{F} + qD_n\nabla n$$

$$\mathbf{J}_p = qn\mu_p\mathbf{F} - qD_p\nabla p$$

Continuity equations

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

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

+

Poisson equation: $\mathbf{F} = -\nabla V$

$$\nabla\cdot\left(\varepsilon_0\varepsilon_r\nabla V\right) = -q\left(p - n + N_D - N_A\right)$$

key parameter: $\mu = \mu(F, T, N_D, N_A, \ldots)$

Low Field

$$\mu(T) = \mu_0 \left(\frac{T}{300} \right)^{\alpha}$$

High field

Silicon-like

$$\mu(F) = \mu_0 \frac{1}{\left(1 + \left(\frac{\mu_0 F}{v_{sat}} \right)^{\beta} \right)^{1/\beta}}$$

GaAs-like

$$\mu(E) = \frac{\mu_0 + \frac{v_{sat}}{F} \left(\frac{F}{F_0} \right)^{\gamma}}{1 + \left(\frac{F}{F_0} \right)^{\gamma}}$$

Doping Dependent

$$\mu(N_D) = \mu_0 - A \ln \left[\frac{N_D}{n_i} \right]$$

Organic transport

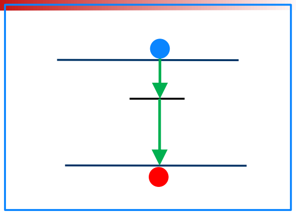
Hopping

$$\mu(F) = \mu_0(T) \exp \left[\sqrt{\frac{F}{F_0}} \right]$$

Band-like

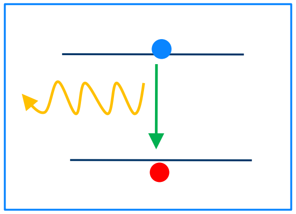
$$\mu(F) = \frac{\mu_0(T)\sqrt{2}}{\left[1 + \sqrt{1 + \frac{3\pi}{8} \left(\frac{\mu_0 F}{v_s} \right)^2} \right]^{\frac{1}{2}}}$$

Generation-Recombinations



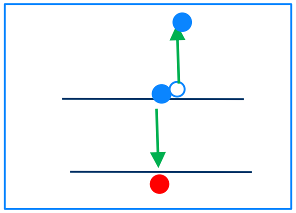
Shockley-Read-Hall (SRH) recombination (non-radiative)

$$R_{SRH}=\frac{pn-n_i^2}{\tau_p\left[n+n_i\exp\left(\frac{E_t-E_i}{kT}\right)\right]+\tau_n\left[p+n_i\exp\left(\frac{E_i-E_t}{kT}\right)\right]}$$



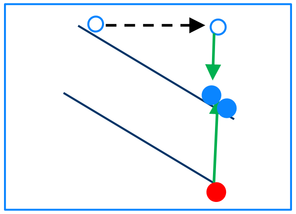
Radiative recombination

$$R_R=C\left(pn-n_i^2\right)$$



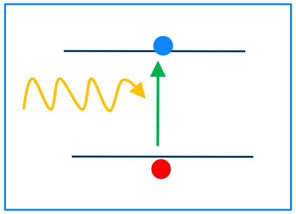
Auger recombination (non-radiative)

$$R_A=D_n\left(pn^2-nn_i^2\right)+D_p\left(np^2-pn_i^2\right)$$



Impact ionization generation (hot-carriers)

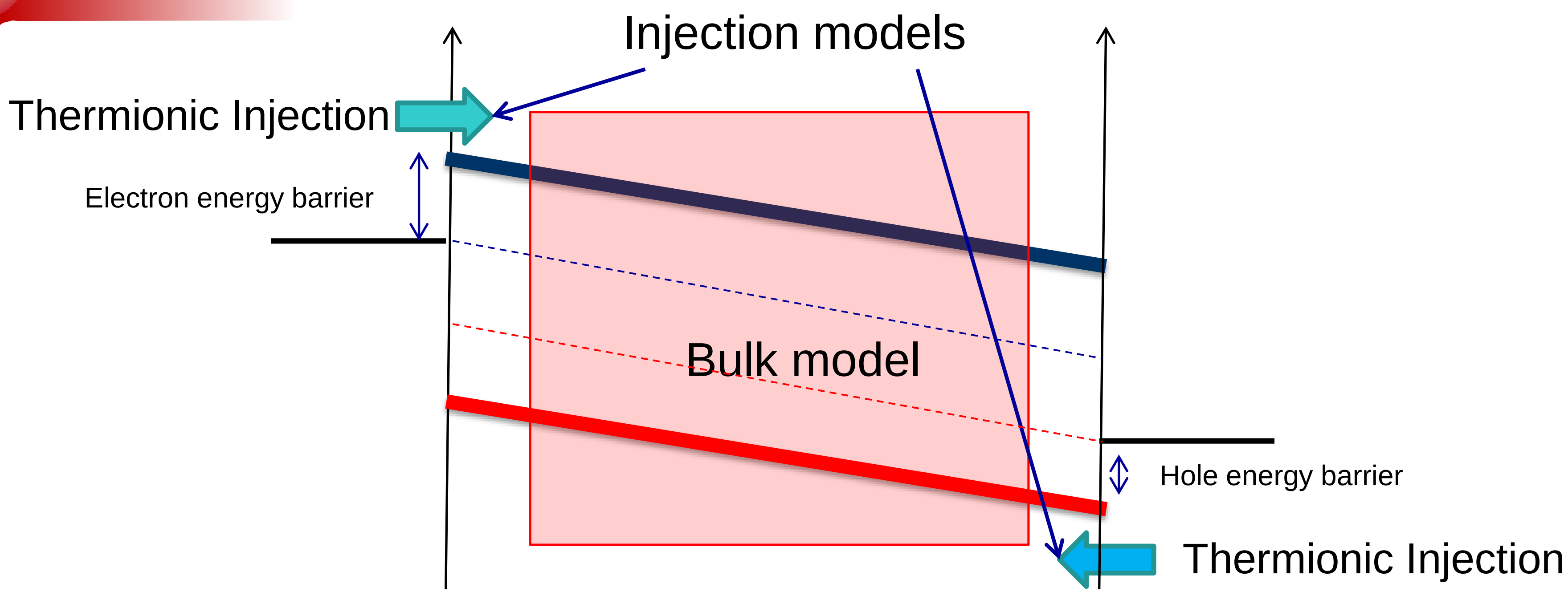
$$G_{II}=\alpha_n\frac{|J_n|}{q}+\alpha_p\frac{|J_p|}{q}\qquad \alpha_{n,p}(F)=\alpha_{n,p}^{\infty}\exp\left[-\left(\frac{F_{n,p}^{crit}}{F}\right)^{\beta_{n,p}}\right]$$

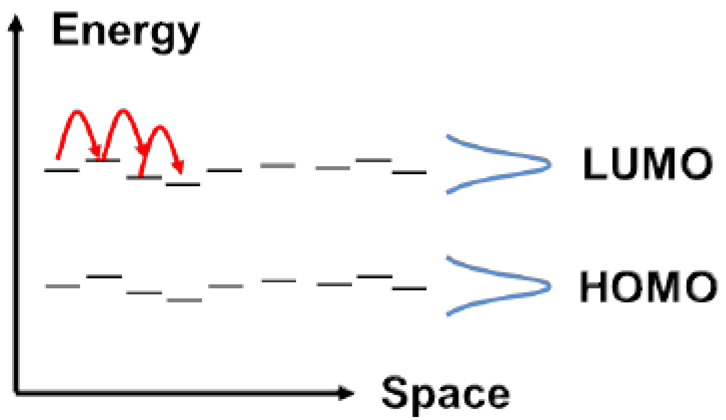


Photoabsorption generation

$$G_{ph}=\alpha|E|^2$$

Special case for organics





Drift-Diffusion Model

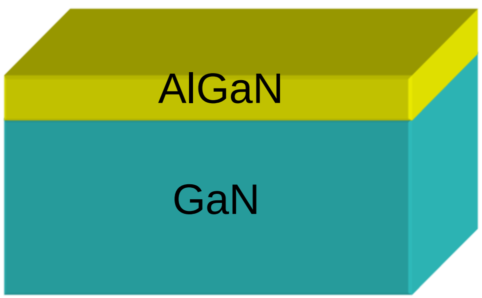
$$\begin{cases} -\nabla\left(\varepsilon_r \nabla \varphi - \mathbf{P}\right) = e\left(p - n - N_d^+ - N_a^-\right) \\ \nabla\left(\mu_n n \nabla \phi_n\right) = G - R \\ -\nabla\left(\mu_p p \nabla \phi_p\right) = G - R \end{cases}$$

F. Santoni, A. Gagliardi, M. auf der Maur, A. Di Carlo, Organic Electronics 15 (2014) 1557–1570

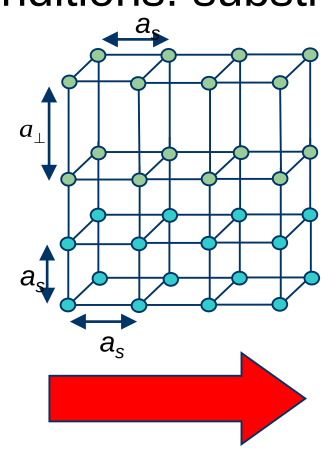
Elasticity and Strain Module

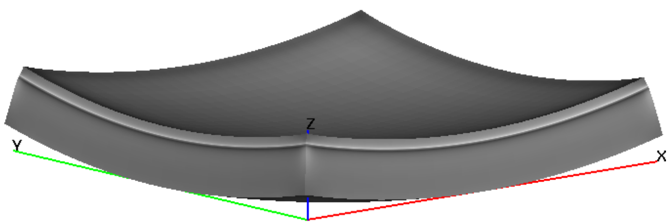
Physical Models: Strain in heterostructures

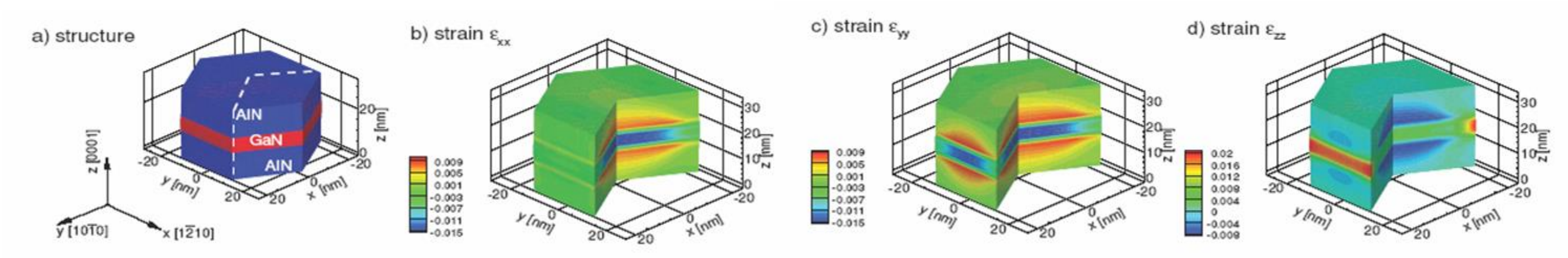
- External mechanical forces can be included as boundary conditions
- We can calculate shape deformation and piezoelectric effect $P_i = e_{i,jk}\varepsilon_{jk}$
- Converse piezoelectric effect can be included $\sigma_{jk} = -e_{i,jk}E_i$
- Thermal stress can be included $\varepsilon_{jk} = -\alpha_{jk}(T - T_0)$
- Several boundary conditions: substrate, plane, free



Free-standing AlGaN/GaN







Grid deformations

Povolotskyi-Di Carlo, JAP 100, 063514 (2006)

define shape

$$\varepsilon_{ij}^{0} = \delta_{ij}\frac{a_i^S - a_i}{a_i}$$

$$\frac{\partial}{\partial x_i}\left(C_{ijkl}(\mathbf{r})\left(\frac{\partial u_k}{\partial x_l} + \varepsilon_{kl}^{n}(\mathbf{r})\right)\right) = 0$$

$$\varepsilon_{ij}^{n} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \varepsilon_{ij}^{n-1}$$

define new shape by moving nodes

$$\vec{r} \rightarrow \vec{r} + \vec{u}$$

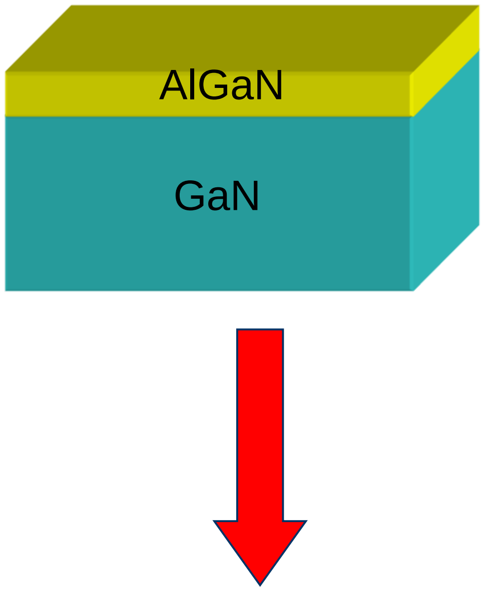
$$\|\vec{u}\| > \delta$$

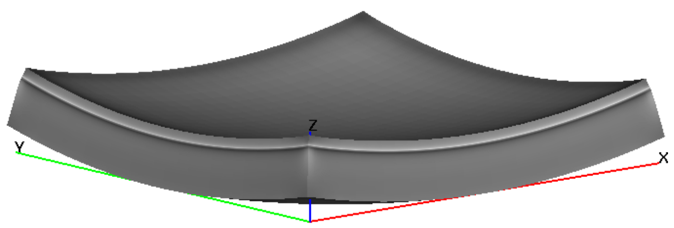
yes

stop

self-consistent cycles

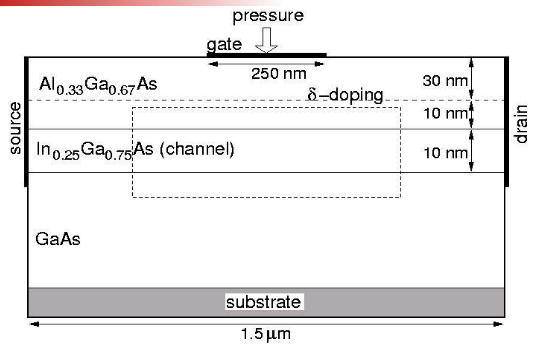
Free-standing AlGaN/GaN



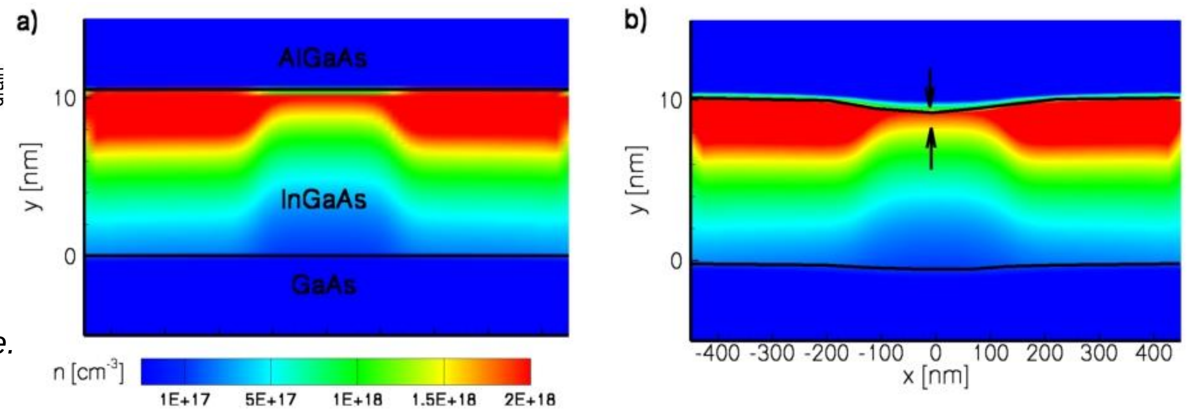


Adaptive grid are used

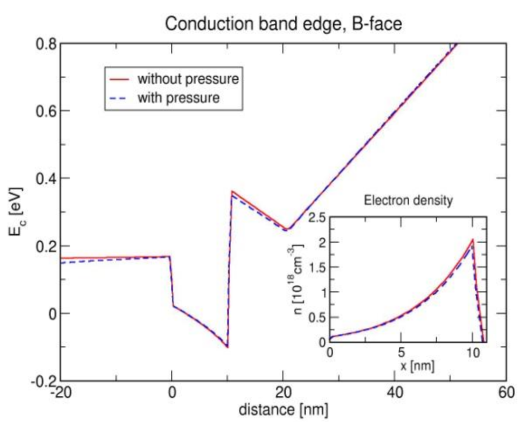
Piezoelectric sensors in InGaAs



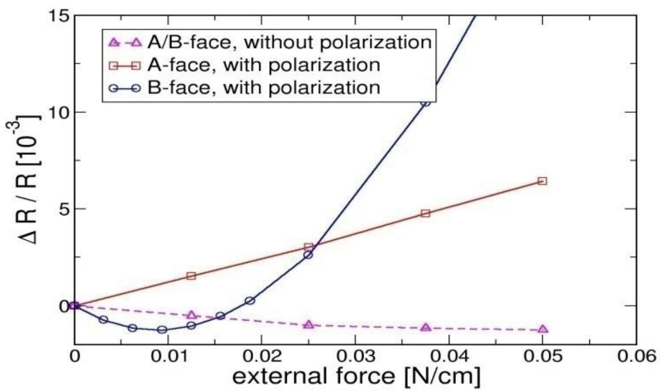
AlGaAs/InGaAs/GaAs HEMT structure. Growth directions [311] (A-face) and [31̄1̄] (B-face) are considered.



Electron density in the AlGaAs/InGaAs/GaAs B-face structure without (a) and with (b) pressure (F = 75mN/cm).



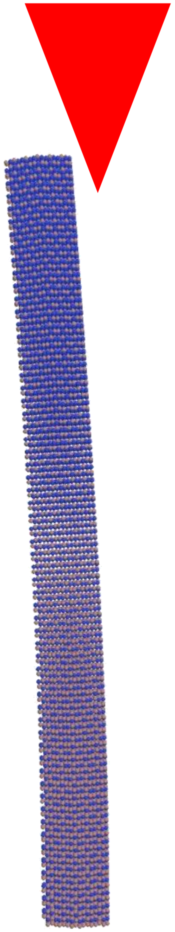
Band profile and classical electron density for the B-face structure with and without pressure.

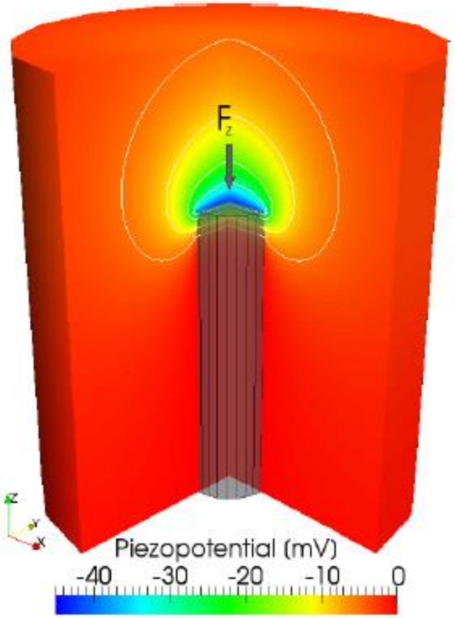


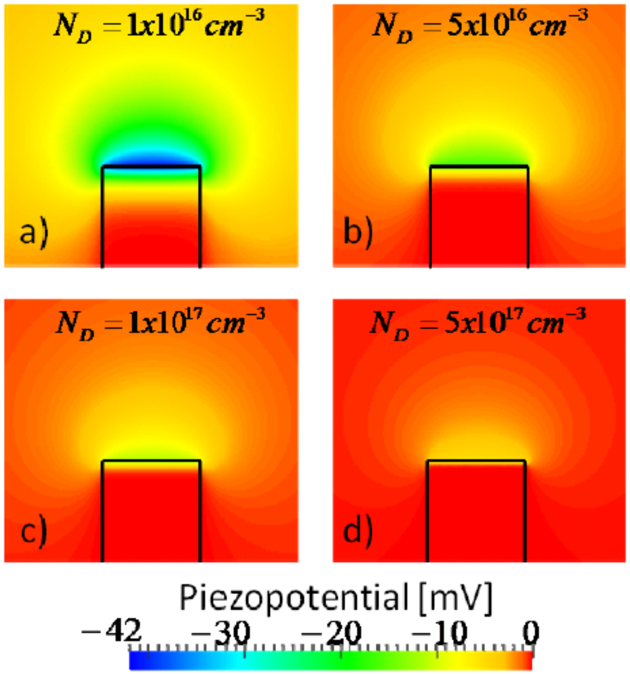
Piezoresistivity for the AlGaAs/InGaAs/GaAs structure. Gate voltage is 0 V.

Piezoelectric nanogenerators

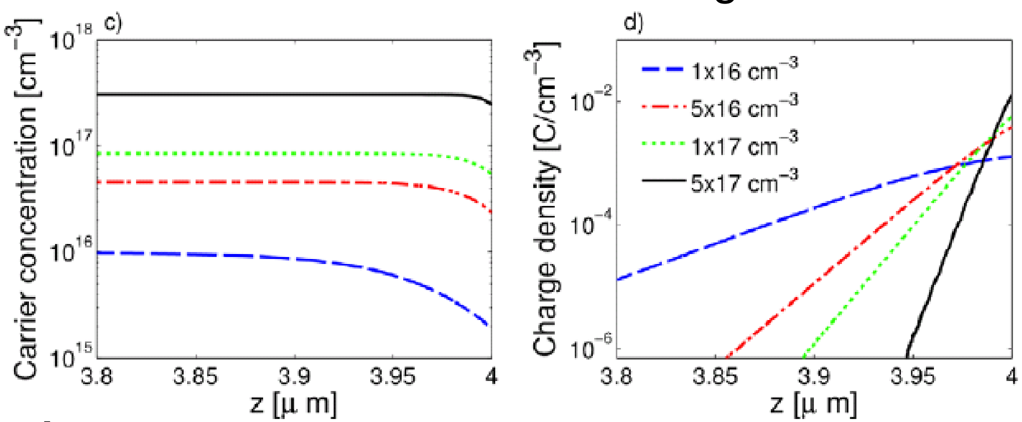
Deformations and compressive stress







Free-carrier screening effects

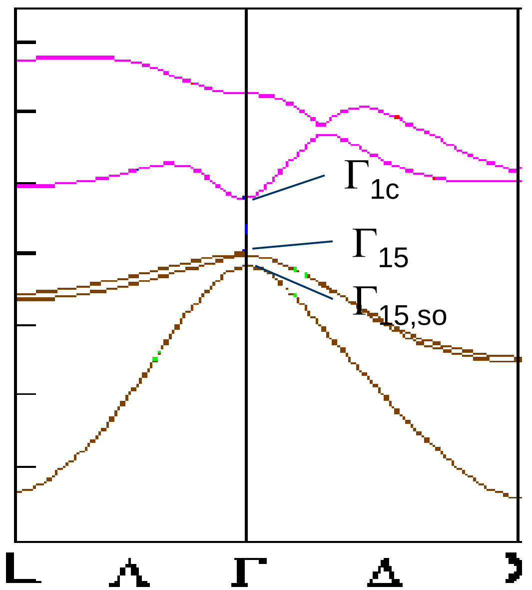


G. Romano et al., Nanotechnology **22 (2011) 465401**

Quantum States

Quantum Models: k·p

Band-structure near k=0



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{cr}(r)\right]\psi_{n\mathbf{k}}(r) = E_n(\mathbf{k})\psi_{n\mathbf{k}}(r)$$

$$\psi_{n\mathbf{k}}(r) = e^{i\mathbf{kr}}u_{n\mathbf{k}}(r)$$

$$\left[\hat{H} + \frac{\hbar}{m}\mathbf{k}\cdot\hat{\mathbf{p}}\right]u_{n\mathbf{k}}(r) = \left[E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m}\right]u_{n\mathbf{k}}(r)$$

$$E_n(\mathbf{k}) \approx E_{\Gamma_{15}} + \frac{\hbar^2 k^2}{2m^2} + \Lambda_n$$

$$H_{rs} = \frac{\hbar^2}{m^2}\sum_{i,j} k_i k_j \sum_{l\alpha\nu} \frac{\langle r|p_i|l\alpha\nu\rangle\langle l\alpha\nu|p_j|s\rangle}{E_{\Gamma_{15}} - E_{l\alpha}}$$

$$H_{3x3} = \begin{bmatrix} Lk_x^2 + M(k_y^2 + k_z^2) & Nk_x k_y & Nk_x k_z \\ Nk_x k_y & Lk_y^2 + M(k_x^2 + k_z^2) & Nk_y k_z \\ Nk_x k_z & Nk_y k_z & Lk_z^2 + M(k_x^2 + k_z^2) \end{bmatrix}$$

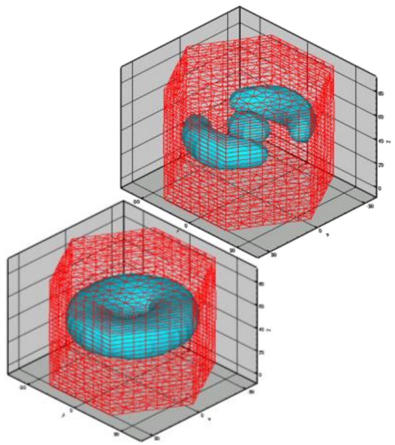
Diagonalize to find Band *n*

Envelope Function Approx

k·p Hamiltonian generalizes single band dispersions

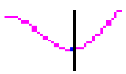
$$\left|\psi^i(r)\right\rangle = \sum_n \left|u_{n\Gamma}(r)\right\rangle \, \phi_n^i(r) \quad \longleftarrow \quad \text{Envelope function}$$

$$\sum_n \left[E_\Gamma \delta_{mn} + \frac{\hbar^2 k^2}{2m^2}\delta_{mn} + H_{mn}(\mathbf{k}) + V(r)\delta_{mn} \right] \phi_n^i(r) = E^i \phi_m^i(r)$$

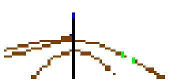


k is interpreted as the usual momentum operator: $k_l \mapsto i\partial_l$

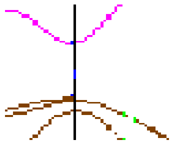
In TiberCAD:



$$H_{2x2}$$

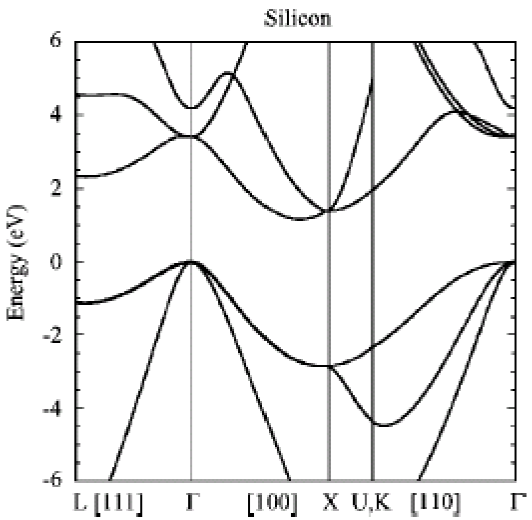


$$H_{6x6} = \begin{bmatrix} H_{3x3} & 0 \\ 0 & H_{3x3} \end{bmatrix} + H_{so}$$



$$H_{8x8} = \begin{bmatrix} H_{4x4} & 0 \\ 0 & H_{4x4} \end{bmatrix} + H_{so}$$

Full Band kp

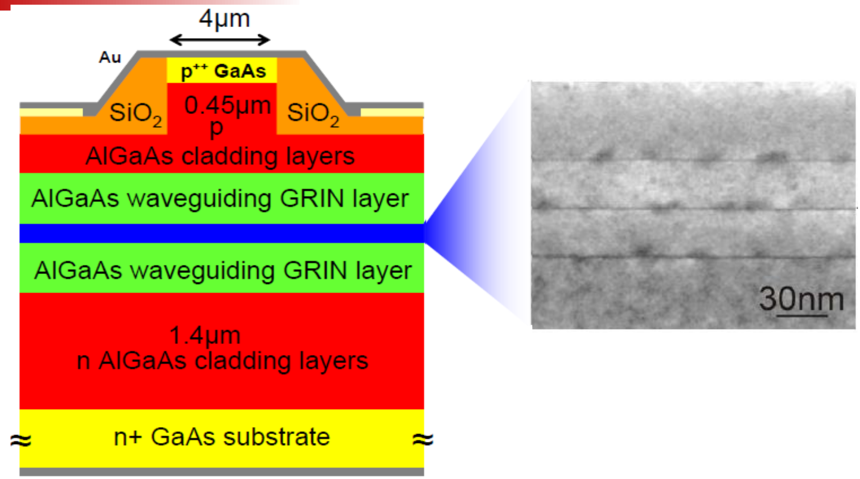


$$H_{30x30} = \begin{bmatrix} H_{15x15} & 0 \\ 0 & H_{15x15} \end{bmatrix} + H_{so}$$

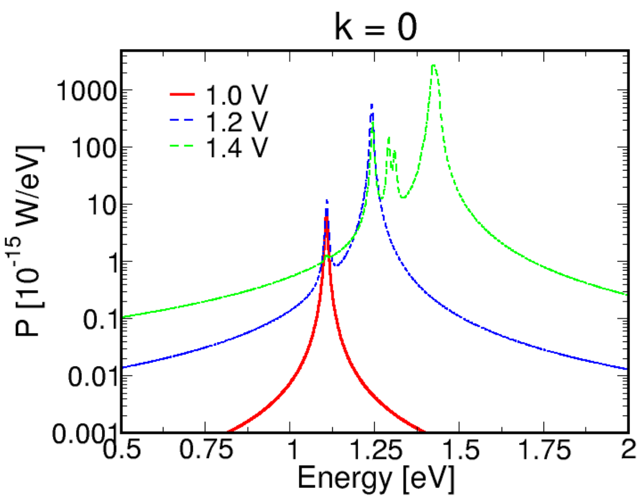
Cardona-Pollak (1966)
G. Fishman (2004)

