NEMO5 Introduction

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Network for Computational Nanotechnology (NCN)

Electrical and Computer Engineering

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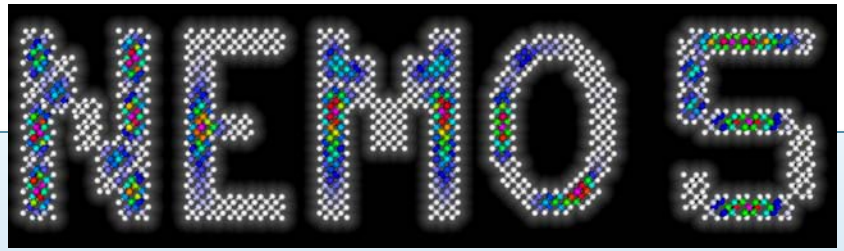
This lecture is about

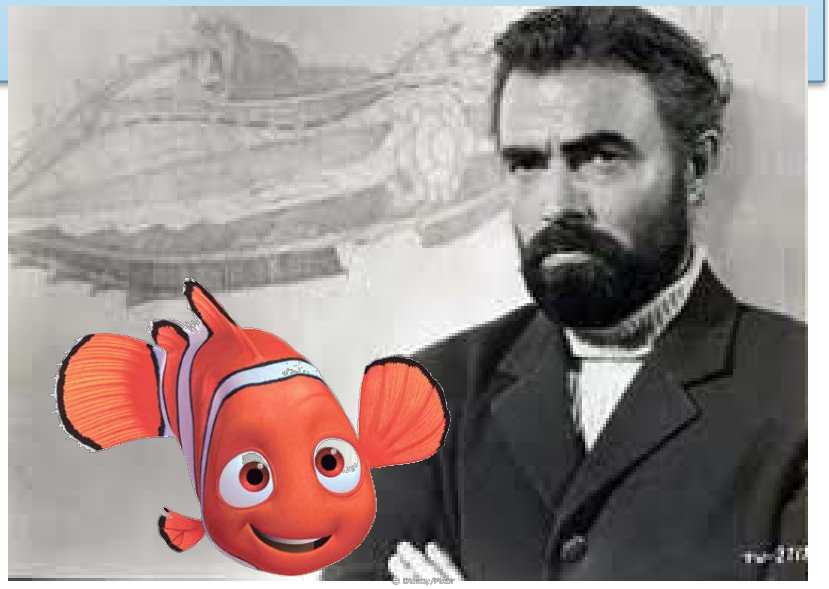


What is NEMO?

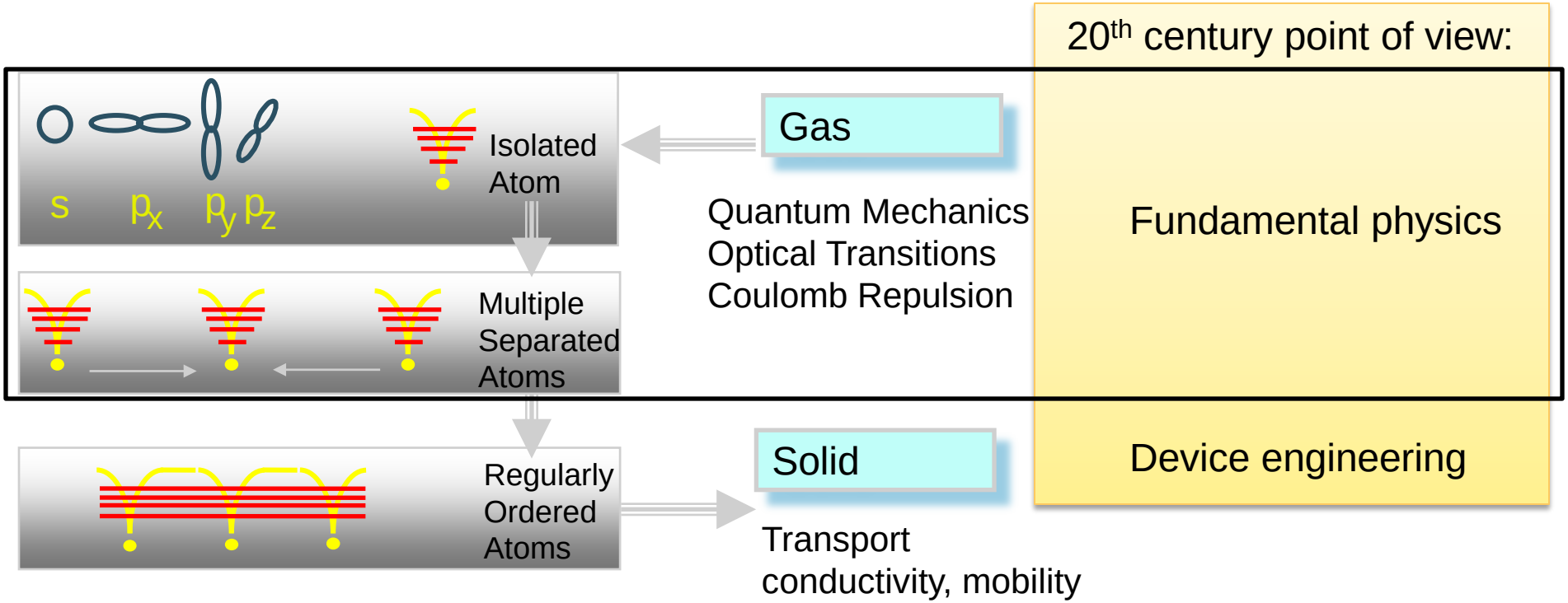
What can NEMO do?

Why NEMO and not something else?

Where can you find NEMO?



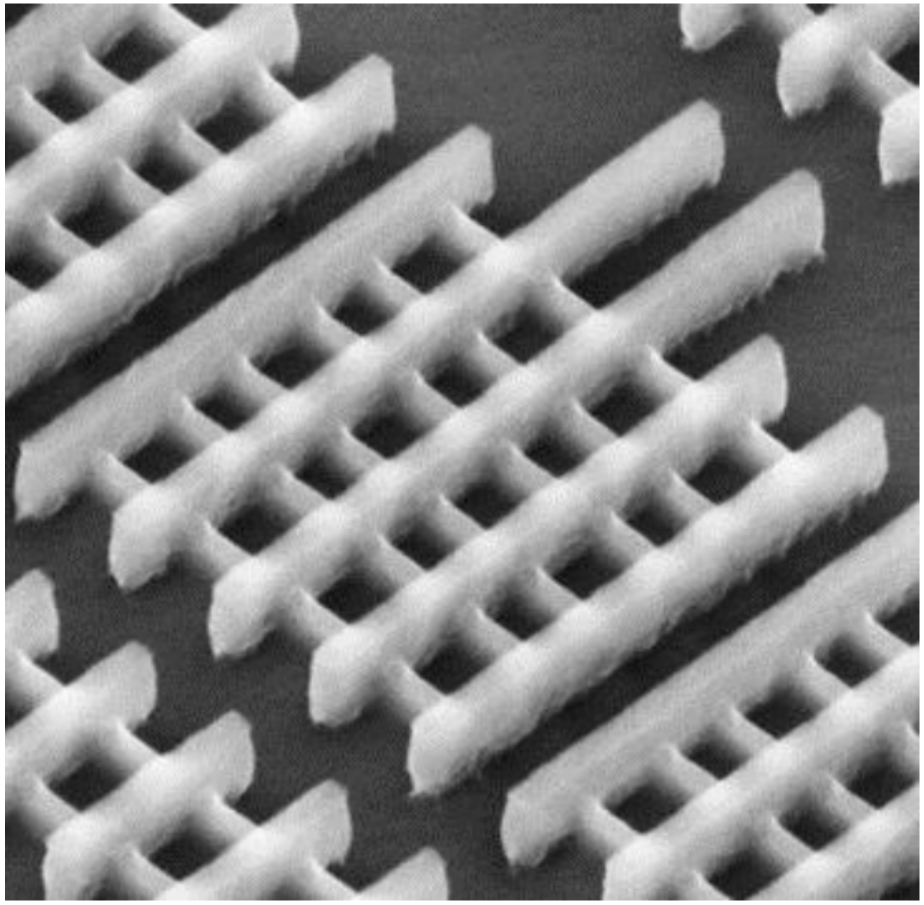
A change in the view of the world



Today:
Devices enter the realm of countable atoms
Distinction of individual bands (e.g. CB, VB) becomes artificial

Today's simulation requirements: industry

Example: Intel's 22 nm Tri-Gate Transistor



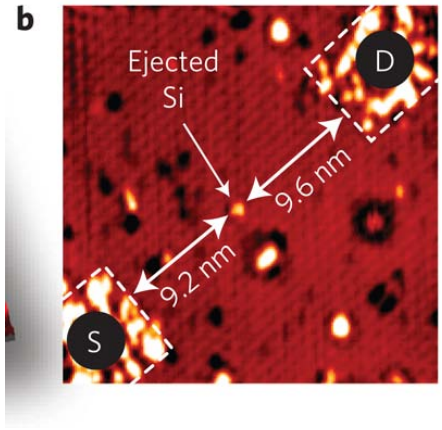
http://newsroom.intel.com/docs/DOC-2035

Real world effects:
Strained structures
Imperfect growth
- Impurities
- Alloy disorder
- Surface and interface roughness

3D geometry affects electrons
Scattering on lattice vibrations
Gate leakage
Contact resistance
Joule heating
…

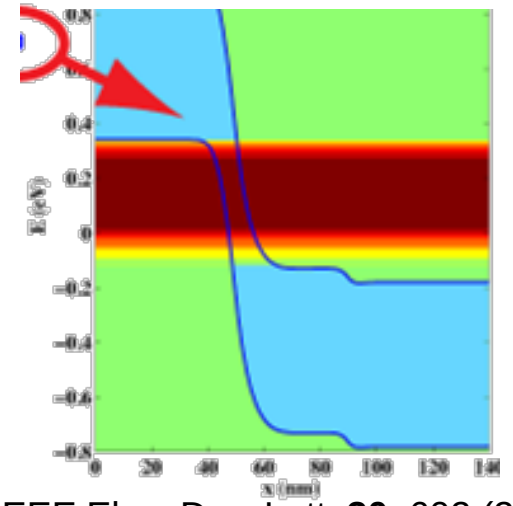
Today's simulation requirements: research

Single atom transistor



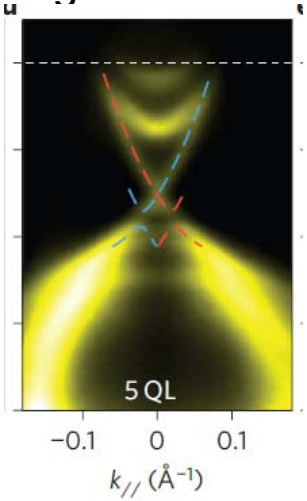
Nature Nanotechnology **7**, 242 (2012)

Band-to-band tunneling



IEEE Elec. Dev. Lett. **30,** 602 (2009)

Topological insulators



Nature Physics **6**, 584 (2010)

Countable device atoms suggest atomistic descriptions
Modern device concepts, e.g.

