Dottorato di Ricerca in Ingegneria dei Sistemi Sensoriali e di Apprendimento

XXII Ciclo del Corso di Dottorato

Development of an atomistic/continuous simulation tool for nanoelectronic devices

Candidato

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Coordinator
Prof. Corrado Di Natale

Outline

- **Multiphysics/Multiscale simulation of nanoelectronic devices: TiberCAD**
- **Optoelectronic properties of a nanostructured device: models and applications**
- **A selfconsistent Schrodinger/Drift-diffusion**
- **Valence Force Field and Continuum Elasticity**
- **Non Equilibrium Green's Function for quantum transport: theory and applications**

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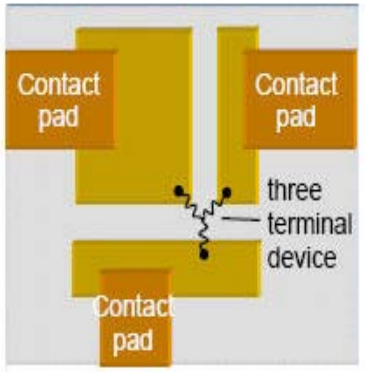
Nanoelectronic devices

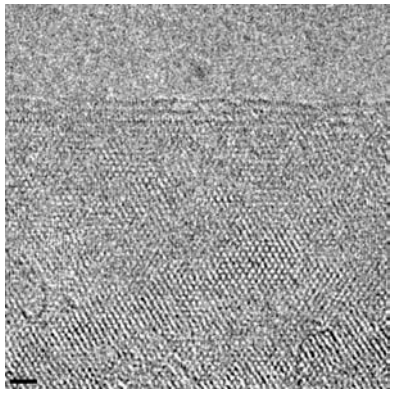
Which future for optoelectronic devices?

Molecular devices

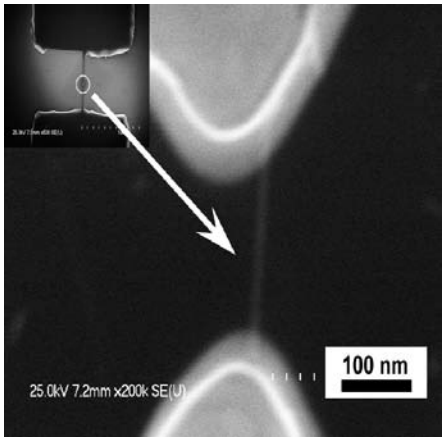
- Organic compounds
- Quasi-1D and 2D structures (nanotubes, graphene)
- Single molecule devices
- Electrochemical devices (DSC)



Macromolecules, 37 (2004) 4740



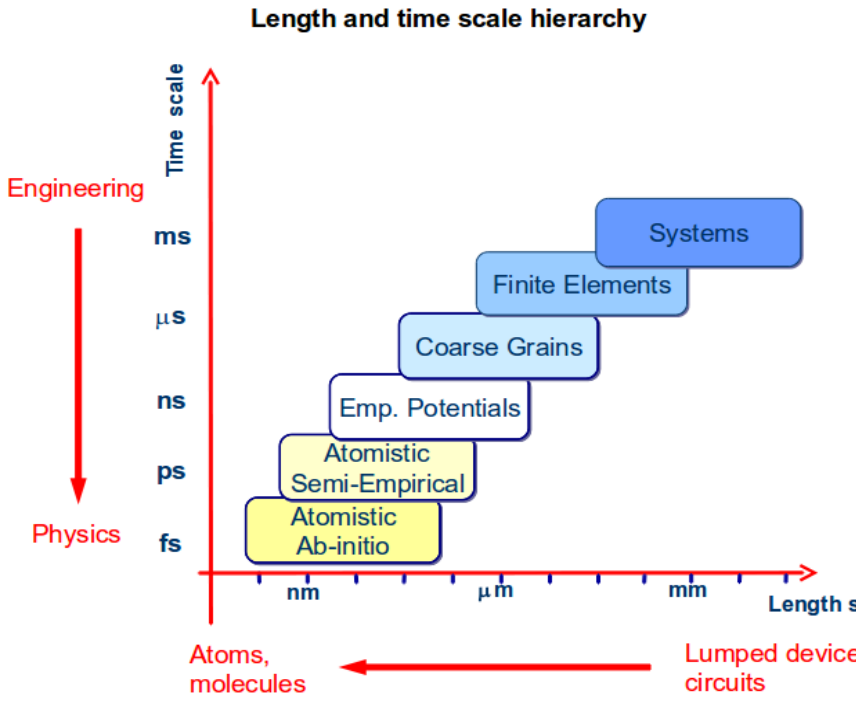
Nature, 446 – 60 (2007)

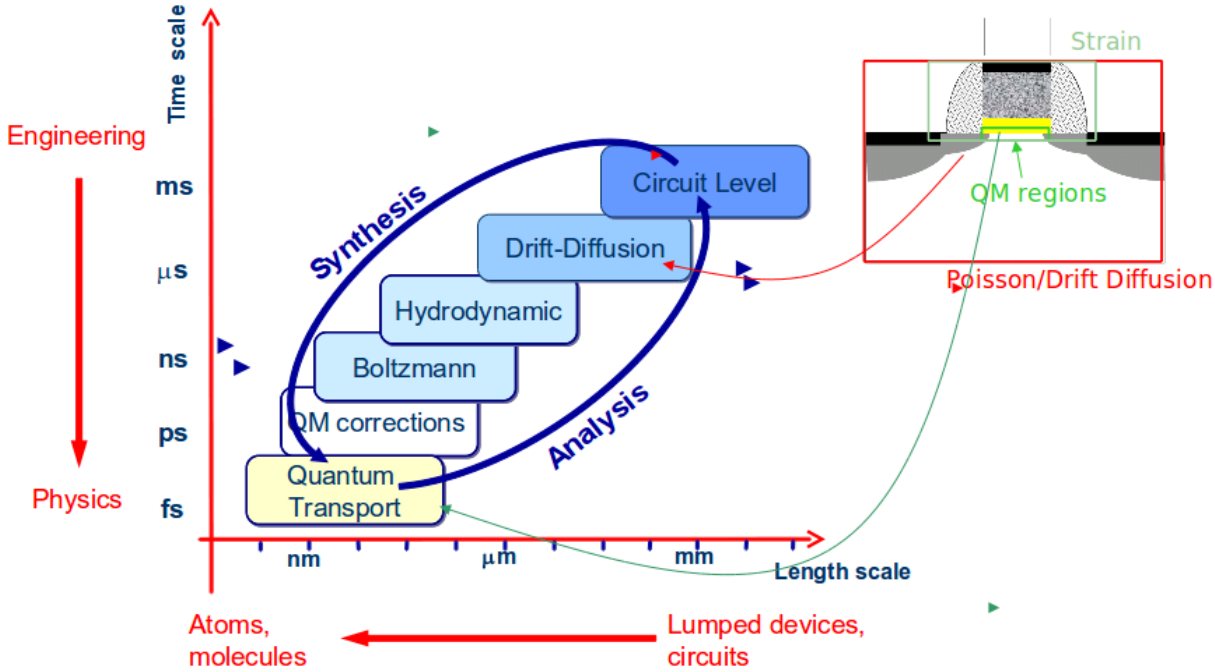


Atomistic or Continuous?

Device physics is described through atomistic or continuous models,

depending on length and time scales involved





Continuous/Atomistic Environment

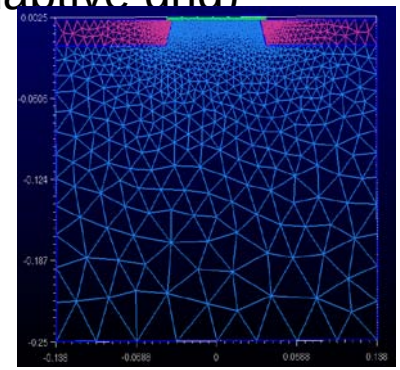
Finite Element Method

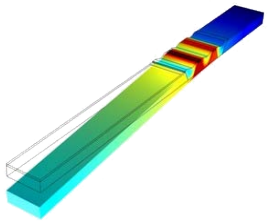
Numerical implementation of PDEs

Best method for solving engineering problems in continuous medium approximation

Equations discretized on elements (tethraedra)

Element dimension is determined by accuracy and convergency issues. It can vary according the calculation itself (adaptive grid)





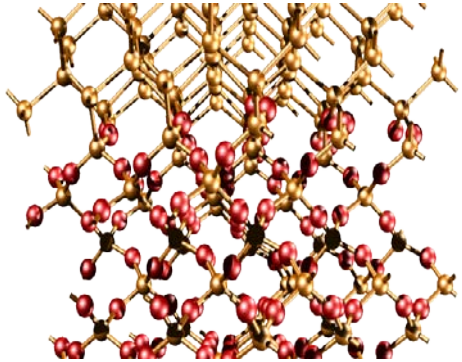
Atomistic local basis

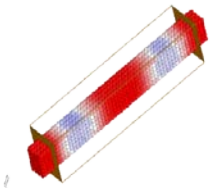
Potential minimization, eigenvalue problems

Beyond continuous medium limitations (molecules, defects, single dopant ecc.)

Equation “discretized” on atoms

Atom distance is a physical quantity: number of atoms depends on geometrical dimensions





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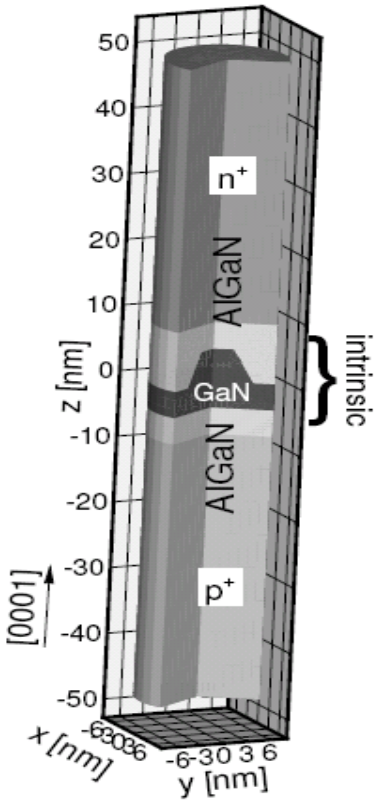
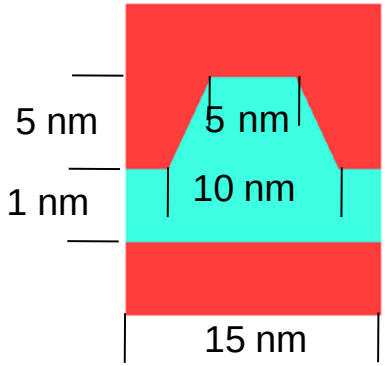
QDOT LED: models and application

We start directly from showing what is needed to calculate optoelectronic properties of a nanostructured device





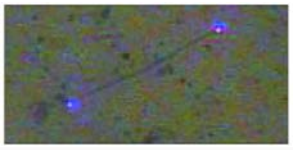
X = 0.3

Doping fraction = 10^{19} cm^{-3}

We want:

Investigate the role of piezoelectric field in (0001) and (000-1) growth direction.

•Calculate current and emission spectrum.