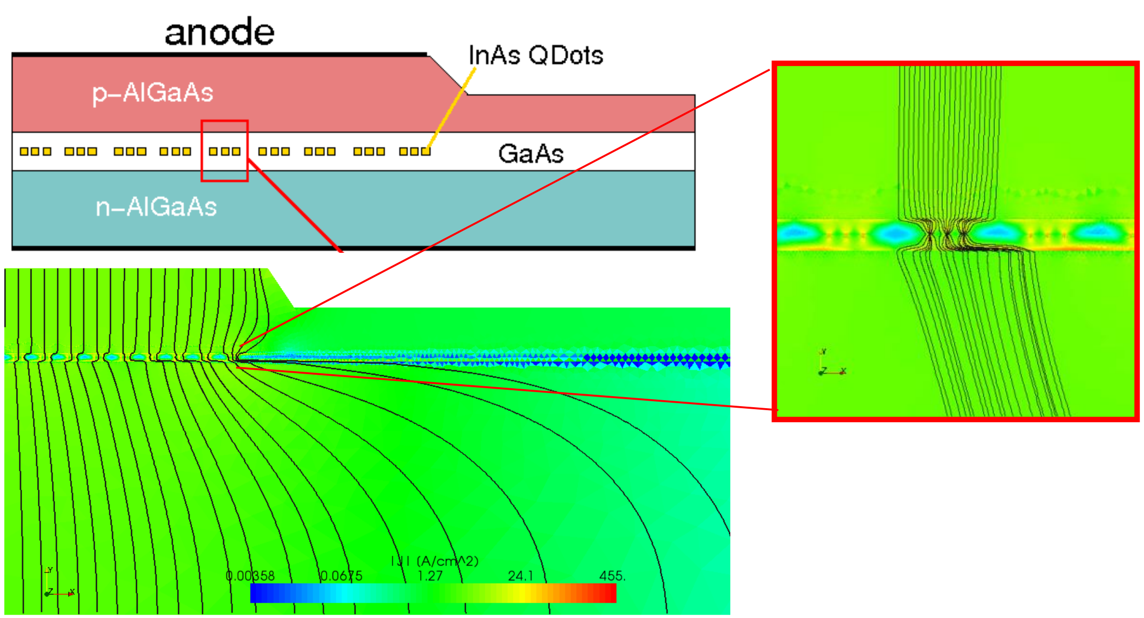
$$H_{14x14}, H_{20x20}, H_{24x24}$$

InAs Qdots

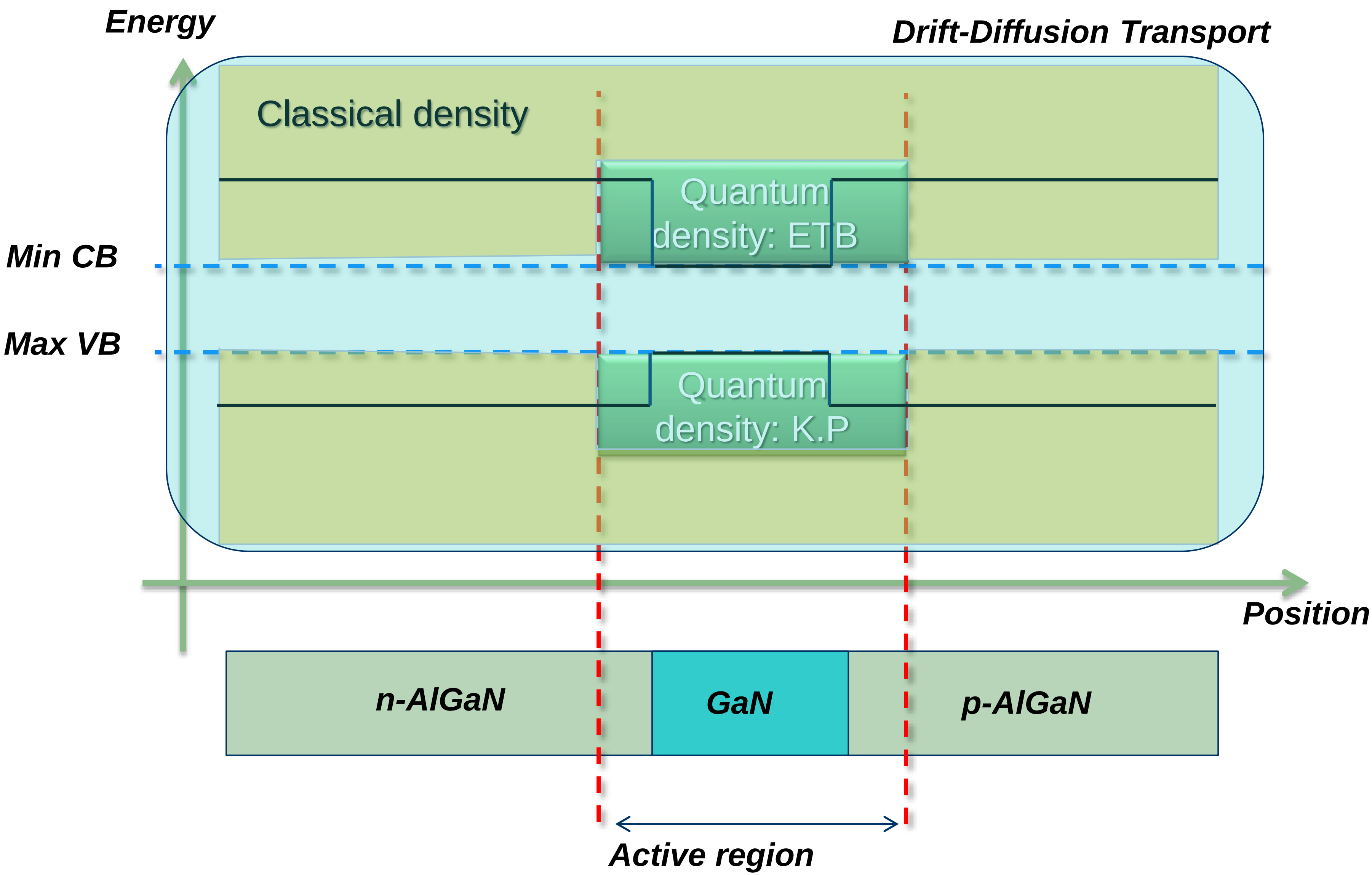


M. Buda et. al., IEEE Journal of Quantum Electronics, 2003

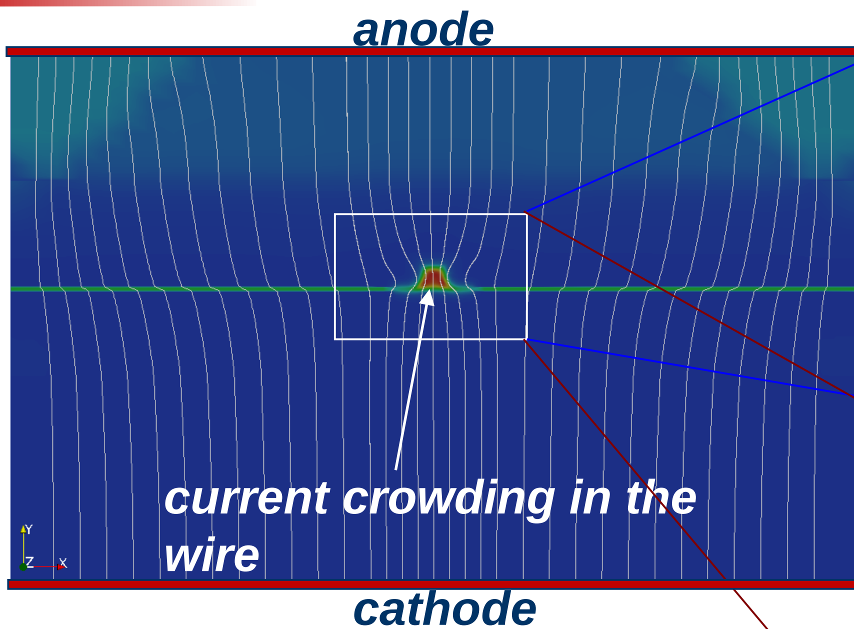


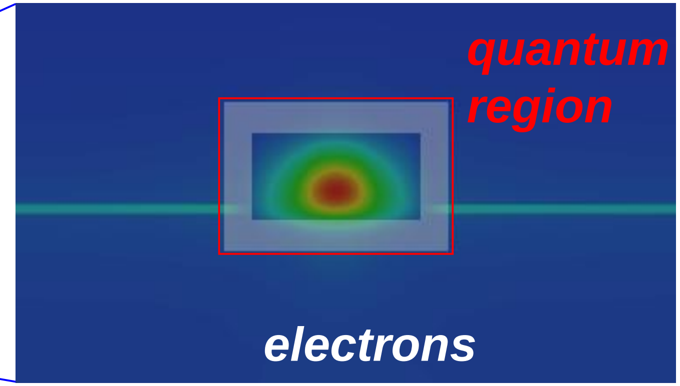


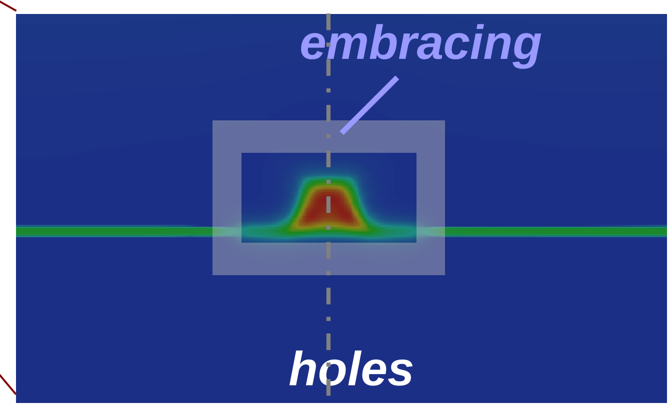
Energy/Position Multiscale

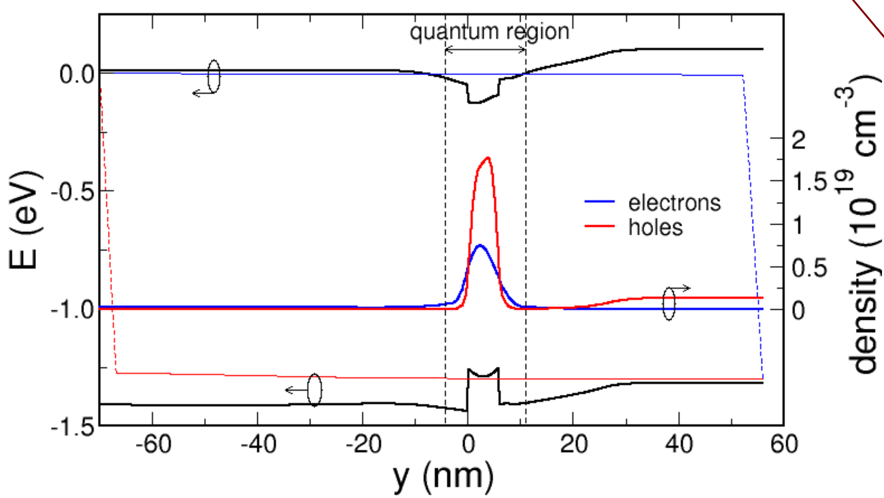


InGaAs Quantum wire: overlap scheme







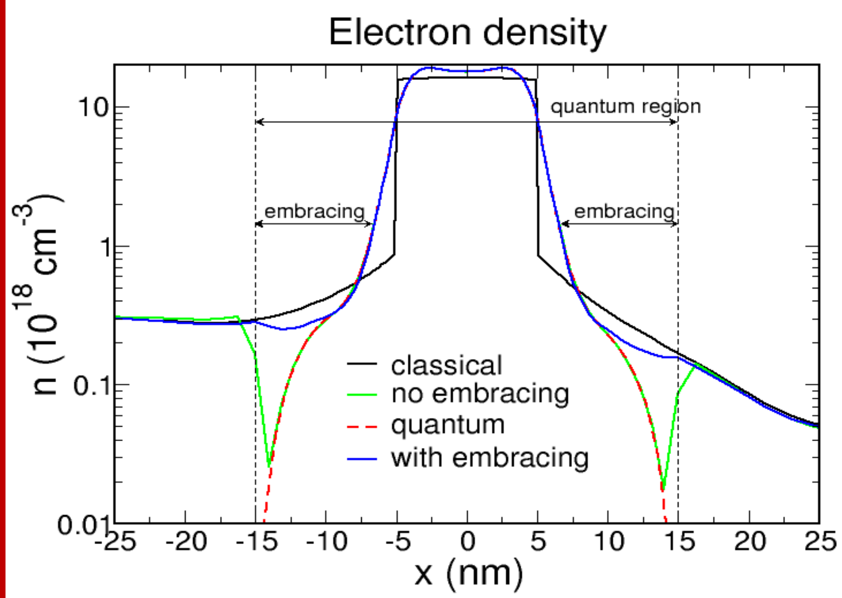


Self-consistent densities at Vb = 1.3 V

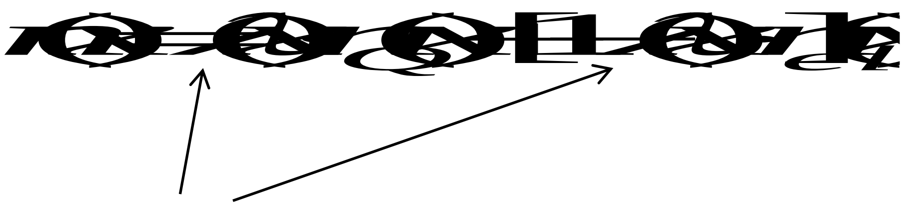
K.P quantum model

Embracing technique

TiberCAD includes a technique for mixing classical and quantum density, acting as a quantum correction to drift-diffusion calculation

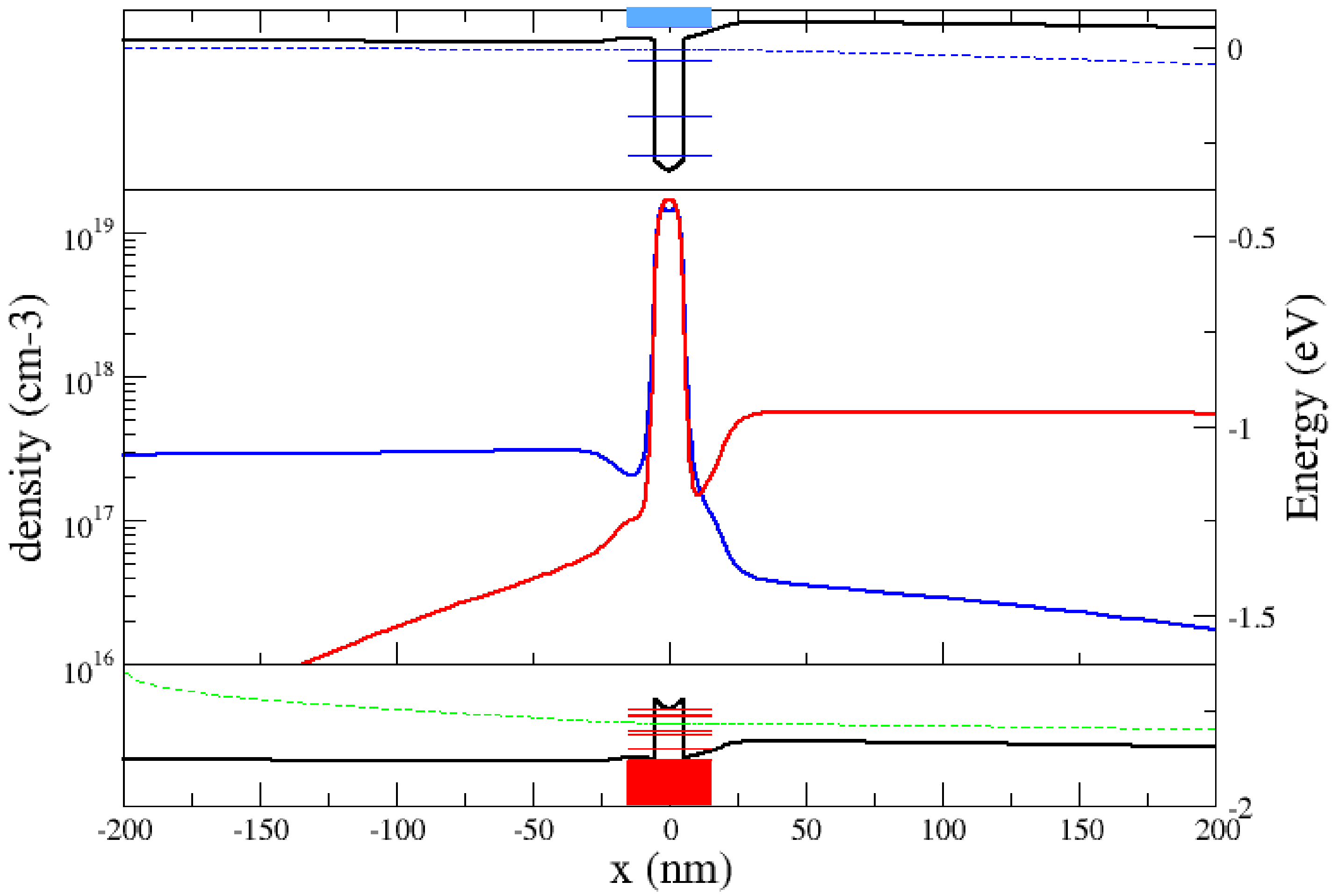


Embracing region where **classical** and **quantum** charge are mixed.



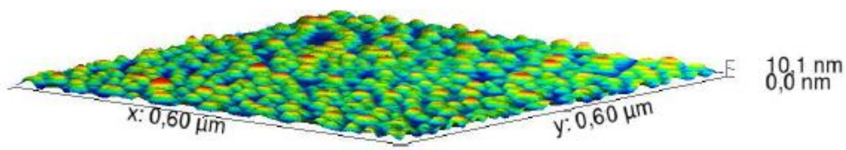
The mixing parmeter is solution of a Laplace equation with Dirichelet boundary conditions 0.0 and 1.0

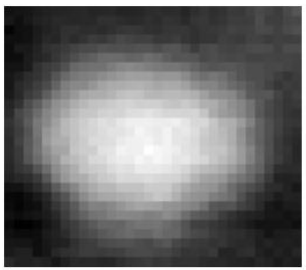
Alternative: Quantum+Classical

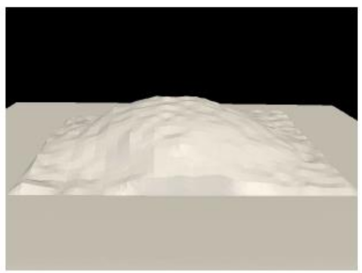


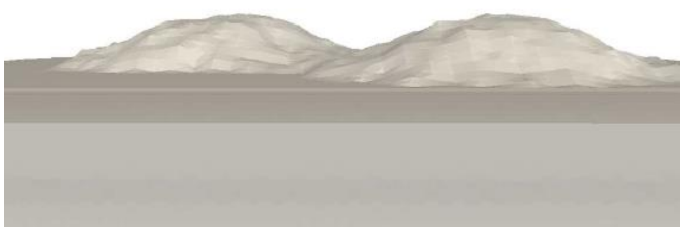
InP dots for gas sensing

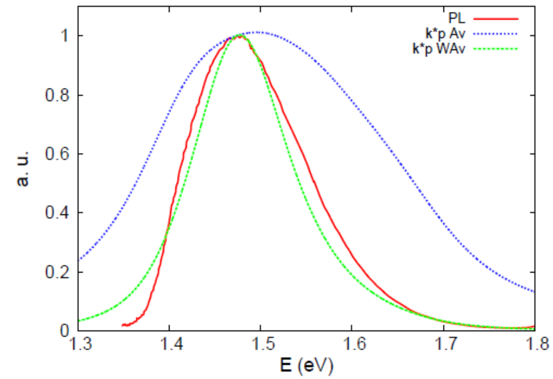
AFM image:



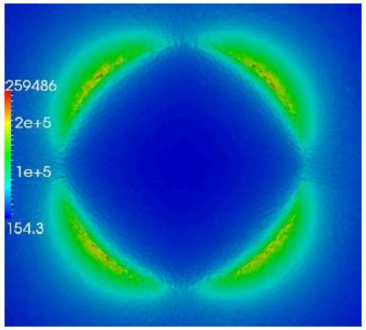




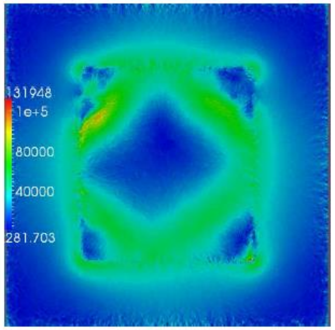




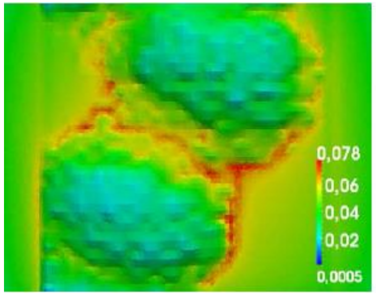
Idealized dot

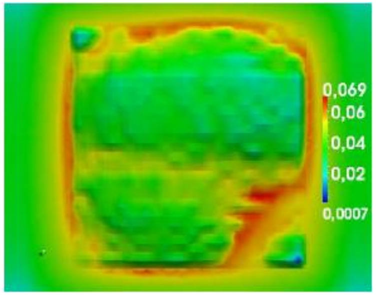


Realistic dot



Strain field maps

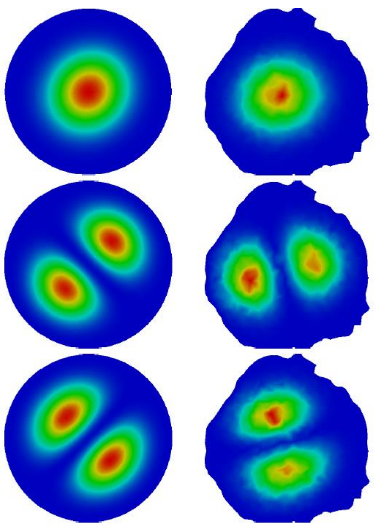




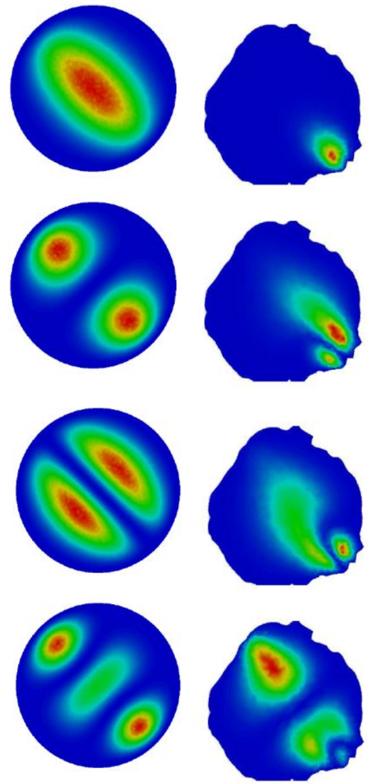
Closely coupled dots

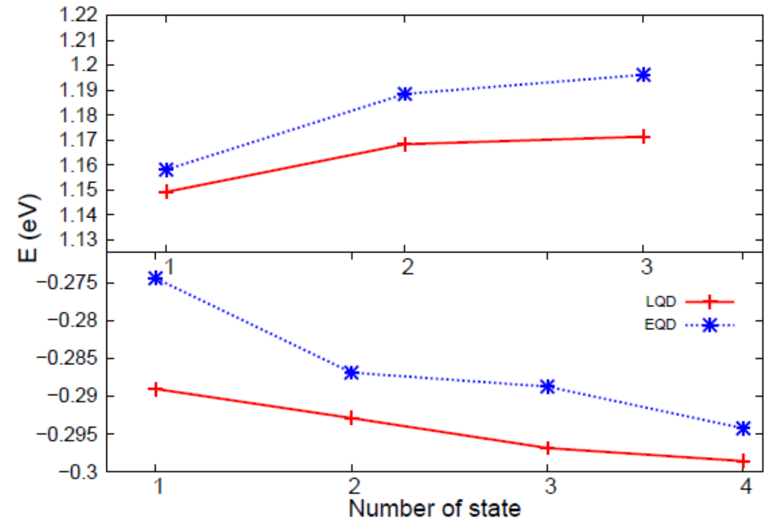
Electronic properties

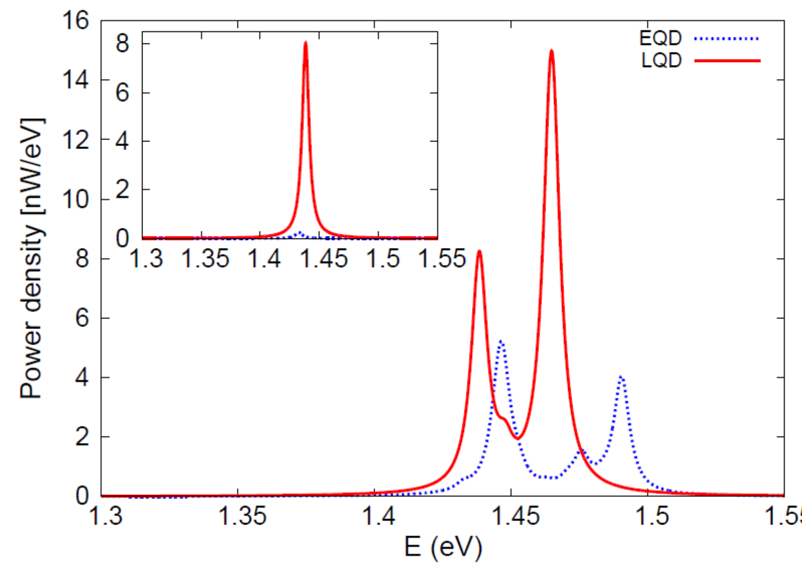
Electron states



Hole states





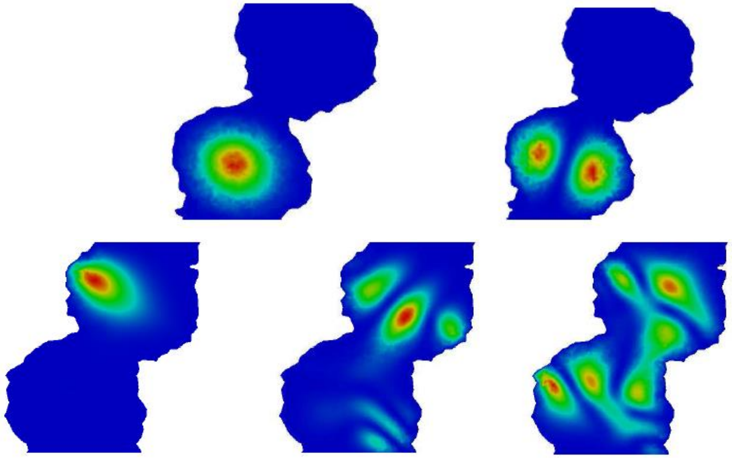


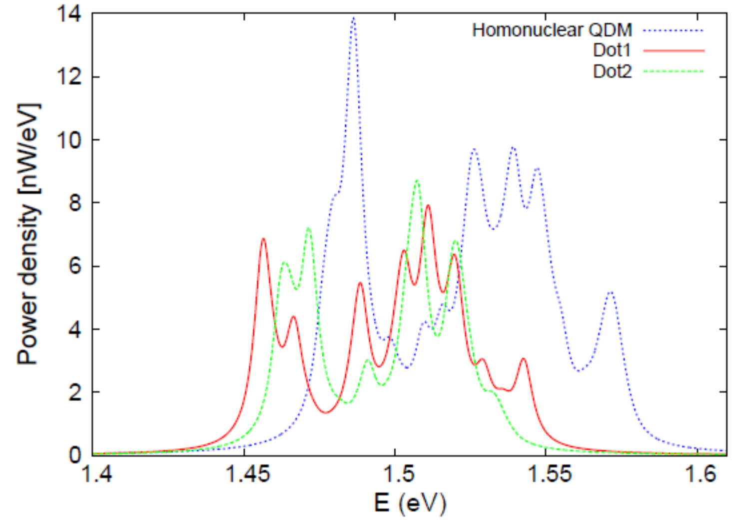
Comparisons between dots

homo-nuclear dots

el:

hl:

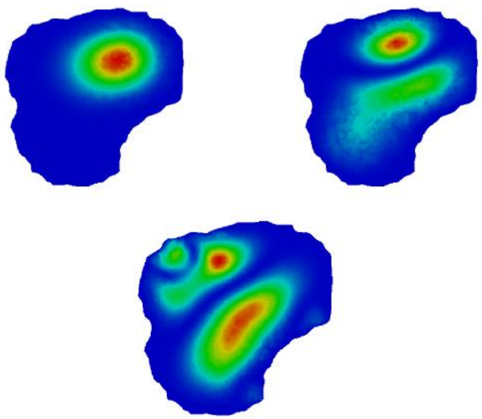


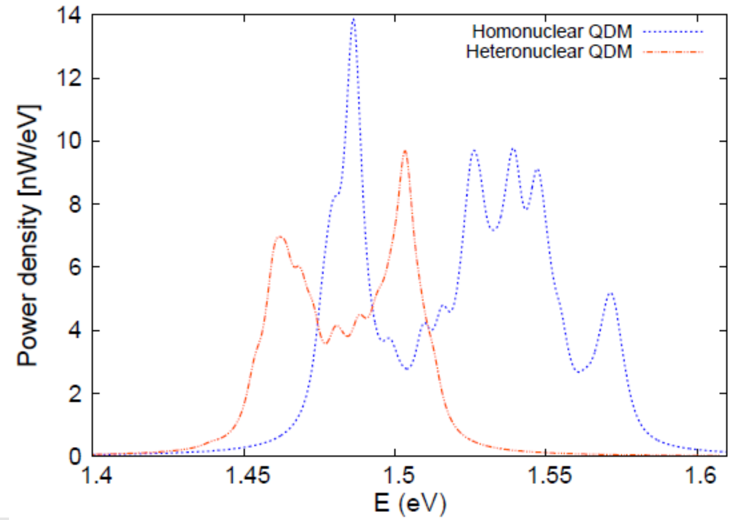


hetero-nuclear dots

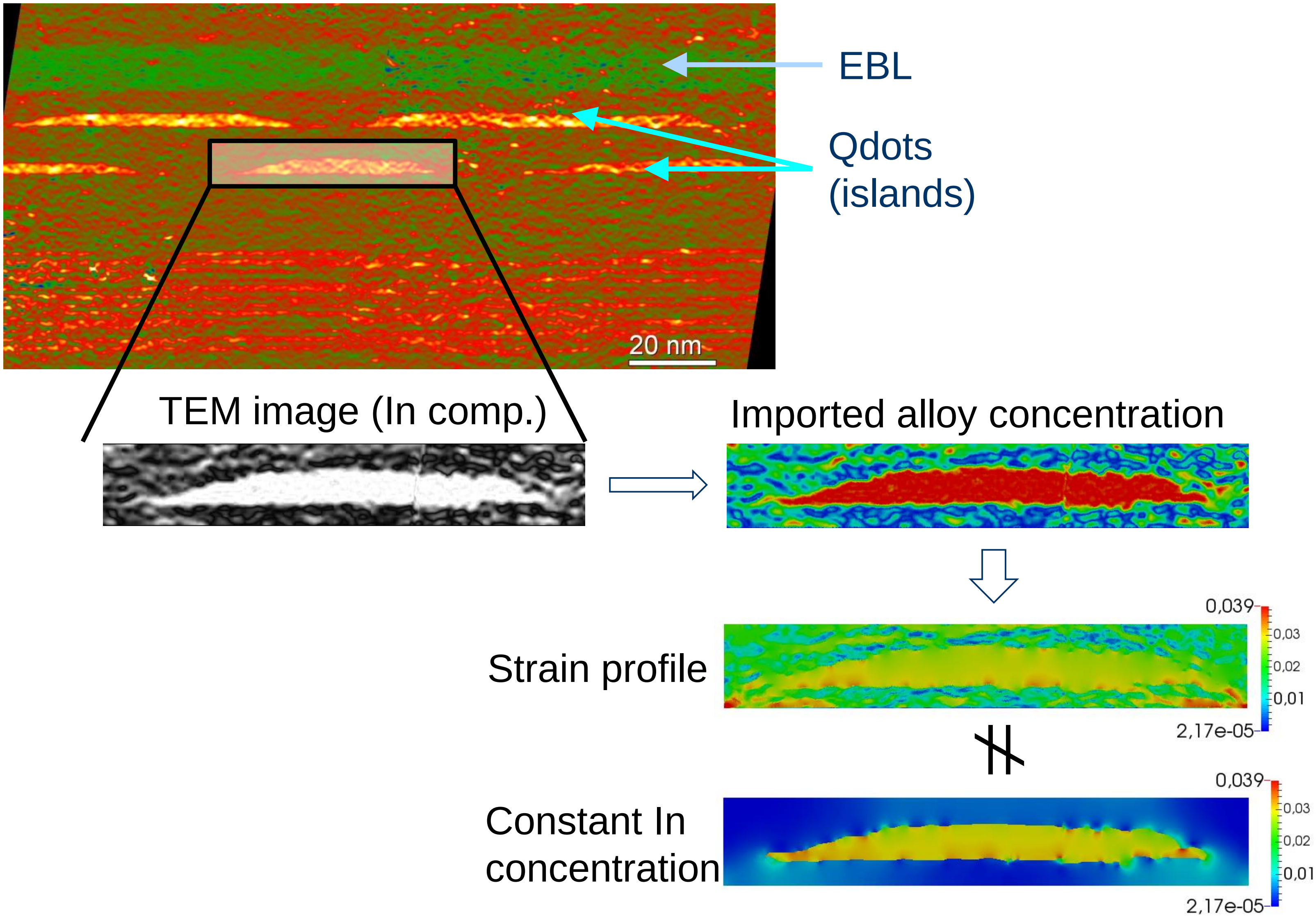
el:

hl:



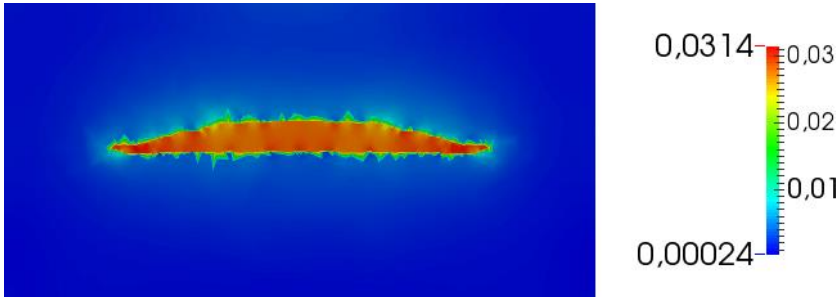


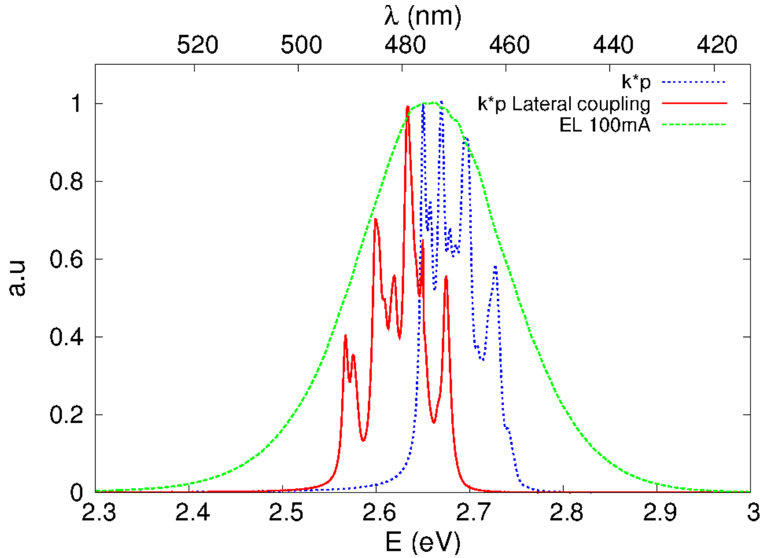
Shape and alloy effects in Qdot system

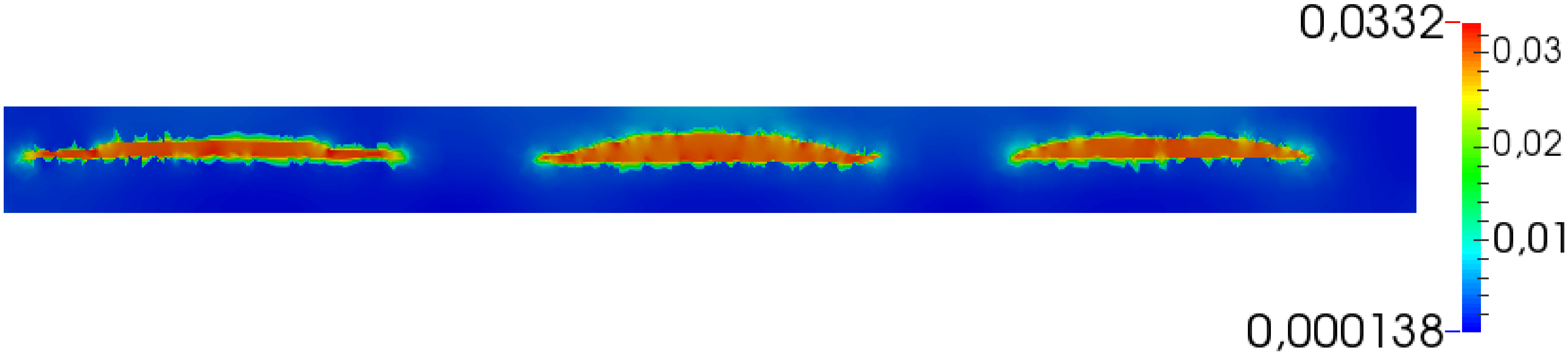


Lateral coupling via strain

Impact of **lateral** coupling given mainly by strain field (continuum and k*p 3D model): **shift** of the spectrum of the central dot of about **90meV**

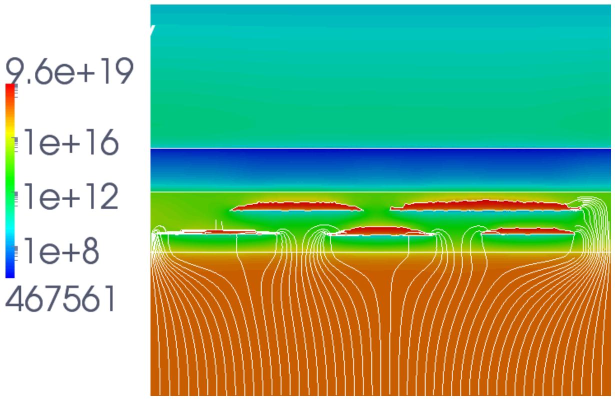




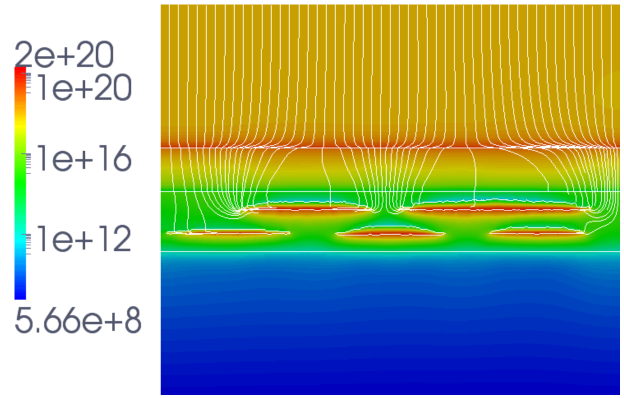


Current densities

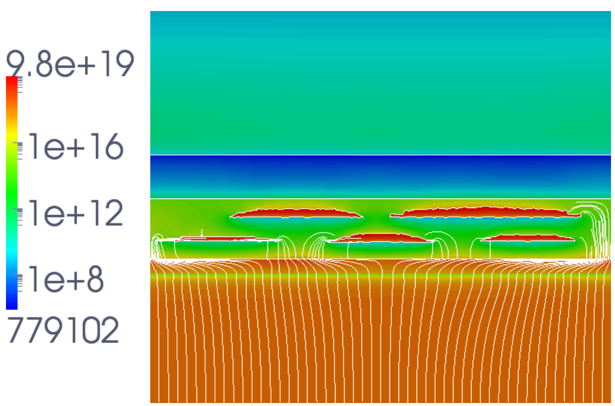
electron current density

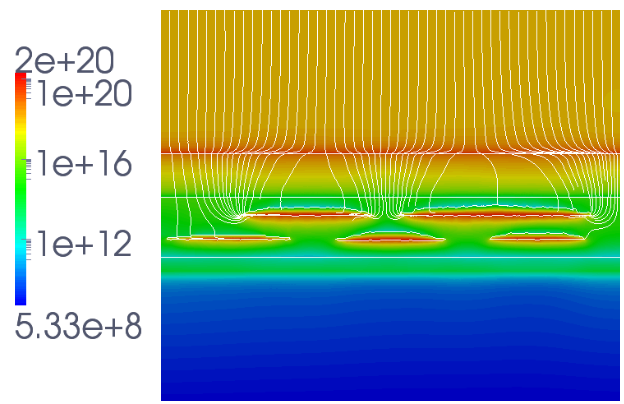


Hole current density



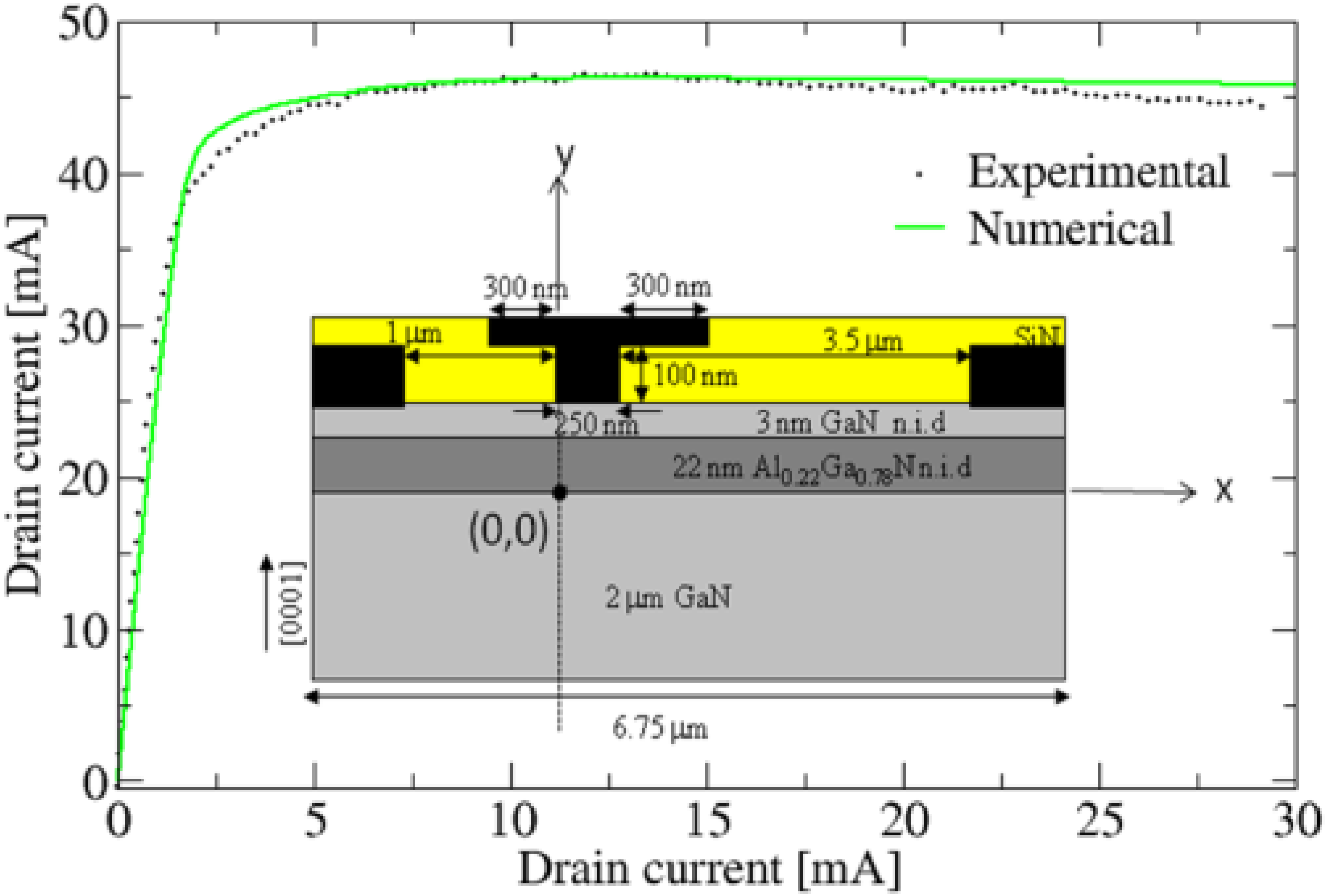
Increasing electron current density with electron-rich layer





Bridge Multiscale

Thermal properties of HEMT



Thermal Models

Fourier Heat Diffusion: $-\nabla \cdot \left(\kappa \nabla T\right) = H$

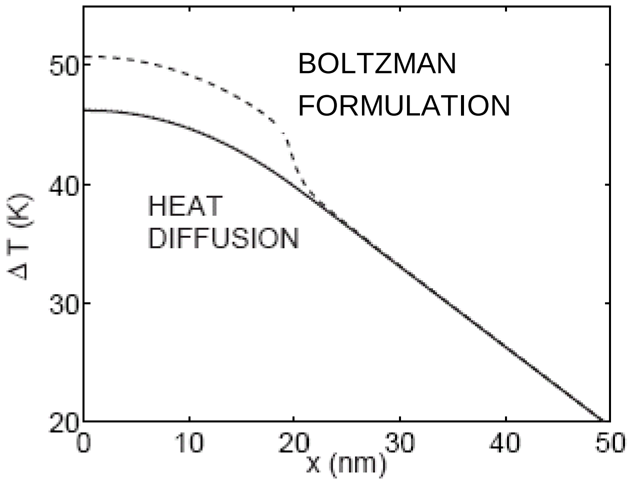
Energy Moment of the Boltzman Transport Equation for phonons

$$\frac{\partial e''}{\partial t} + \mathbf{v} \cdot \nabla e'' = -\frac{e'' - e^0}{\tau}$$

$$e'' = \int \hbar \omega [N - \bar{N}(T_{ref})] g(\omega) d\omega$$

A gray model assume isotropic and constant phonon velocity:

$$\frac{\partial e''}{\partial t} + v_g \nabla \cdot \mathbf{s} e'' = -\frac{e'' - e^0}{\tau}$$



Fourier/Gray bridge method

Drift Diffusion

$$H = -\nabla\cdot\left(\mathbf{J_n}\varphi_n\right) - \nabla\cdot\left(\mathbf{J_p}\varphi_p\right)$$

Gray model

$$e^0 = \frac{4\pi(T - T_0)}{C_V}$$

$$v_g \nabla\cdot\left(\mathbf{s}e''\right) = \frac{e^0 - e''}{\tau} + H$$

$$e^0 = \frac{1}{4\pi}\int_{4\pi} e'' d\Omega$$

$$T = T_0 + \frac{C_V}{4\pi}e^0$$

$$\mathbf{J_q} = \int_{4\pi} \mathbf{s}e'' d\Omega$$

Temperature

Heat flux

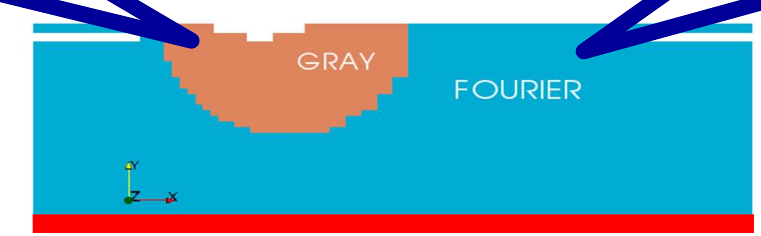
Fourier model

$\mathbf{J_q}$ as B.C.

$$-\nabla\cdot\left(\kappa\nabla T\right) = H$$

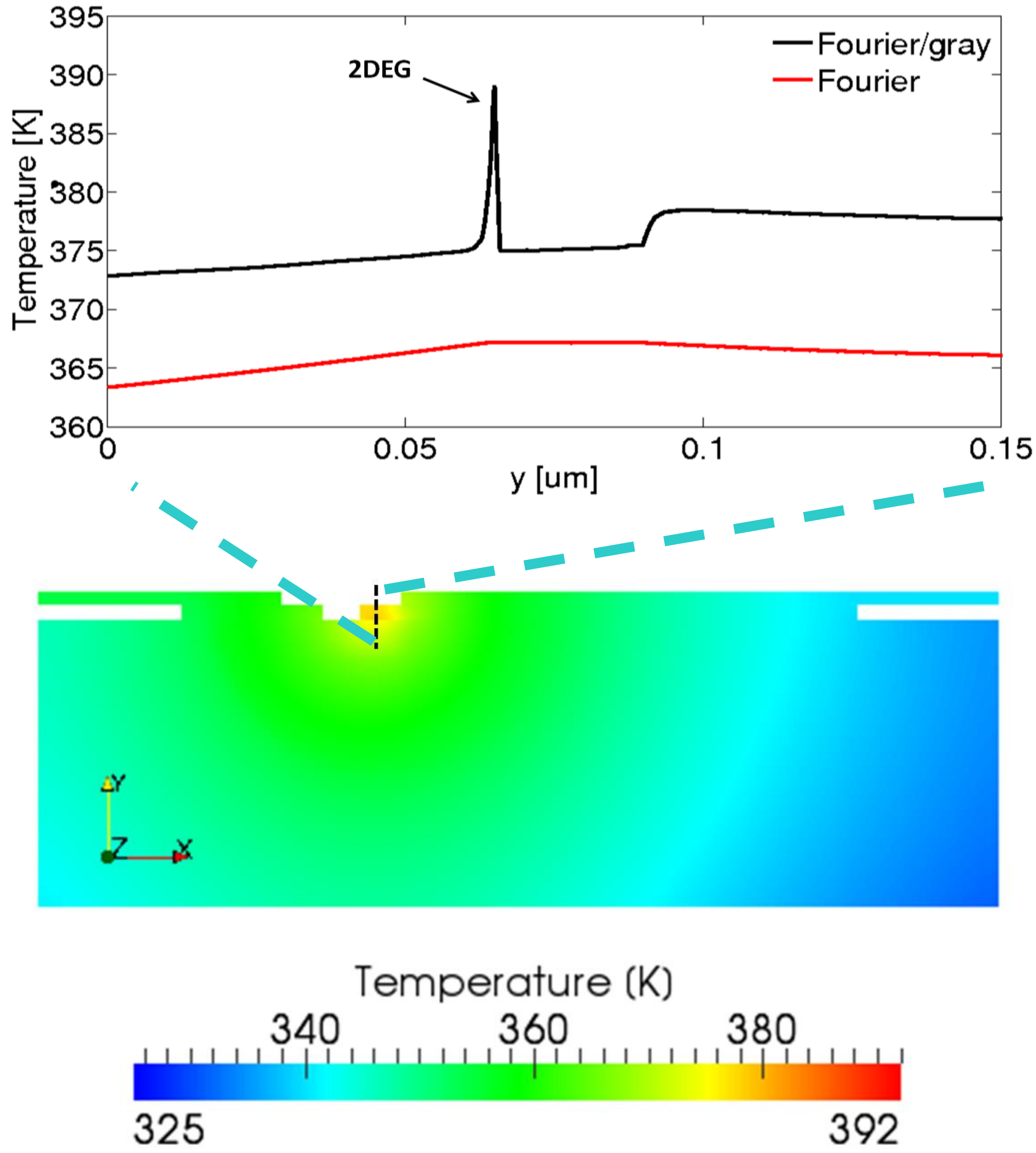
$$T$$

$$\mathbf{J_q} = -\kappa\nabla T$$



$$R_T = 0.8\ \mathrm{mWcm^2/K}$$

Temperature profile



Special self-consistence scheme

```
Module selfconsistent
{
  solve = (fourier, gray)

  Multiscale bridge {
    macromodel = fourier
    micromodel = gray
    restrict_variables = (temperature)
  }
  max_iterations = 10
  absolute_tolerance = 1e-3
  relative_tolerance = 1e-9
}
```

macromodel
is solved everywhere

micromodel is solved

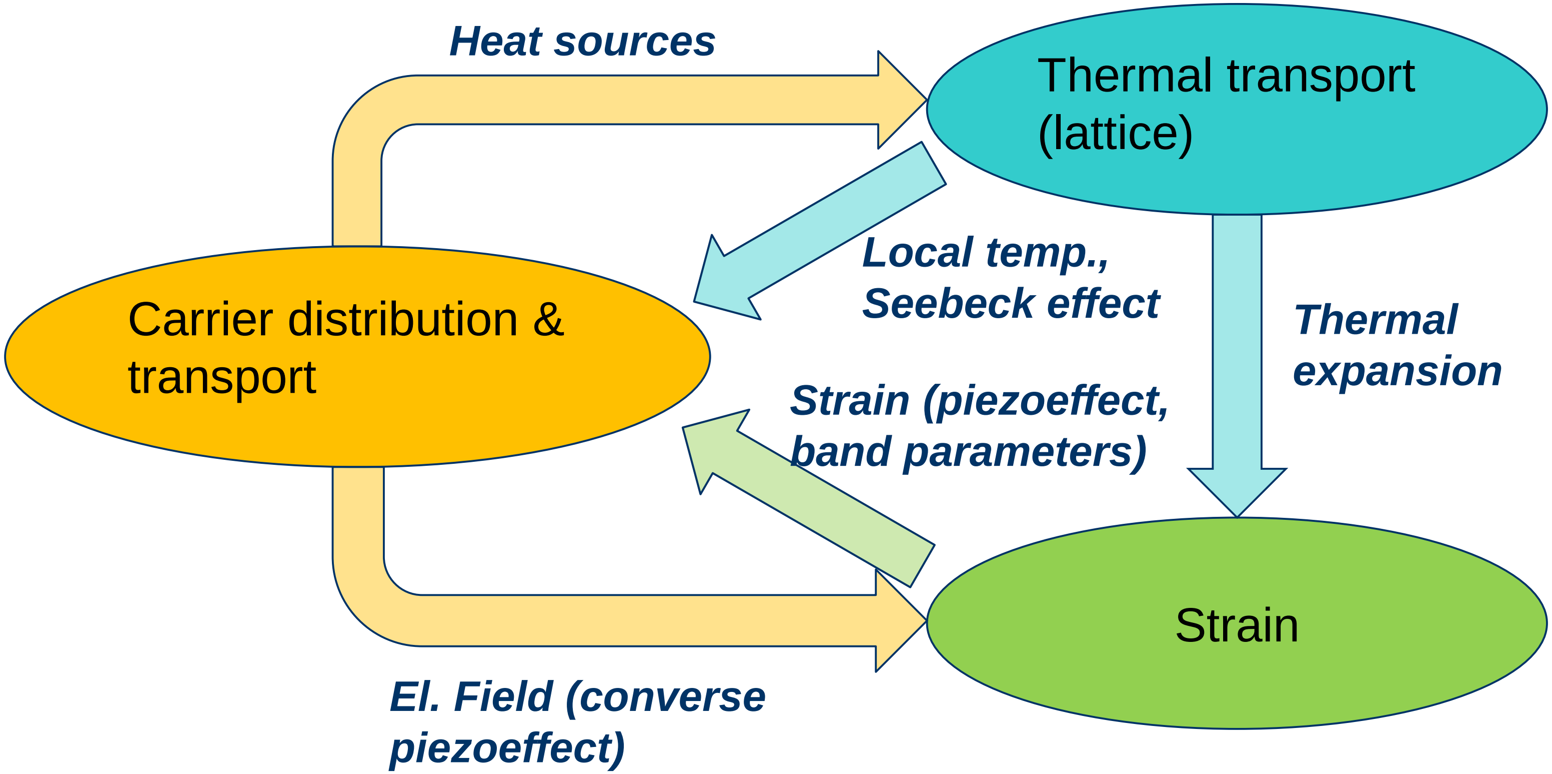
macromodel is solved

temperature is not solved
on fourier ∩ gray

Electro-thermal and Strain

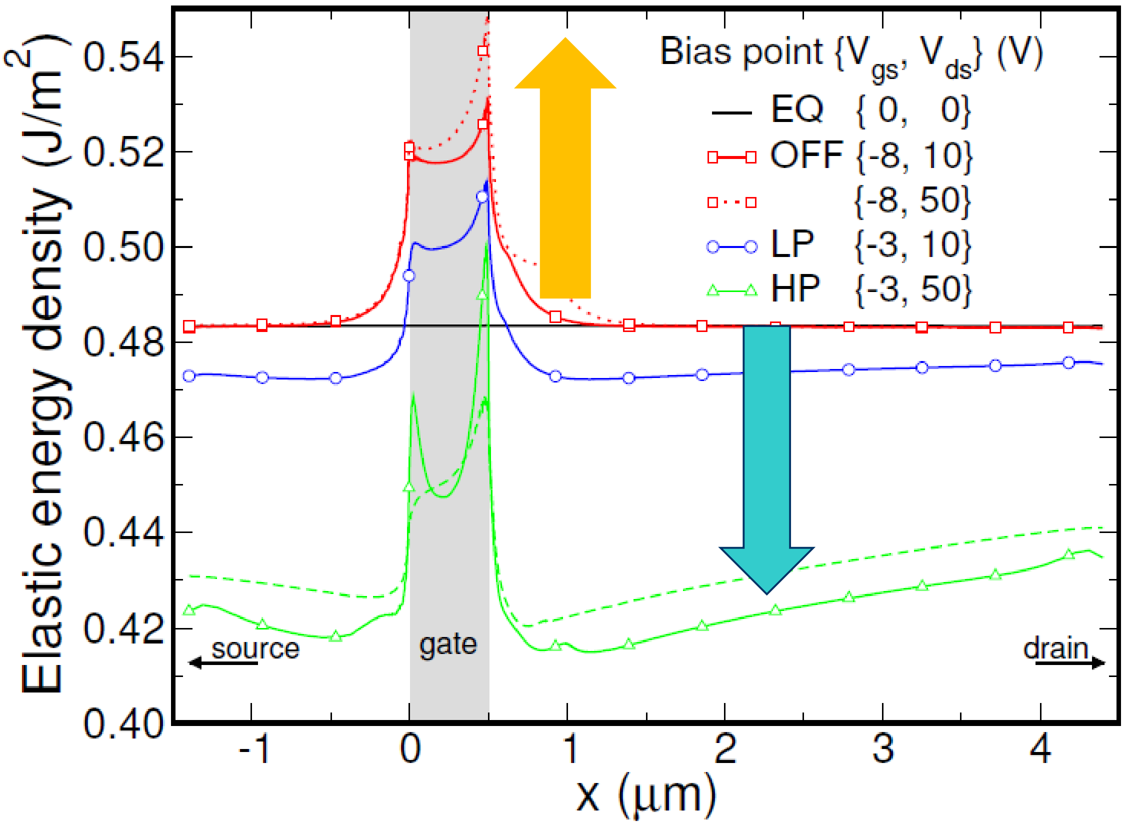
Electro-thermo-mechanical simulation

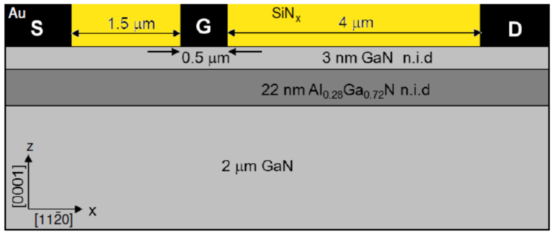
- How does mechanical stress in a HEMT depend on operating conditions?
- Electrical, thermal and mechanical device behavior are interconnected:



Simulation Results: mechanical energy

Mechanical energy density, integrated along [0001]:





- Converse piezoelectric effect increases locally mechanical stress
- Self-heating decreases overall mechanical stress

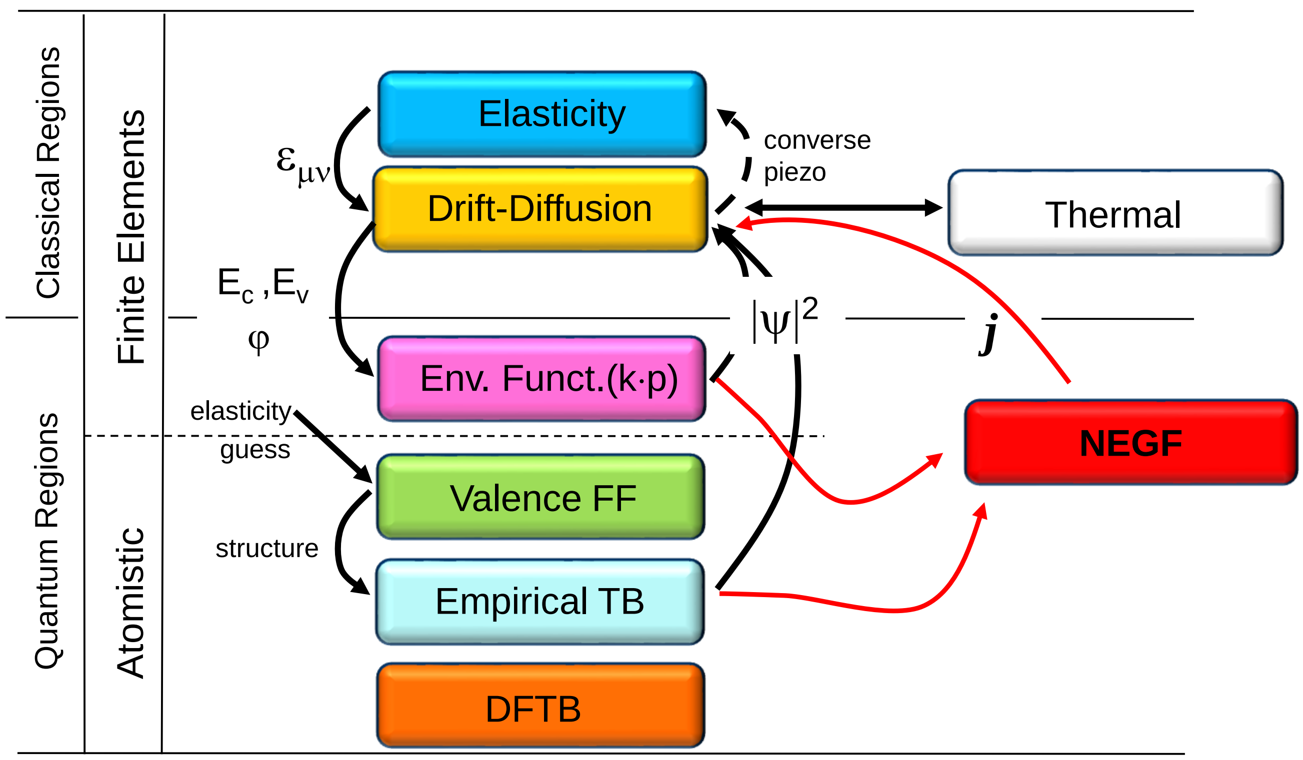
Critical planar energy densities are given in the range of 0.49 ~ 0.7 J/m^2