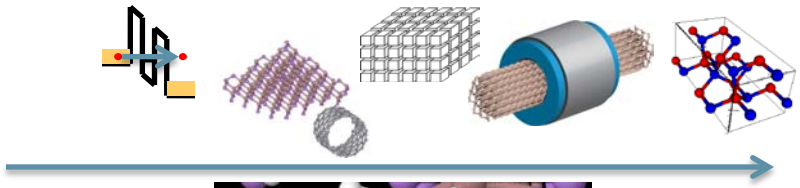
- Band to band tunneling
- Topological insulators (gap less materials)
- Band/Valley mixing etc.

require multi band representations

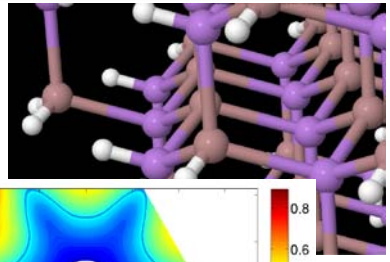
Academic and industrial research&development is and has been the driver of NEMO

NEMO5 lecture - overview

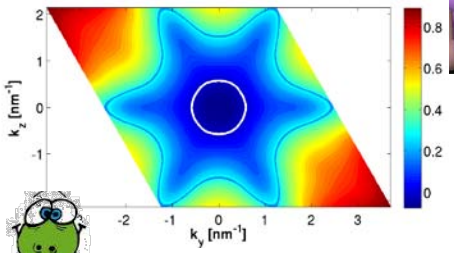
NEMO5 origins + history



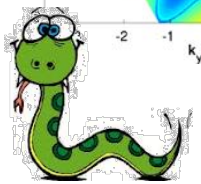
NEMO5 and atomic representations



NEMO5 solvers + physics



NEMO5 expandability + flexibility

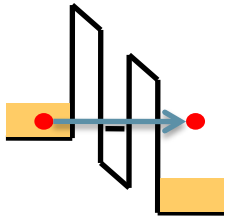


NEMO5 on supercomputers (scalability and compatibility)

NEMO5 support (for output and users)

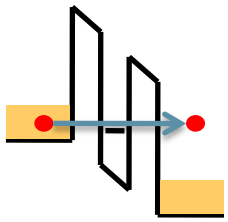
Evolution of Nanoelectronics Tools NEMO and OMEN

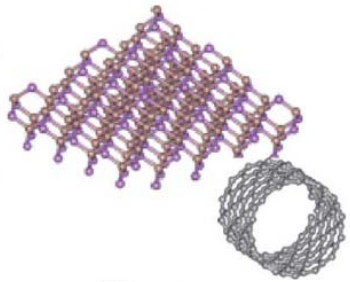
	NEMO-1D
Transport	Yes
Dim.	1D
Atoms	~1,000
Crystal	[100] Cubic, ZB
Strain	-
Multi-physics	-
Parallel Comp.	3 levels 23,000 cores



Evolution of Nanoelectronics Tools NEMO and OMEN

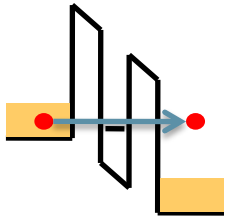
	NEMO-1D	NEMO-3D
Transport	Yes	-
Dim.	1D	any
Atoms	~1,000	50 Million
Crystal	[100] Cubic, ZB	[100] Cubic, ZB
Strain	-	VFF
Multi-physics	-	
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores

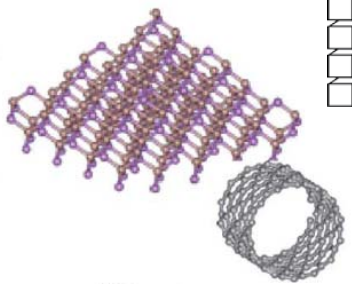


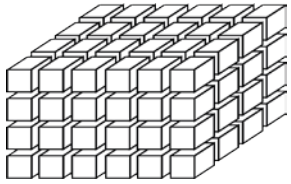


Evolution of Nanoelectronics Tools NEMO and OMEN

	NEMO-1D	NEMO-3D	NEMO3Dpeta
Transport	Yes	-	-
Dim.	1D	any	any
Atoms	~1,000	50 Million	100 Million
Crystal	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic,ZB, WU
Strain	-	VFF	VFF
Multi-physics	-		
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores

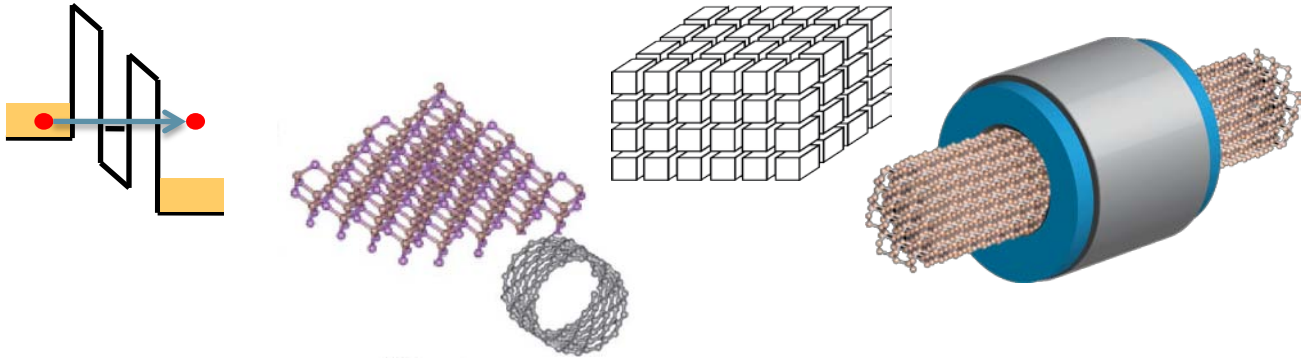






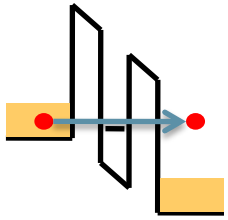
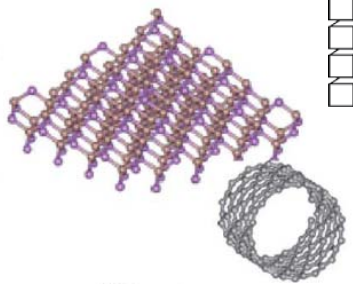
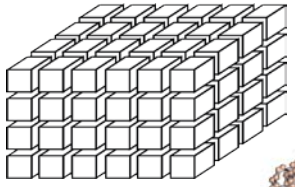
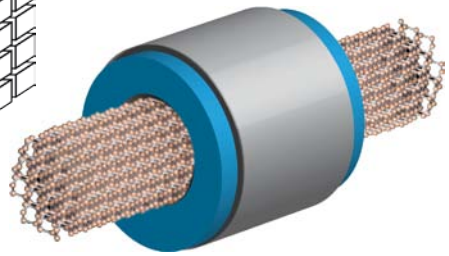
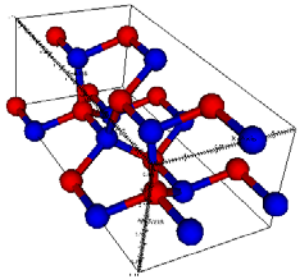
Evolution of Nanoelectronics Tools NEMO and OMEN

	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN
Transport	Yes	-	-	Yes
Dim.	1D	any	any	Almost any
Atoms	~1,000	50 Million	100 Million	~140,000
Crystal	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic,ZB, WU	Any Any
Strain	-	VFF	VFF	-
Multi-physics	-			
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co



Evolution of Nanoelectronics Tools NEMO and OMEN

	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	Yes	-	-	Yes	Yes
Dim.	1D	any	any	any	any
Atoms	~1,000	50 Million	100 Million	~140,000	100 Million
Crystal	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic,ZB, WU	Any Any	Any Any
Strain	-	VFF	VFF	-	MVFF
Multi-physics	-				Spin, Classical
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co	4 levels 100,000 cores

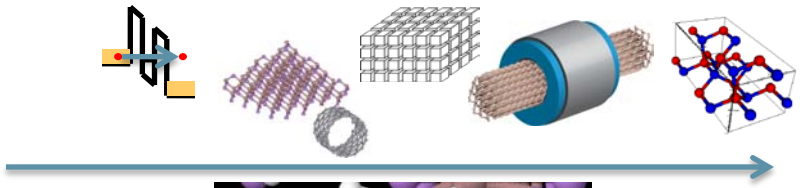






Core Code / Theory Development

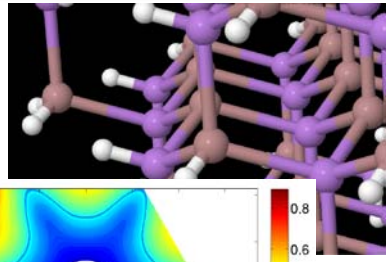
- NEMO-1D (Texas Instruments '94-'98, JPL '98-'03)
  - »Roger Lake, R. Chris Bowen, Dan Blanks, Gerhard Klimeck
- NEMO3D (NASA JPL, Purdue, '98-'07)
  - »R. Chris Bowen, Fabiano Oyafuso, Seungwon Lee, Gerhard Klimeck
- NEMO3D-peta (Purdue, '06-'11)
  - »Hoon Ryu, Sunhee Lee, Gerhard Klimeck
- OMEN (ETH, Purdue, '06-'11)
  - »Mathieu Luisier, Gerhard Klimeck
- NEMO5 (Purdue, '09-'12)
  - »Michael Povolotsky, Hong-Hyun Park, Sebastian Steiger, Tillmann Kubis, Jim Fonseca, Jean Michel Sellier, Gerhard Klimeck
  - »Zhengping Jiang, Lang Zeng, Daniel Mejia, Yu He Sunhee Lee, Mehdi Salmani, Hesam Ilati, Ganesh Hegde

NEMO5 lecture - overview

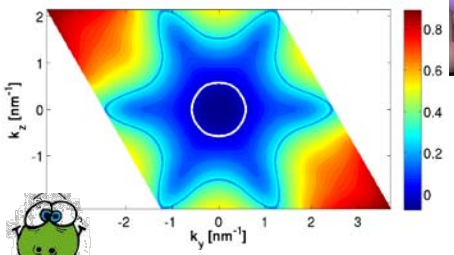
NEMO5 origins + history



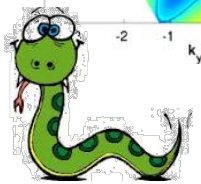
NEMO5 and atomic representations



NEMO5 solvers + physics



NEMO5 expandability + flexibility



NEMO5 on supercomputers (scalability and compatibility)

NEMO5 support (for output and users)

Challenge: large variety of materials

"Is Silicon approaching the end of it's scalability?"