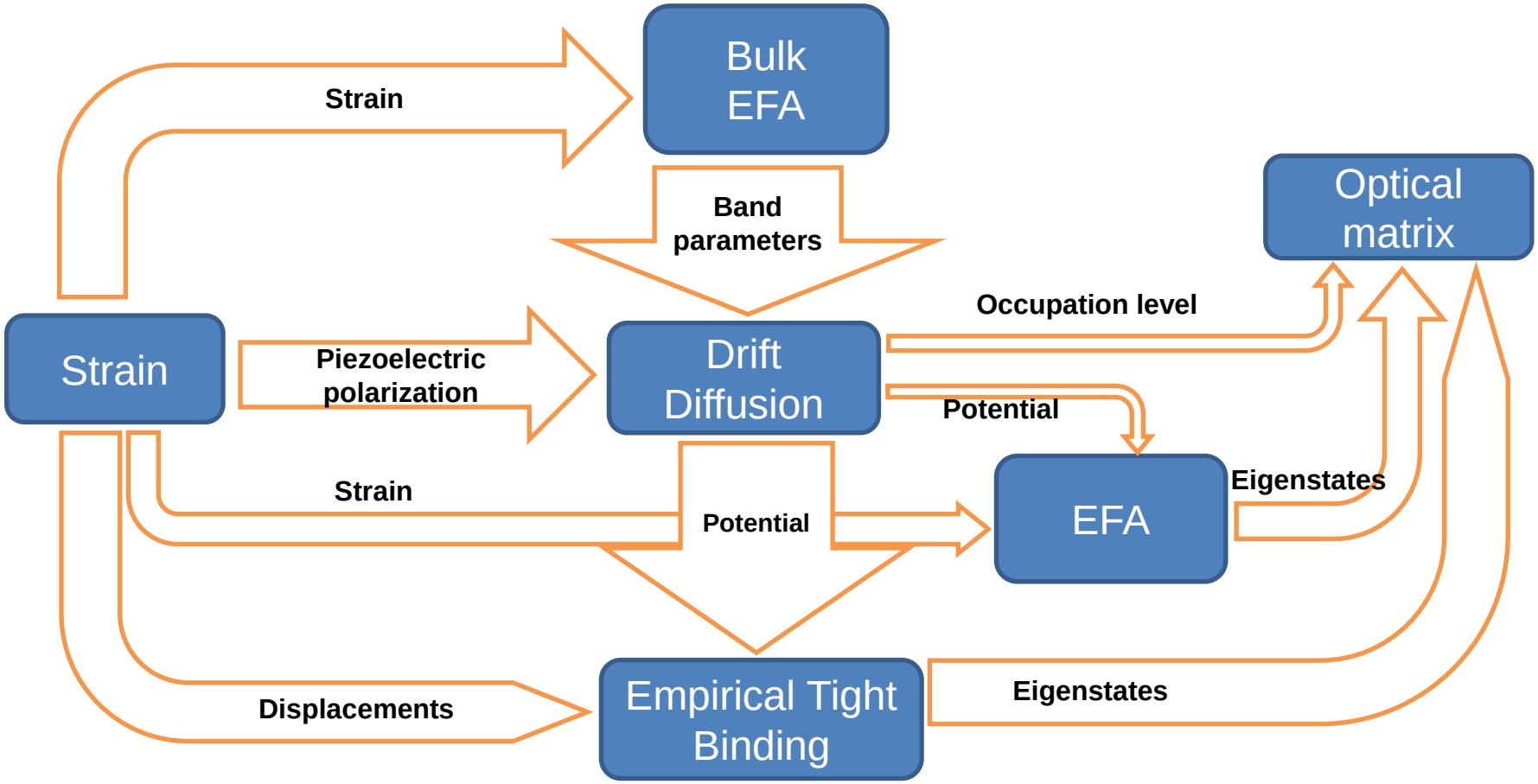


Johnson et al. Nature materials 1, 106 (2002)

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

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

GaN/AlGaN QDOT simulation scheme



Quantum models: EFA

We solve the Schrödinger equation in the intrinsic region. We assume that the system is in local equilibrium (low bias) and apply infinite wall boundary conditions.

EFA (Envelope Function Approximation): wavefunction is expressed in a Bloch function basis

$$\left[-\frac{\hbar^2}{2}\nabla_r\left(\frac{1}{m}\nabla_r\right)+V_{eff}(\boldsymbol{r})\right]\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

$$\psi(\boldsymbol{r})=\sum_n F_n(\boldsymbol{r})u_n(\boldsymbol{r}) \qquad F_n(\boldsymbol{r})=\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}}C_{n,\boldsymbol{k}}$$

$$H^{\varepsilon}_{3\times 3}=$$

$$\begin{pmatrix} l_1\varepsilon_{xx}+m_1\varepsilon_{yy}+m_2\varepsilon_{zz} & n_1\varepsilon_{xy} & n_2\varepsilon_{xz} \\ n_1\varepsilon_{xy} & m_1\varepsilon_{xx}+l_1\varepsilon_{yy}+m_2\varepsilon_{zz} & n_2\varepsilon_{yz} \\ n_2\varepsilon_{xz} & n_2\varepsilon_{yz} & m_3\varepsilon_{xx}+m_3\varepsilon_{yy}+l_2\varepsilon_{zz} \end{pmatrix}$$

Quantum models: Tight Binding

Tight Binding: wavefunction is expressed in a atomic orbitals basis (LCAO)

$$|\Psi\rangle = \sum_{\alpha \boldsymbol{R}} C_{\alpha \boldsymbol{R}} |\alpha, \boldsymbol{R}\rangle$$

$$\sum_{\alpha' \boldsymbol{R}'} C_{\alpha' \boldsymbol{R}'} \left[H_{\alpha' \boldsymbol{R}' \alpha \boldsymbol{R}} - E S_{\alpha' \boldsymbol{R}' \alpha \boldsymbol{R}} \right] = 0$$

$$H_{n'\alpha',n\alpha} = \langle n'\alpha' | H | n\alpha \rangle$$

$$S_{n'\alpha',n\alpha} = \langle n'\alpha' | n\alpha \rangle$$

$$H_{n'\alpha',n\alpha} = \int \psi^*_{\alpha'}(\boldsymbol{r} - \boldsymbol{R}_{n'}) \left[\frac{\boldsymbol{p}^2}{2m} + \sum_{n''} V_{n''}(\boldsymbol{r} - \boldsymbol{R}_{n''}) \right] \psi_{\alpha}(\boldsymbol{r} - \boldsymbol{R}_{n}) \, \mathrm{d}\boldsymbol{r}$$

The technique used to write the hamiltonian matrix elements and the overlap distinguish between different Tight Binding implementations.

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The technique used to write the hamiltonian matrix elements and the overlap distinguish between different Tight Binding implementations.

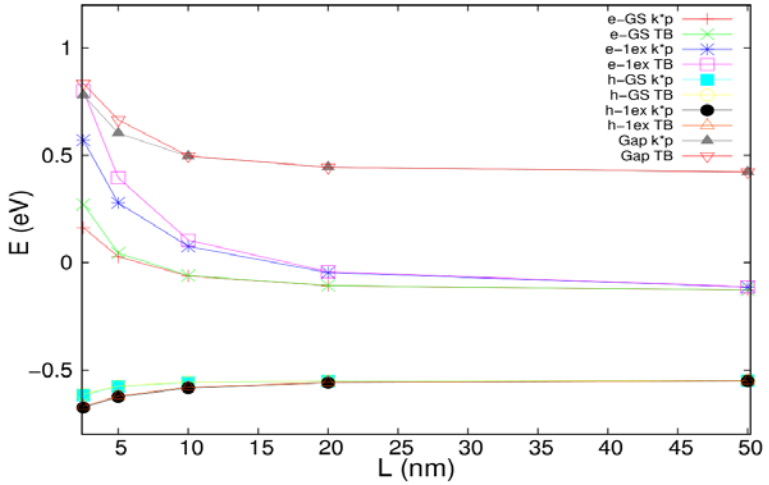
Empirical Tight Binding (ETB):
Matrix element obtained by fitting relevant quantities in bulk crystal structures.
Two-center approximation.
Orthogonal basis.

Density Functional Tight Binding(DFTB):
Matrix element obtained byab-initio DFT calculations.
Two-center approximation.
Non-orthogonal basis.

ETB vs EFA

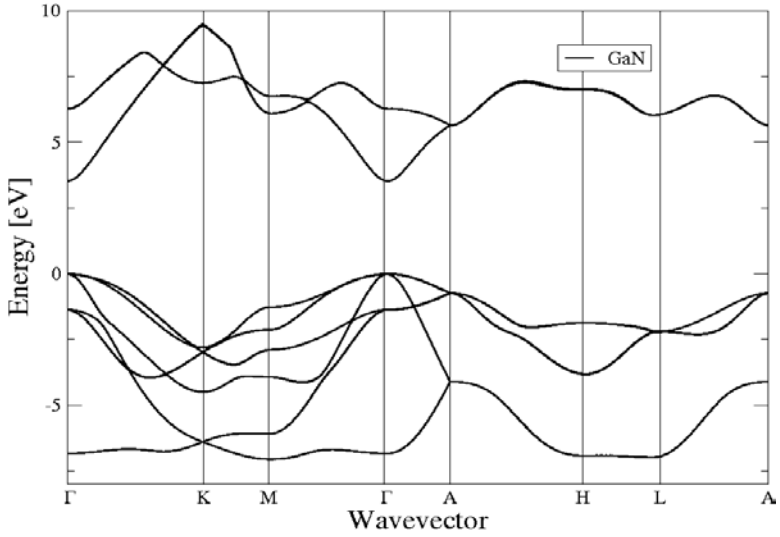
EFA advantages:
- Fast and easier technique.
- FEM implementation.
- Can include easily strain effects.
- Multi-band perturbative approach.

EFA drawbacks:
- Good description of bands only near valleys.
- Not a full band description.
- Fails for highly confined structures.
- Limited to effective medium descriptions.



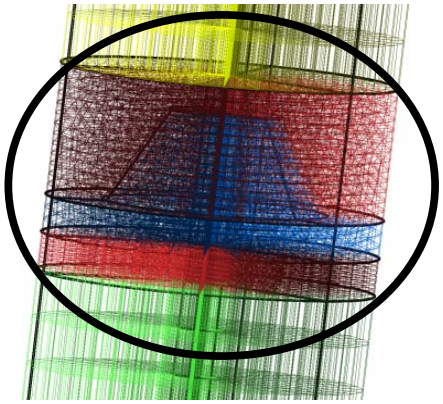
ETB advantages:
- Best accuracy for crystal nanostructurs.
- Full band approach.
- Beyond effective medium (random alloys).

ETB drawbacks:
- Very high computational effort (respect to EFA).
- Limited to crystals..

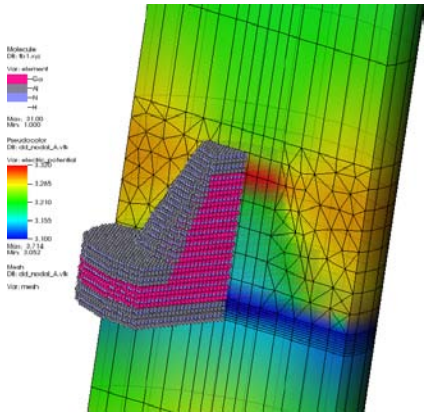


Device design

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



Atomistic structure is innerly generated. Atoms and elements connected within the same environment



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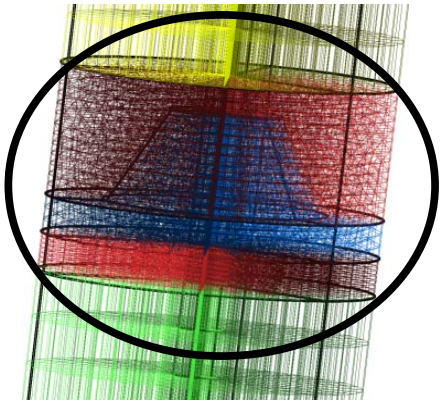

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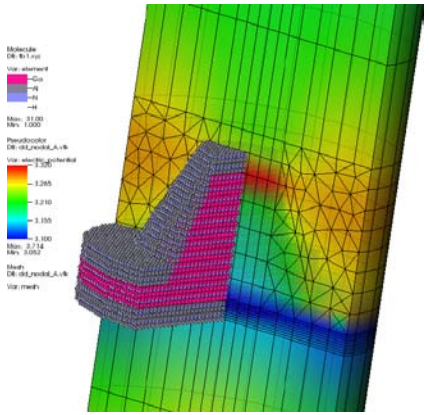

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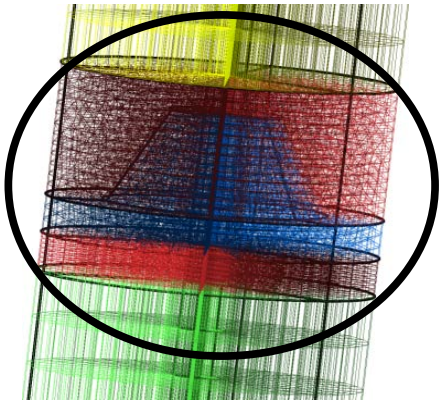

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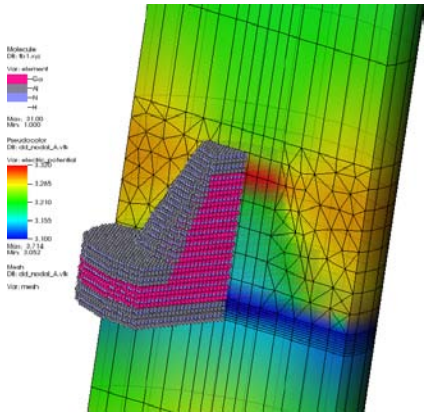


Atomistic Generator

Manage fcc, cubic, bcc, hexagonal lattices
Any atom basis can be added in database
O(N) bond map
Automatic hydrogen passivation
Heterostructures

Atomistic Structure Handler

List of atoms (position, specie, material)
Periodicity
Atom/Elements map for data exchange
Projection techniques

FEM/ETB data exchange

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

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

Tight Binding parameters calculated according to Harrison scaling rule:

Potential:

Use FEM potential solution to provide Hamiltonian shifts.

$$V_i = V(r_i)$$

- 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.