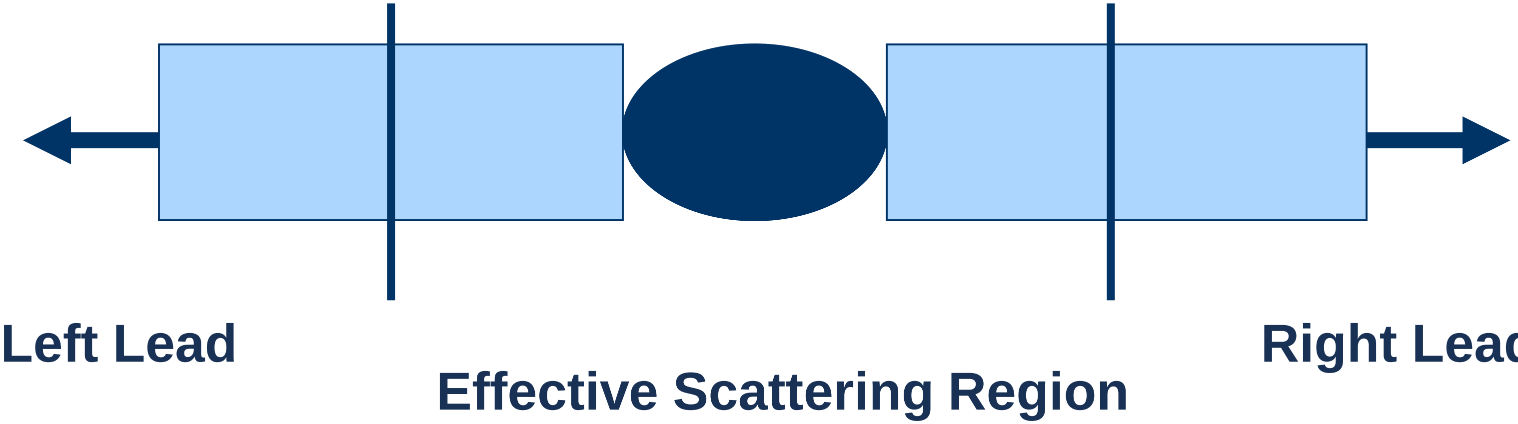
Joh et al. Microelectronics Reliability, 50, 767, 2010

J. Floro et al. J. Appl. Phys., 96, 7087, 2004

Quantum Transport: NEGF

Models overview

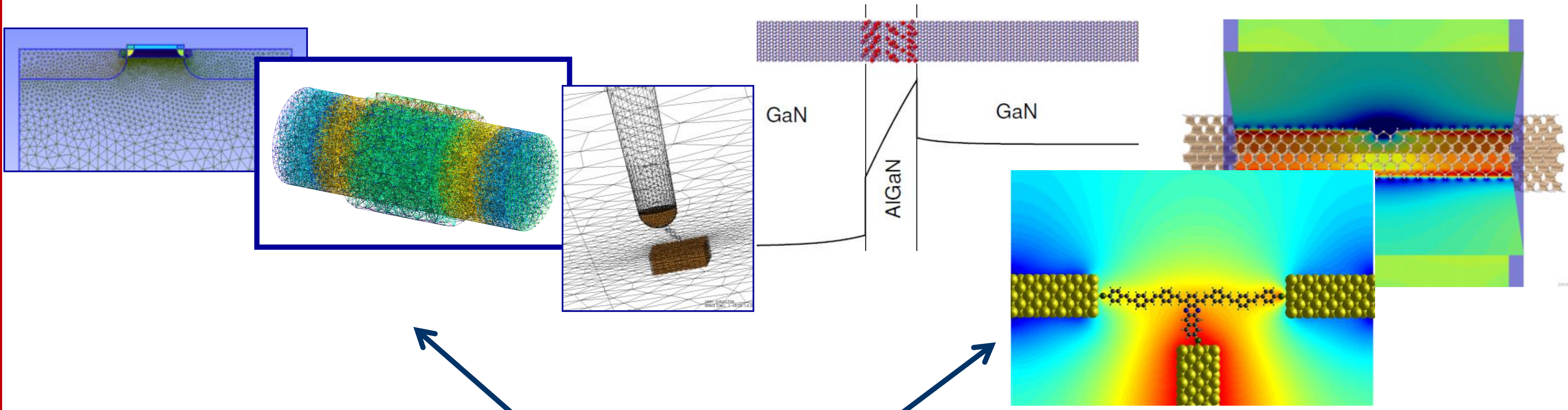




$$[E - H + \Sigma^r(E)]G^r(E) = \mathbf{I}$$

$$D(\mathbf{r}, E) = 2i\,\mathrm{Im}\,G^r(\mathbf{r}, \mathbf{r}, E)$$

Continuous — Quantum-classical interfaces — Atomistic



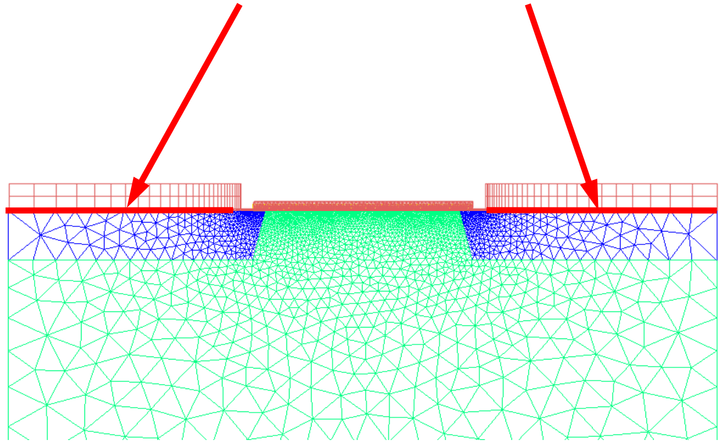
libNEGF

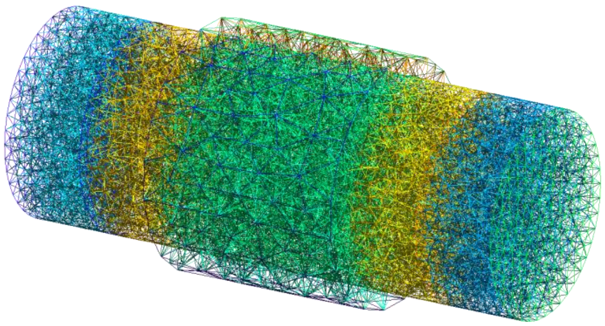
Bitbucket

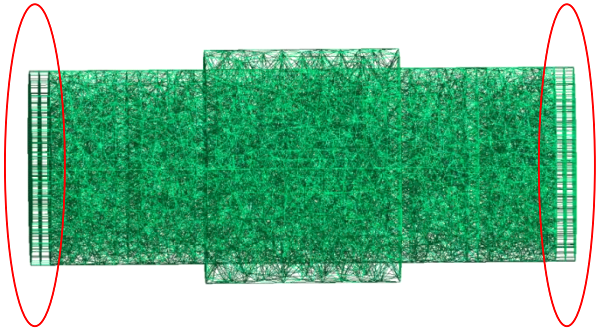
http://www.bitbucket.org

NEGF: contact generation

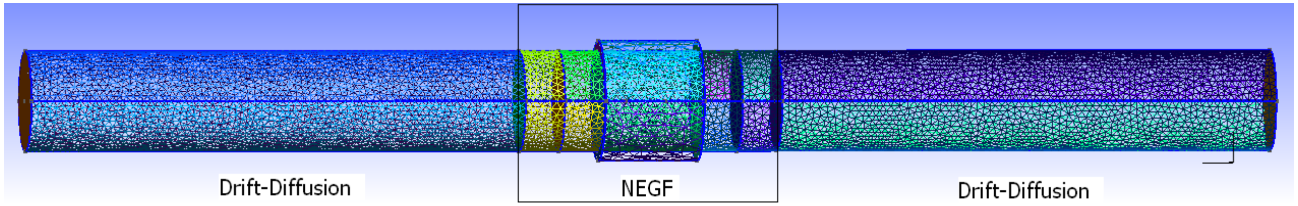
N-1 dimensional Contacts



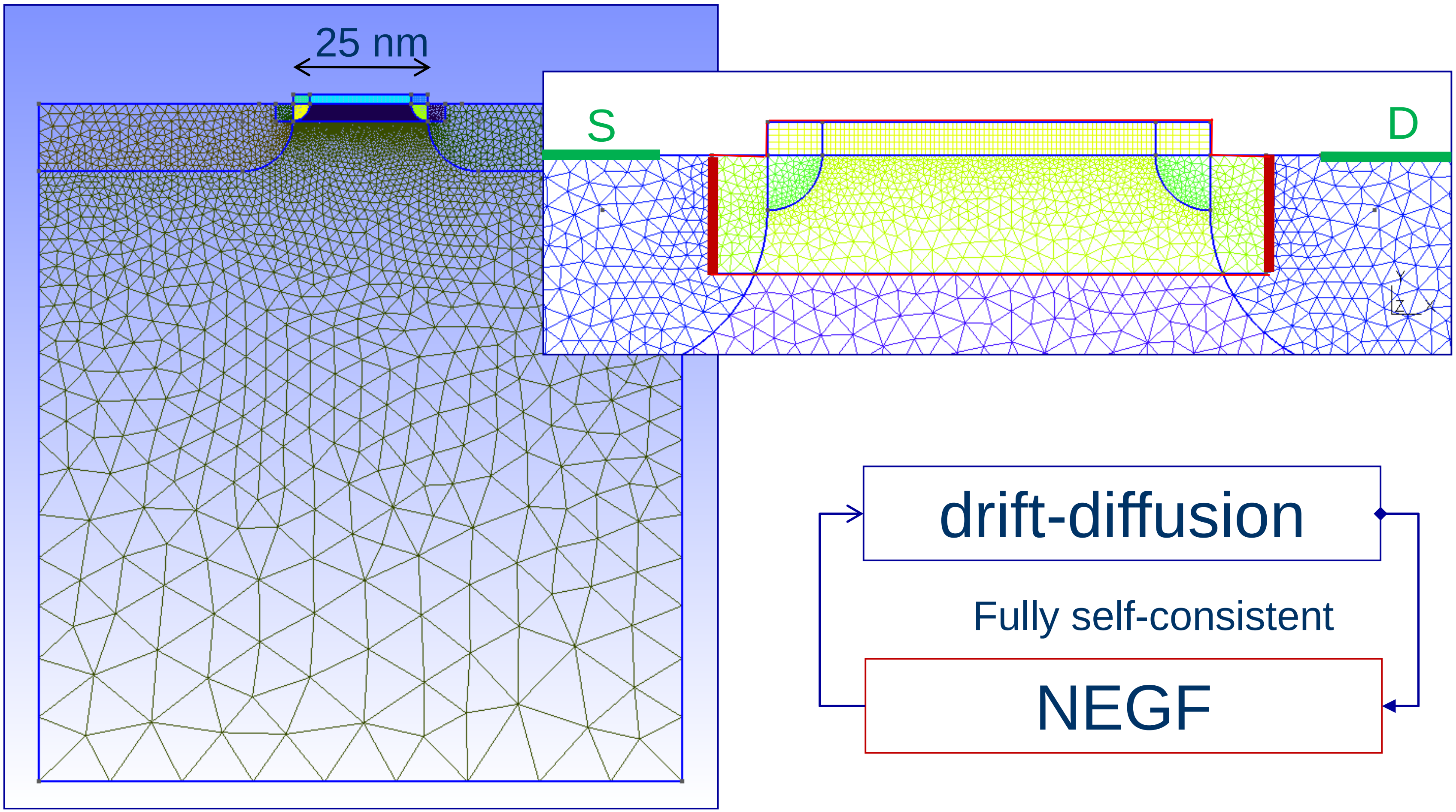




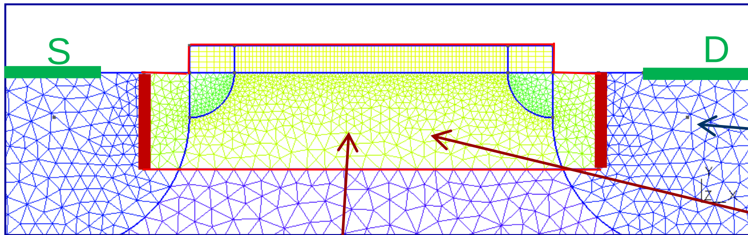
- Automatic mesh creation using *lib*MESH classes
- General extrusion of planar contacts in 1,2,3D



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



NEGF: input file



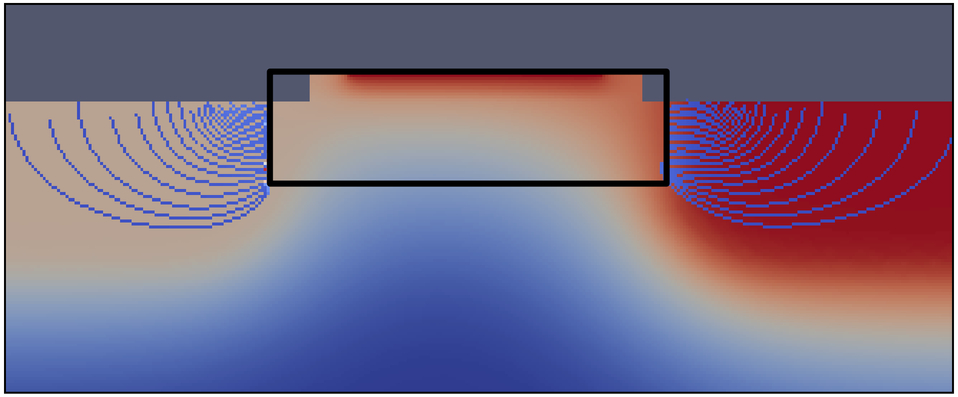
$$
\begin{cases}
\mathbf{J}_n = en\mu_n \mathbf{F} + eD_n \nabla n \\
\nabla \cdot \mathbf{J}_n = e(R - G) \\
\nabla \cdot \left(\varepsilon_0 \varepsilon_r \nabla V \right) = e\left(n - N_D \right)
\end{cases}
$$

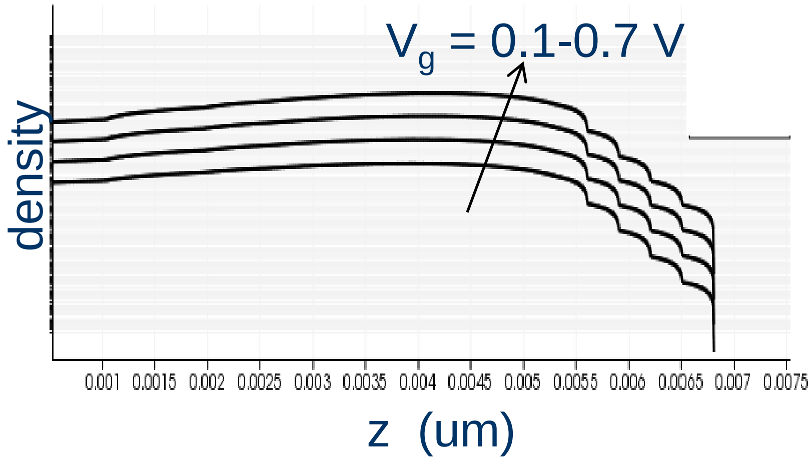
```
Module negf{
    regions = channel
    Physics{
      Hamiltonian efa {}
    }
}
```

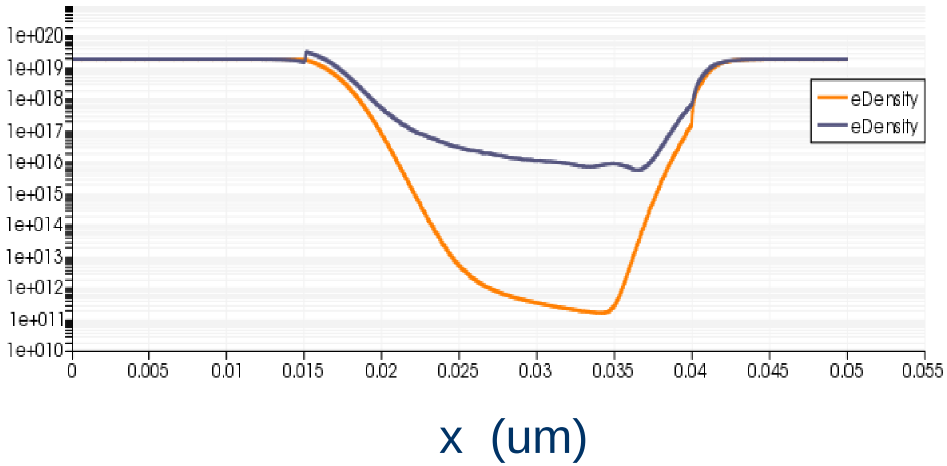
In negf regions, solve only for electrostatic potential, (not for electron current)

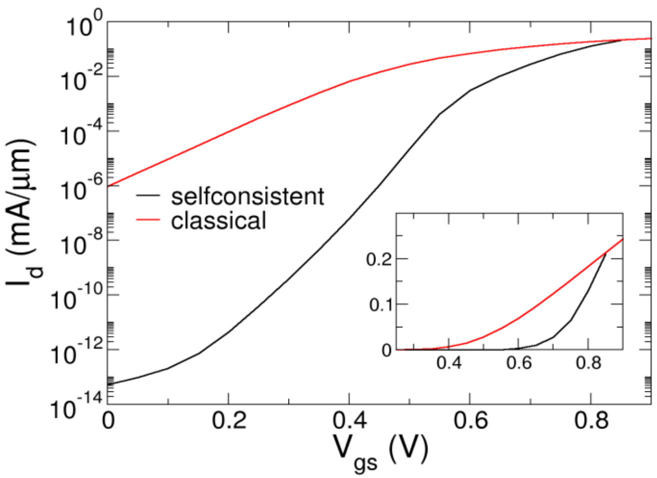
```
Module selfconsistent
{
  solve = (negf, driftdiffusion)

  Multiscale bridge {
    macromodel = driftdiffusion
    micromodel = negf
    restrict_variables = (fermi_e)
  }
  max_iterations = 10
  absolute_tolerance = 1e-3
  relative_tolerance = 1e-9
}
```

MOS: quantum/classical





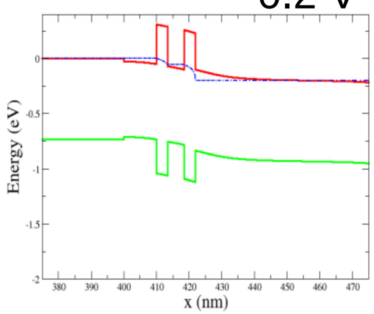


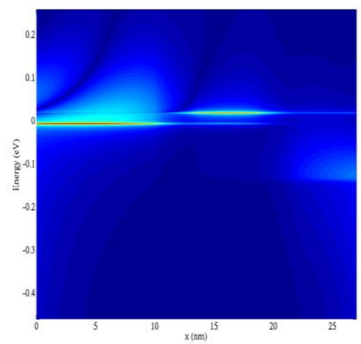


RTD structure

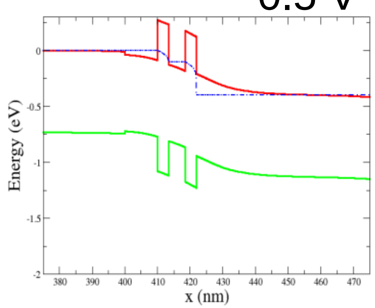
500A	n+	$In_{0.53}Ga_{0.47}As$	Contact
500A	n	$In_{0.53}Ga_{0.47}As$	Emitter
50A	i	$In_{0.53}Ga_{0.47}As$	Spacer
35A	i	$In_{0.7}Ga_{0.3}P$	Barrier
50A	i	$In_{0.6}Ga_{0.4}As$	Strained well
35A	i	$In_{0.7}Ga_{0.3}P$	Barrier
100A	i	$In_{0.6}Ga_{0.4}As$	Strained layer
1000A	i	$In_{0.53}Ga_{0.47}As$	Collector
3000A	n+	$In_{0.53}Ga_{0.47}As$	Contact
S.I.-InP substrate			

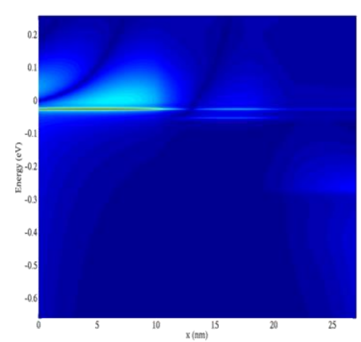
0.2 V

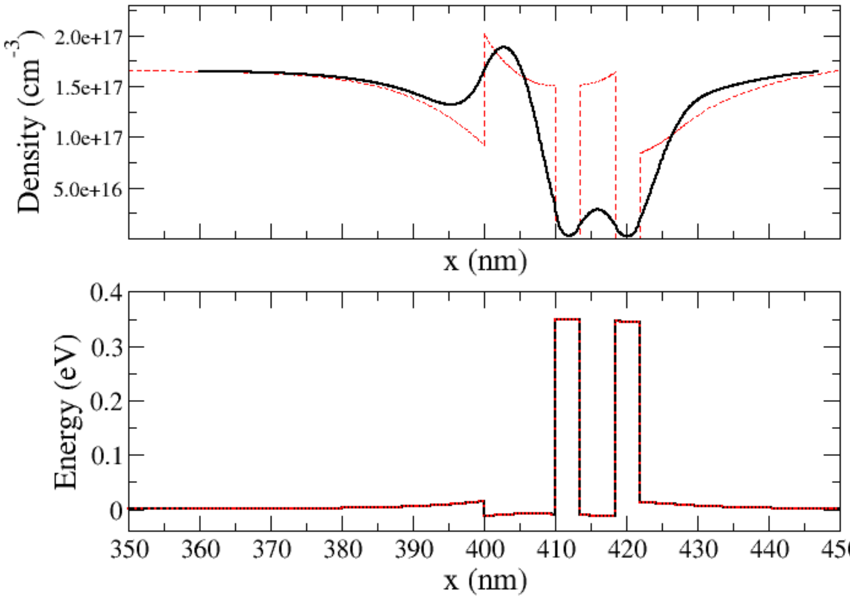


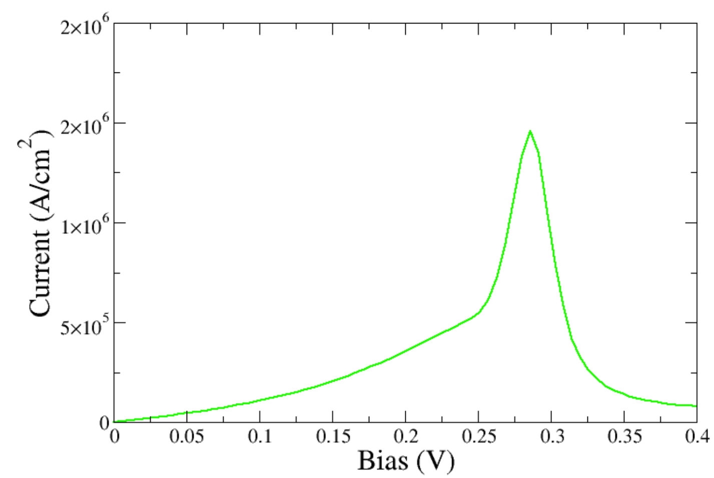


0.5 V

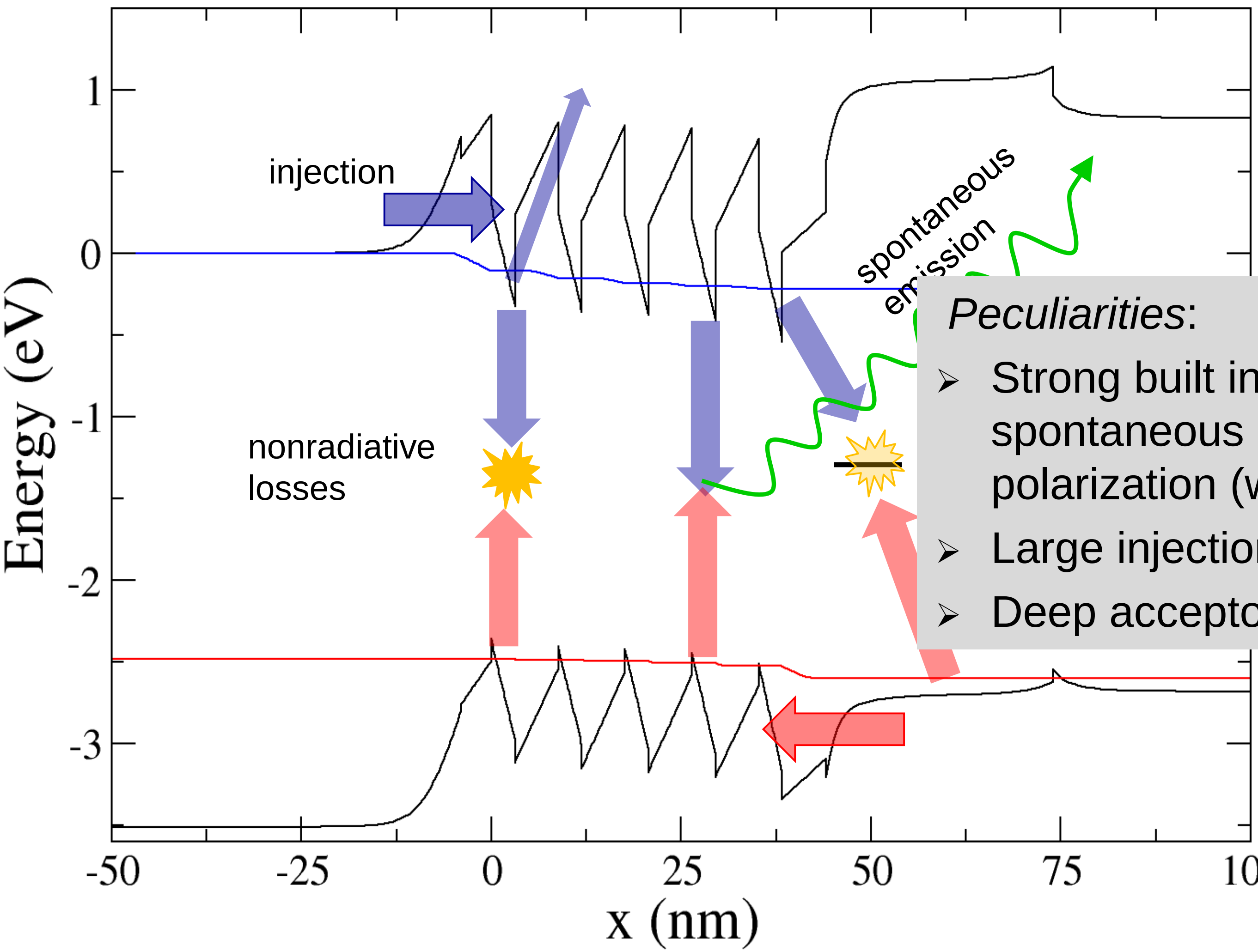








InGaN/GaN multi QW



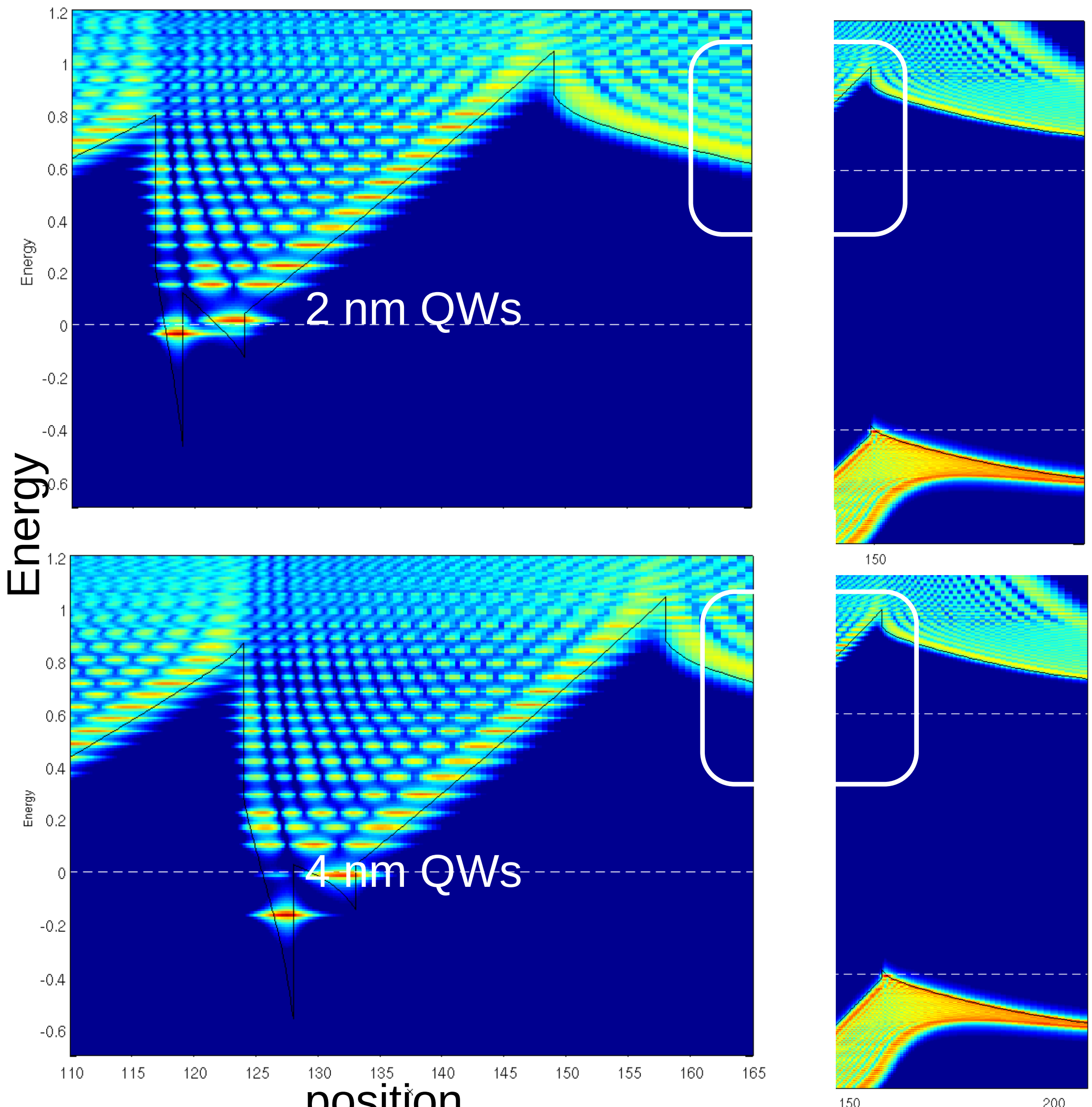
Peculiarities:

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

$$IQE = \frac{radiative\ rec}{radiative\ rec + nonradiative\ rec.}$$

Example: excited states

- Here we use (NE)GF to calculate the LDOS, on top of a DD simulation (no selfconsistency)



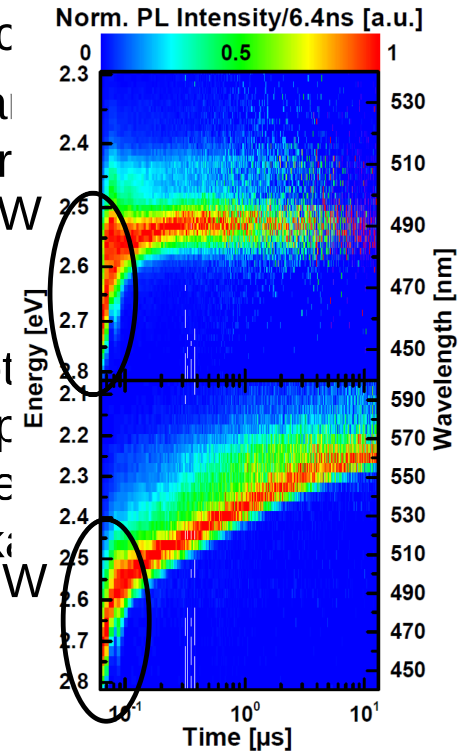
- NEGF based LDOS give more insight into spatio-spec
- «sta appr

2 nm QW

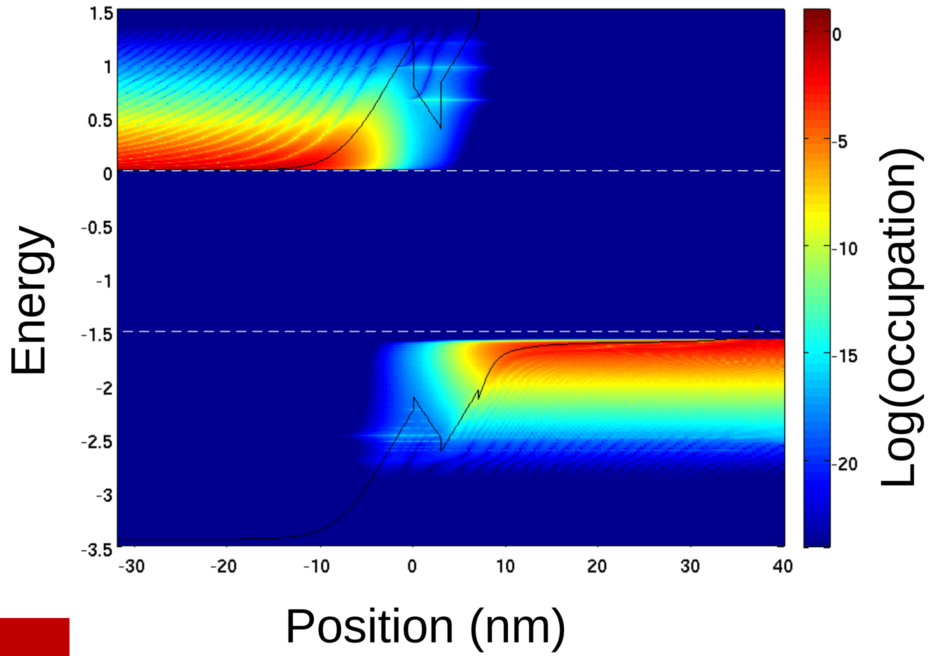
Future:

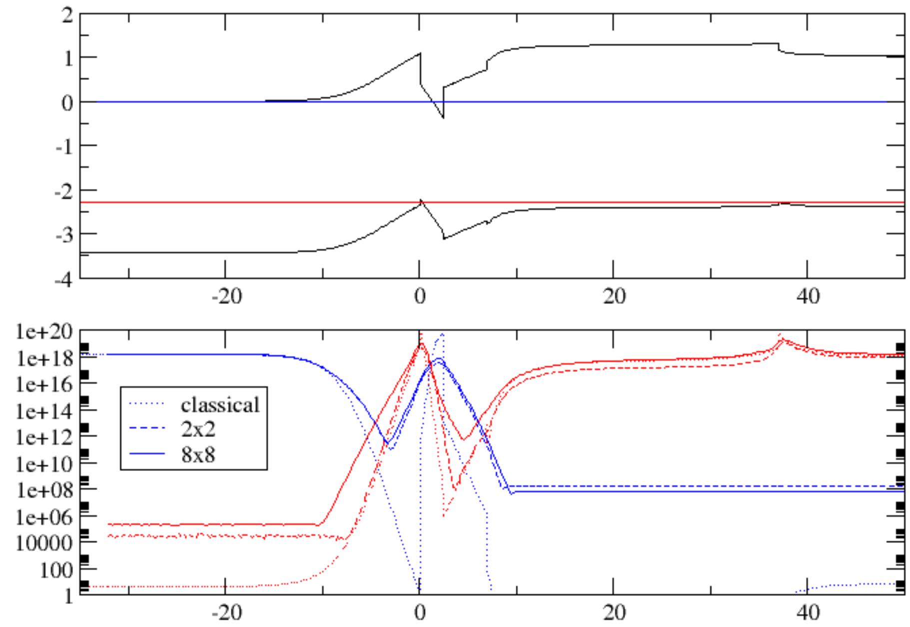
- Phot coup asse leak

4 nm QW



- Difficulties: separate n/p densities near equilibrium
- Below knee voltage the minority carrier densities become extremely low
- Reproduce non-radiative recombinations in NEGF (Auger, SRH)
- Introduce el-γ coupling in NEGF

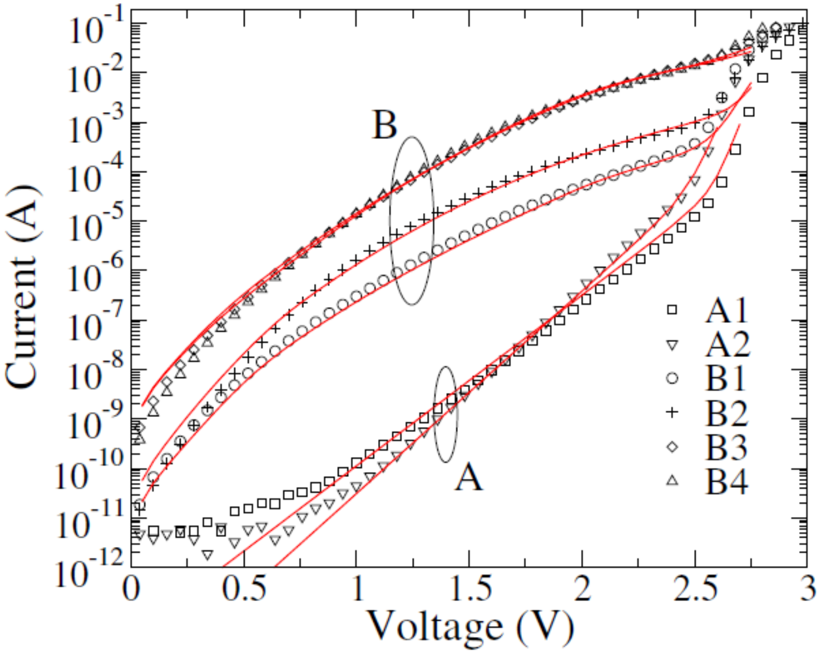


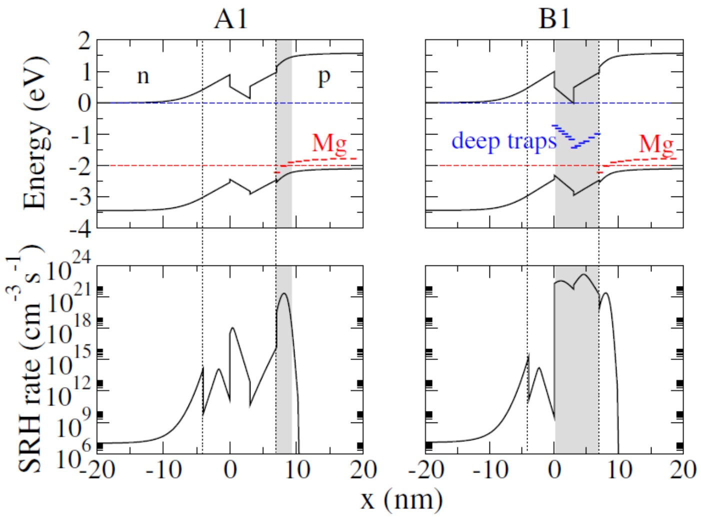


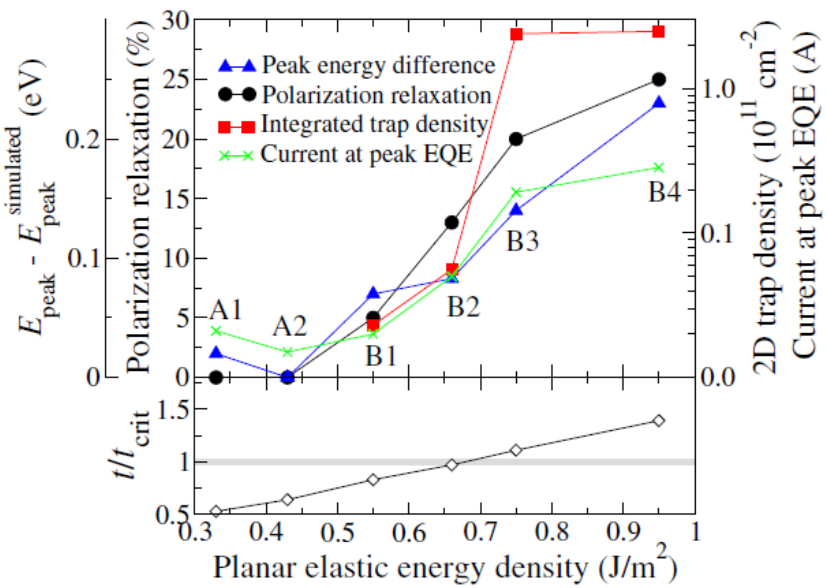
⇒ *work in progress*

Importance of non-radiative losses

- Forward current at low injection, for different devices (different QW thickness, different In content)

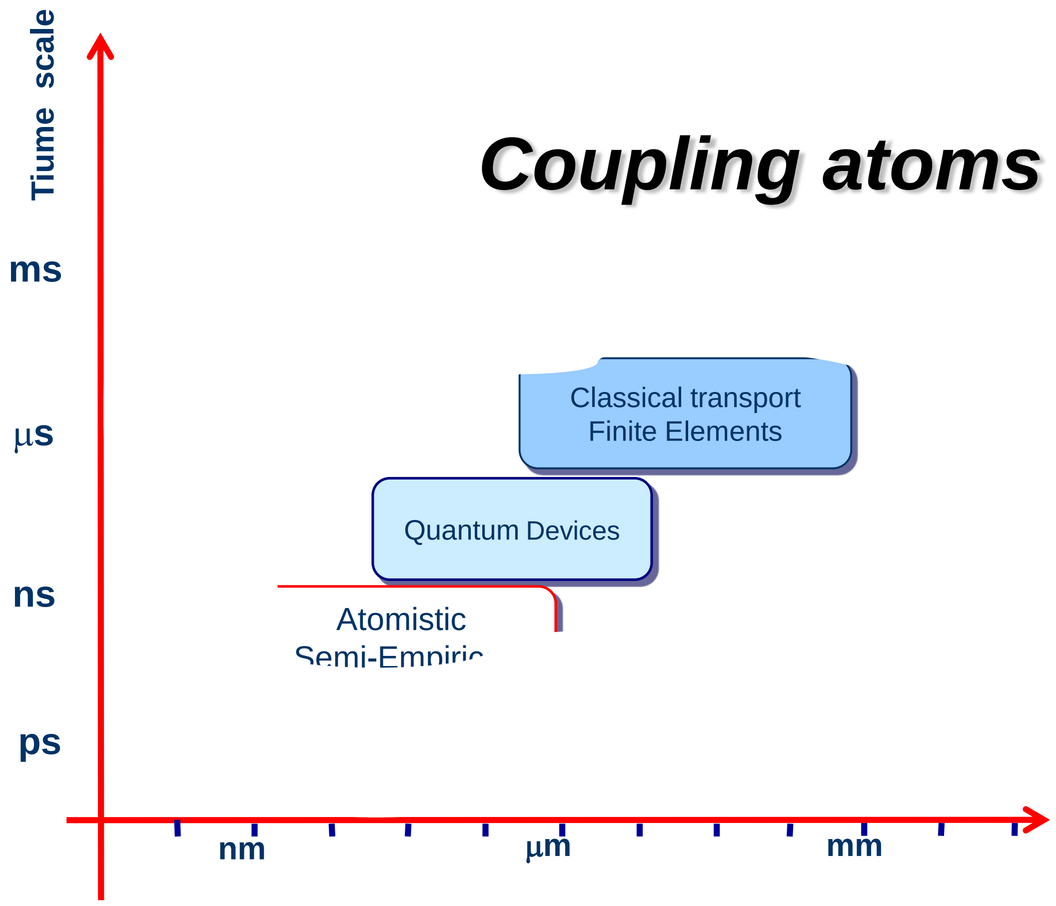






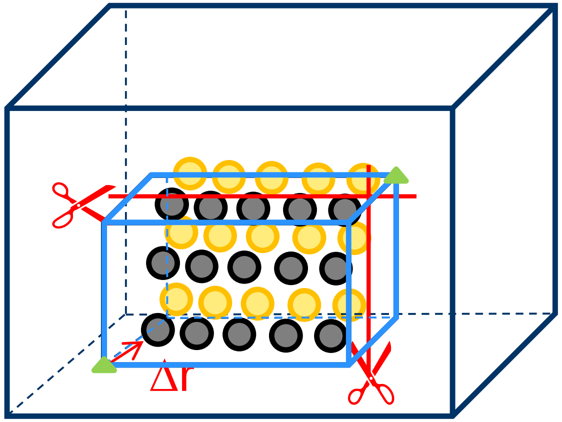
Correlation between fitting parameters and independent mechanical data

Coupling atoms with finite elements



Atomistic structure generation

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

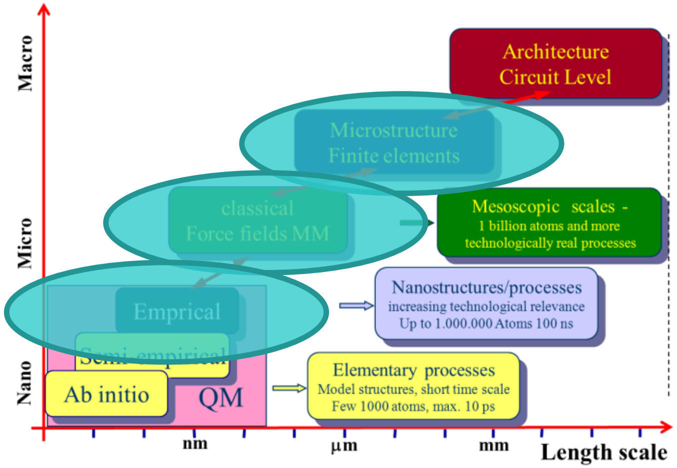


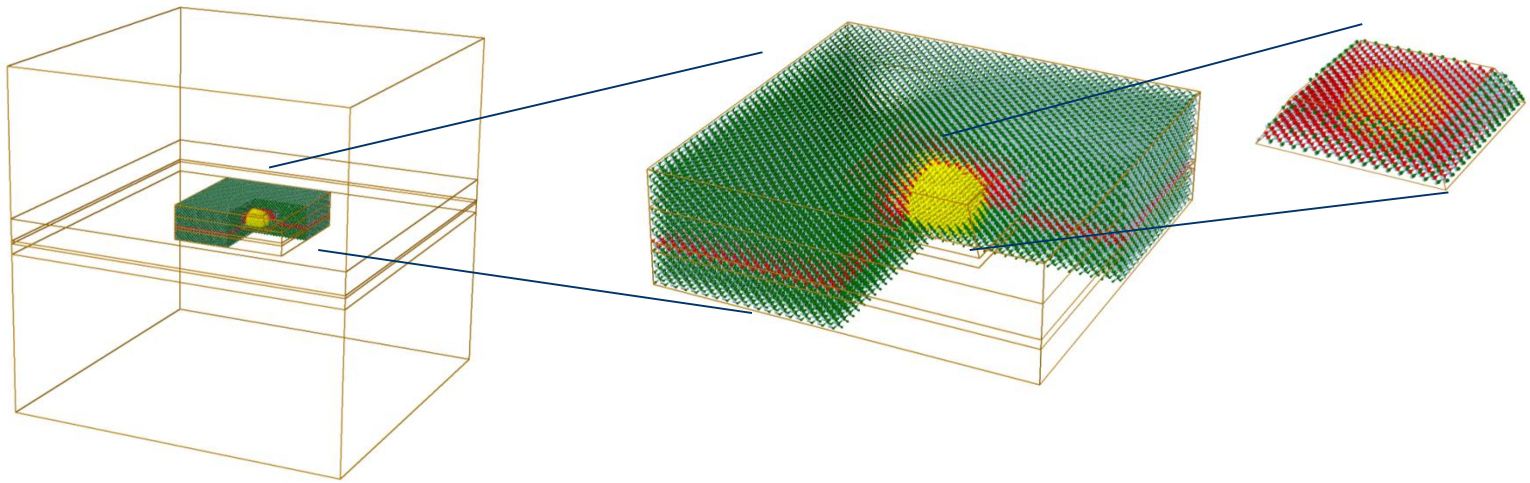
1. Identify relevant volume
2. Shift origin slightly inside
3. Fill up with atoms using the crystal basis
4. Cut atoms outside of the structure

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

- we assume pseudomorphic structures with commensurate interfaces

The multiscale problem



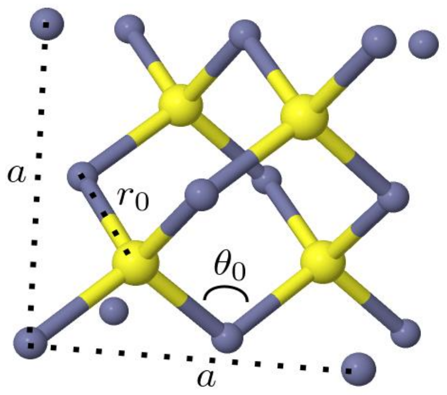


Drift-diffusion
Elasticity

Force Field

ETB

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



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

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

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

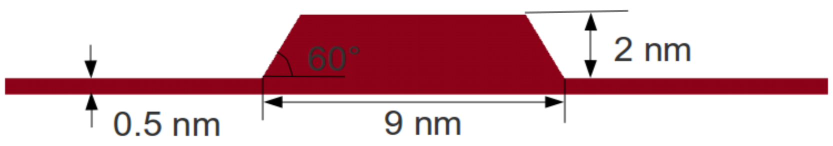
The equilibrium position is that one which minimizes U
We use a nonlinear conjugate gradient minimization technique

Keating (1966)
D. Camacho, Y. M. Niquet (2009)
Penazzi Gabriele, PhD. Thesis (2010)

VFF vs Elasticity

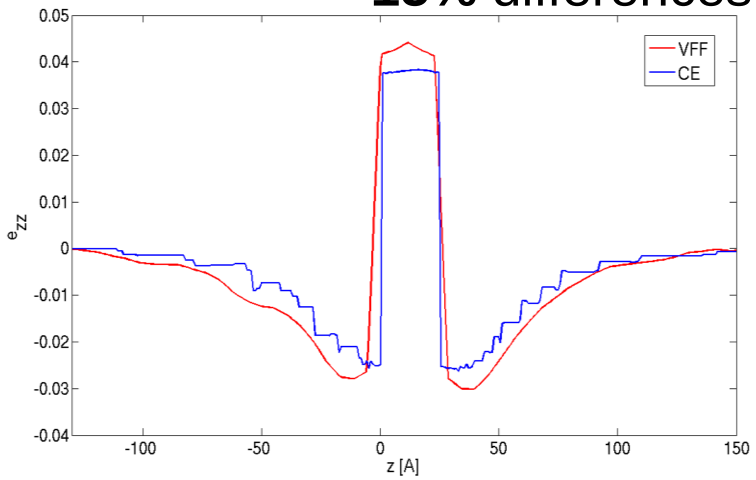
Evaluating when Continuum Elasticity failures is not trivial.
It depends on structure geometry. In general, it fails near interfaces

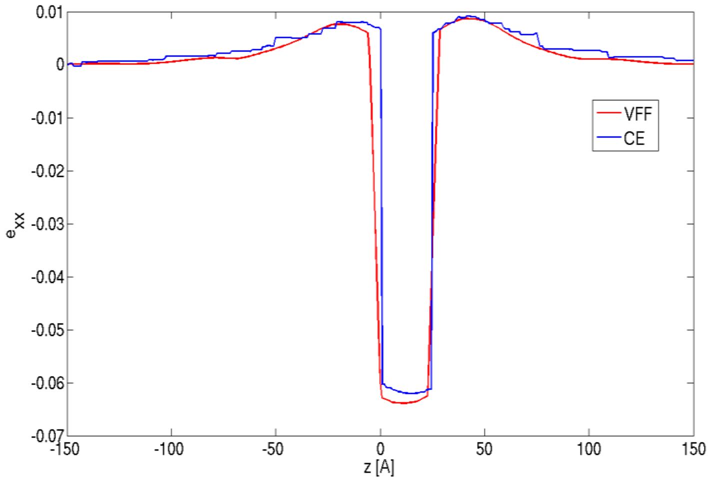
InAs quantum dot on GaAs substrate



Self assembled by strain relaxation
High lattice mismatch (about 7%)

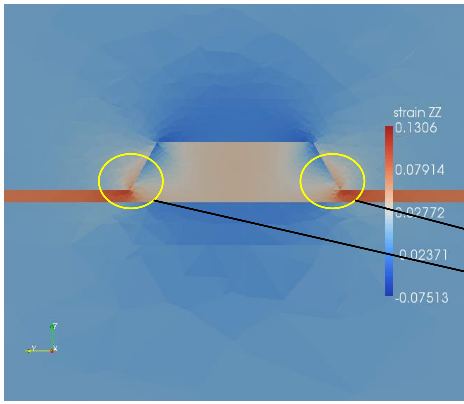
15% differences



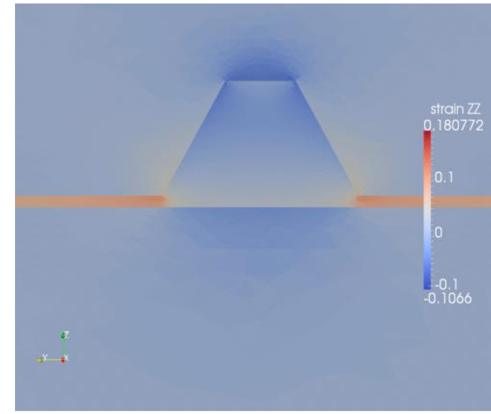


VFF vs Elasticity II

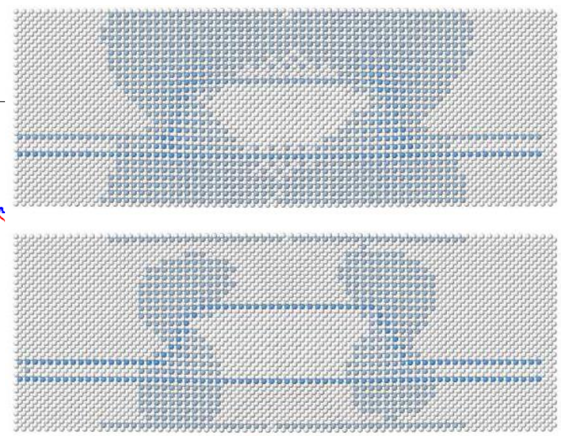
Smaller differences on low aspect/ratio structures

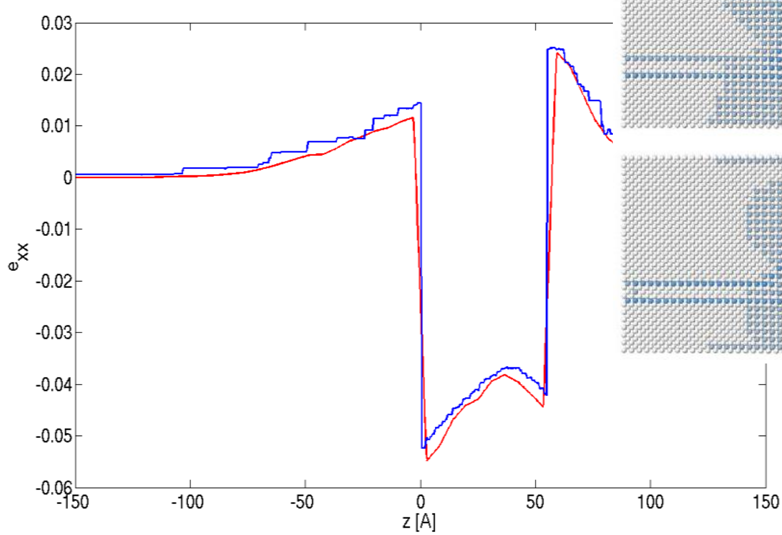


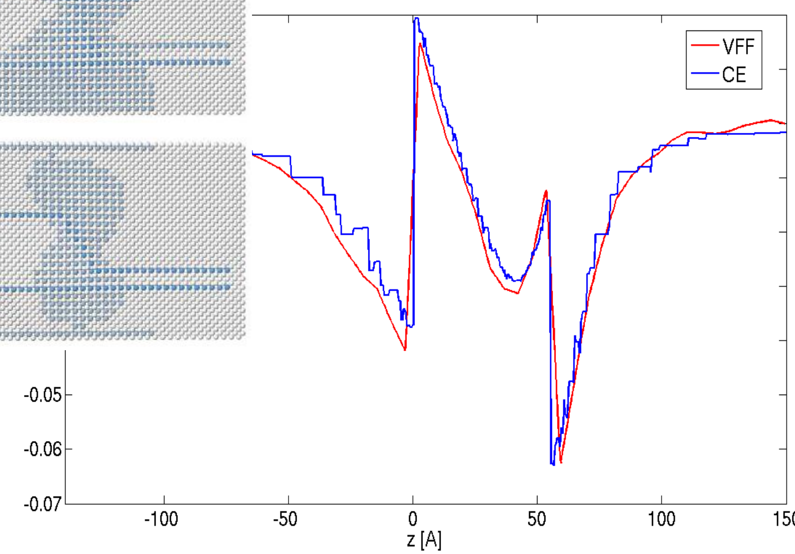
Increase height up to 5 nm

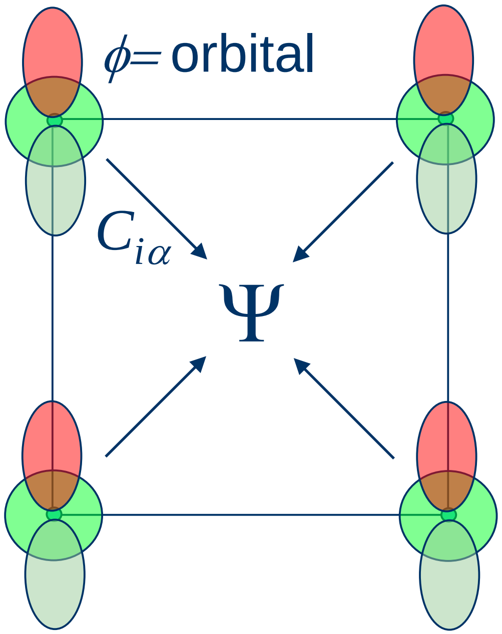


VFF is **fundamental** also to include **internal strain** here!









$$\psi(\mathbf{r}) = \sum_{\substack{\text{atomic} \\ \text{site, } i}} \sum_{\text{orbitals, } \alpha} C_{i\alpha}\, \phi_{i\alpha}(\mathbf{r} + \mathbf{R}_i)$$

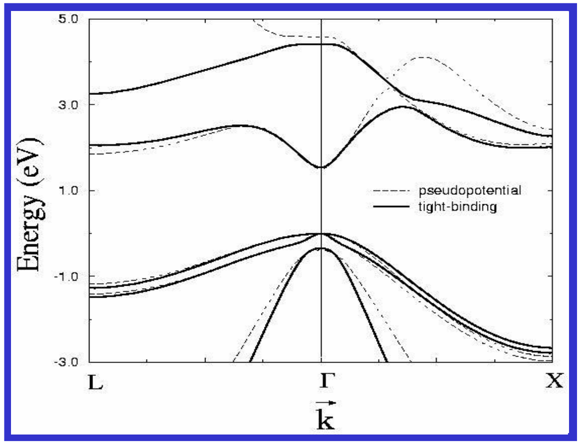
$$\langle \phi_{i\alpha} | \phi_{j\beta} \rangle = S_{i\alpha, j\beta} = \delta_{ij} \delta_{\alpha\beta}$$

$$\sum_{\substack{\text{atomic} \\ \text{site, j}}} \sum_{\text{orbitals, } \beta} \left[H_{i\alpha, j\beta} - E_n \right] C_{j\beta} = 0$$

matrix notation:

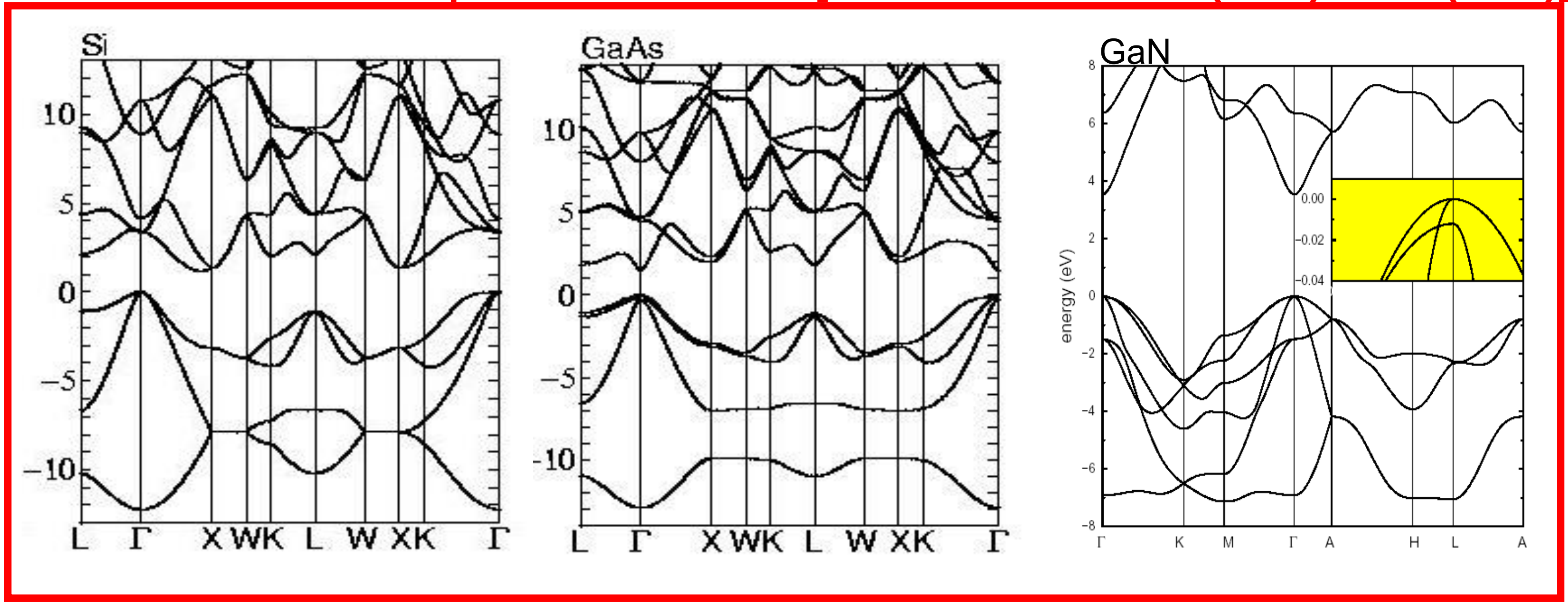
HC=EC

Empirical Tight-Binding

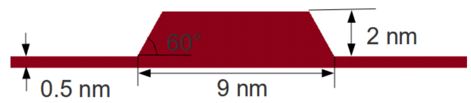


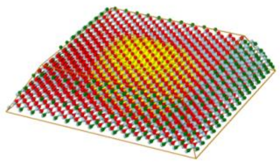
The sp^{3}s* Hamiltonian
[Vogl et al. J. Phys. Chem Sol. 44, 365 (1983)]

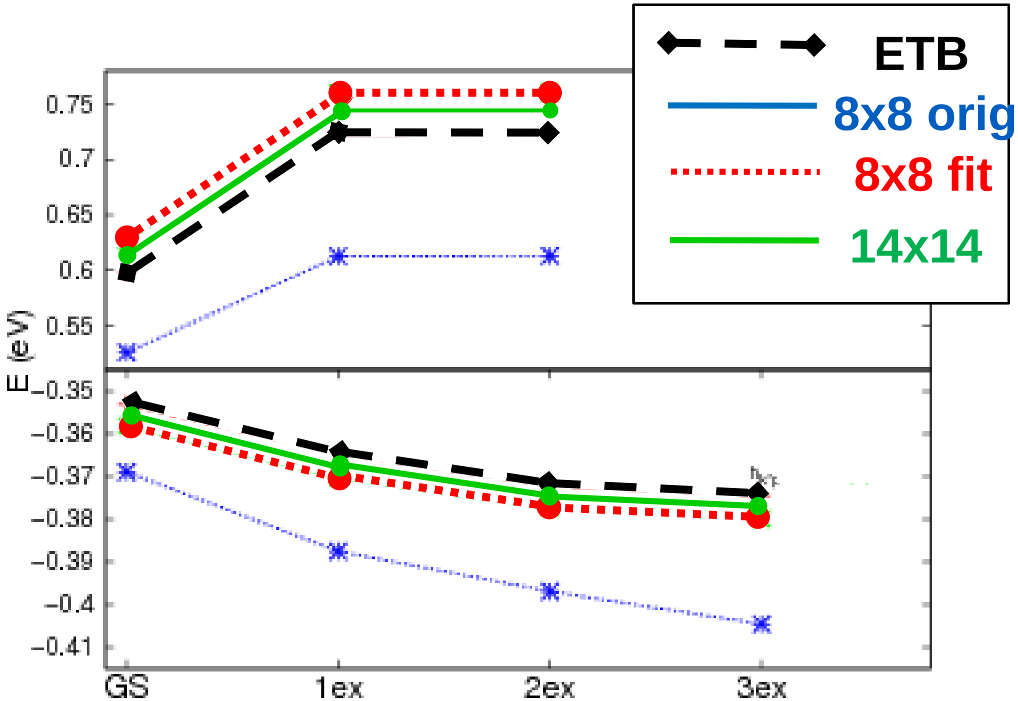
The sp^{3}d^{5}s* Hamiltonian [Jancu et al. PRB 57 (1998); PRB (2001)]

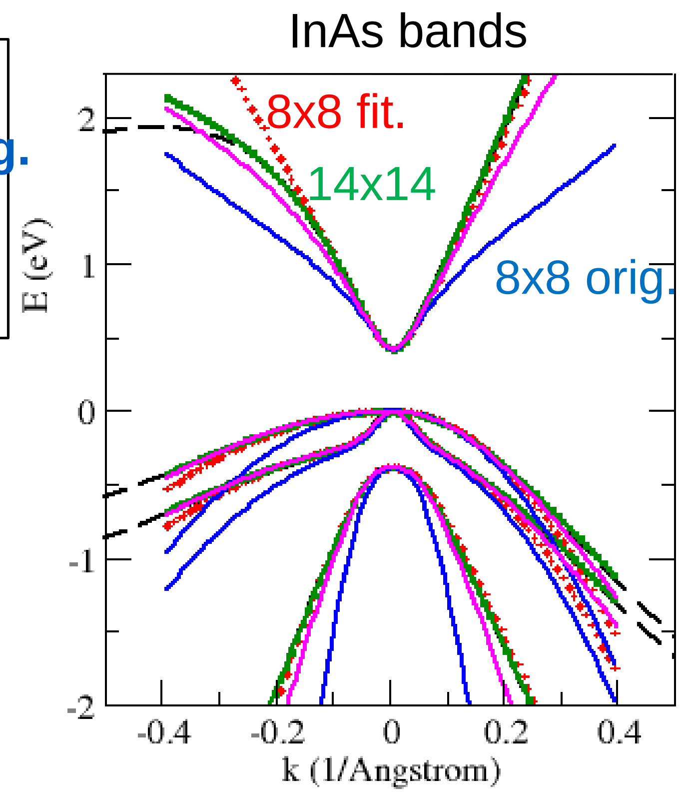


k.p vs TB









Residual difference can be due to **interface effects**

Alloys

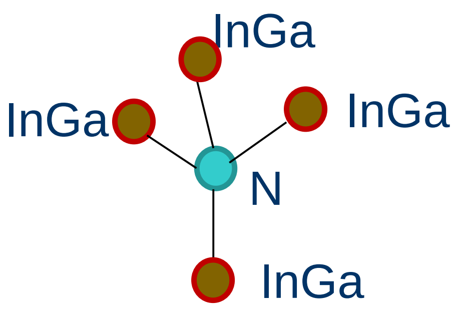
Can treat alloys in two ways: VCA (virtual crystal approximation, effective material) or ‘real’ structure (e.g. random alloy)

- In VCA matrix elements are taken as mean values:

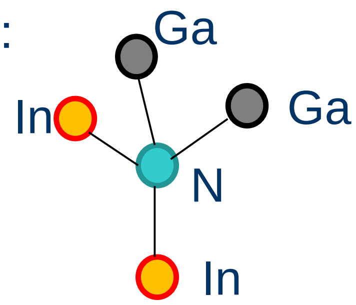
  $In_xGa_{1-x}N$ = x*(InN) + (1-x)*(GaN)

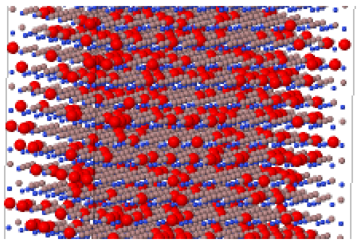
- otherwise onsite elements according to the atom and hopping element according to the pair

VCA:



‘real’:



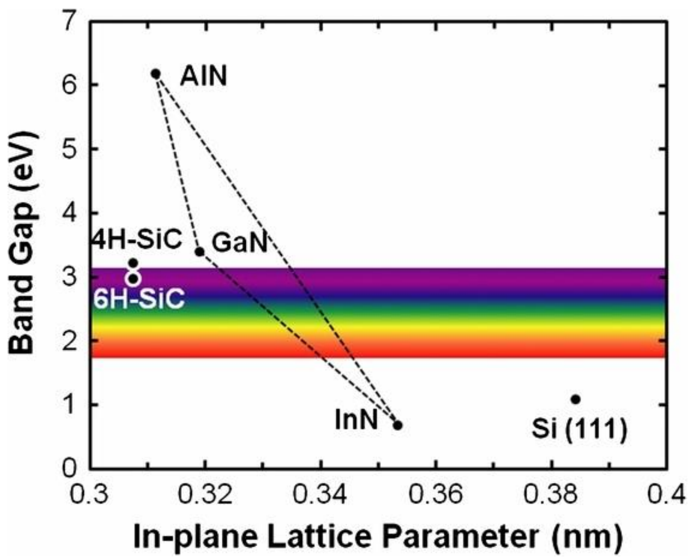


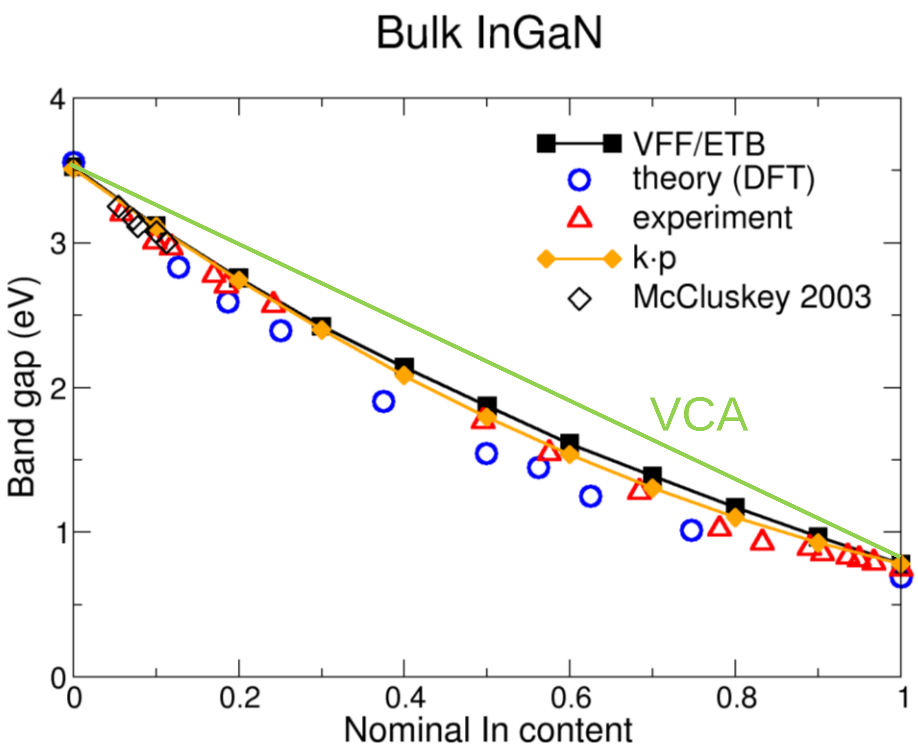
requires supercell + statistical ensemble

Note: we like parameter sets where the common atom (N) is consistent between InN and GaN

- Tunable gap across visible: high efficiency/efficacy LEDs
- Theoretically could allow for all-nitride phosphor-free white light
- Challenge: InN GaN are 10% lattice mismatched !

Kaun et al, Semicond. Sci. Technol. 28 074001,2013

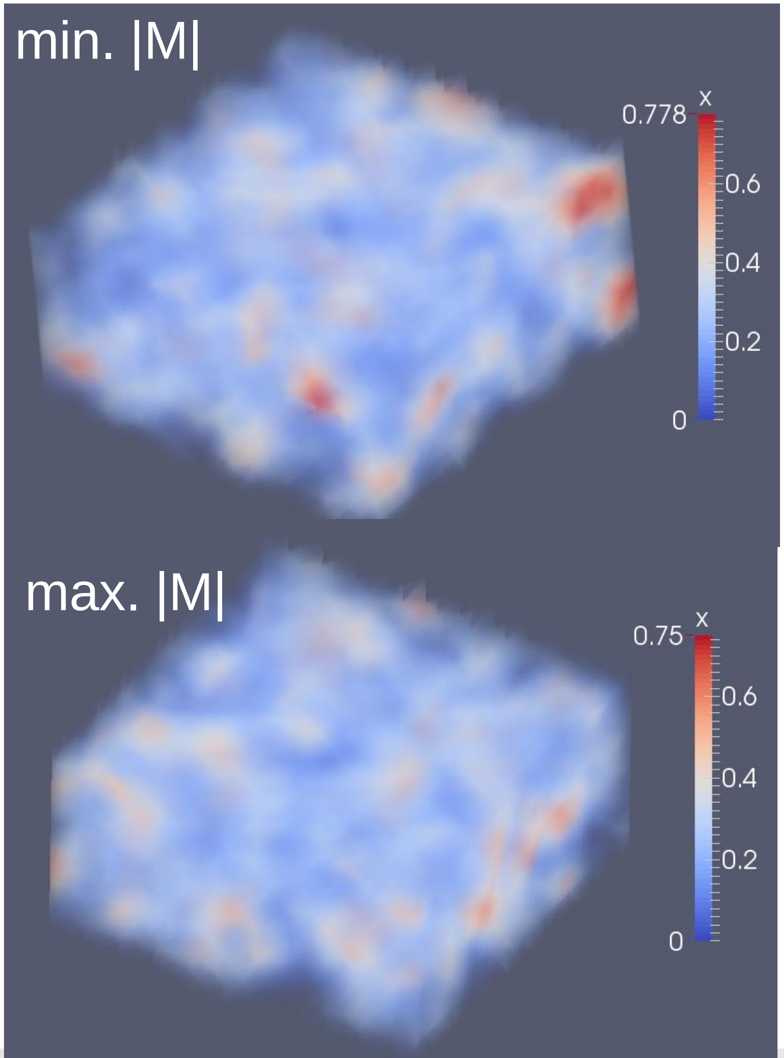


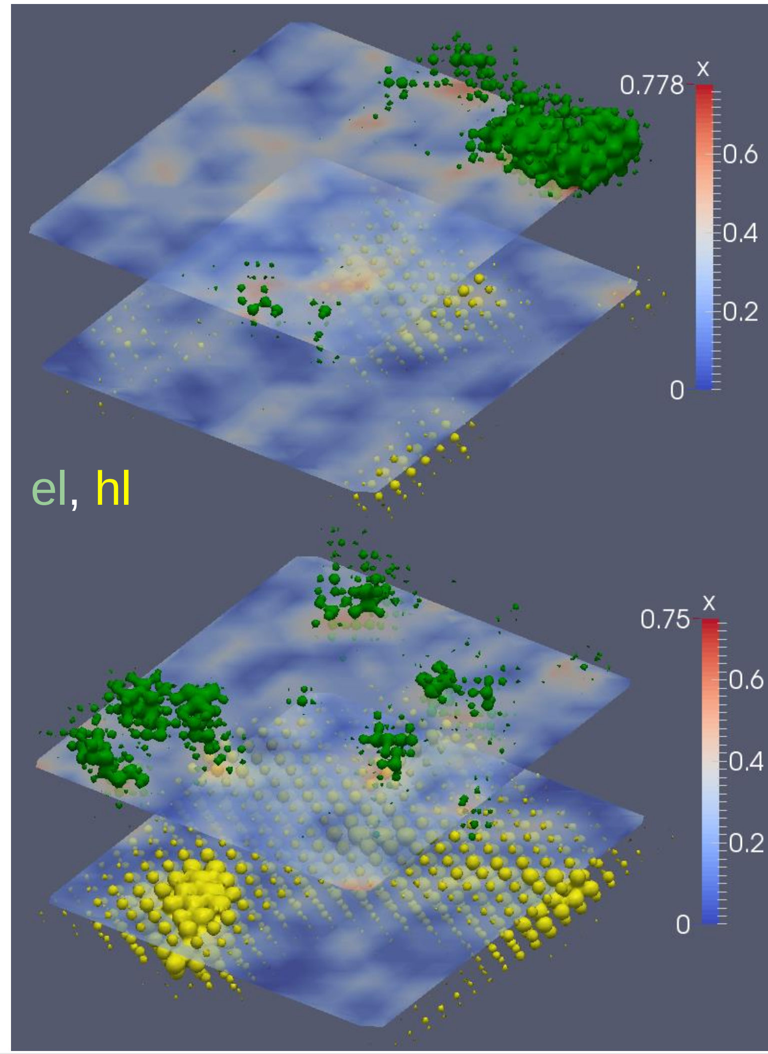


Localization behavior in InGaN QW

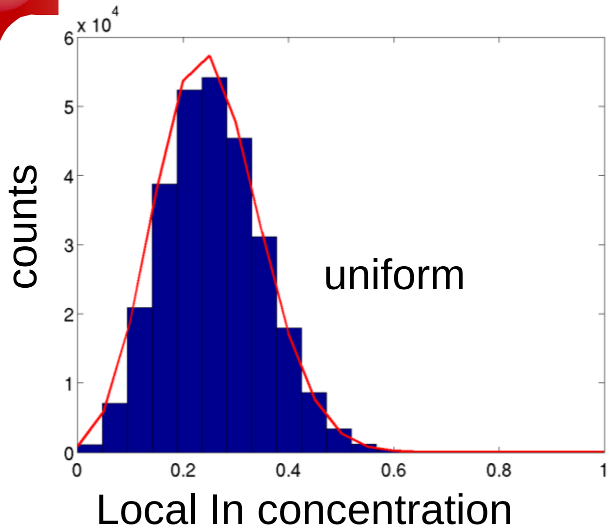
Correlation of local In concentration with wave function localization

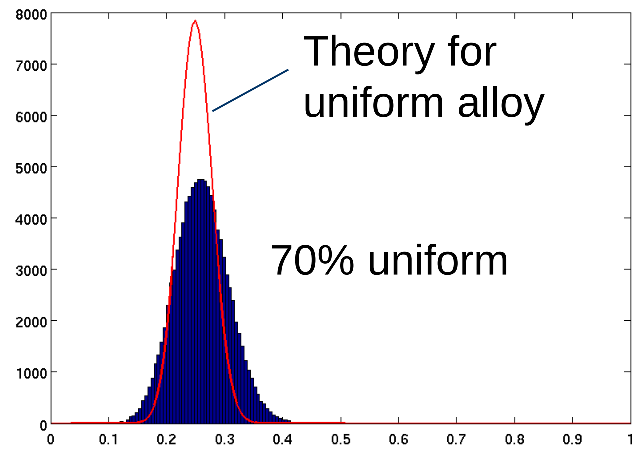
Electrons and holes subject to different In fluctuations planes



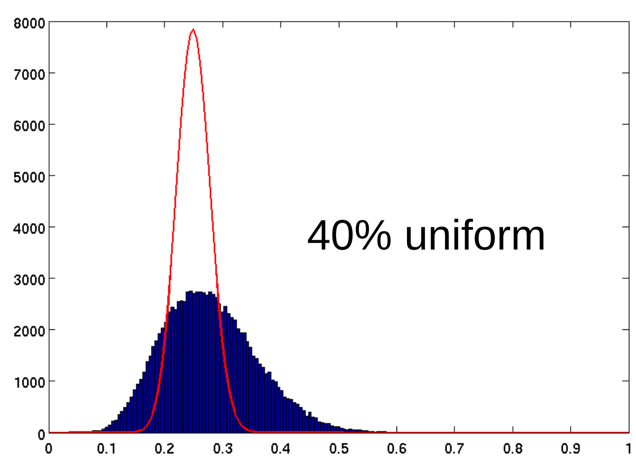


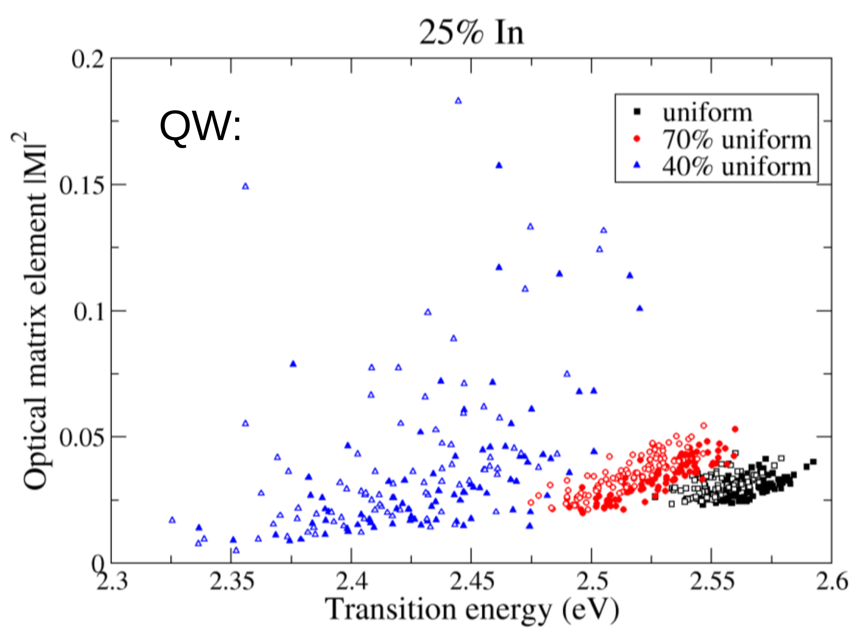
Effect of non-uniformity





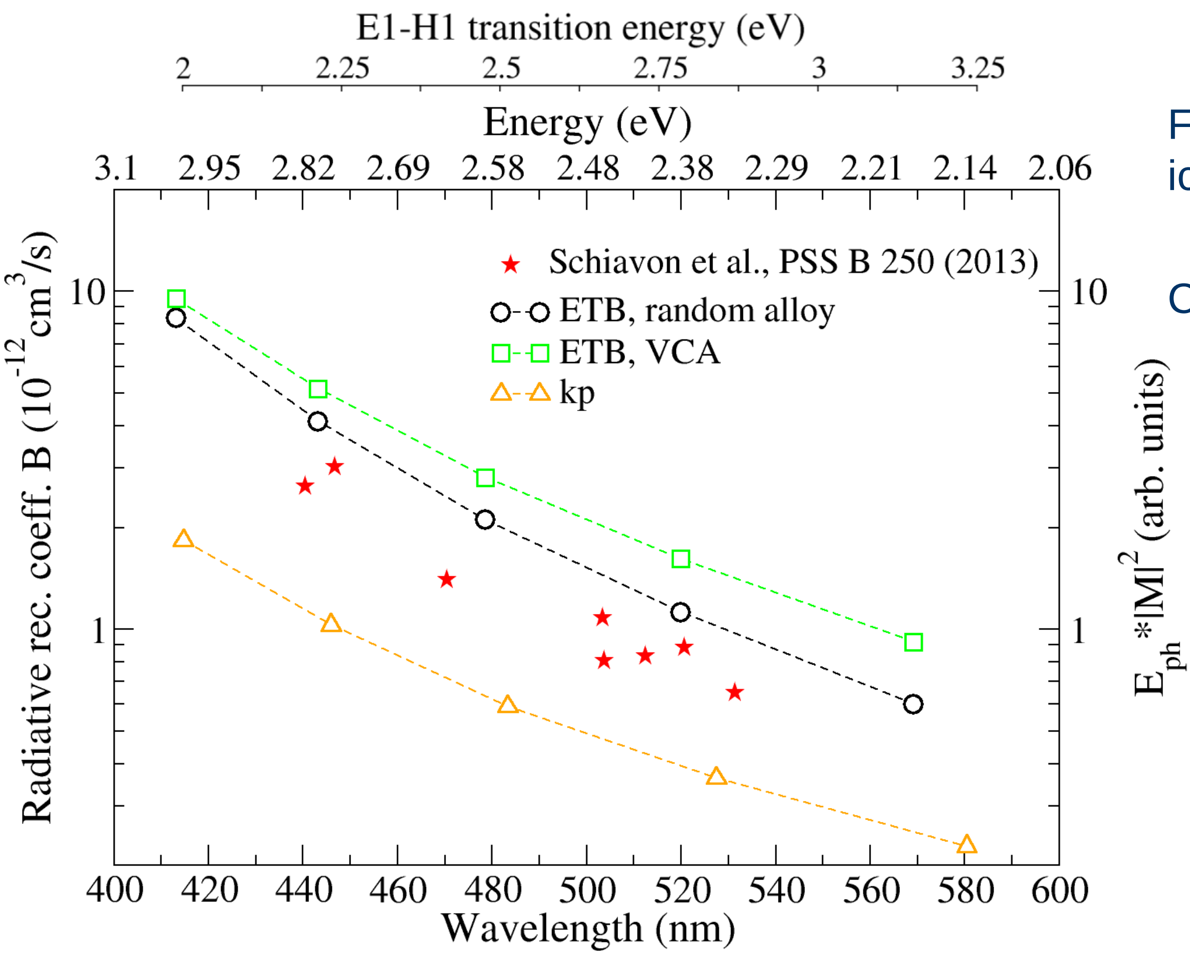
Environment dependent substitution probability





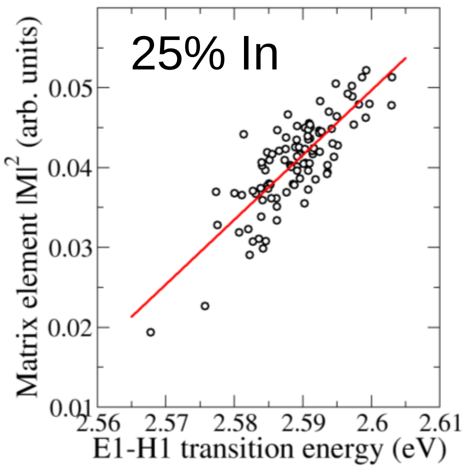
InGaN QW: optical matrix element

Lateral localization leads to strong fluctuations in optical matrix elements



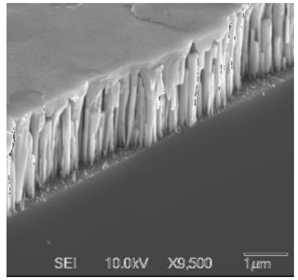
Fluctuation both in energy and M, icreasing with In concentration

Correlation between E_g and MME

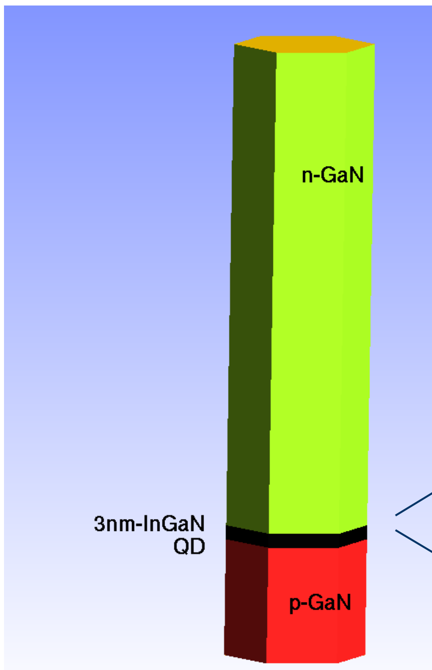


Increasing deviation from VCA values

Modelling nanopillars

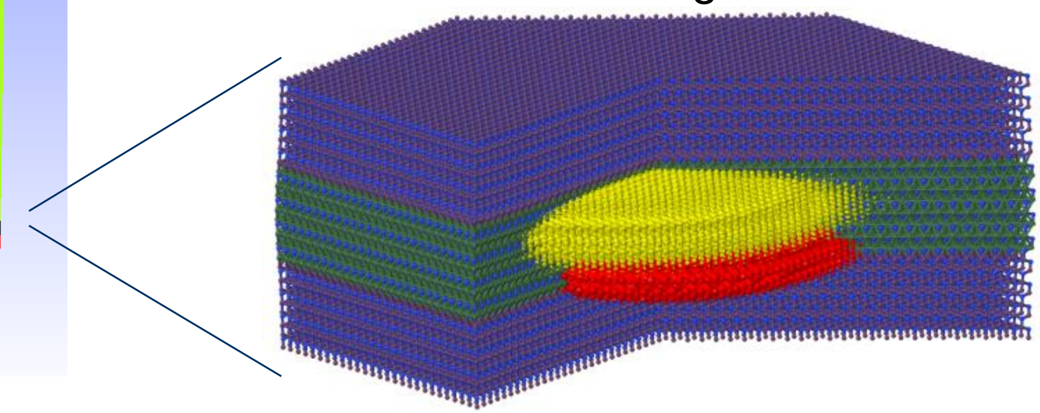


- small footprint on the substrate, allows:
- **defect-free** material
- growth on various substrates (Silicon)
- growth on large area substrates without lattice strain



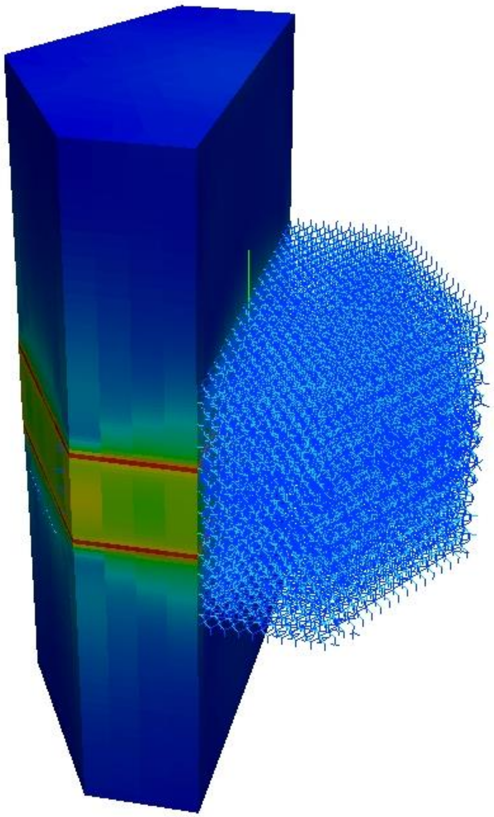
Empirical Tight binding model $sp^3d^5s^*$+SO