Ongoing discussions:

- **III-V** materials might outperform Si (higher mobilities), but Silicon has higher density of states
- Optically active materials are usually **polar** (III-V, II-VI)
- **Graphene** provides native 2D transport
- **Topological insulators** offer unique transport properties
- "Exotic" materials (e.g. **MgO**) might replace today's dielectric barriers
- Devices are so small, transport quality in **metallic** interconnects is important
- …

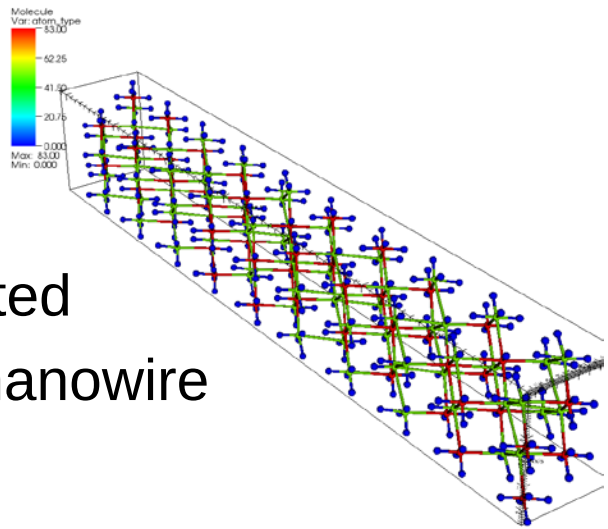
NEMO5 sets up atomistic structures

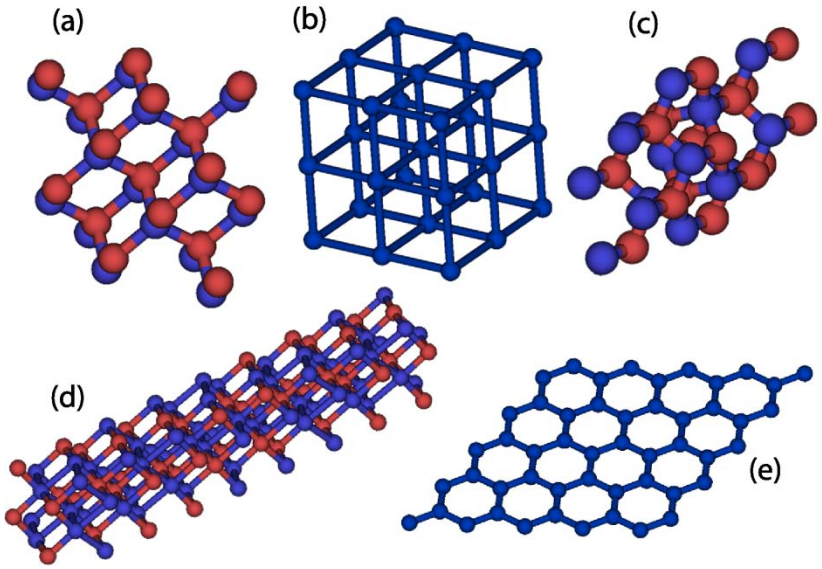
NEMO5: atomistic representation of devices

- Simple-Cubic (for effective-mass band structure)
- Diamond (Si, Ge → MOSFETs, UTBs, …)
- Zincblende (GaAs, InSb, … → TFETs, HEMTs, QDs)
- Wurtzite (nitrides → HEMTs, LEDs)
- Rhombohedral (Bi_2Te_3 → thermoelectrics)
- Graphene

passivated

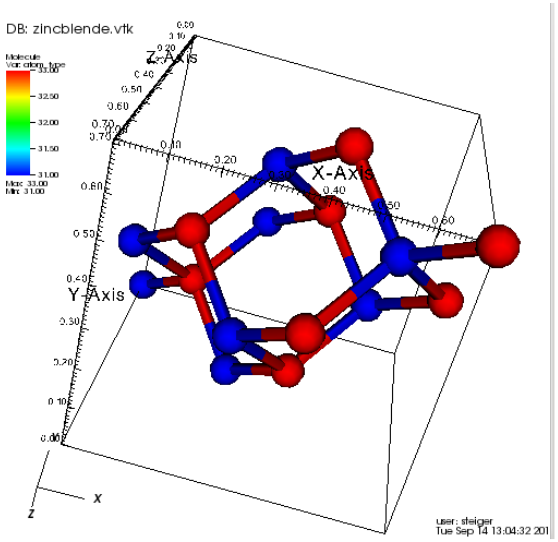
Bi_2Te_3 nanowire

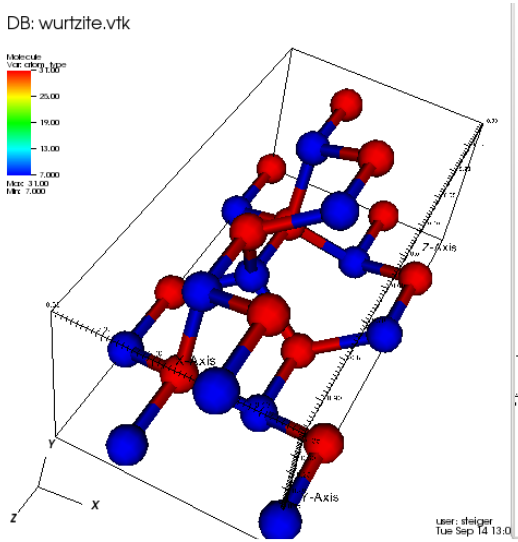


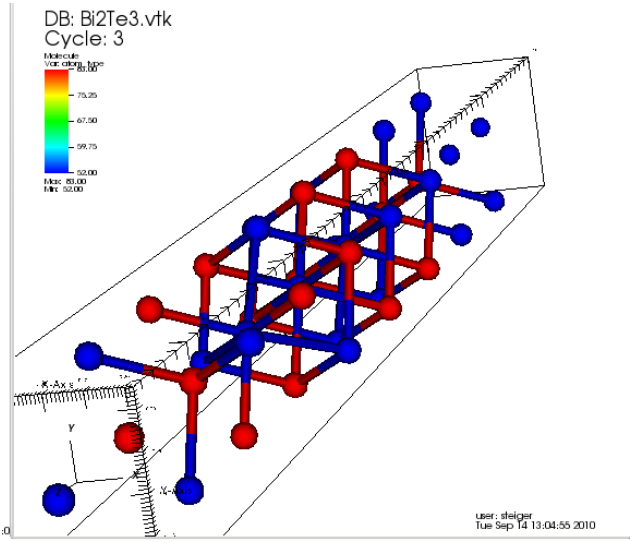


Zincblende, Wurtzite and Rhombohedral Crystals

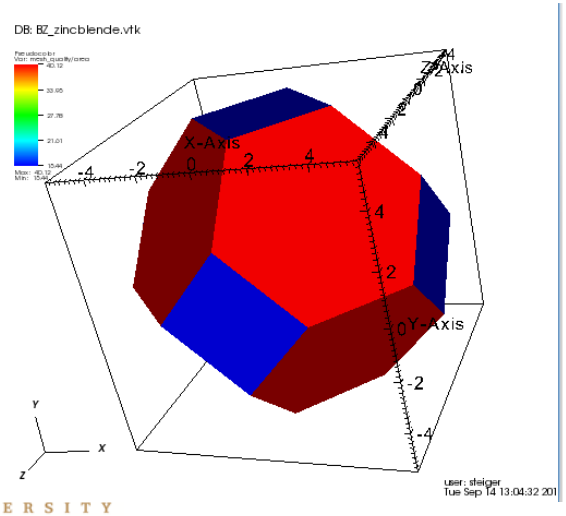
Some crystal structures in NEMO5:

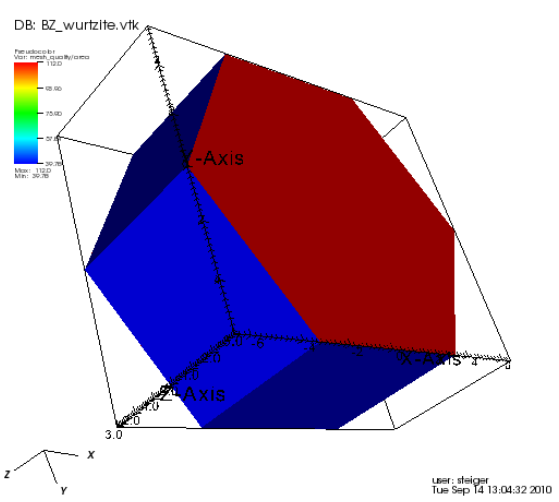


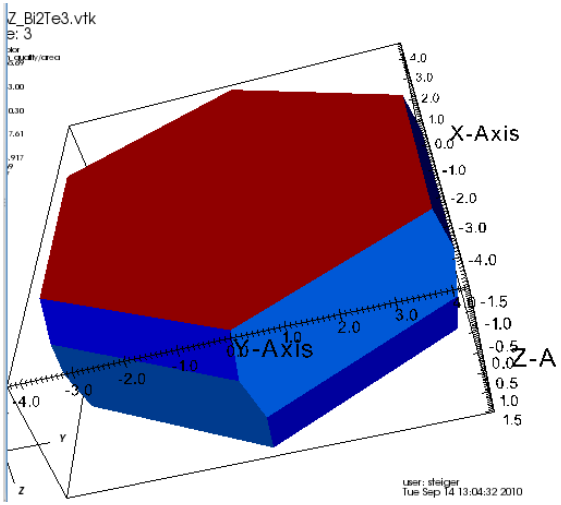




Corresponding Brillouin zones:







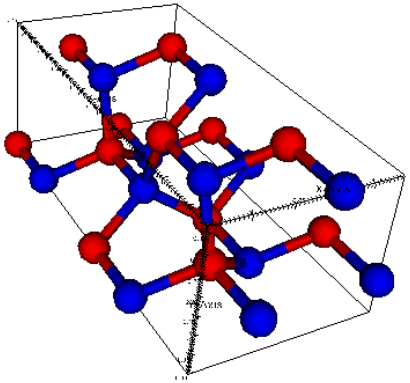
3 steps to add yet another cyrstal structure

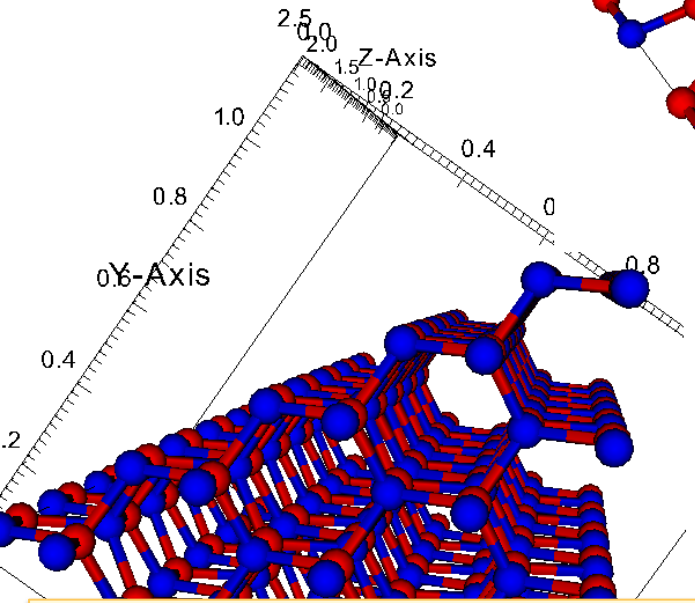
B4 (ZnS)
Primitive Vectors

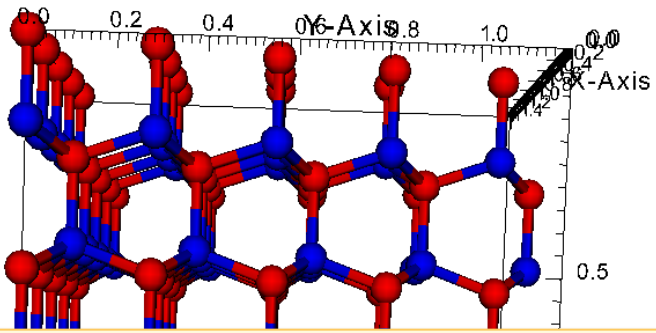
$$\vec{a}_1 = \frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{2}a\hat{y}$$
$$\vec{a}_2 = \frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$$
$$\vec{a}_3 = c\hat{z}$$