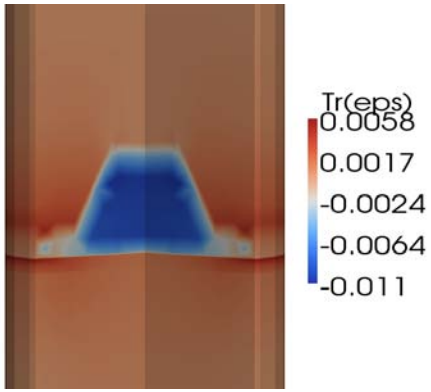
$$V_i = \frac{\tau_i^3}{8\pi}\int V(r_i) e^{-\tau|r-r_i|} d$$

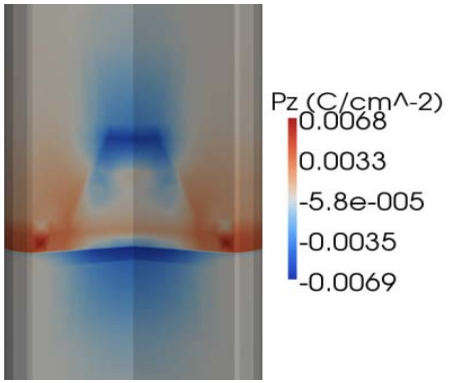
Charge:

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

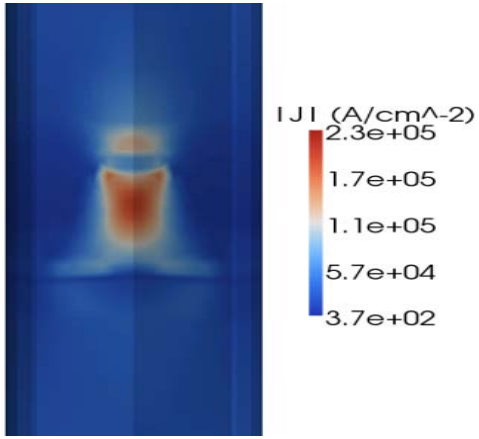
$$n(r) = \sum_i \frac{\tau_i^3}{8\pi}\int \Delta q_i e^{-\tau|r-r_i|} d$$

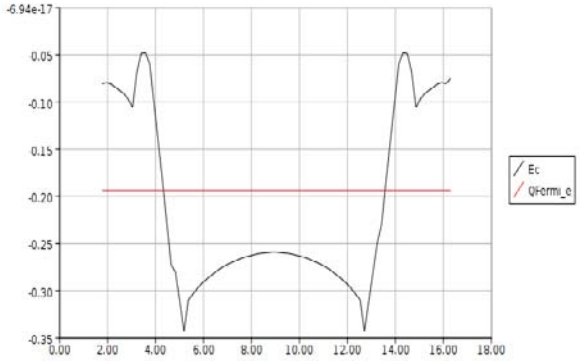
Strain and current

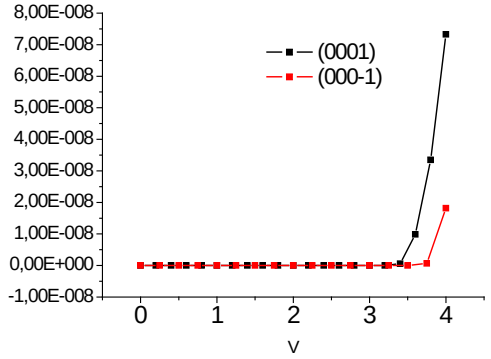




Piezoelectric effect plays a crucial role, affecting both electrical and optical properties

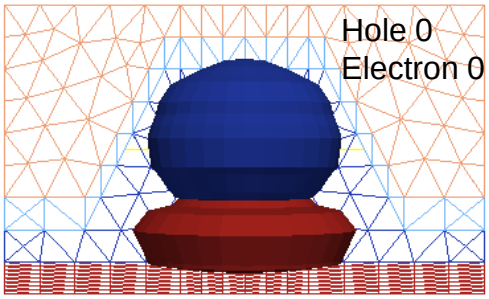


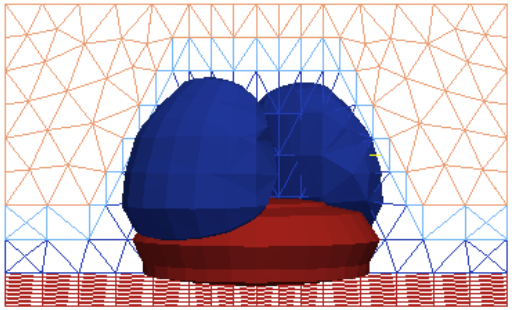




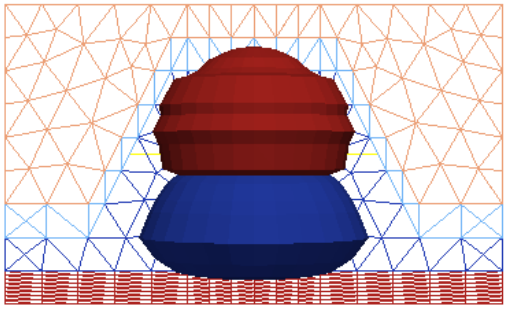
EFA: spectra and states

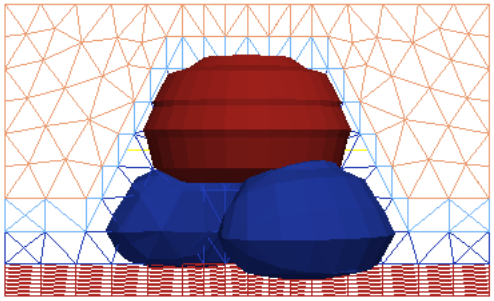
(0001)

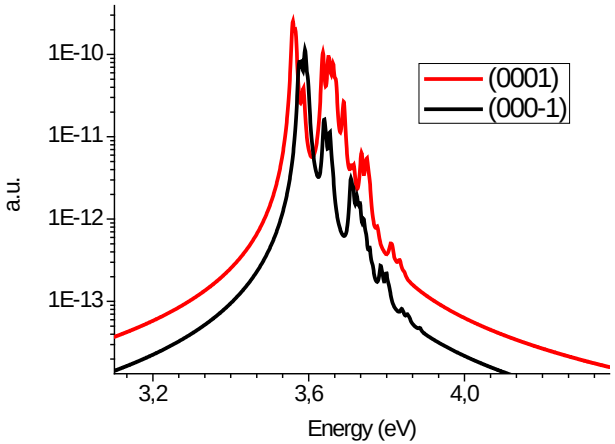




$(000\bar{1})$







(0001)

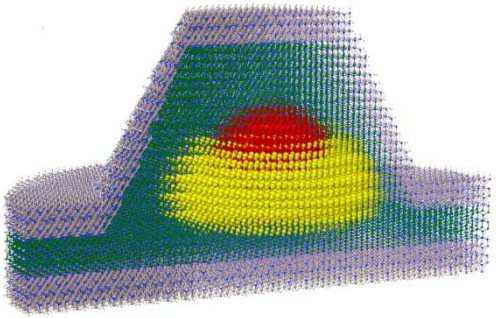
E-HH1	3.559
E-HH2	3.565

$(000\bar{1})$

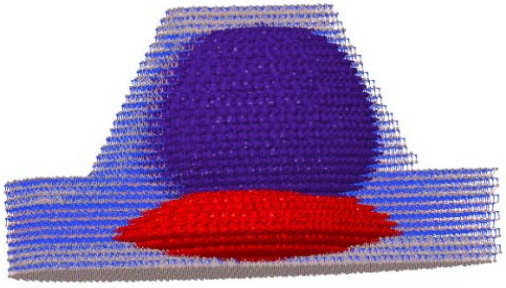
E-HH1	3.574
E-HH2	3.577

Blu: electron state
Red: hole state

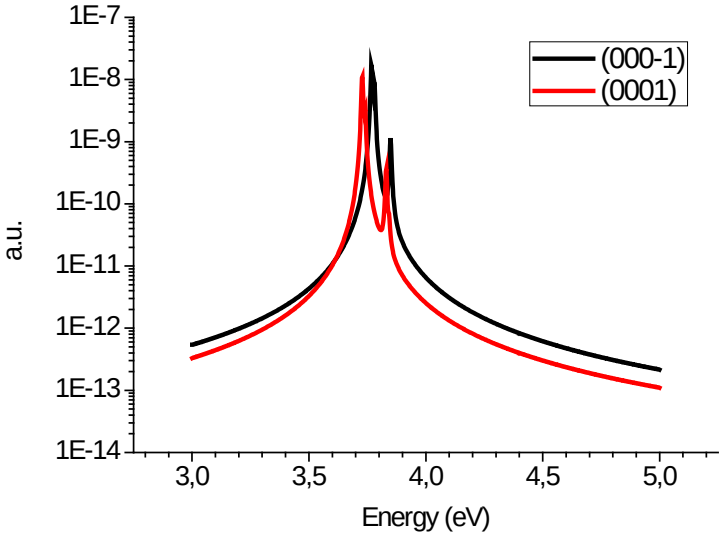
ETB: spectra and states

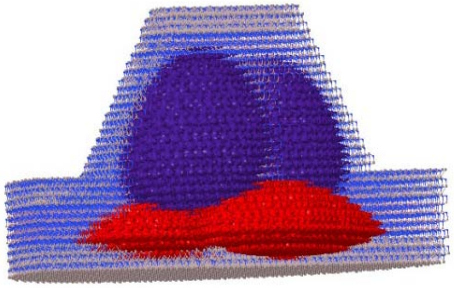


Ground states at equilibrium, without external bias applied

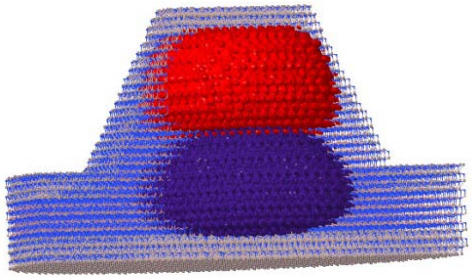


(0001) ground states





(0001) 2nd hole and electron states



(000-1) ground states

(0001)

E-HH1	3.728
E-HH2	3.740

$(000\bar{1})$

E-HH1	3.905
E-HH2	3.908

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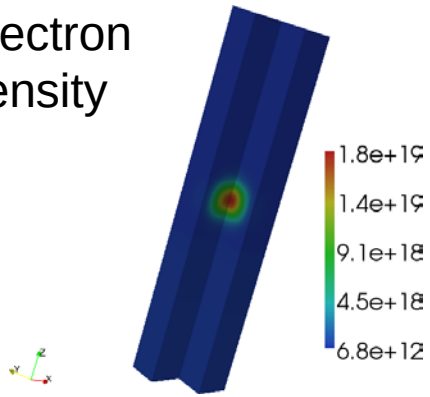
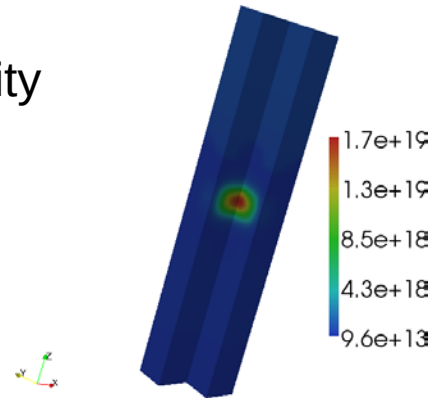
EFA/drift-diffusion

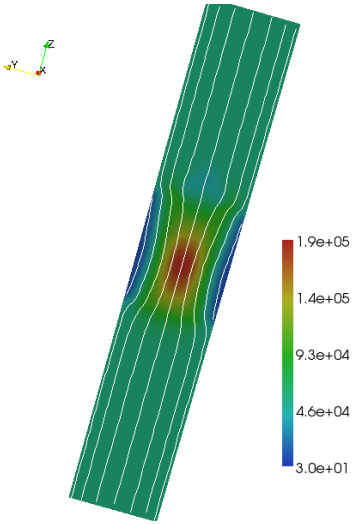
The selfconsistent scheme is general and it can be applied to 3D structures