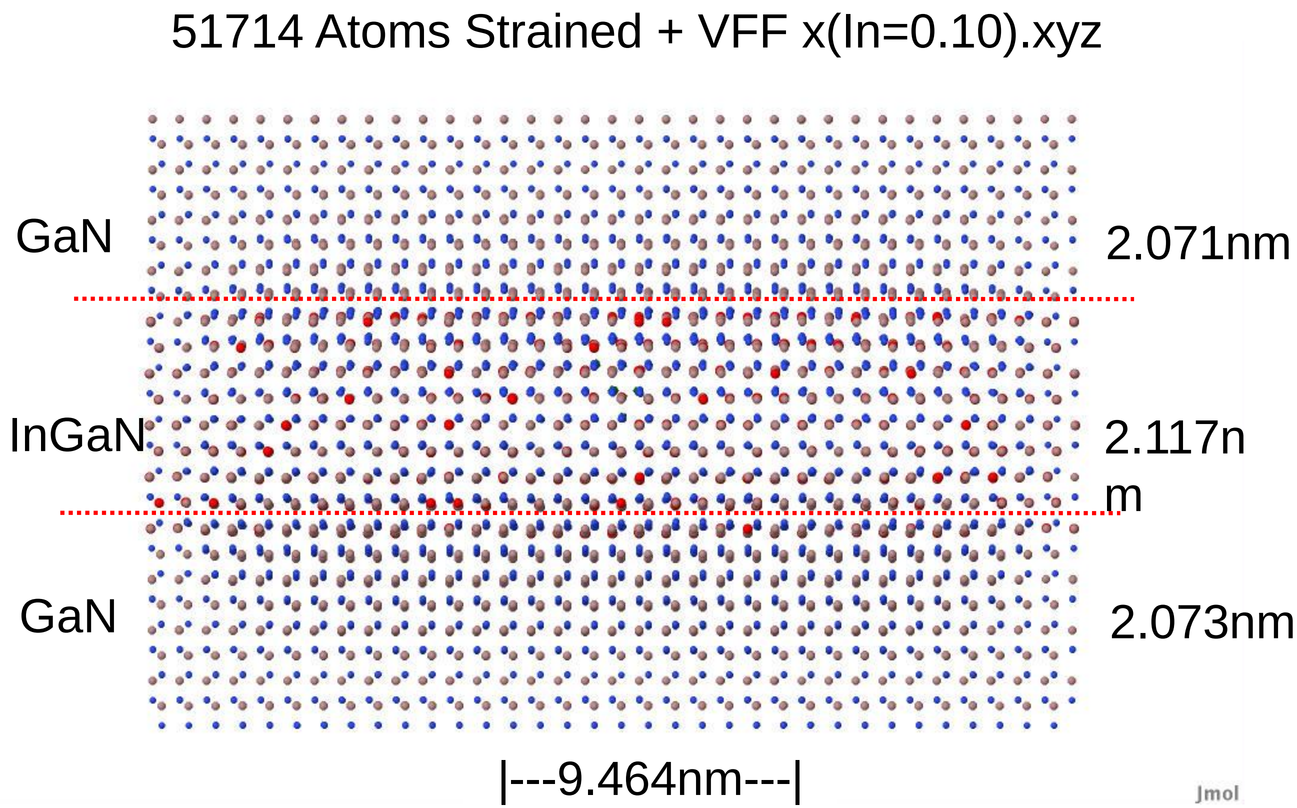
Solve few states using Lanczos



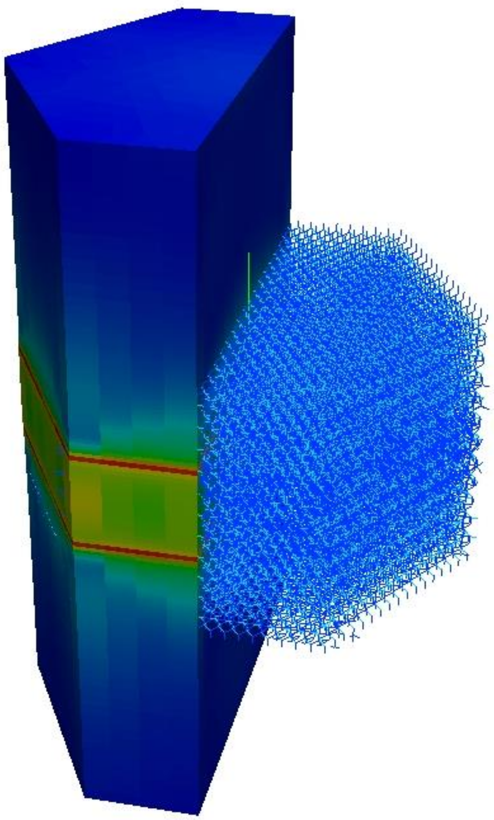
M. Auf der Maur IEEE TED (2011)

InGaN nanocolumns

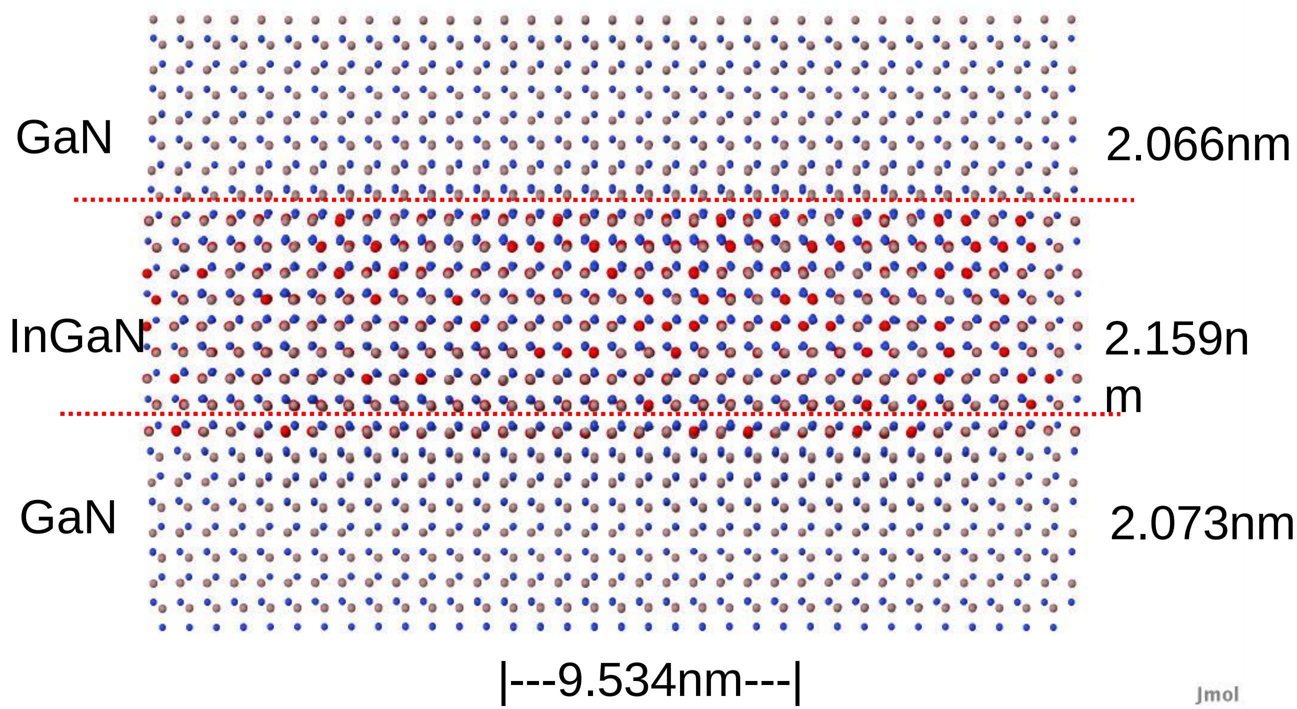




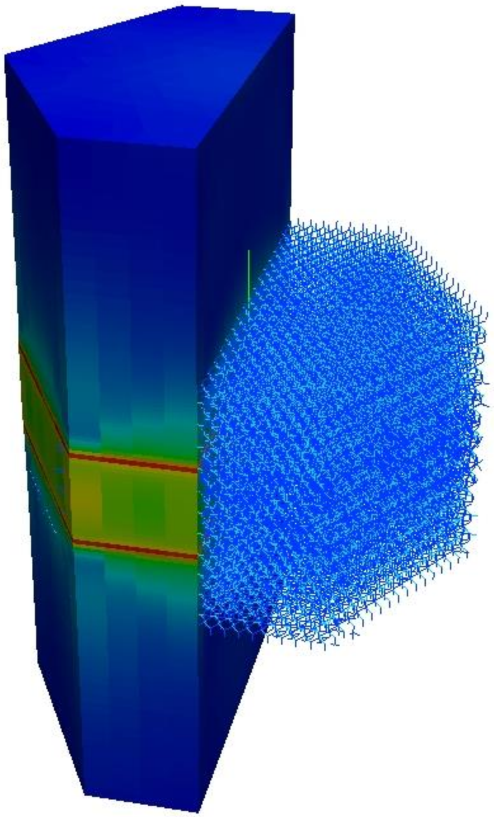
InGaN nanocolumns



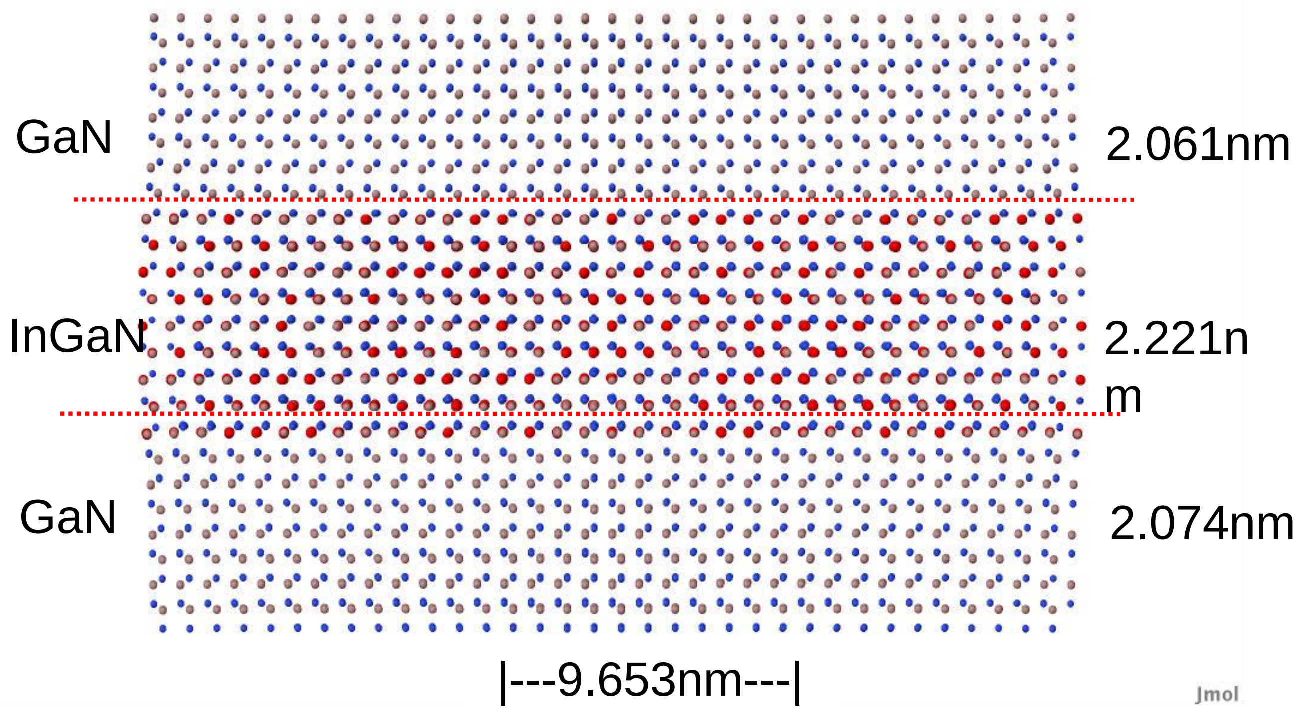
51714 Atoms Strained + VFF x(In=0.20).xyz

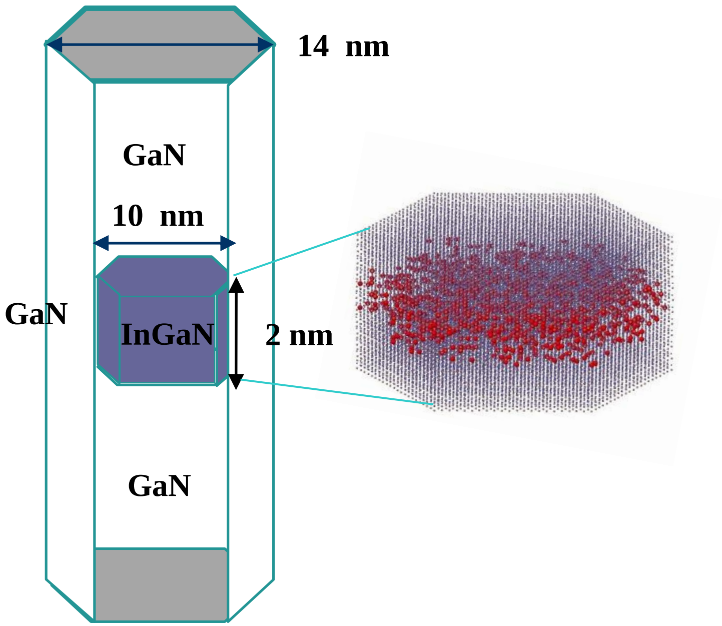


InGaN nanocolumns



51714 Atoms Strained + VFF x(In=0.35).xyz





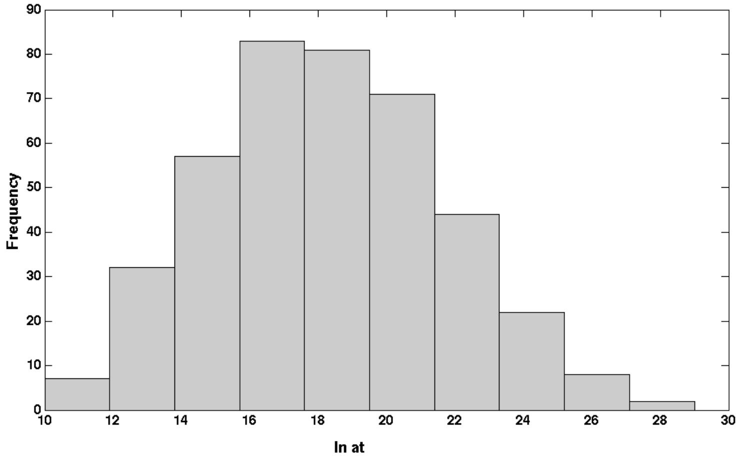
- VCA
- Random uniform
- Random with clustering

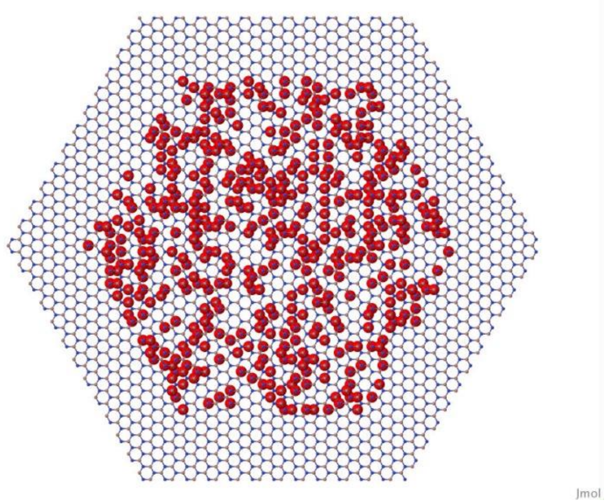
Uniform distribution is first applied to the structure (e.g. 70% uniform and 30% clustering)

Probability of Substitution of a Ga atom in GaN with In is higher if other In atoms are already in a sphere of 1nm radius around the atom.

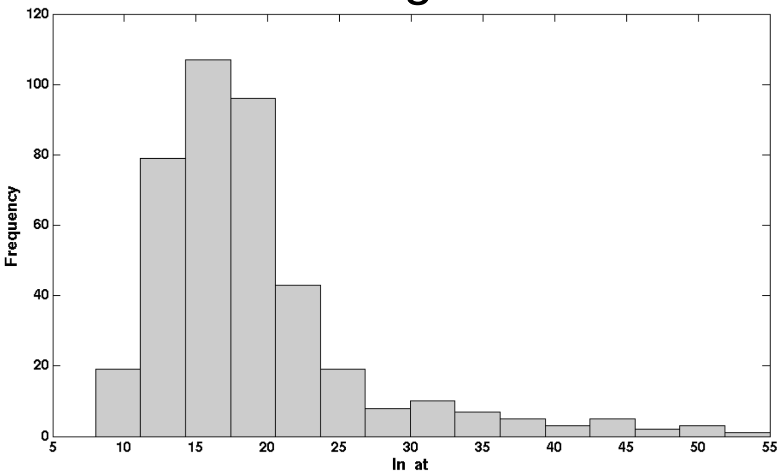
Modelling nanopillars

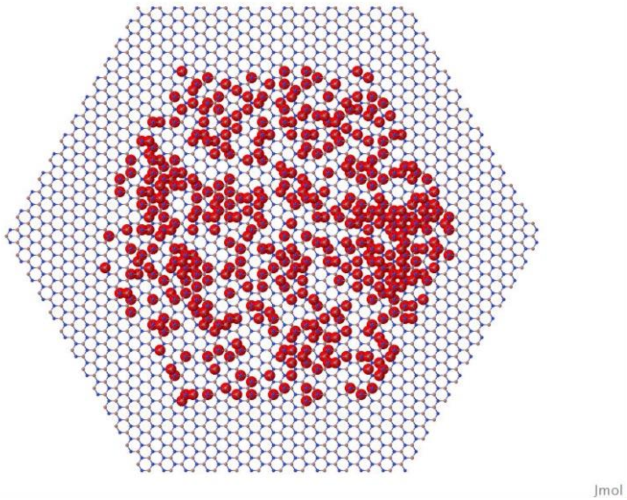
No clustering



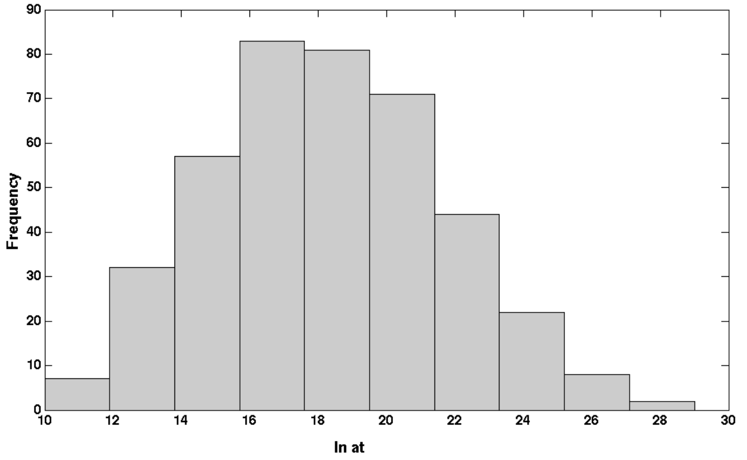


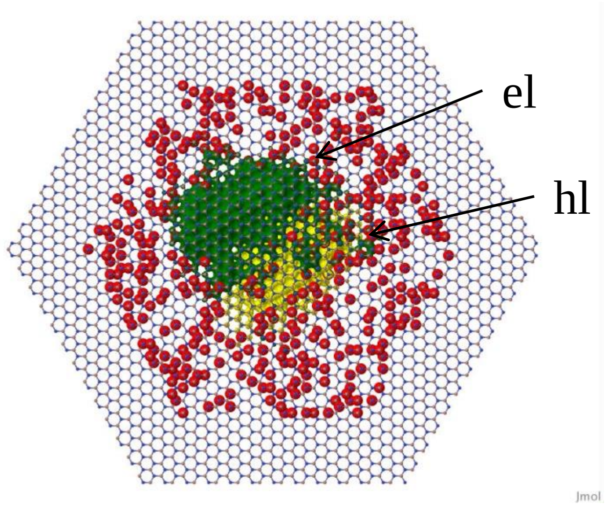
30% clustering



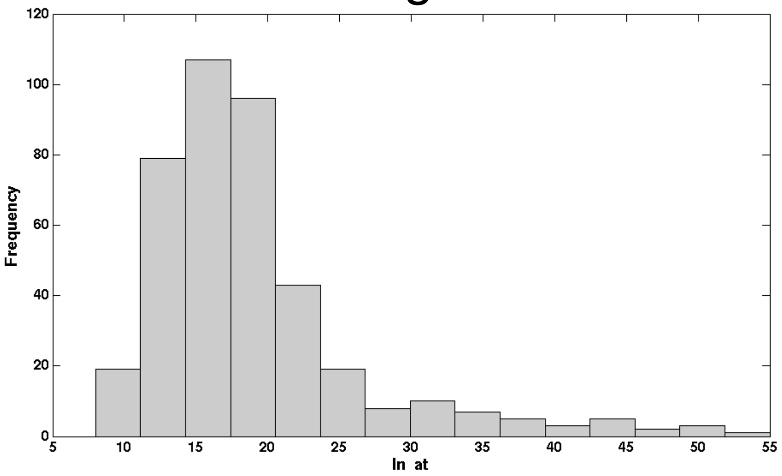


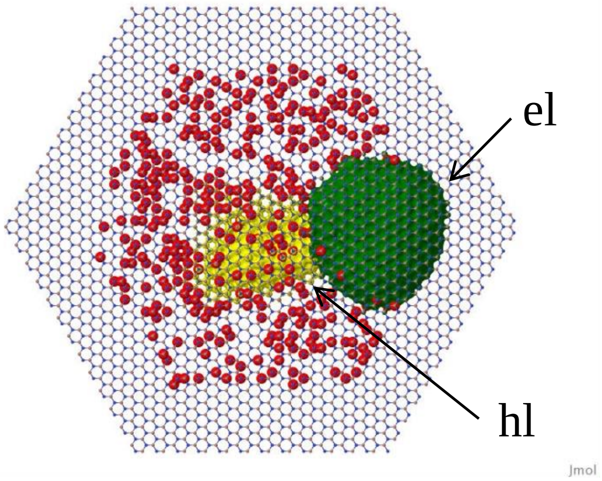
No clustering



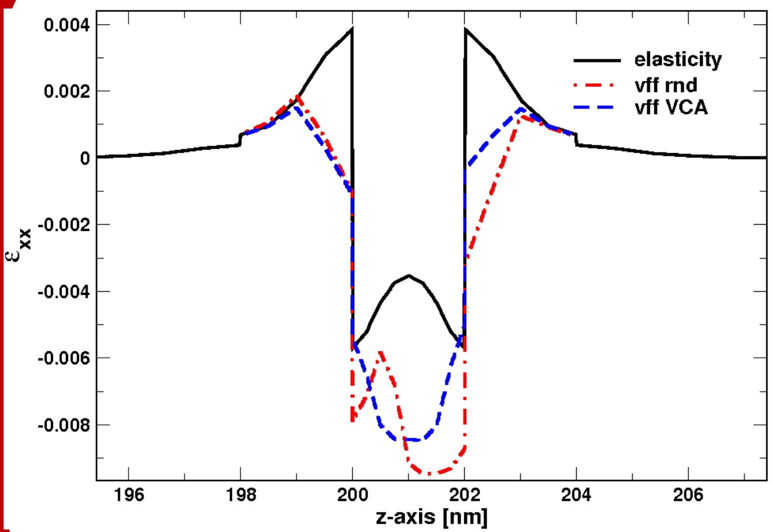


30% clustering

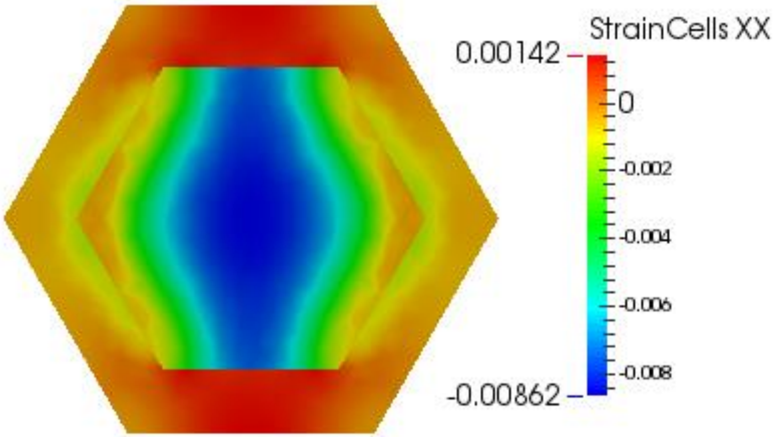


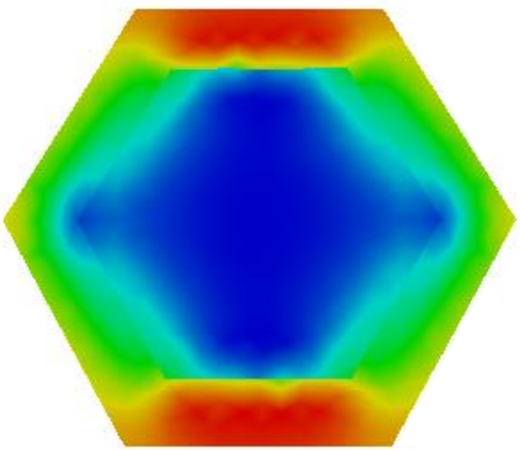


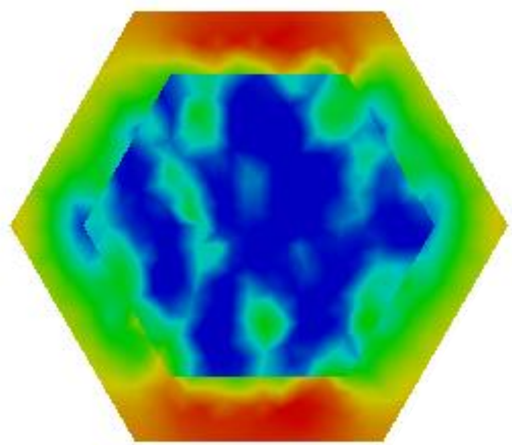
VFF and elasticity models



ε_{xx} strain from elasticity macroscopic model (VCA)