Basis Vectors

$$\vec{b}_1 = \frac{1}{3}\vec{a}_1 + \frac{2}{3}\vec{a}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2\sqrt{3}}a\hat{y} \quad (Zn)$$
$$\vec{b}_2 = \frac{2}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + \frac{1}{2}\vec{a}_3 = \frac{1}{2}a\hat{x} - \frac{1}{2\sqrt{3}}a\hat{y} + \frac{1}{2}c\hat{z} \quad (Zn)$$
$$\vec{b}_3 = \frac{1}{3}\vec{a}_1 + \frac{2}{3}\vec{a}_2 + u\vec{a}_3 = \frac{1}{2}a\hat{x} + \frac{1}{2\sqrt{3}}a\hat{y} + uc\hat{z} \quad (S)$$
$$\vec{b}_4 = \frac{2}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + (\frac{1}{2}+u)\vec{a}_3 = \frac{1}{2}a\hat{x} - \frac{1}{2\sqrt{3}}a\hat{y} + (\frac{1}{2}+u)c\hat{z} \quad (S)$$





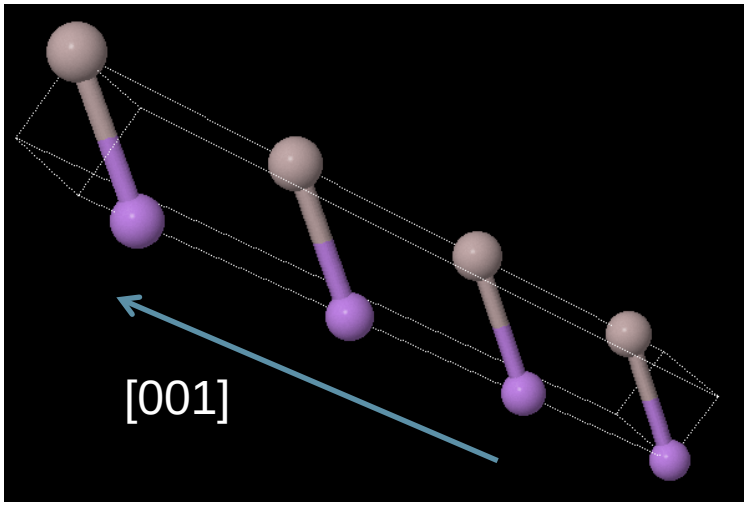


How is it done in NEMO5:

1) Define primitive vectors -> Bravais lattice
2) Define basis (atoms in 1 unit cells) -> crystal structure
3) Define bond radius -> connectivity
4) (optional) Define conventional Miller notation
   (e.g. in wurtzite: (0001) = (001) in the primitive basis)

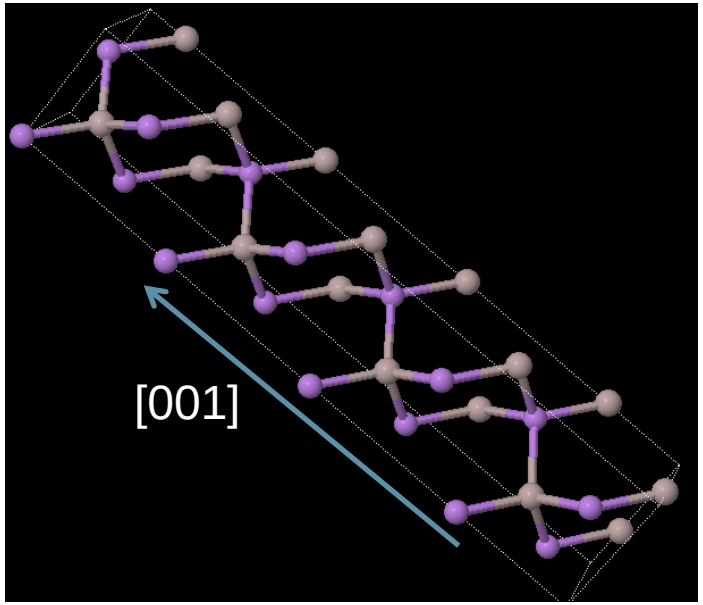
NEMO5: Primitive and conventional unit cells

Example: 4 unit cell zincblende material quantum well, [001] growth



The minimal elementary cell (2 atoms)

$\mathbf{b}_1$= [001] (growth direction)
$\mathbf{b}_2$ = [110]
$\mathbf{b}_3$ = [101]



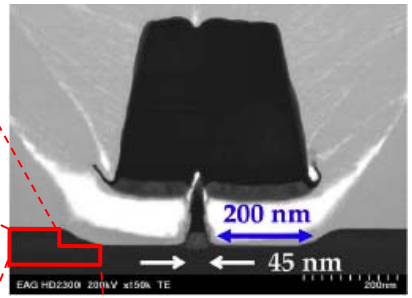
The typical conventional cell (8 atoms)

$\mathbf{b}_1$= [001] (growth direction)
$\mathbf{b}_2$ = [010]
$\mathbf{b}_3$ = [100]

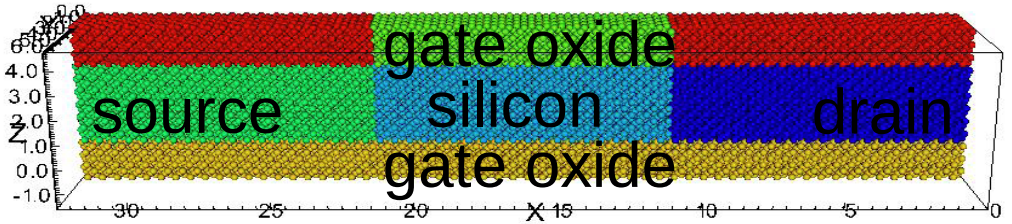
NEMO5 allows to define your conventional unit cell in inputdecks

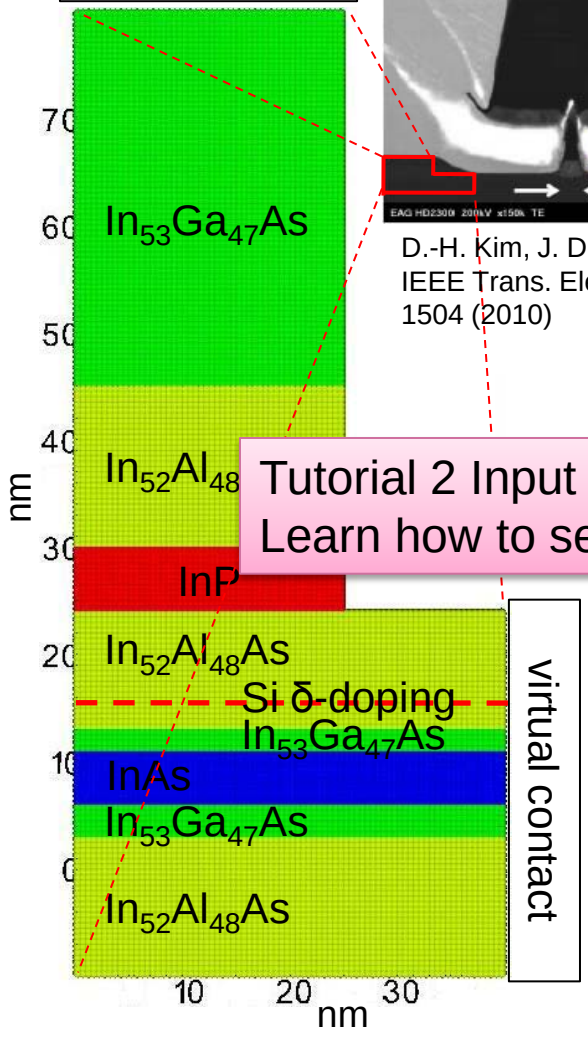
NEMO5: arbitrary geometries

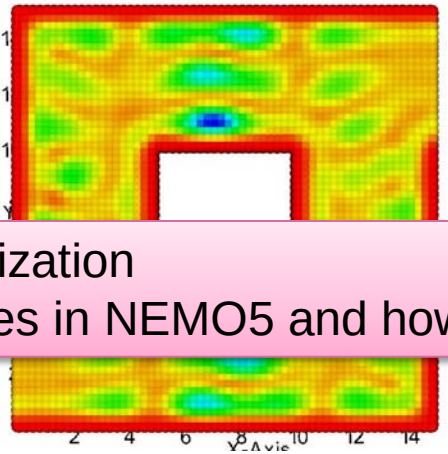
real contact

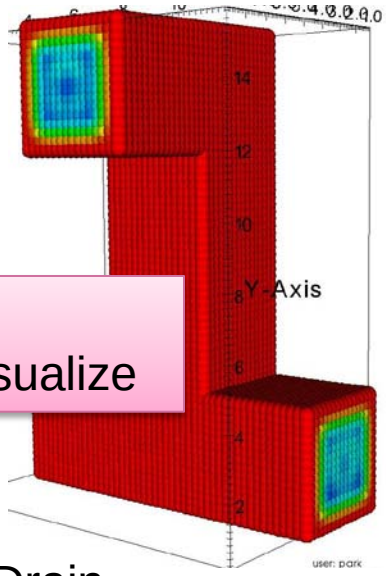


D.-H. Kim, J. D. A. del Alamo, IEEE Trans. Elec. Dev. 57, 1504 (2010)

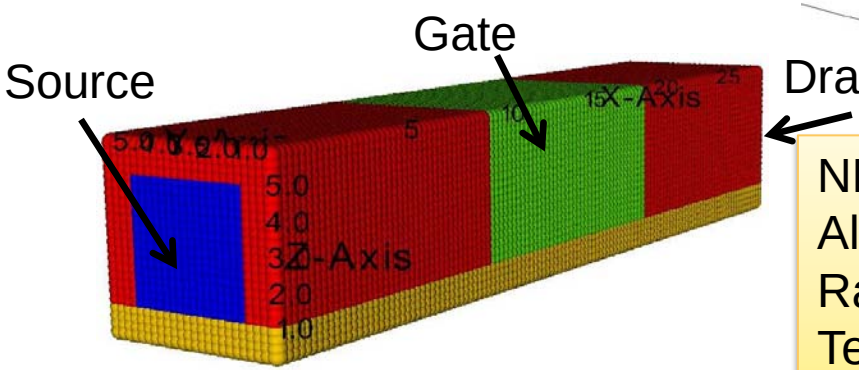








Tutorial 2 Input and Visualization
Learn how to set up devices in NEMO5 and how to visualize



NEMO5 also covers:
Alloy disorder
Random dopants
Ternary alloys

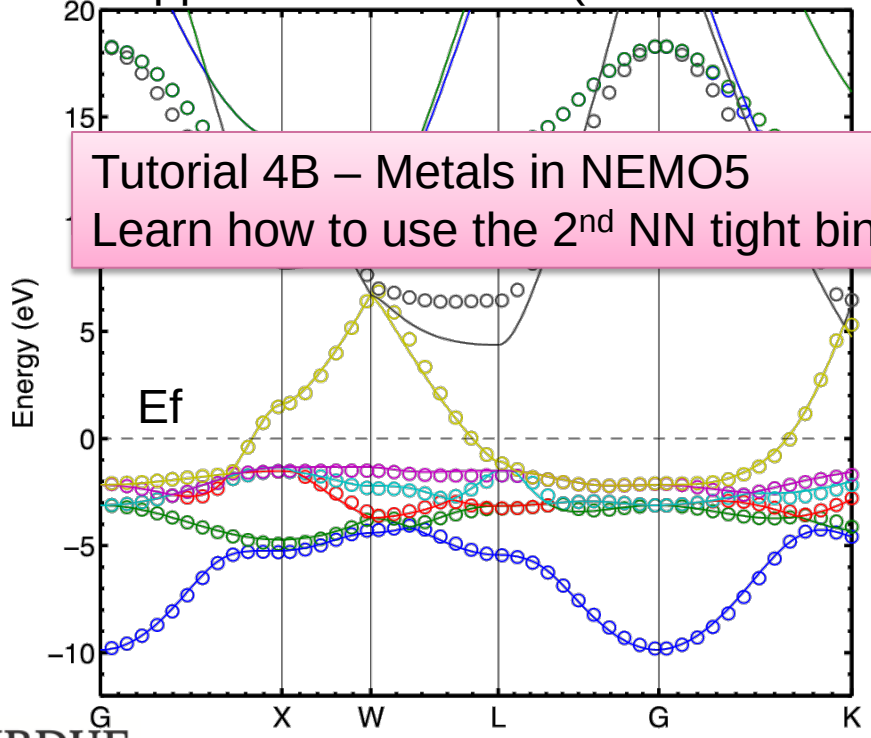
All models within NEMO5 can handle 1D, 2D, 3D and arbitrary geometries