Electron density

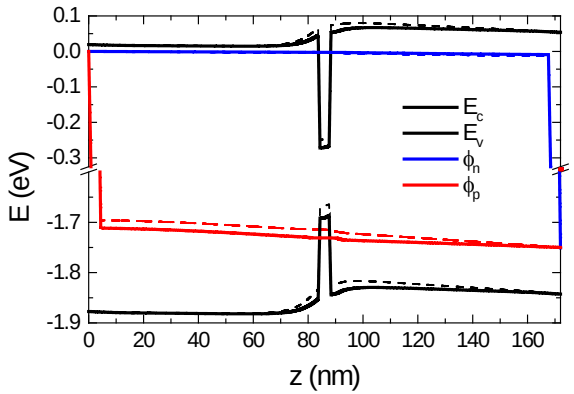


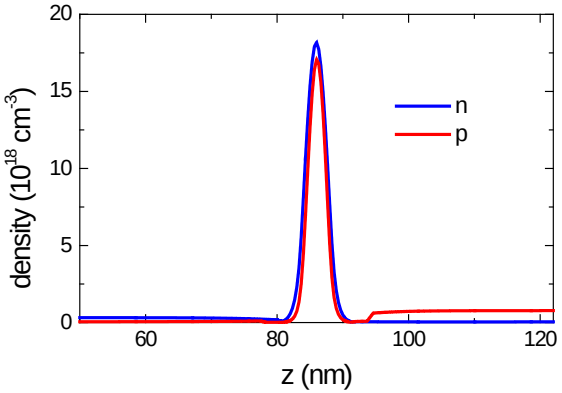
Hole density

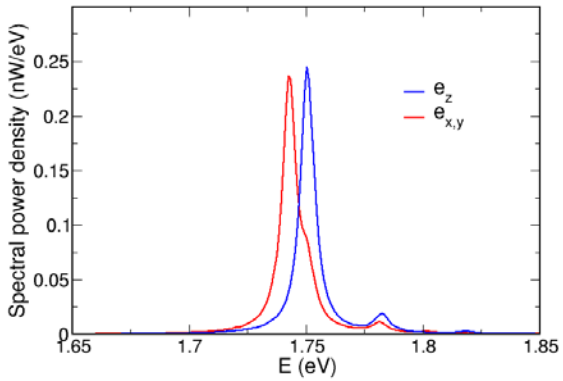




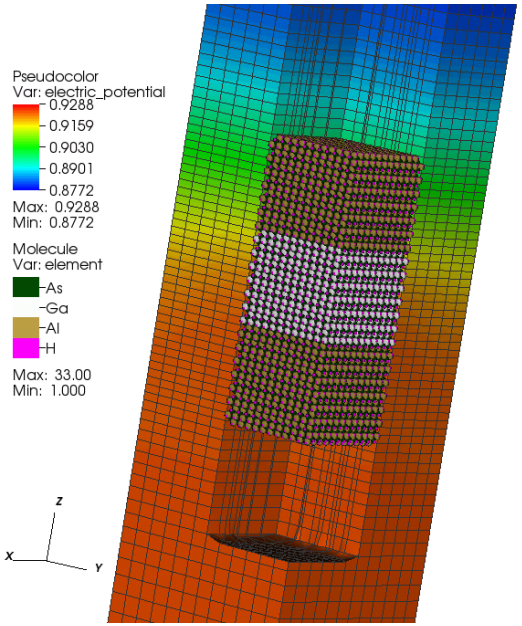
Total current





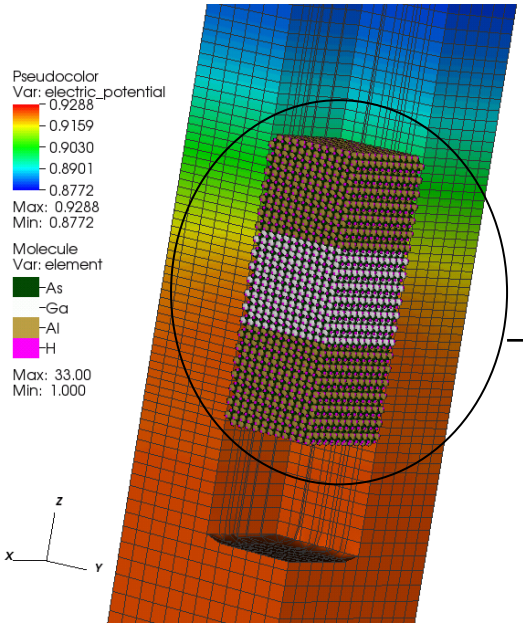


ETB/drift-diffusion



The crystal is generated in the same region where we calculated EFA. Strain is included and potential is projected in the Hamiltonian in a selfconsistent way

ETB/drift-diffusion



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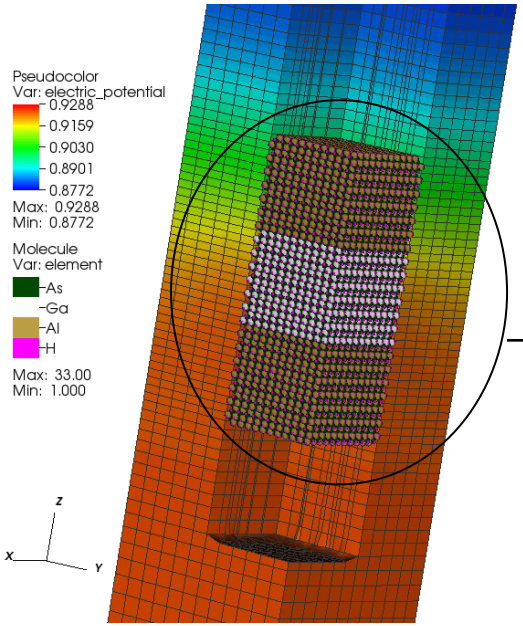
50 000 atoms
20 orbital per atom
1 000 000 orbitals (2h per state)
5 selfconsistent iteration expected
1 electron state confined, many hole states

ETB for electron states – EFA for valence states

ETB/drift-diffusion



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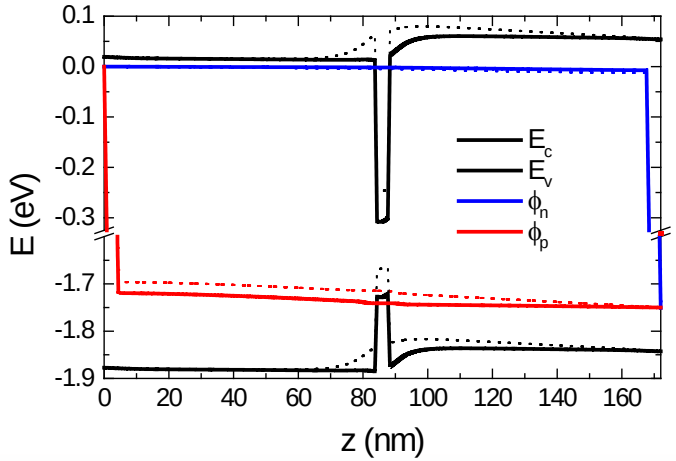

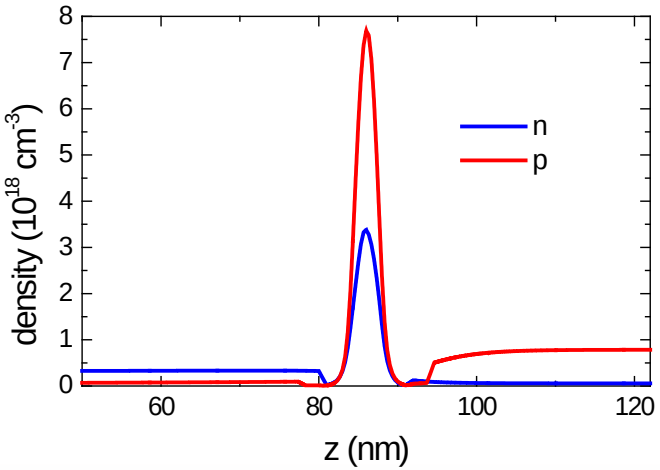

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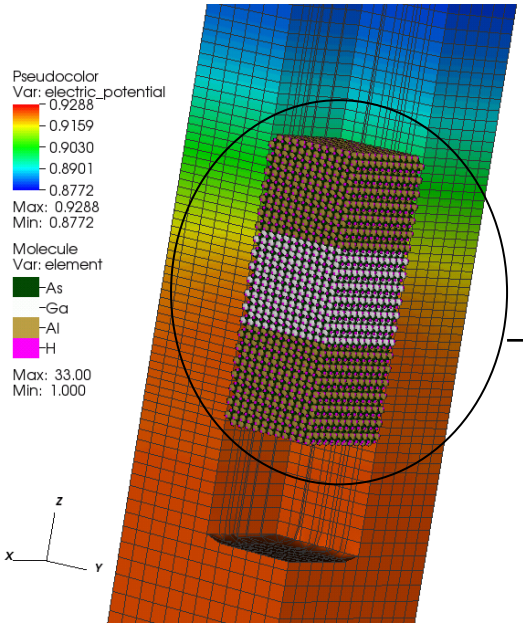

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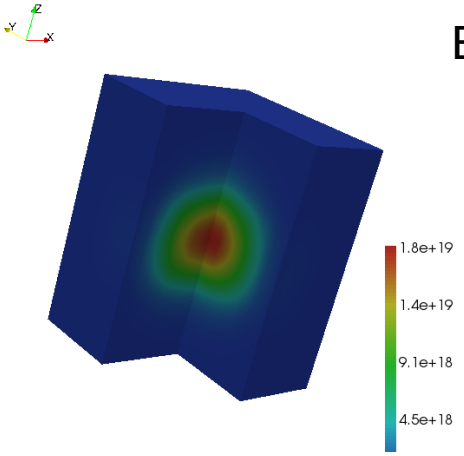
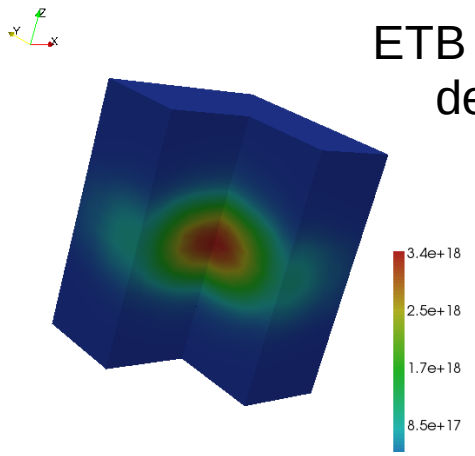
EFA electron density

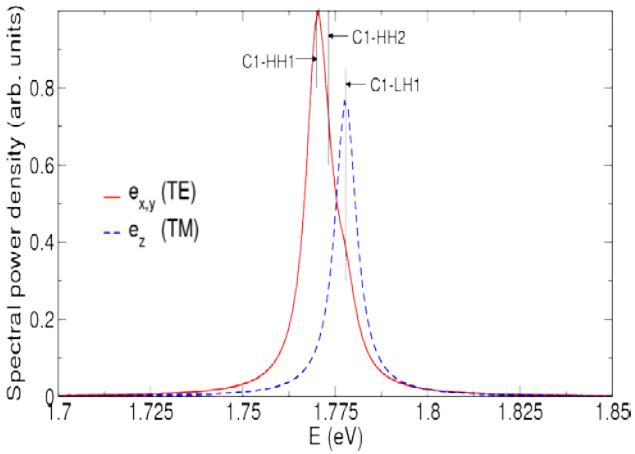


ETB electron density

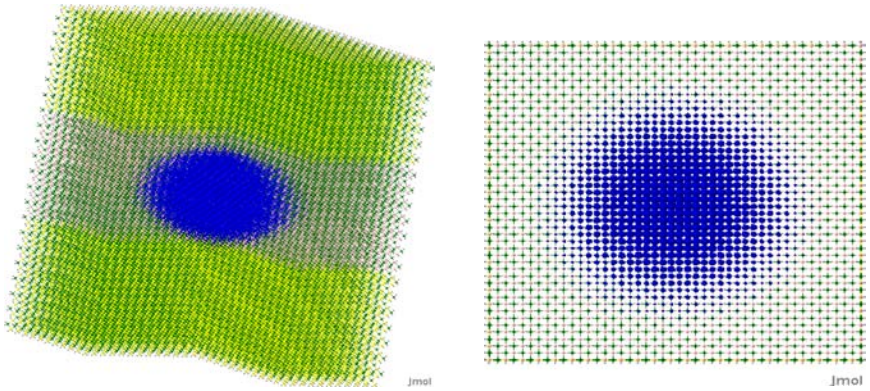


ETB/drift-diffusion

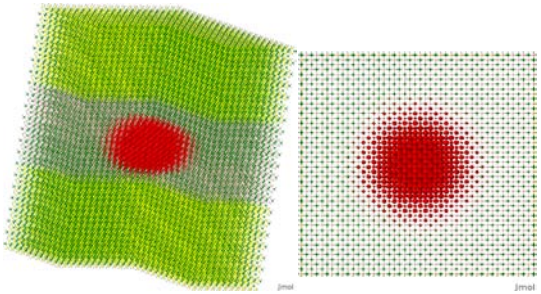
We can use the final potential profile and calculate the first three hole states and the spontaneous emission spectrum.