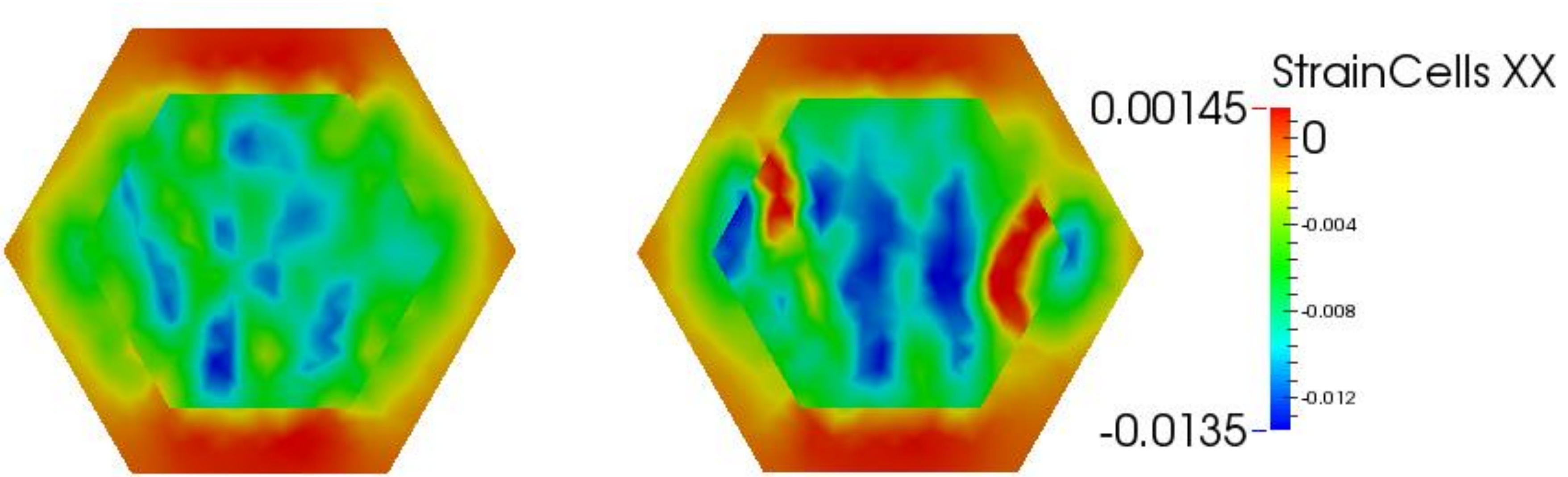


xy plane in the InGaN region

VFF on a VCA structure

VFF on a random sample

Strain from VFF on a random sample

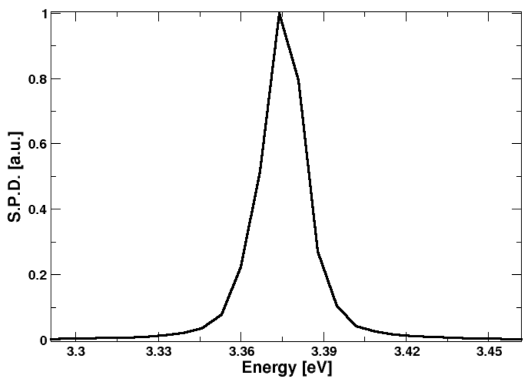


uniform distribution

clustering

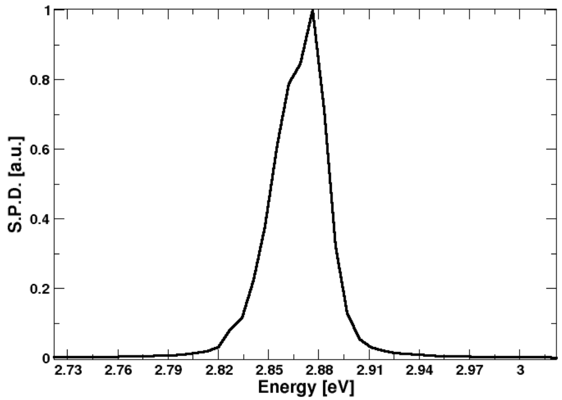
Optical Spectrum – no clustering

In 10%

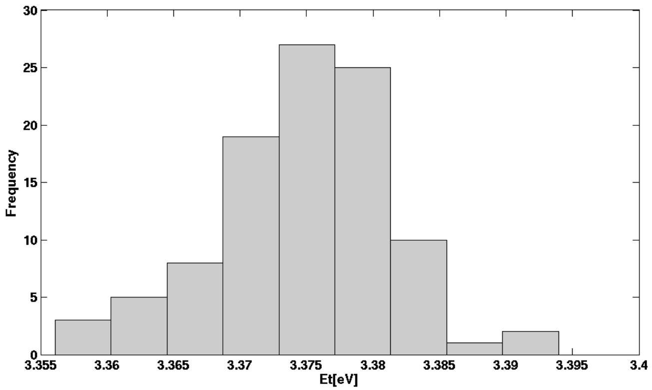


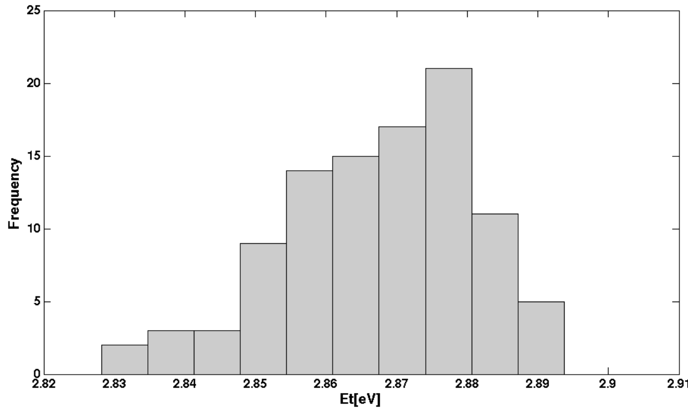
FWHM = 18 meV

In 30%



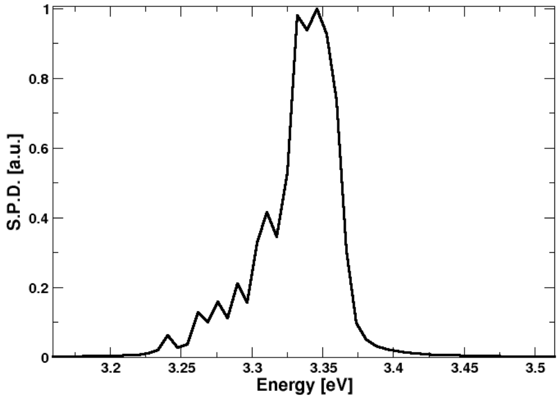
FWHM = 35 meV



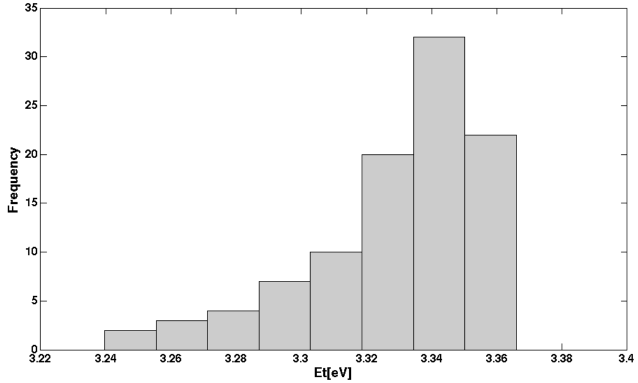


Optical Spectrum – 30% clustering

In 10%



FWHM = 20 meV broadening



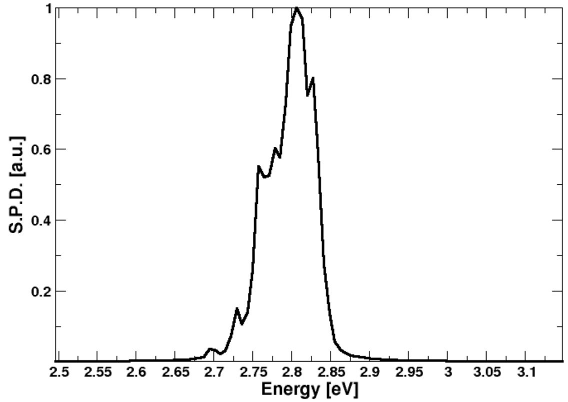
Distribution of energy gaps

Mean = 3.329

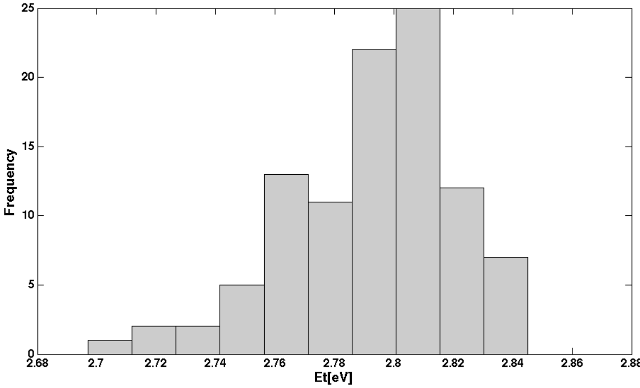
Std = 0.0278

skew = -1.242

In 30%



FWHM = 45 meV broadening

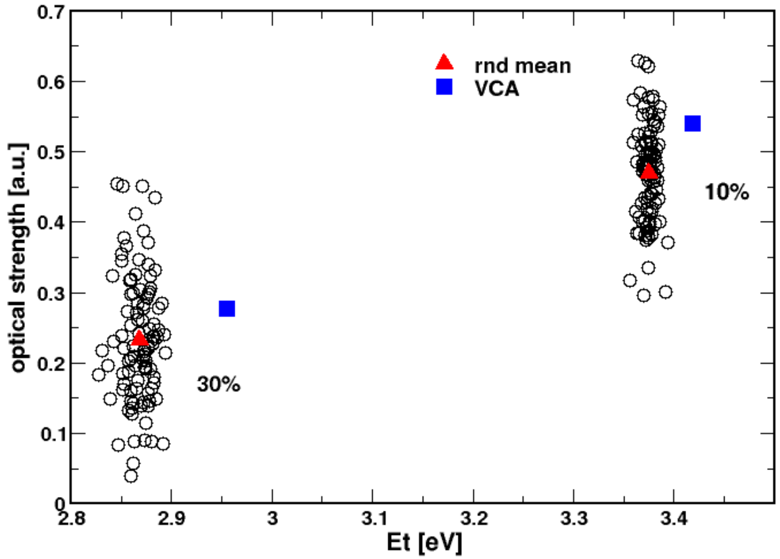


Distribution of energy gaps

Mean = 2.793

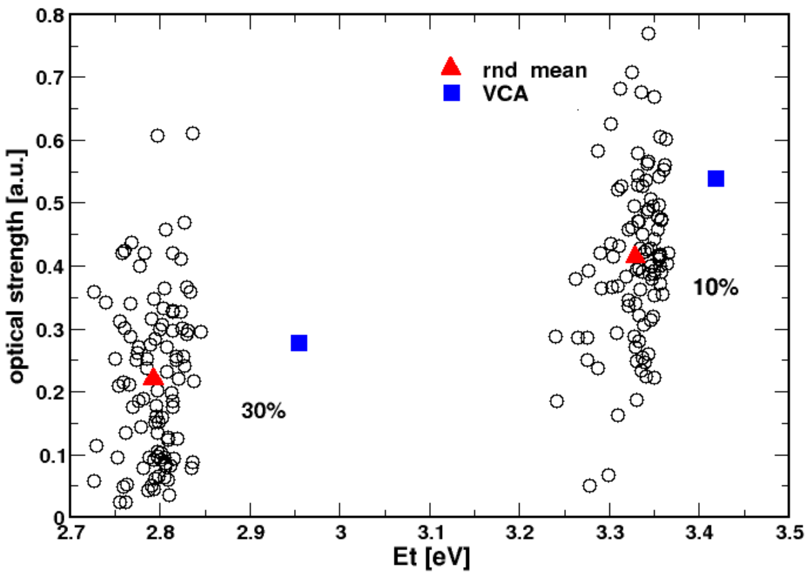
Std = 0.028

skew = -0.708



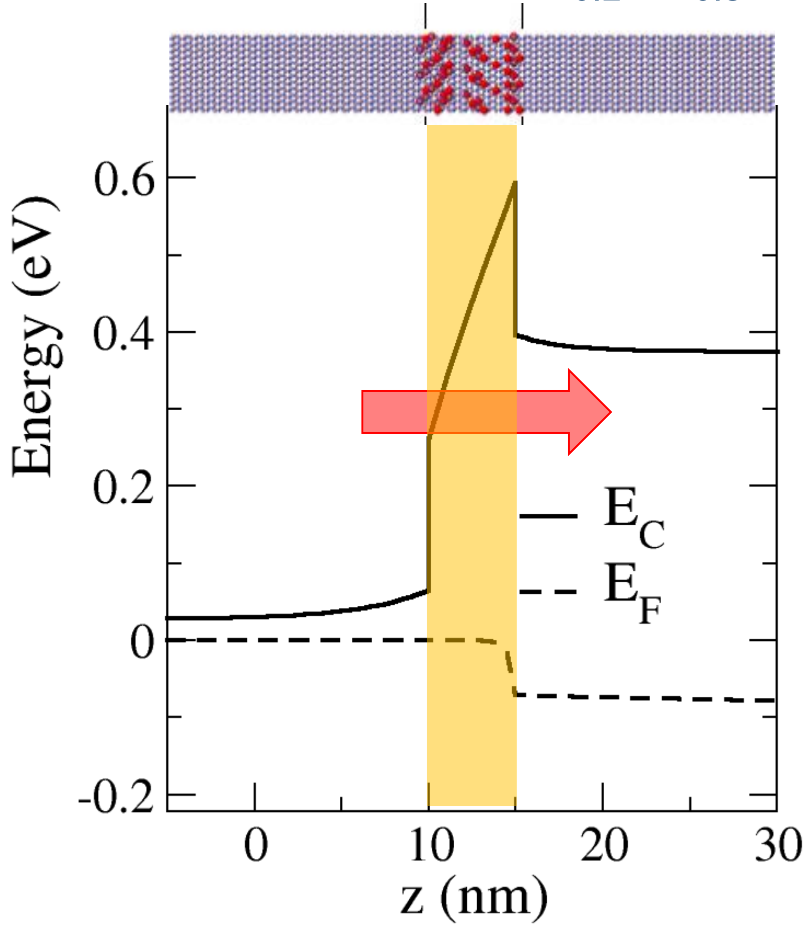
- Correlation between ground state transition energy and optical strength
- Increasing spread in random distribution with higher x(In)
- VCA overestimates Et and Opt.strength

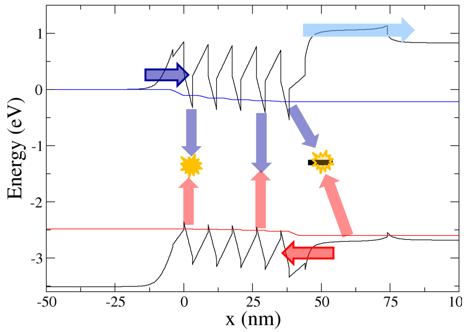
- Clustering effect:
- Larger spread in random distribution
- Lowering of mean Et

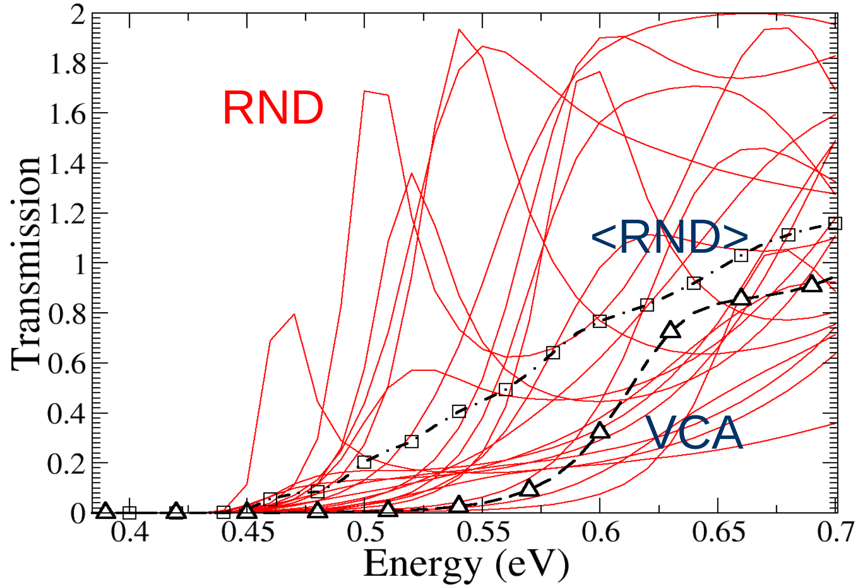


Transport across EBL

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

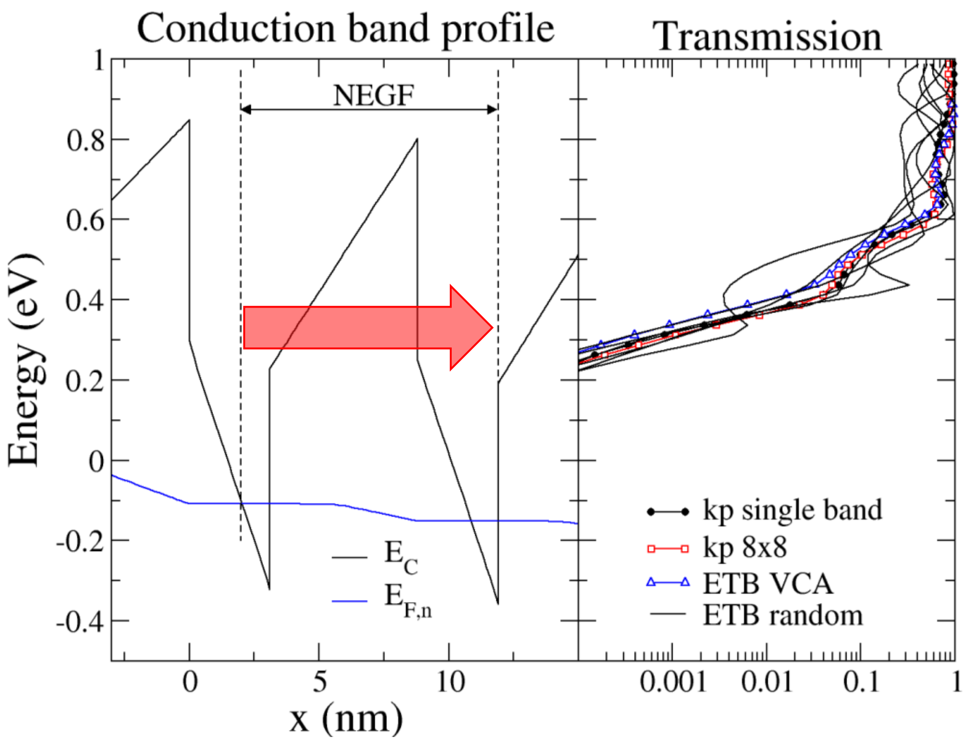






Considerable fluctuations due to random alloy: similar to defect assisted tunneling

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



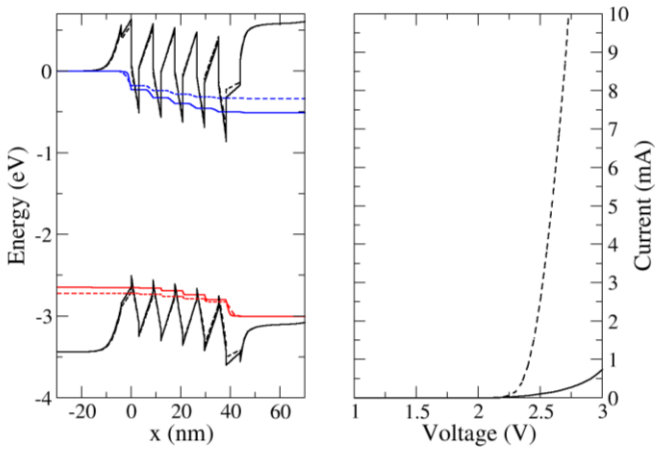
Extracted barrier resistivity:

Pure drift-diffusion: 15 Ωcm^2

8 band k·p: 1.33 Ωcm^2

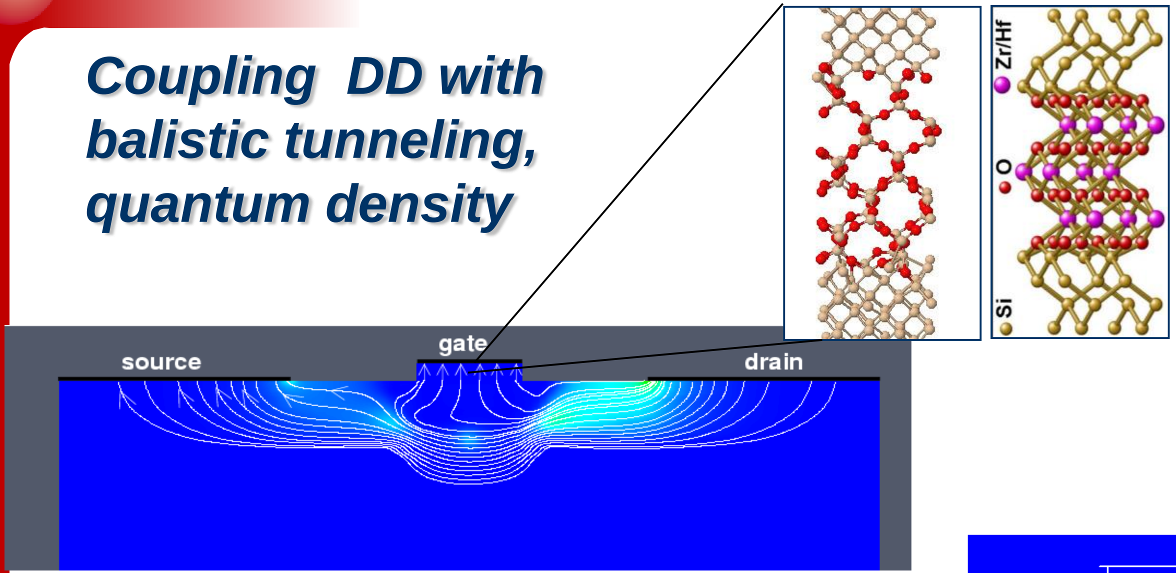
Random alloy: 0.28 – 1.26 Ωcm^2

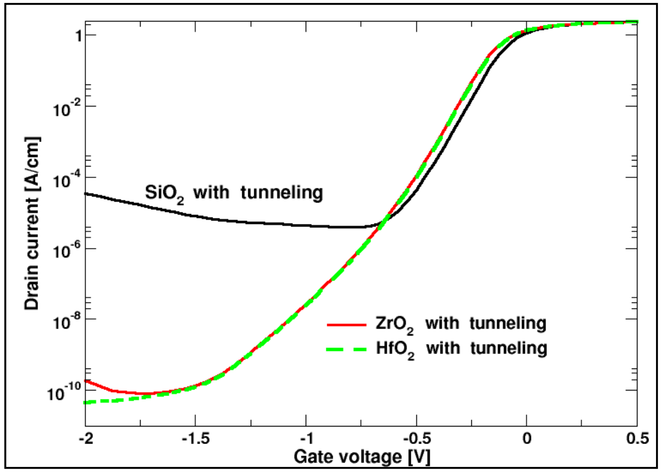
⇒ More realistic ON current:

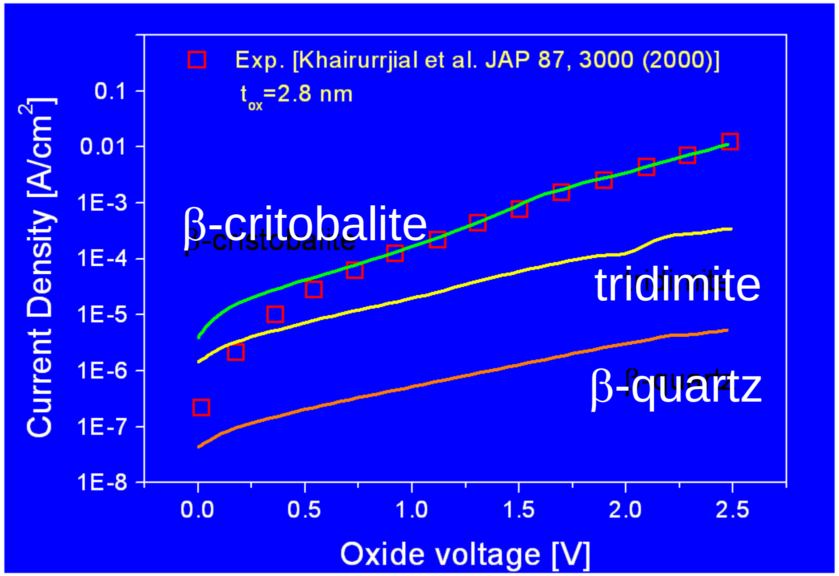


Oxide-tunneling

Coupling DD with balistic tunneling, quantum density



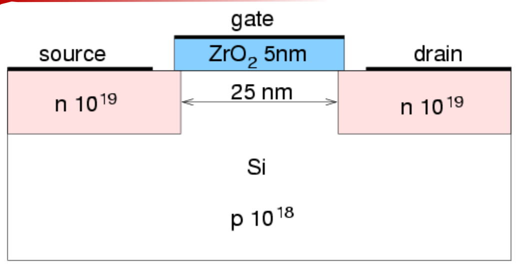


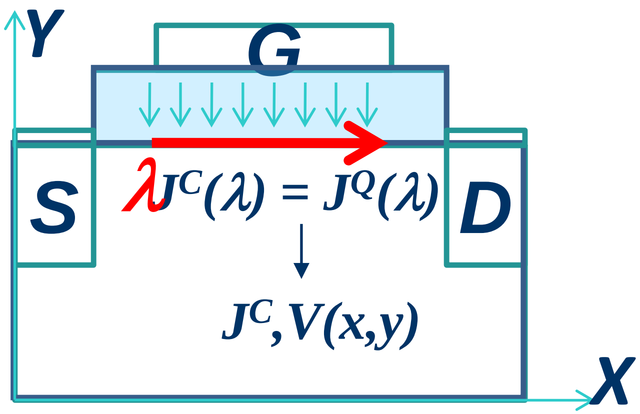


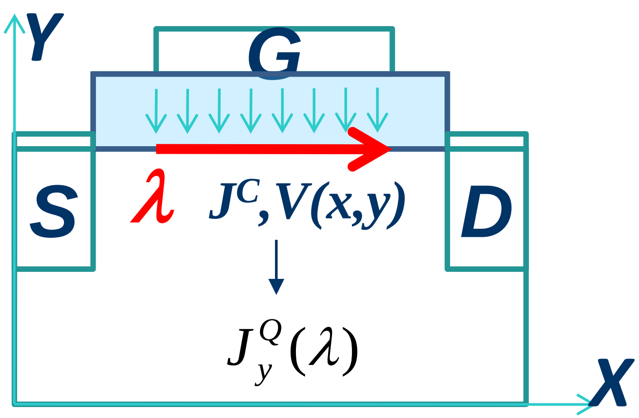
Sacconi et al IEEE TED 2004 and 2007

M. Auf der Maur et al. J. Comp. Elect., 7 398 (2008)

Bridge method: flux continuity







$$J_y^C(\lambda) = 0$$

$$\mathbf{J}^C = \mu_n n \nabla \phi_n$$

$$\nabla \cdot \mathbf{J}^C = G - R$$

$$\nabla \cdot (\varepsilon \nabla V) = -\rho$$

$$V(\lambda)$$

$$J_y^Q(\lambda) = f(V(\lambda) - V_G)$$

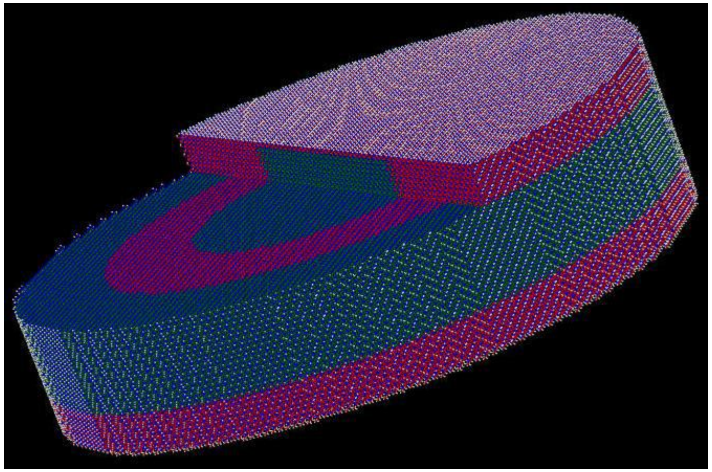
$$J_y^C(\lambda) = J_y^Q(\lambda)$$

Poisson-Drift-Diffusion is solved in the whole device

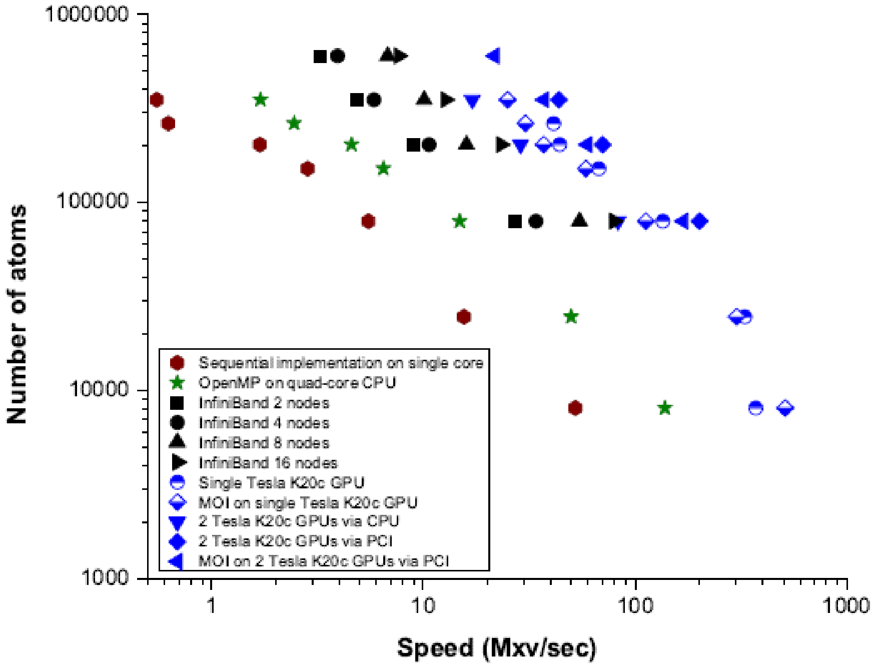
Self consistent cycle

Tunneling current calculated with atomistic tight-binding model is taken as a boundary condition for electron continuity at Si/oxide interface

CUDA developments



1,000,000 atoms on a WS!



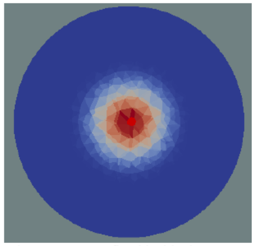


Fig 3:State 1 confined inside the Dot

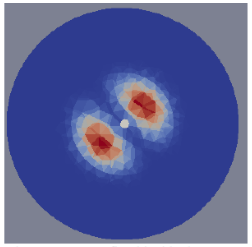


Fig 4:State 3 confined inside the Dot

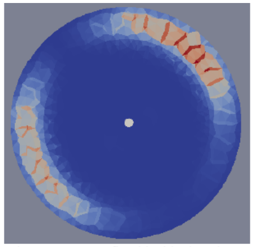
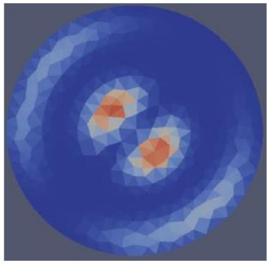


Fig 5:State 8 confined inside the Ring



Lambda state

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

Software Development ToolKit

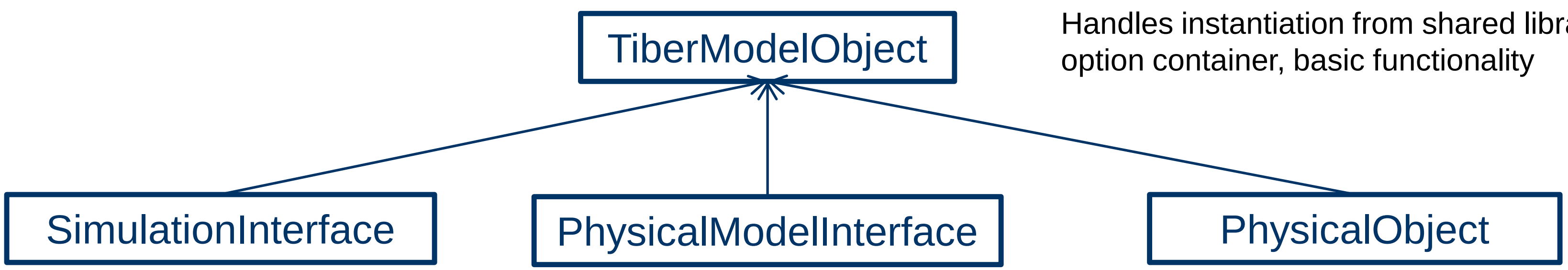
Software Development toolKit

⇒ Allows to add new modules by user without relinking core

```
Module somename
{
  Physics {
    mobility constant { }
  }
}
```

library name *somename.so*

library name *mobility_constant.so*



Handles instantiation from shared libraries, option container, basic functionality

```
Module driftdiffusion
{
}
```

```
Physics {
    mobility constant { }
}
```

Base class of all physical entities
bulk, interface, edge, node

Example: Poisson

```
#include "SimulationInterface.h"

class Poisson : public SimulationInterface
{
  public:
    static Poisson* create(options);

  protected:
    virtual void do_init(void);
    virtual void parse_options(void);
    virtual void do_setup_solution_variables(void);
    virtual void do_solve(void);
    virtual PhysicalModel* create_bulk_model(options, material);
    virtual PhysicalModel* create_boundary_model(options, boundary);
    virtual void get_solution_secure(element, data, points);

  private:


};
```

```
Module poisson {
  Physics {
    charge_density constant {


    }
  }
}
```

Conclusions

- Multiscale/multiphysics is requested for simulation of real modern electronic devices where electronics, optics, chemistry are linked together
- We have seen the most important physical models implemented in tiberCAD
- We have discussed the basics of how to couple atomistic and classical simulations
- Much effort is still needed to arrive at a true multiscale integration for transport simulations

*Additional info about **TiberCAD**:*
http://www.tibercad.org

Download <u>free trial version</u>:

tiberlab

www.tiberlab.com
info@tiberlab.com

THANK YOU !