Realistic contact material: Metals in NEMO5

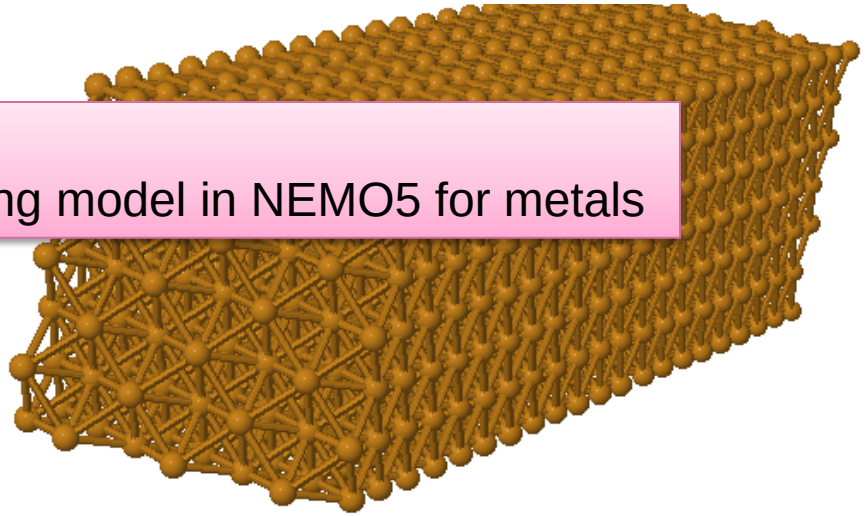
Challenges:
Shrinking semiconductor device dimensions enhance influence of metallic leads
Metals have long range interactions beyond standard 1st nearest neighbor tight binding models

NEMO5:
Extended neighbor interactions included
Bandstructure and transport in ideal metal structures verified (Cu, Ag, Au, Al, Pb)

FCC Copper bandstructure (DFT vs. NEMO5)



Cu nanowire in NEMO5



Tutorial 4B – Metals in NEMO5
Learn how to use the 2nd NN tight binding model in NEMO5 for metals

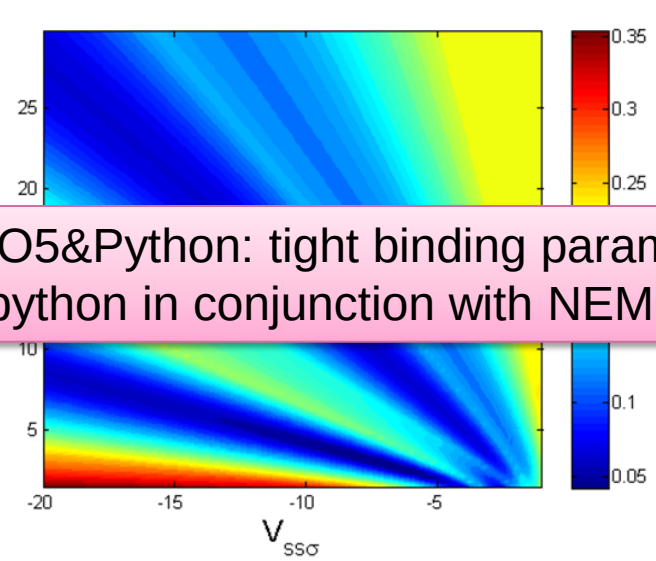
Lines: FP-LAPW- DFT*

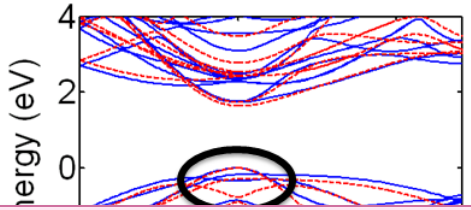
* Full Potential Linear Augmented Plane Wave Density Functional Theory

Circles: NEMO5 fitted to FP-LAPW-DFT

NEMO5: how to do parameter fitting

Results of Example





Band structure of Si UTB:
Blue lines: DFT results
Red lines: nemo5 results

100 different values for Vspσ_H_Si and Vssσ_H_Si → 10000 samples
DFT result is generated by ABINIT

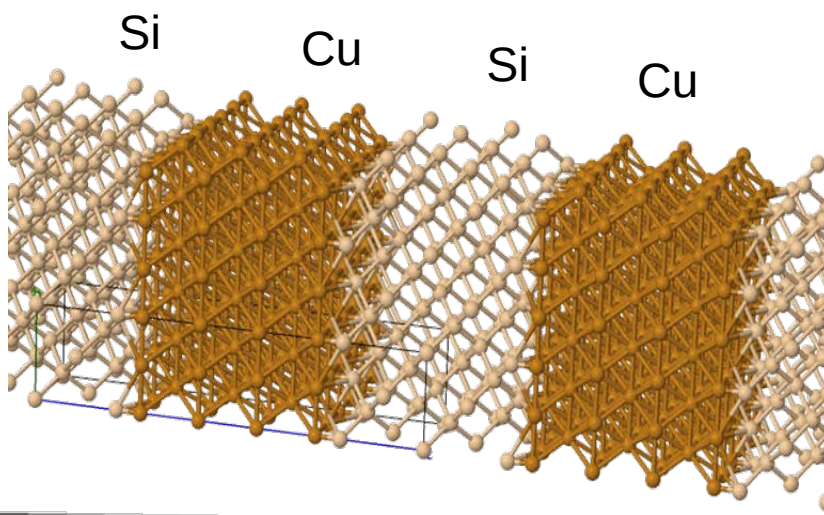
PURDUE UNIVERSITY

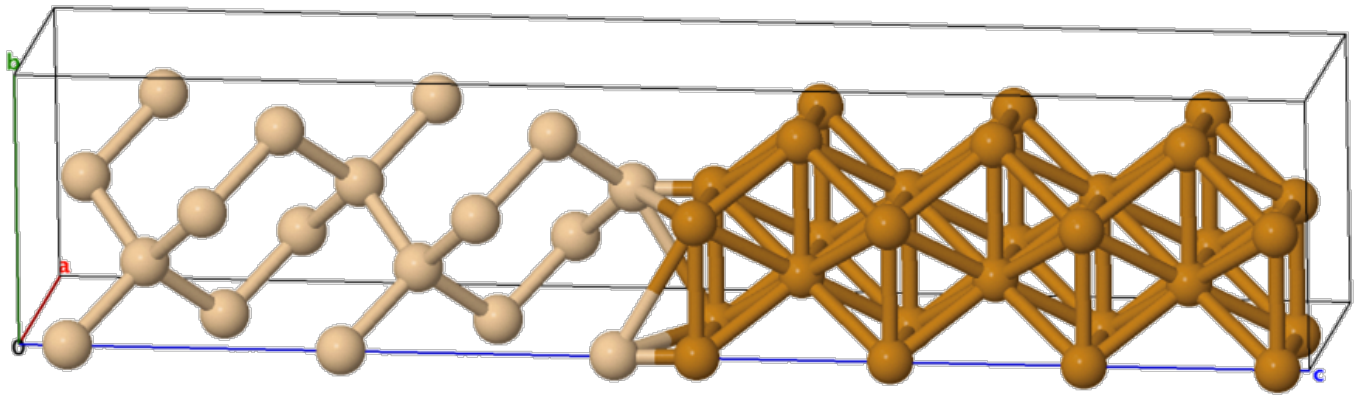
Tutorial 4D – NEMO5&Python: tight binding parameter fitting
Learn how to use python in conjunction with NEMO5 to fit tight binding parameters

Realistic interfaces: NEMO5 and external solvers

Challenges:
Metals have different crystal structures than typical semiconductors

NEMO5:
Pseudomorphic interfaces available
Read in incommensurate heterostructures from external simulators possible (e.g. Reaxff)





Large strain on the surface might require sophisticated molecular dynamics calculations – NEMO5 is compatible to that

Many materials require a sophisticated database

Semiconductor research spans over a huge variety of materials
Simulators have to provide a database that is…

- Universal: many different parameter sets (bandgap, effective mass, strain constants, TB constants…
- General: allow different parameters given by different authors
- Flexible: expandable to cover new parameter sets (for new models,…)
- Editable: easy to read and edit (avoid “getting lost”, no double entries,…)

NEMO5 database:
One ascii file; default: NEMO/prototype/materials/all.mat
Directly editable via inputdecks (convenient for test purposes)

```
#SO_P_Ge       = 0.20264;
#SO_D_Ge       = 0;
V_S_P_Sigma_Ge_Ge = 2.73135;
V_P_D_Sigma_Ge_Ge = -2.00115;
V_Sstar_P_Sigma_Ge_Ge = 2.68638;
V_S_D_Sigma_Ge_Ge = -2.64779;
V_P_D_Pi_Ge_Ge  = 2.10953;
V_Sstar_D_Sigma_Ge_Ge = -1.12312;
V_S_S_Sigma_Ge_Ge = -1.39456;
V_Sstar_S_Sigma_Ge_Ge = -2.0183;
V_S_Sstar_Sigma_Ge_Ge = -2.0183;
V_Sstar_Sstar_Sigma_Ge_Ge = -3.5668;
V_P_P_Sigma_Ge_Ge = 4.28921;
```

Many materials require a sophisticated database

Joseph Weinbub (http://www.iue.tuwien.ac.at/pdf/ib_2010/CP2010_Weinbub_1.pdf) (ViennaIPD):
"Applications for scientific computing require a powerful control language to satisfy the need of control parameters, e.g. material properties, models to take into account, model parameters, process definitions, simulation modes, iteration schemes, and numerical behavior. **As a result, control files grow in size, which results in decreased maintainability.**
Therefore a powerful control language has been developed …" *
(* 2010 ViennaIPD - An Input Control Language for Scientific Computing, Josef Weinbub, Karl Rupp, Siegfried Selberherr, Institute for Microelectronics, Technische Universität Wien)

NEMO5 database:
Capable to handle formulas (control language developed)

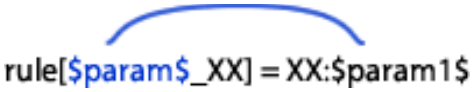
Snapshot of all.mat: Simple example for a database formula

```
Ec       = Ec_X + VBO;
Ec_ref   = "definition";
Eg       = Ec-Ev;
Eg_ref   = "def: Eg = Ec - Ev";

mstar_c_dos = (ml_X*mt_X^2)^(1.0/3.0)*(6.0^(2.0/3.0));
mstar_v_dos = (ml_X*mt_X^2)^(1.0/3.0)*(6.0^(2.0/3.0));

# heavy holes
Ev_hh = 0.0;
ml_hh = 0.49;
```