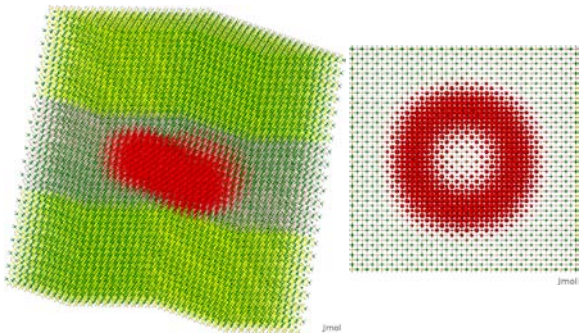
First conduction state



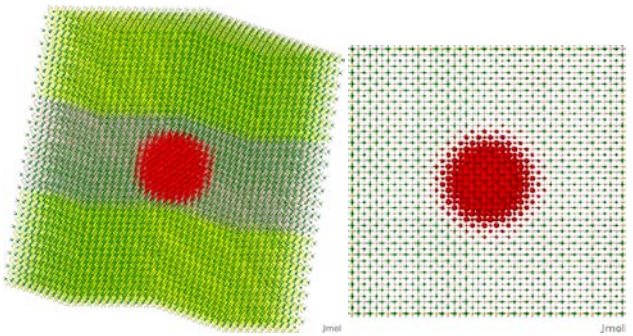
First HH state



Second HH state



First LH state

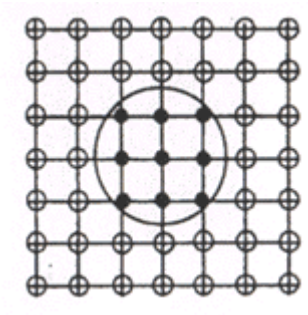


Outline

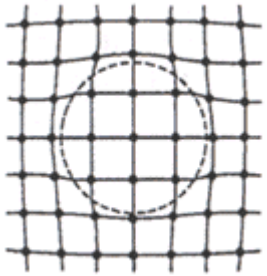
- Multiphysics/Multiscale simulation of nanoelectronic devices: TiberCAD
- Optoelectronic properties of a nanostructured device: models and applications
- A selfconsistent Schrodinger/Drift-diffusion
- **Valence Force Field and Continuum Elasticity**
- Non Equilibrium Green's Function for quantum transport: theory and applicationa

Continuum elasticity

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



Lattice match



Lattice mismatch

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

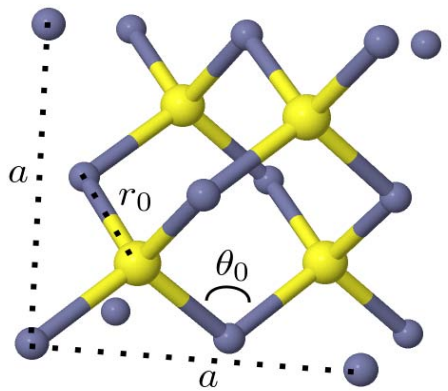
$$\varepsilon_{ij}(\boldsymbol{r}) = \tilde{\varepsilon}_{ij}(\boldsymbol{r}) + \varepsilon^0_{ij}(\boldsymbol{r})$$

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

PDE is solved with FEM technique

Valence Force Field

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

Advantages:

Most efficient atomistic technique

Description beyond effective medium (random alloy)

Include internal strain

More accurate for some classes of nanostructures

VFF vs CE

Evaluating when CE fails 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%)

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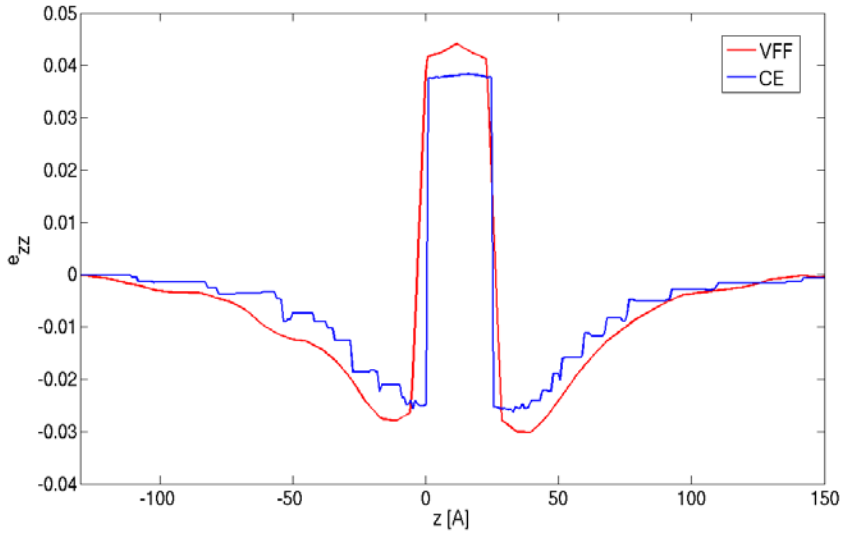

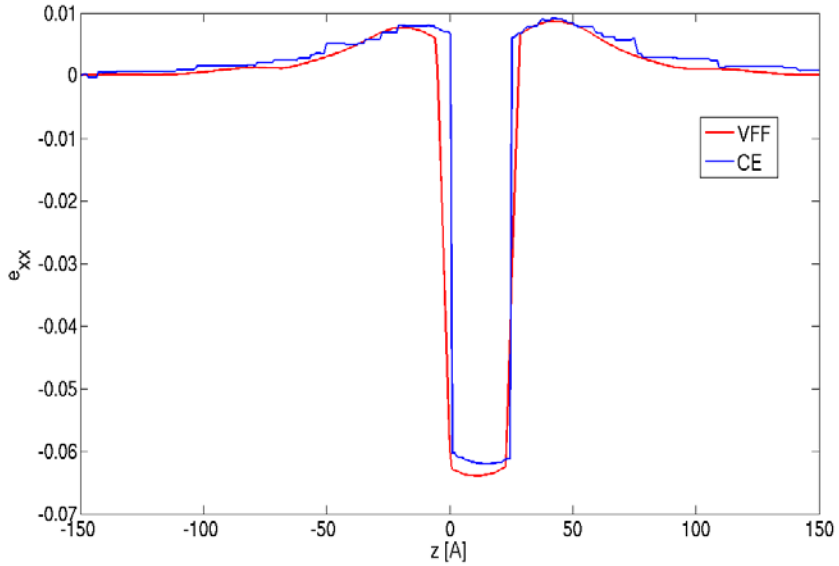

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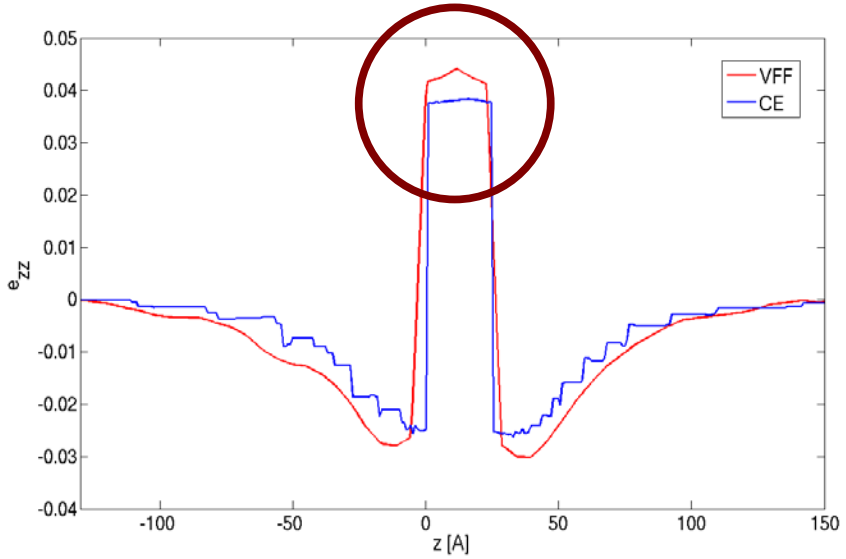
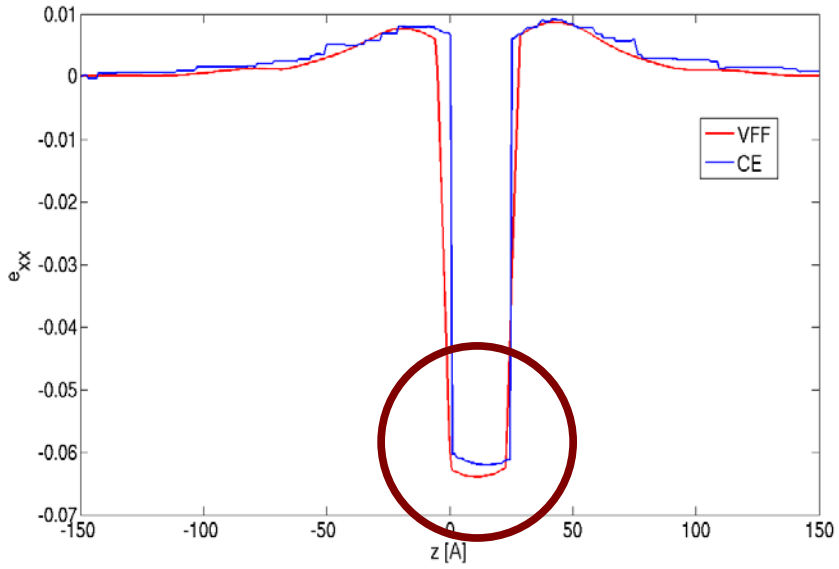


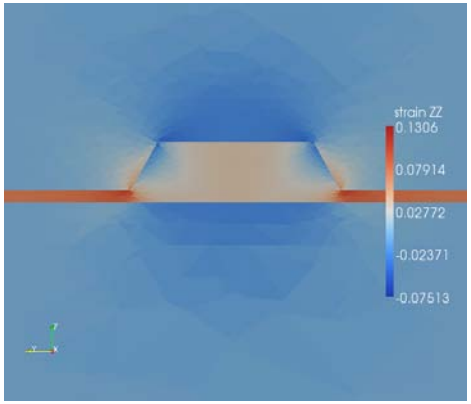
Self assembled by strain relaxation
High lattice mismatch (about 7%)
High aspect ratio

Big difference! (14% - 5%)

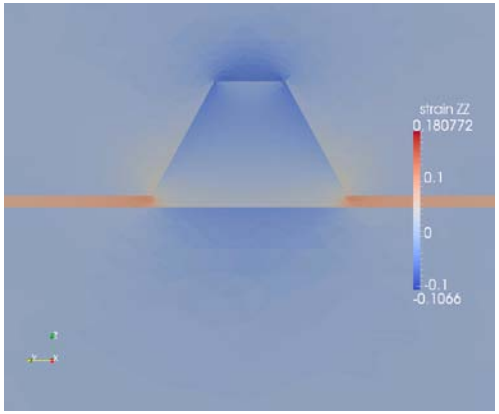


VFF vs CE

In literature smaller differences are reported, but on structure with smaller aspect ratio



Increase height up to 5 nm



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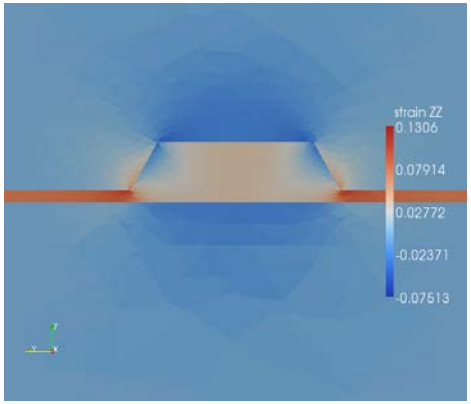