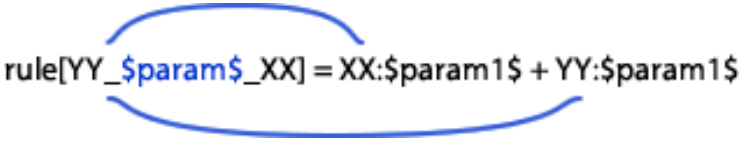
NEMO5: Database Rules

NEMO5 database:
Sophisticated formulas/rules are supported

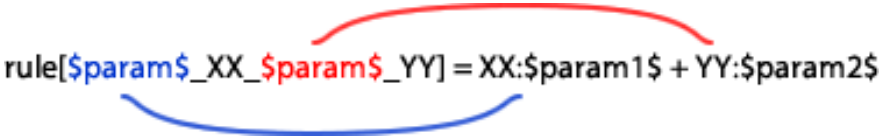
NEMO/prototype/tests/test_database_regex_nemo/DatabaseTutorial.pdf



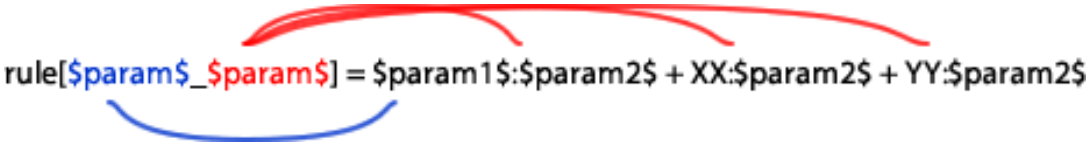
Basic Parameters



Complex Parameter



Multiple Parameters



Multiple Complex Parameters

Si:Bands:TB:sp3d5sstar_SO:param_Boykin (all.mat)

```
rule[$param$_SiGe_Si] = 0.5 * SiGe:Bands:TB:sp3d5sstar_SO:param_Boykin:$param1$_SiGe_SiGe + 0.5 * Si:Bands:TB:sp3d5sstar_
rule[$param$_SiGe_Ge] = 0.5 * SiGe:Bands:TB:sp3d5sstar_SO:param_Boykin:$param1$_SiGe_SiGe + 0.5 * Ge:Bands:TB:sp3d5ssta
rule[$param$_Si_Ge] = SiGe:Bands:TB:sp3d5sstar_SO:param_unknown:$param1$_Si_Ge;
rule[$param$_Ge_Si] = SiGe:Bands:TB:sp3d5sstar_SO:param_unknown:$param1$_Ge_Si;
```

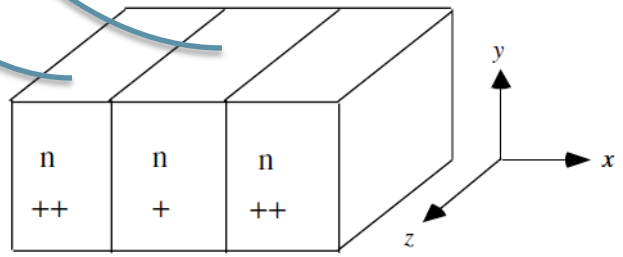
NEMO5: Database Multiple Views

NEMO/prototype/examples/Transport/TEST/datta.in

```
Material
{
  tag                          = n
  name                         = Si
  Lattice:a_lattice            = 0.3
  …
  doping_type                  = N
  doping_density               = 1e20
}
Material
{
  tag                          = nplus
  name                         = Si
  Lattice:a_lattice            = 0.3
  …
  doping_type                  = N
  doping_density               = 5e19
}
```

Original image from: http://www.imvis-eu.org/

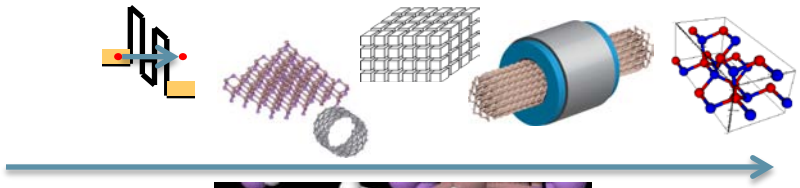
NEMO5 allows to use materials as templates
Change material parameters in the inputdeck to design your own material



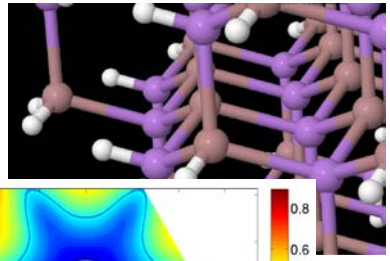
Original image from: Datta, Superlatt. and Microstruct. **28**, 253 (2000)

NEMO5 lecture - overview

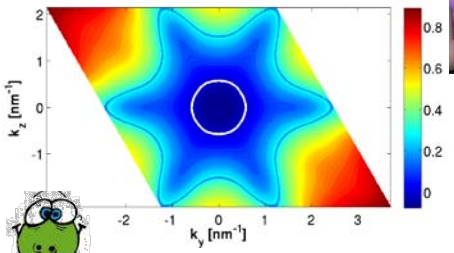
NEMO5 origins + history



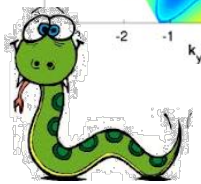
NEMO5 and atomic representations



NEMO5 solvers + physics



NEMO5 expandability + flexibility



NEMO5 on supercomputers (scalability and compatibility)

NEMO5 support (for output and users)

Challenge: various physics involved

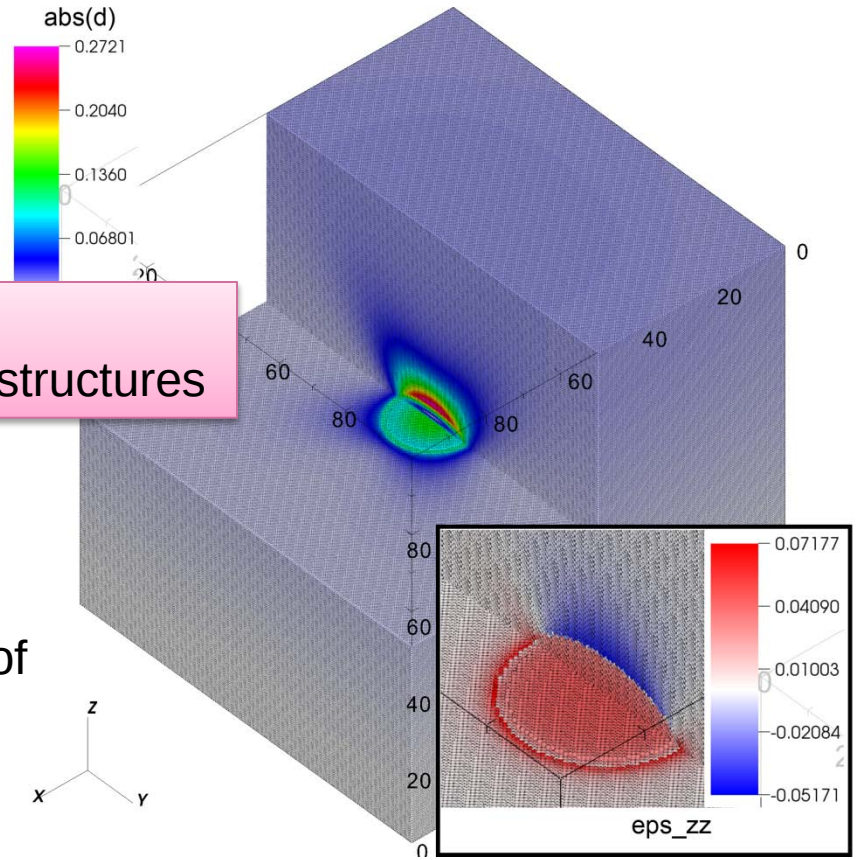
Original question “What happens in that device?” yields lots of follow-up questions:

- What is the atomic structure?
  Heterostructures are usually lattice mismatched (strained)
- What are the electron and phonon states?
  Devices often produce confinement and interference effects (sophisticated bandstructures)
- How are the electrons distributed?
  Doping and charge distribution require solutions of the electrostatics
- How reliable are the device properties?
  Imperfect device growth, randomness and finite temperature deteriorate the ideal device performance
- How large will be the current density for a given gate and supply voltage?
  Concrete transport properties depend on all other questions

NEMO5: strain in nanostructures

- Atomistic description using valence force field (VFF) method
- Structure relaxation by minimizing an energy functional that depends on bond angles and bond lengths
- Various models for energy functional available

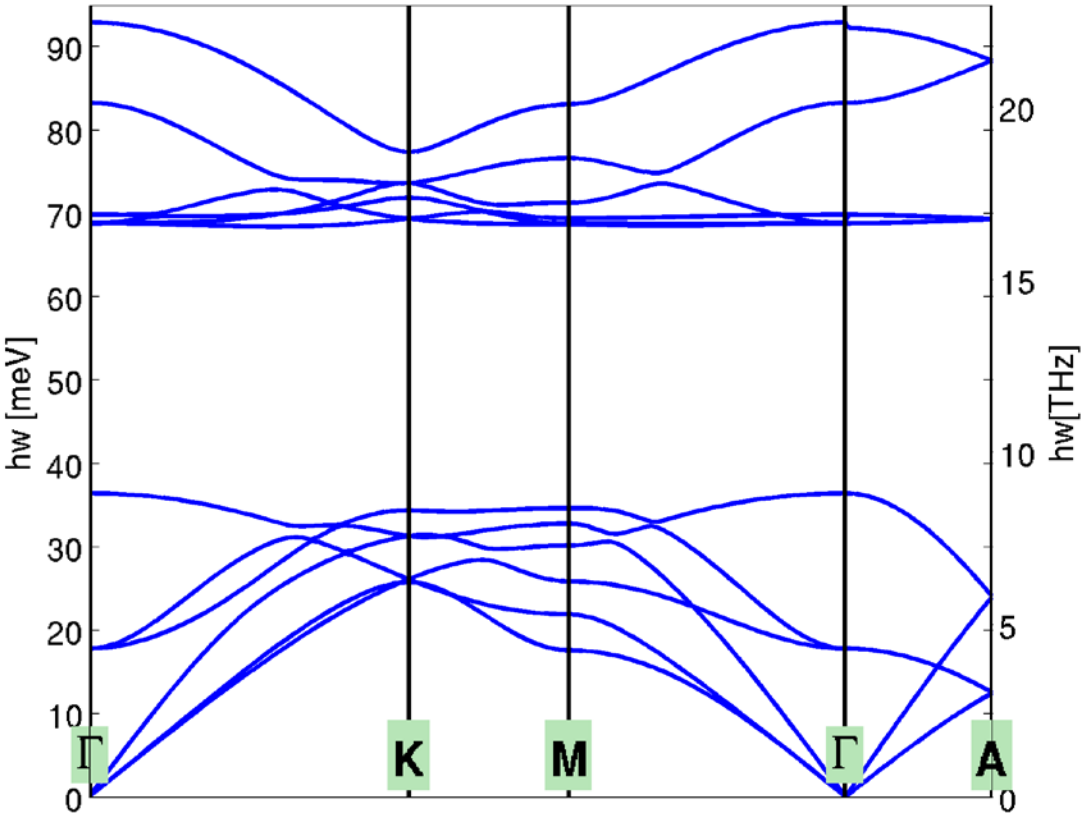
Tutorial 5B Strain in NEMO5
Learn how to use NEMO5 to relax heterostructures



displacement vector and zz-component of strain tensor in a InAs lens-shaped quantum dot (~50 million InAs atoms)

NEMO5: phonon modes

- Same physical model as strain relaxation
- Hessian of energy functional is reused as dynamical matrix