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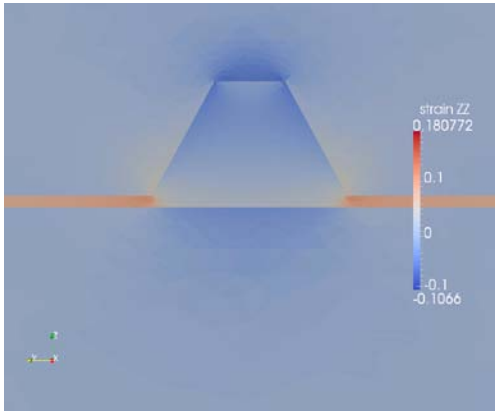
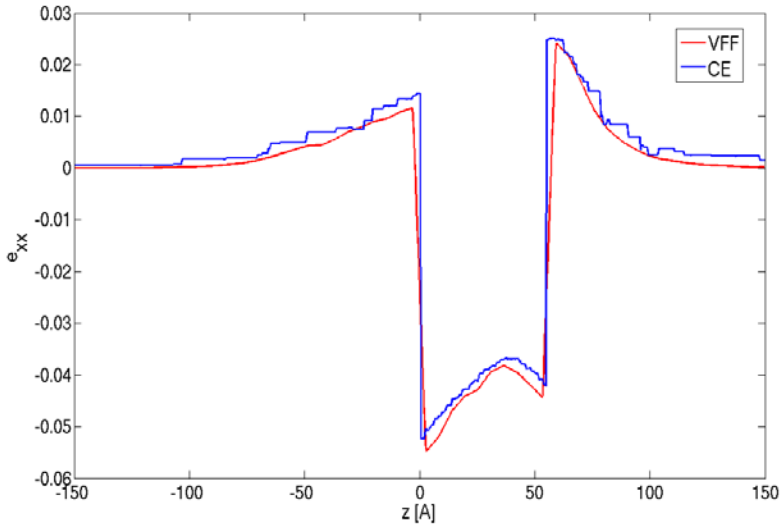
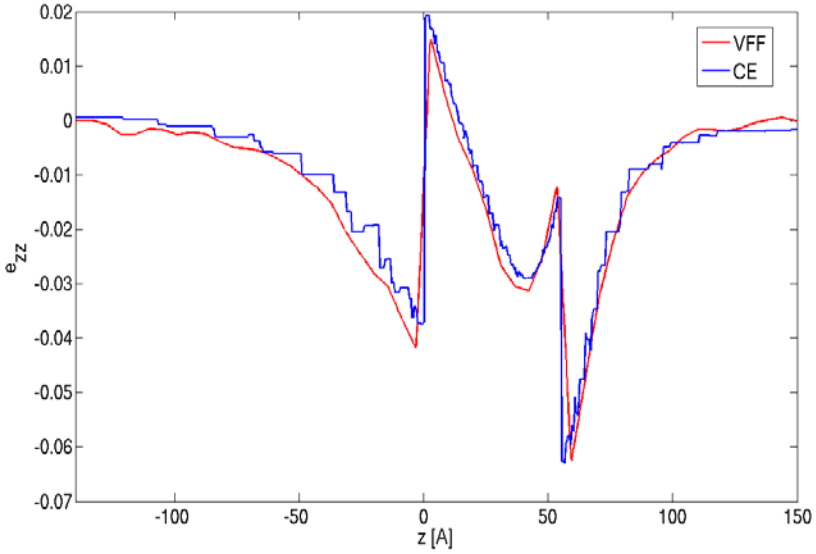


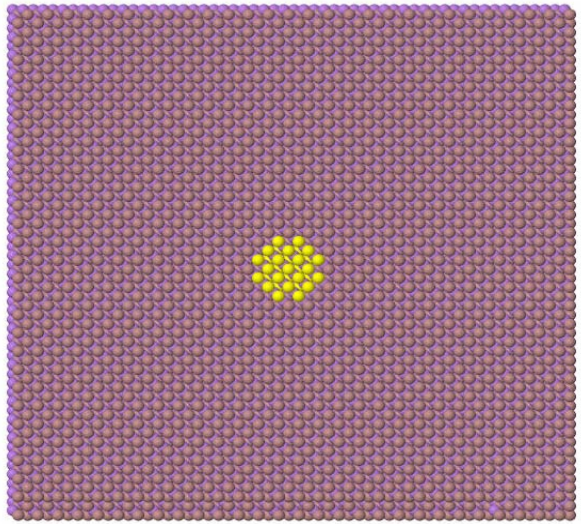


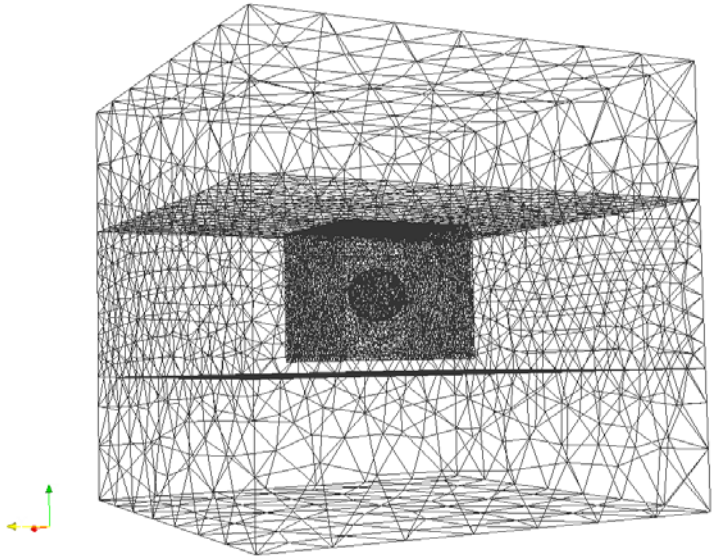


Multiscale strain

We have both CE and VFF in TiberCAD. We have methods to make them exchange data. Let's try a novel scheme!

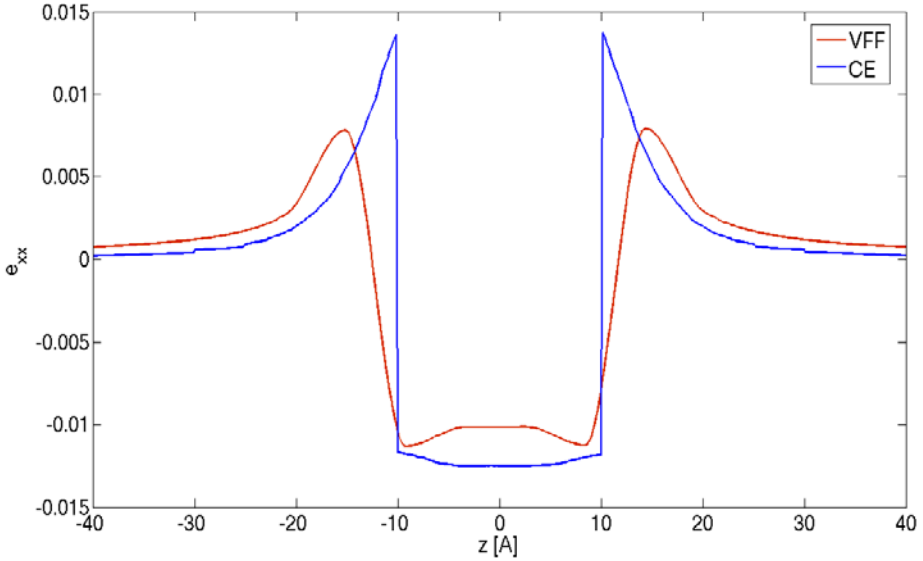
Test structure: spherical InAs quantum dot in GaAs box (GaAs substrate)

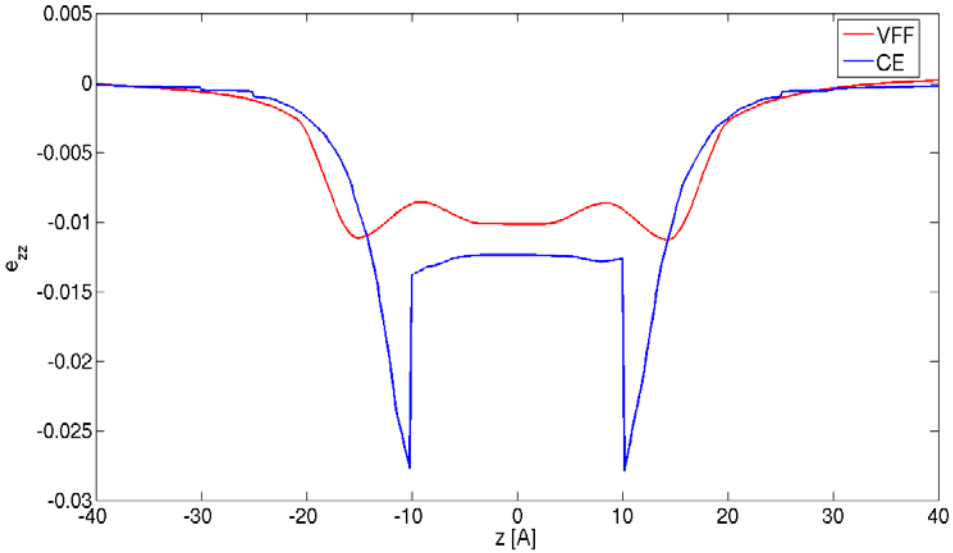




16 nm cubic box (200 000 atoms)
Full CE and Full VFF
GaAs substrate boundary condition

Multiscale strain

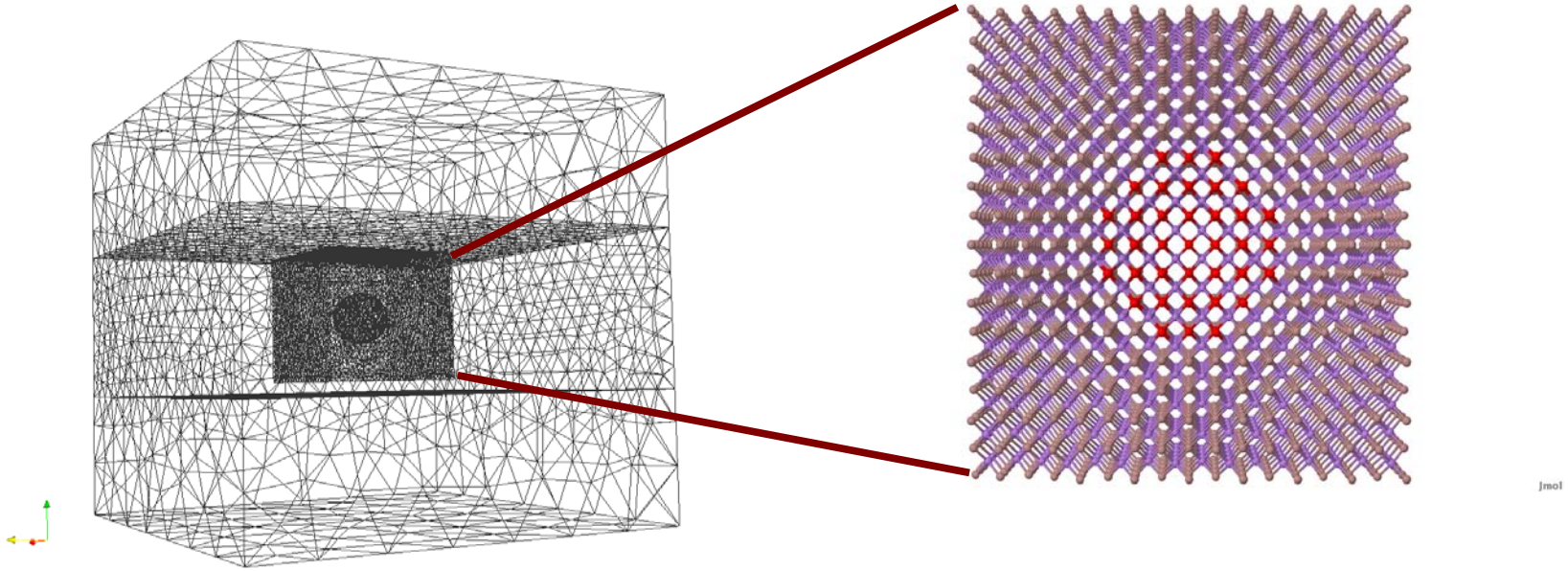




They differ a lot (up to 15% inside dot), CE model fails
Good agreement a few nanometers outside the dot
CE takes a few seconds
VFF takes about 15 minutes

Multiscale strain

We can try a multiscale approach



Atomistic structure is only defined in a smaller box (5nm): 4000 atoms

Multiscale strain

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
4)Solve VFF in the smaller structure
5)Join results

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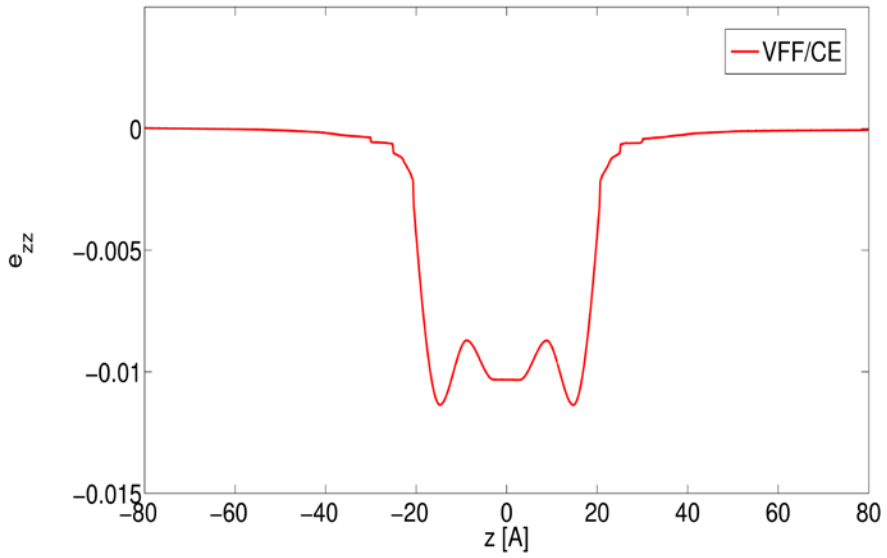

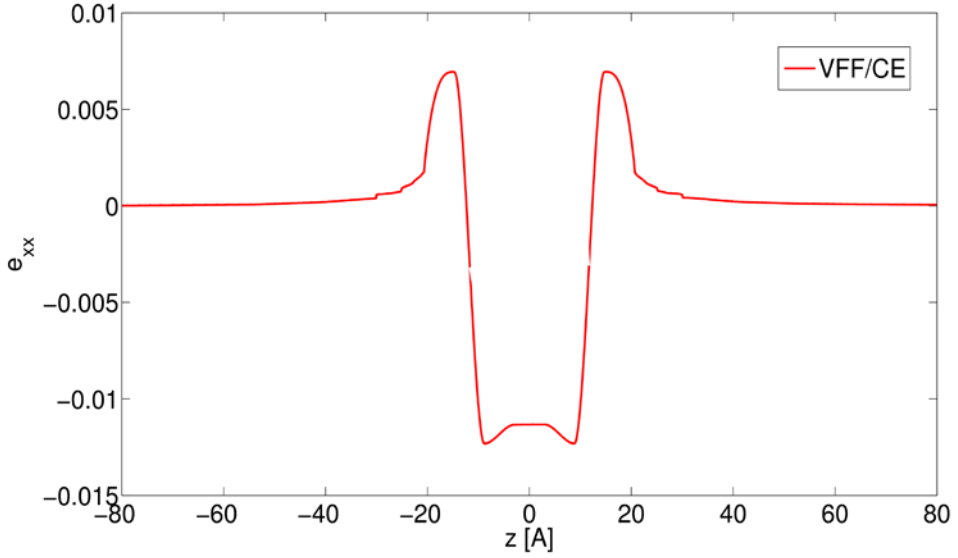

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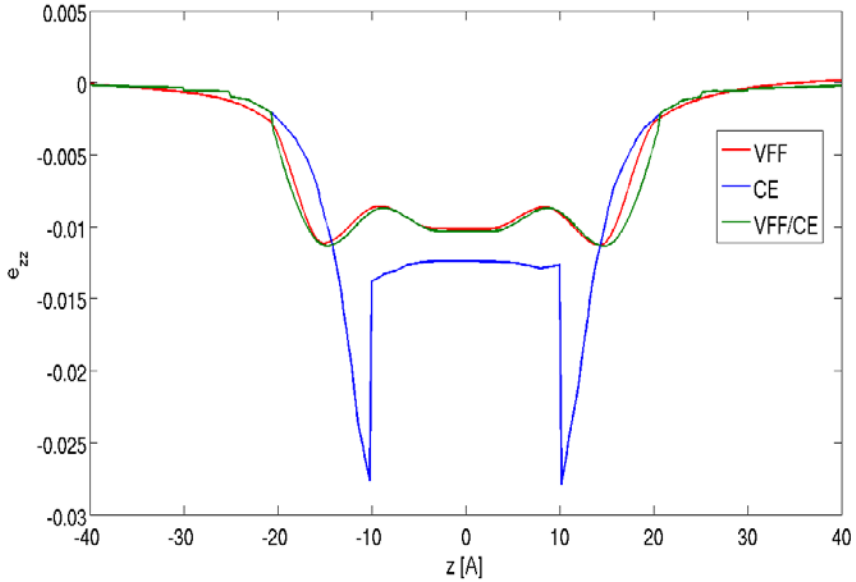

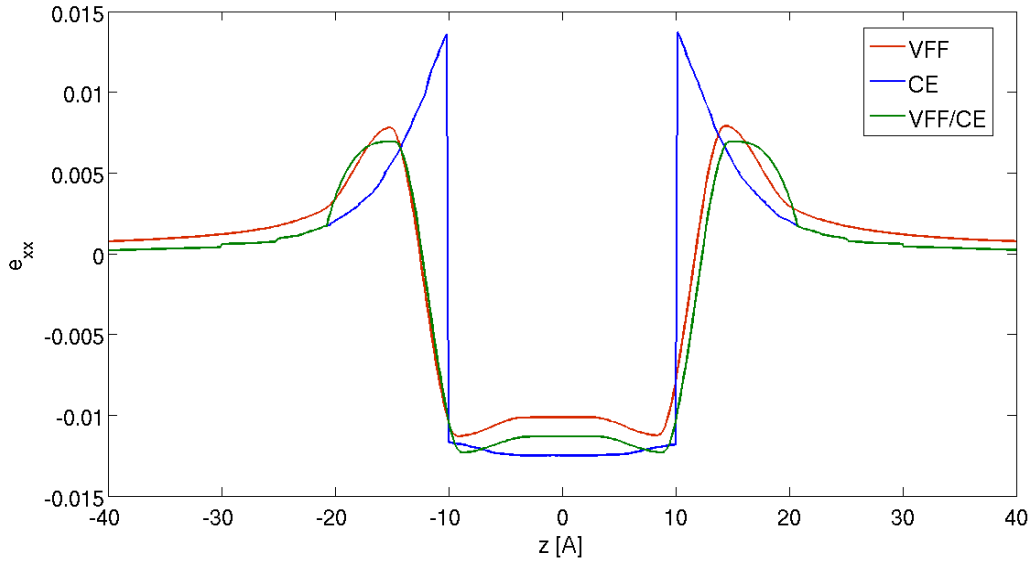

VFF/CE approach: a few seconds

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- **Non Equilibrium Green's Function for quantum transport: theory and applications**

What is a Green's function

Let's consider a quantum system plus a constant perturbation

$$H|\psi\rangle = E|\psi\rangle + |v\rangle$$

$$|\psi\rangle = -(E - H)^{-1}|\psi\rangle = -G(E)|v\rangle$$

$$G^{R,A} = [(E \pm i\delta)I - H]^{-1}$$

The Green's function is the system response to this perturbation
If we consider the contact as a perturbation, we can include injection effects as Self Energies

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$$H = \begin{pmatrix} H_c & -\tau \\ -\tau^\dagger & H_d \end{pmatrix} \Rightarrow \begin{pmatrix} G_c & G_{cd} \\ G_{dc} & G_d \end{pmatrix} = \begin{pmatrix} (E+i\delta)I - H_c & +\tau \\ +\tau^\dagger & (E+i\delta)I - H_d \end{pmatrix}^{-1}$$

$$g_c^R = [(E+i\delta)I - H_c]^{-1} \Rightarrow \Sigma_c^R = \tau^\dagger g_c^R \tau$$

$$G_d = \left[(E+i\delta)I - H_d - \Sigma_d^R\right]^{-1}$$

What is a Green's function

These are the equilibrium Green's function, including the effect of contacts. From G(E) we can derive density of states and transmissione coefficient

$$A = i\left(G^R - G^A\right) \Rightarrow$$ Spectral function

$$N(E) = \frac{1}{2\pi} Tr\left[A(E)\right] \Rightarrow$$ Density of States (DOS)

$$\rho = \frac{1}{2\pi}\int_{-\infty}^{+\infty} F_0(E-\mu)[A(E)]dE \Rightarrow$$ Density matrix

$$T_{1,2}(E) = Tr\left[\Gamma_1 G^R \Gamma_2 G^A\right] \Rightarrow$$ Transmission coefficient

What is a Green's function

What if we are out of equilibrium? In general, Fermi level is not well defined!
Keldysh formalism is needed (NEGF)

$$\Sigma_\alpha^< = f(E-\mu_\alpha)\Gamma_\alpha$$
$$\Sigma_\alpha^> = (1-f(E-\mu_\alpha))\Gamma_\alpha = f(-E+\mu_\alpha)\Gamma_\alpha$$

In-scattering / Out-scattering sources

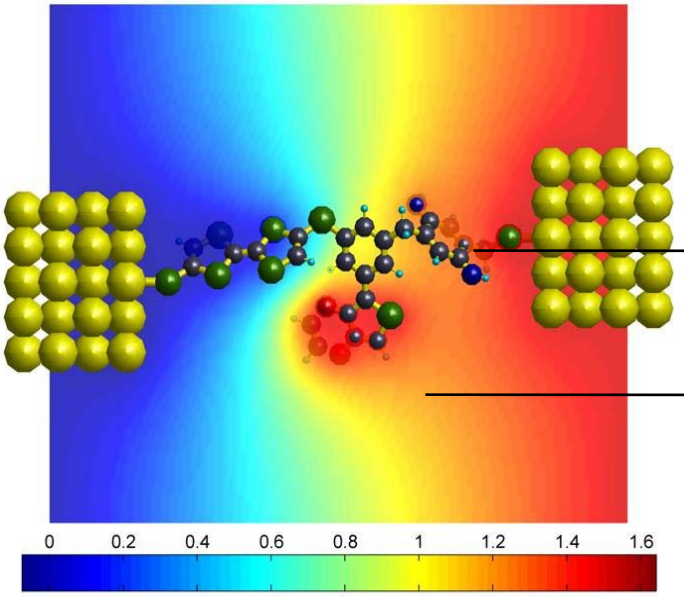
$$G^< = G^R\Sigma^< G^A$$
$$G^> = G^R\Sigma^> G^A$$

Keldysh Green's functions

$$\rho = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} G^<(E)dE$$

Density matrix

Application: molecular device



Tetrathialfulvalene (TTF) – donor-like
(HOMO -4.2 eV LUMO -2.1 eV)

Benzo-quinone-diimine (BQD) – acceptor-like
(HOMO -4.8 eV LUMO -2.8 eV)

Ethyl-dioxy-thiophene (EDT)

A phenil ring connect the molecules

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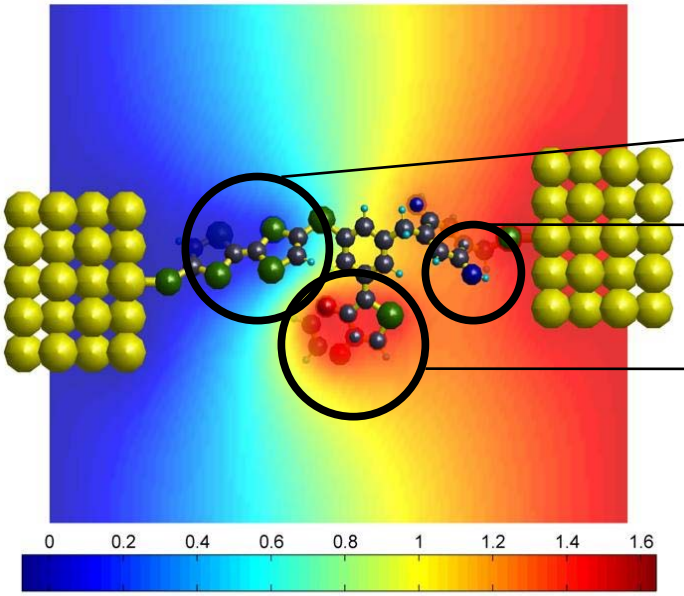

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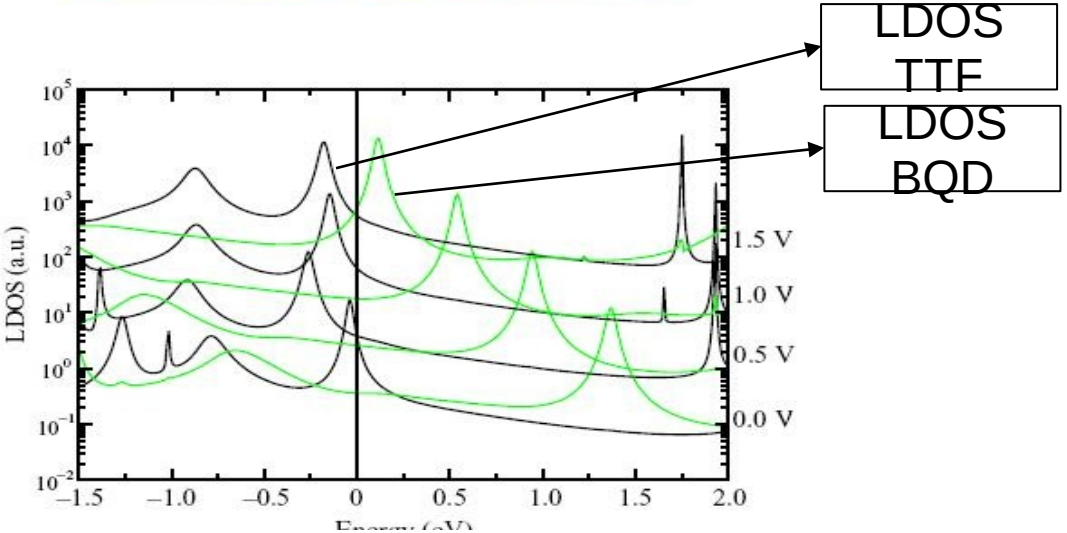
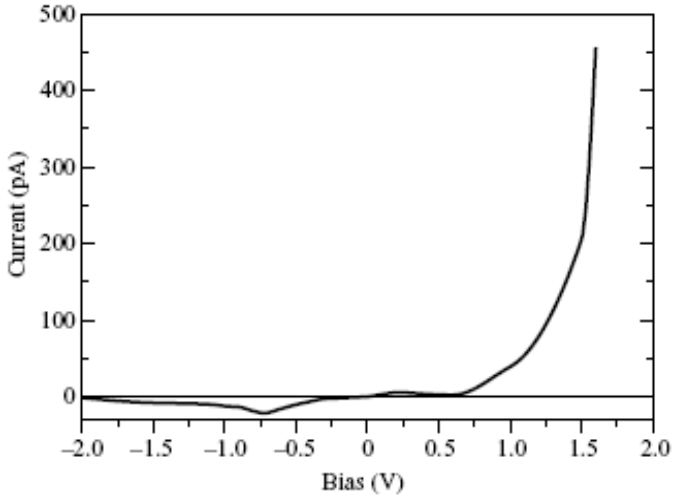
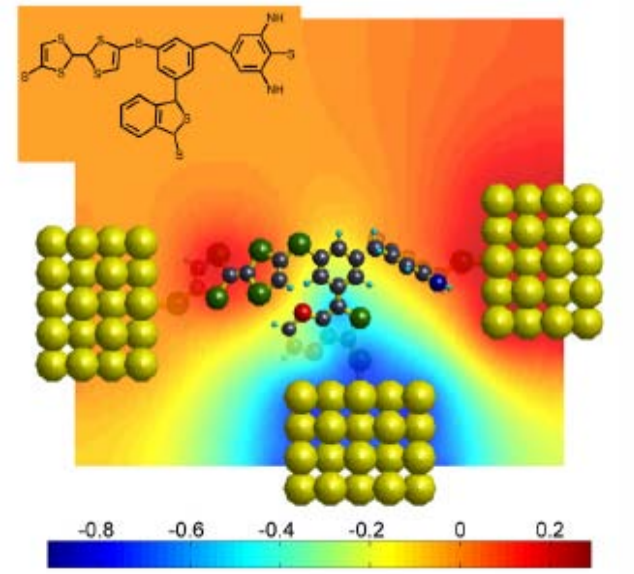
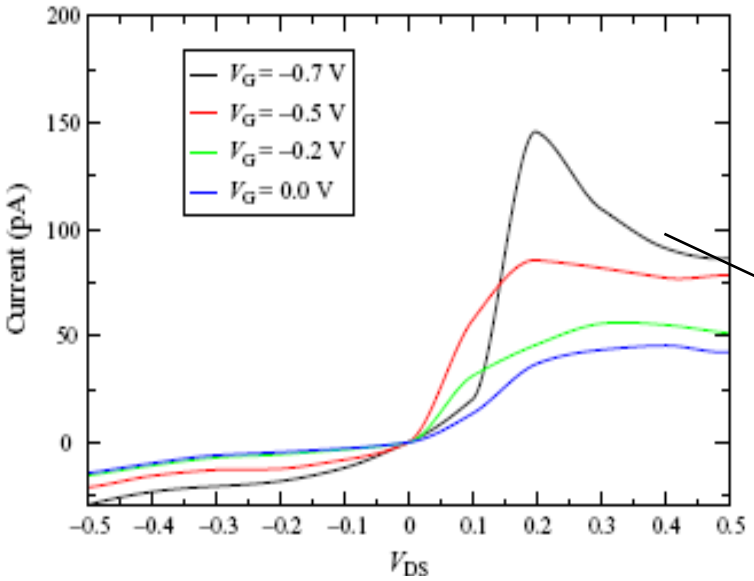
A phenil ring connect the molecules



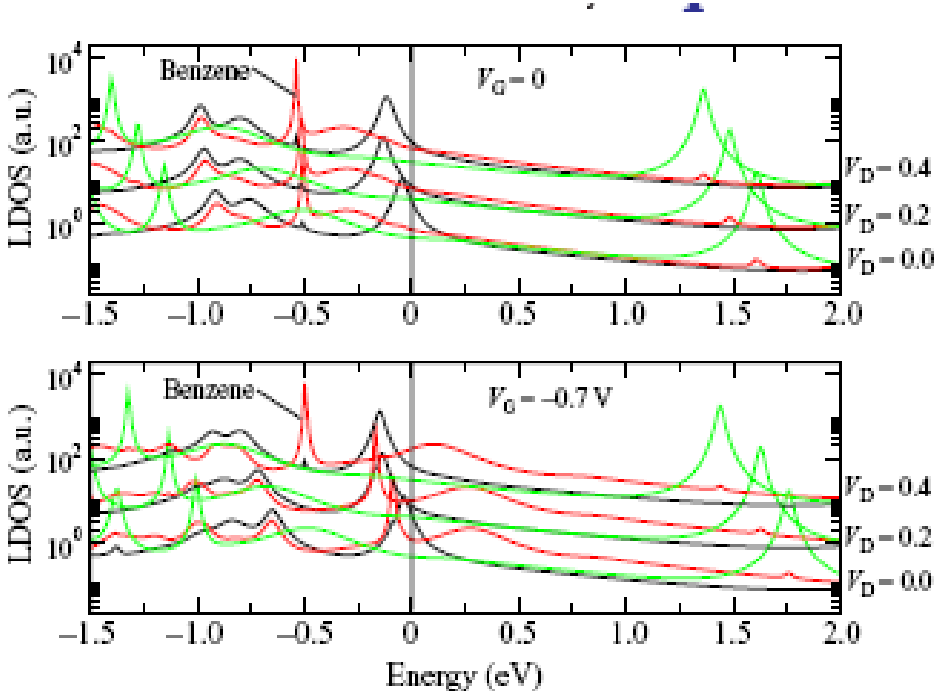


Molecular transistor





NEGF code allows multiterminal analysis



Drain Induced Barrier Lowering (DIBL)
Benzene coupling with BQD too high

Conclusion

We included atomistic description within a FEM code (TiberCAD)

We included Tight Binding models for the calculation of optoelectronic properties

We developed methods for data exchange between continuous and atomistic models

We applied novel simulation schemes to semiconductor nanodevices and demonstrate the need for atomistic modeling

We developed a VFF code and proposed a multiscale scheme for strain calculation

We developed a state-of-the-art NEGF iterative library and applied it to a molecular device

Publications

Journal articles

1) M. Auf der Maur, F. Sacconi, G. Penazzi, M. Povolotskyi, G. Romano, A. Pecchia and A. Di Carlo, *Coupling atomistic and finite element approaches for the simulation of optoelectronic devices,* **Optical and Quantum Electronics**, doi: 10.1007/s11082-010-9375-1

2) G. Penazzi, A. Pecchia, F. Sacconi, and A. Di Carlo, *Calculation of optical properties of a quantum dot embedded in a gan/algan nanocolumn,* **Superlattices and Microstructures**, 47(1) (2010) - pages 123 – 128

3) Matthias Auf Der Maur, Michael Povolotskyi, Fabio Sacconi, Alessandro Pecchia, Giuseppe Romano, Gabriele Penazzi, and Aldo Di Carlo, *Tibercad: Towards multiscale simulation of optoelectronic devices,* **Optical and Quantum Electronics**, 40(14-15 SPEC. ISS.) (2008) - pages 1077 – 1083

4) A. Pecchia, L. Salvucci, G.Penazzi and A. Di Carlo, *Non-equilibrium Green 's functions in density functional tight binding: method and applications,* **New Journal of Physics** 10 (2008) - pages 065022

Pubblications

Proceedings

1) G. Penazzi, A. Pecchia, F. Sacconi, M. Auf Der Maur, M. Povolotskyi, G. Romano, and A. Di Carlo
Multiscale-multiphysics simulation of nanostructured devices: The tibercad project. 2009
13th International Workshop on Computational Electronics, IWCE (2009)

2) M. Auf Der Maur, M. Povolotskyi, F. Sacconi, A. Pecchia, G. Romano, G. Penazzi, A. Di Carlo
TiberCAD: Towards multiscale simulation of optoelectronic devices
International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD (2008) - pages 43 - 44

3) F. Sacconi, G. Romano, G. Penazzi, M. Povolotskyi, M. Auf Der Maur, A. Pecchia, and A. Di Carlo
Electronic and transport properties of gan/algan quantum dot-based p-i-n diodes
International Conference on Simulation of Semiconductor Processes and Devices, SISPAD (2008)

4) A. Di Carlo, M. Auf der Maur, F. Sacconi, A. Pecchia, M. Povolotskyi, G. Penazzi, and G. Romano
Multiscale atomistic simulations of high-k mosfets
8th IEEE Conference on Nanotechnology (NANO) (2008)

Pubblications

Conferences

1) Oral presentation and poster at Gruppo Elettronica 2010, Roma (IT). G. Penazzi, A. Pecchia, M. Auf Der Maur, F. Sacconi, A. Di Carlo, ”Development of an atoistic/continuous simulation tool for optoelectronic devices”.

2) Oral presentation at Theory, Modelling and Computational methods for Semiconductors 2, York 2010
(UK). G. Penazzi, A. Pecchia, M. Auf Der Maur, A. Di Carlo, ”TiberCAD: a multiscale/multiphysics simulation tool for optoelectronic properties of novel devices”.

3) Oral presentation at 13th International Workshop on Computational Electronics, IWCE, Beijing 2009 (China). G. Penazzi, A. Pecchia, F. Sacconi, M. Auf der Maur, M. Povolotskyi, G. Romano, A. Di Carlo,
”Simulations of Optical Properties of a GaN Quantum Dot Embedded in a AlGaN Nanocolumn within a Mixed FEM/atomistic Method”.

4) Poster presentation at International Conference on Physics of Light-Matter Coupling in Nanostructures, PLMCN 9, Lecce, (IT). G. Penazzi, A. Pecchia, F. Sacconi, A. Di Carlo,
”Calculation of optical properties of a quantum dot embedded in a gan/algan nanocolumn”.

Pubblications

Conferences

5) Poster presentation at International Conference on Simulation of Semiconductor Processes and 2007 Devices 12, SISPAD, Vienna, (AU). A. Pecchia, G. Penazzi, A. Di Carlo, ”Efficient Green’s Function Algorithms for Atomistic Modeling of Si Nanowire FETs”.

6) Oral presentation at Italian Workshop on Carbon Nanotubes for Electronics, ICNTE 1, Bologna, 2007 Italy. G. Penazzi, L. Latessa, A. Pecchia, A. Di Carlo, ”Atomistic Simulation of CNT MOSFETs”.