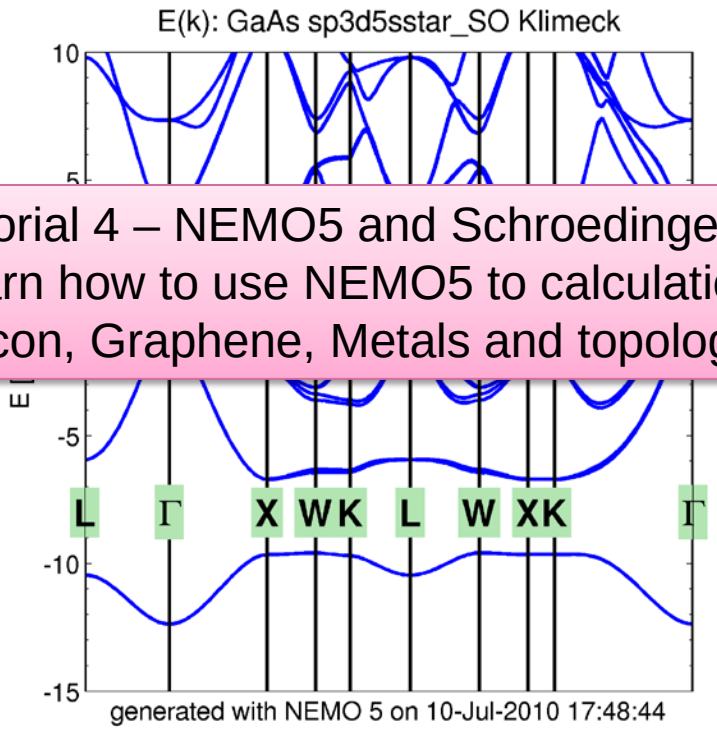


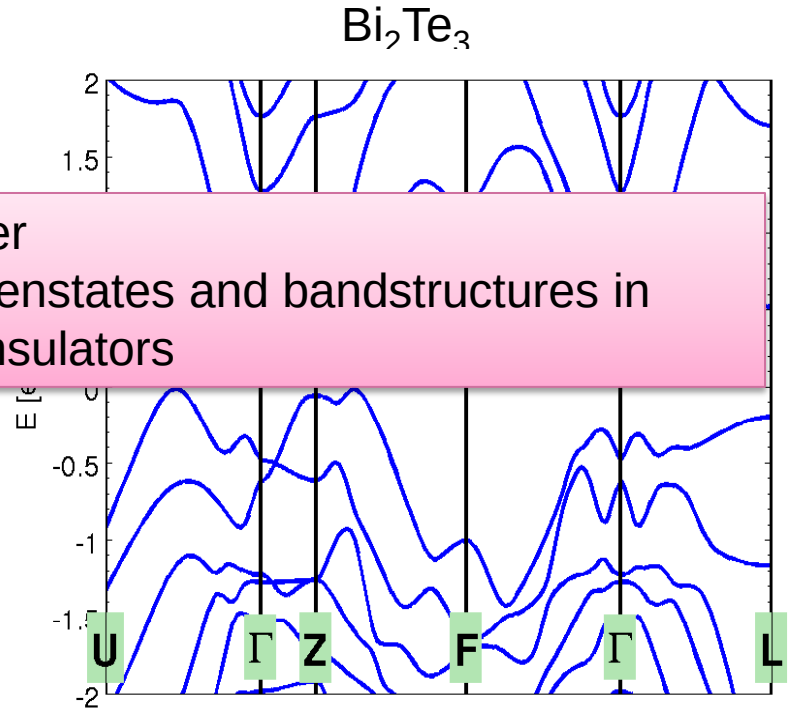
Bulk phonon dispersion for GaN in wurtzite phase

calculated using Keating VFF model + Coulomb interaction

NEMO5: electronic band structures

- Any nearest-neighbor tight-binding model available (s,p,d,f,g,…)
- Any Nth nearest-neighbor tight-binding model possible (2nd nearest neighbor TB used for metals)
- Many parametersets included in the database

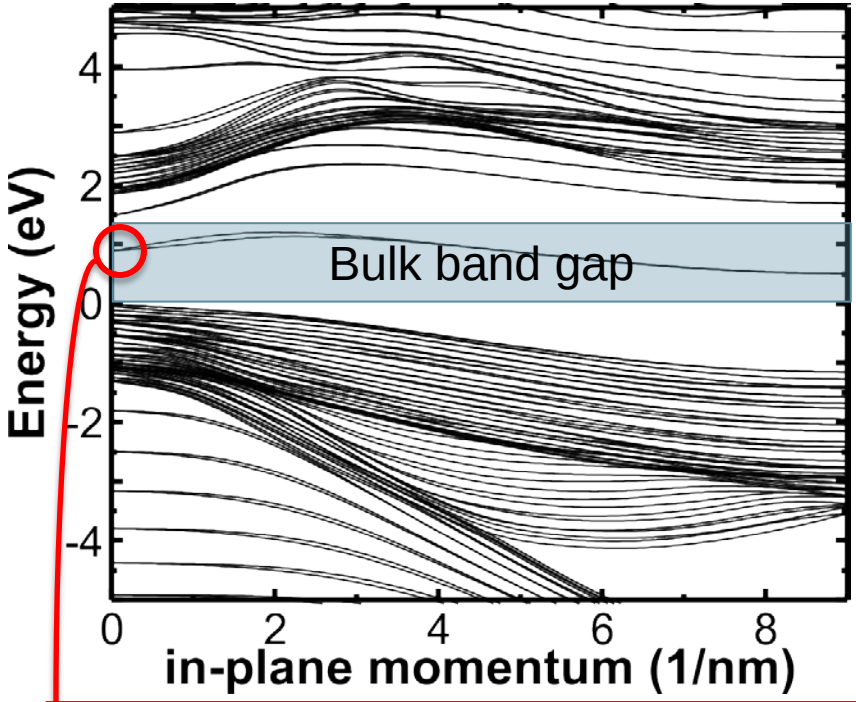




Tutorial 4 – NEMO5 and Schroedinger solver
Learn how to use NEMO5 to calculation eigenstates and bandstructures in Silicon, Graphene, Metals and topological insulators

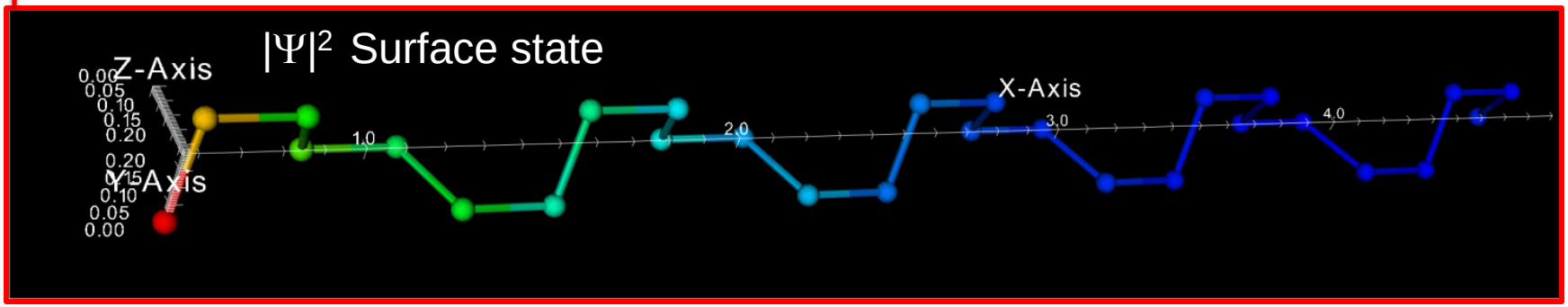
NEMO5: heterostructure band structures

In-plane [111] GaAs quantum well bandstructure



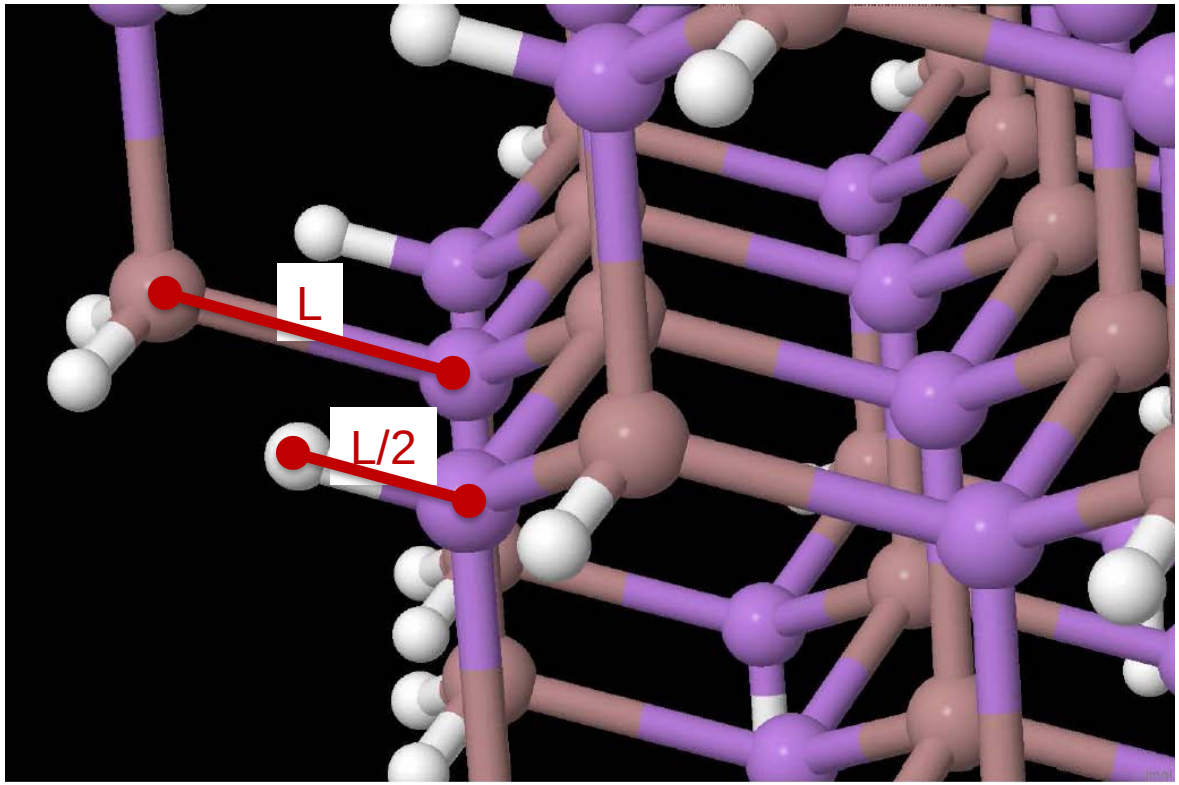
Dangling bonds result in surface states
Without further treatment:
Surface states lie within interesting energy intervals (such as band gap)

In reality:
Surface passivation or surface reconstruction shifts surface states out of relevant energy range



NEMO5: Passivation of surfaces

During device construction:
Hydrogen atoms are added half way to the next (missing) semiconductor atom
Only bonding direction is relevant for the passivation model

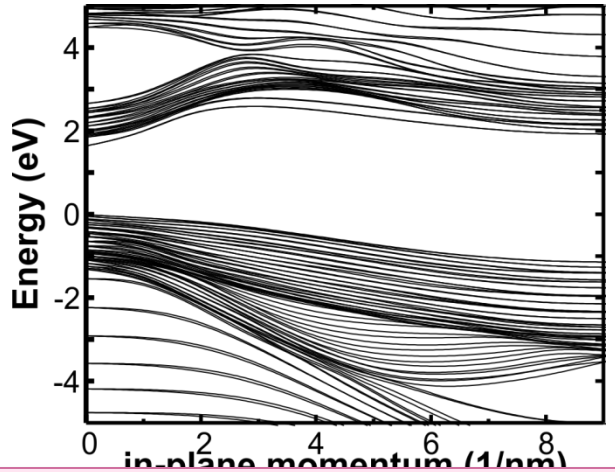


General and fast:

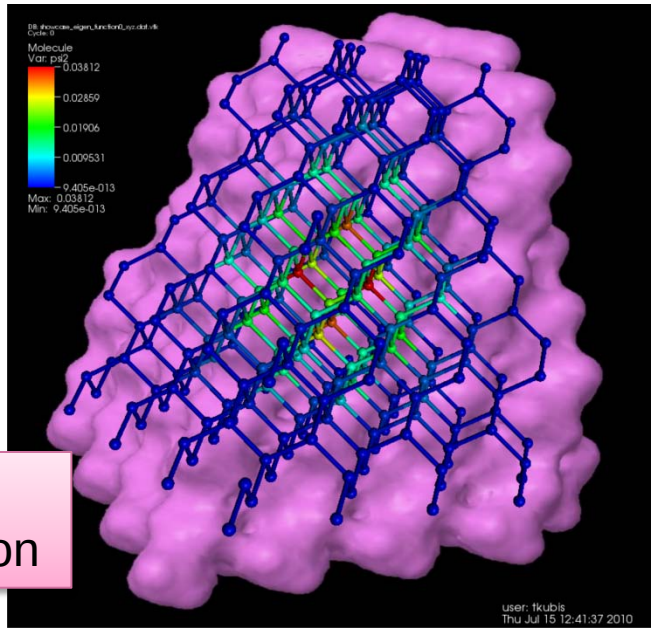
- Allows any kind of surface
- No transformation required (surface hybridization is given automatically)

NEMO5: Passivation of general surfaces

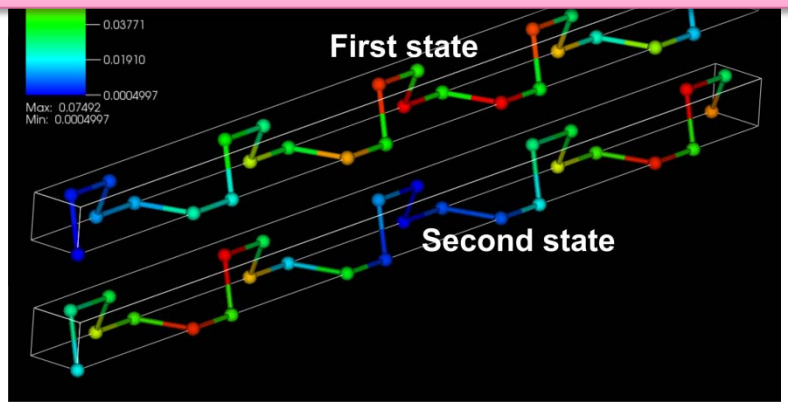
- GaAs [111] quantum well



- GaAs quantum dot



Tutorial 4D – Graphene in NEMO5
Learn how to correctly set up NEMO5 for passivation

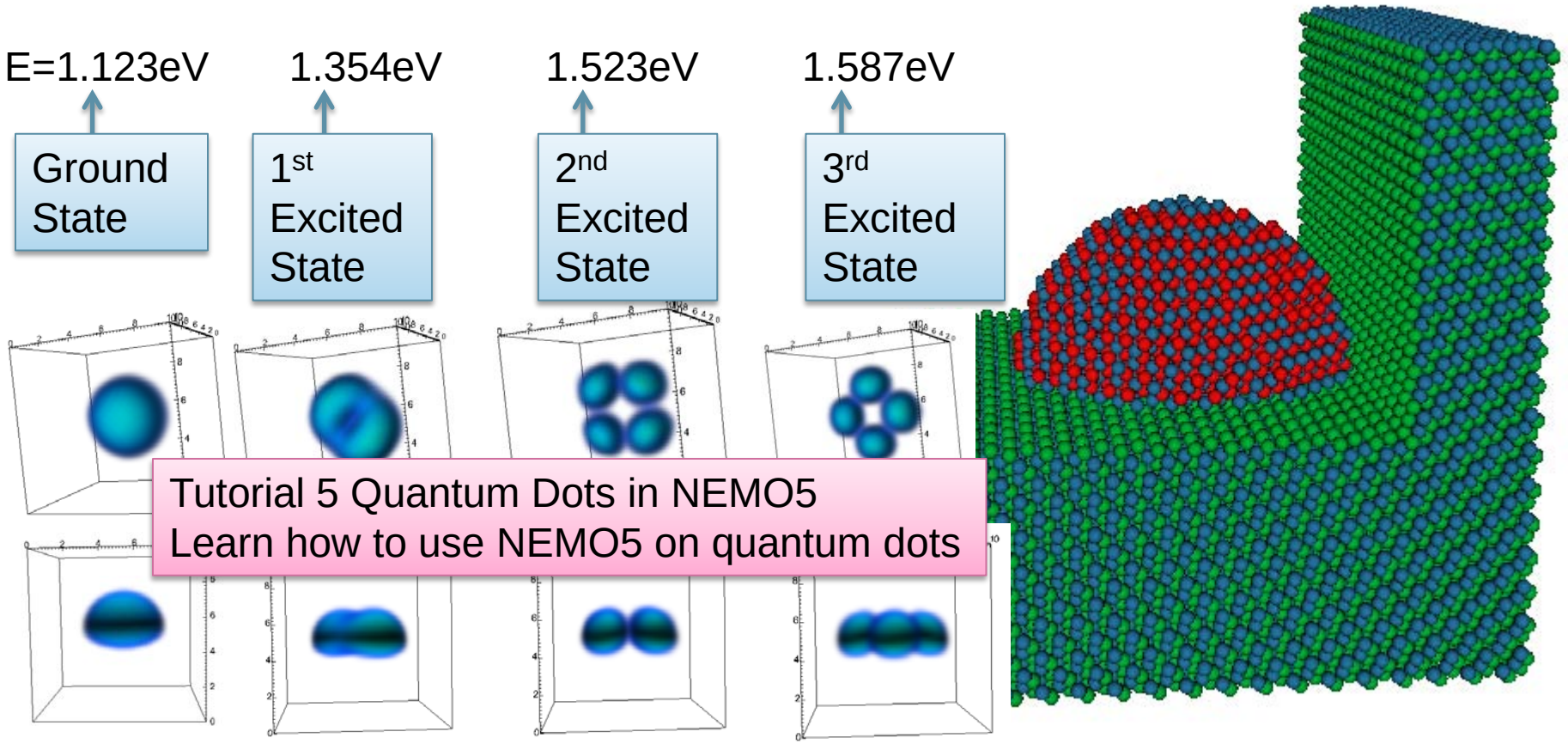


Important: **Surface passivation**

NEMO 5 has general passivation scheme

NEMO5: wave functions in quantum dots

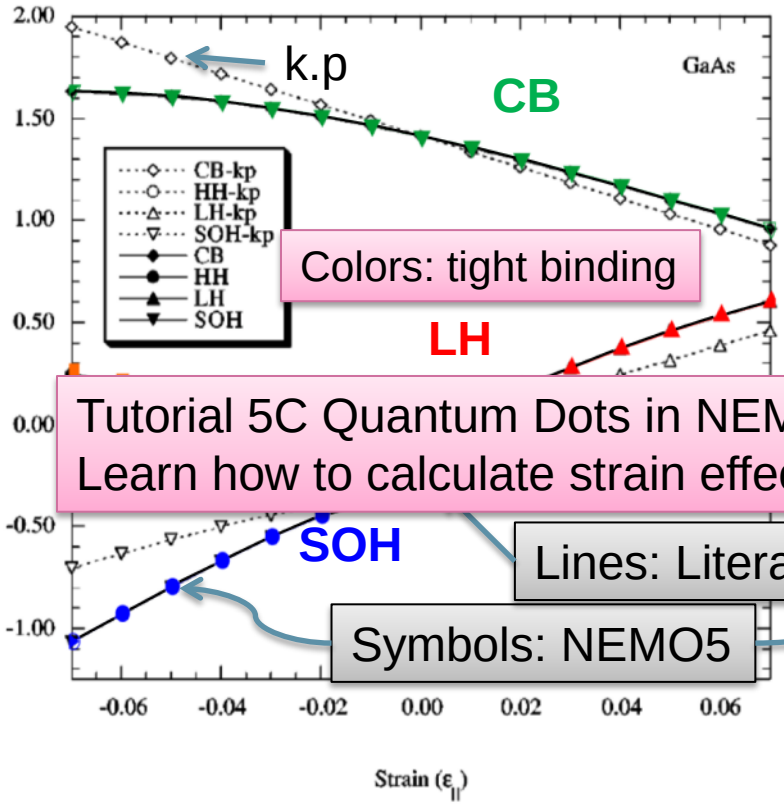
NEMO5: InAs quantum dot embedded in GaAs



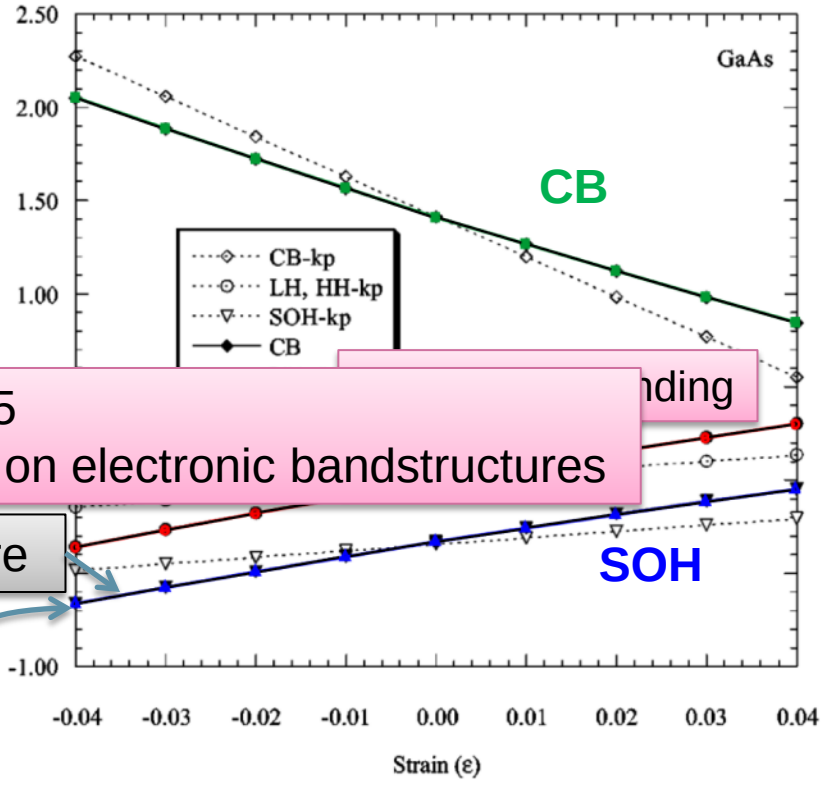
Tutorial 5 Quantum Dots in NEMO5
Learn how to use NEMO5 on quantum dots

NEMO5: strain corrections to tight-binding

Biaxial strain



Hydrostatic strain



Tutorial 5C Quantum Dots in NEMO5
Learn how to calculate strain effects on electronic bandstructures

Lines: Literature

Symbols: NEMO5

- ✓ External strain definable in input deck (via full epsilon matrix)
- ✓ Strain in TB according to Boykin et al. 2002 implemented and tested
- ✓ Strain in TB according to Boykin et al. 2010 implemented, and tested

Exact agreement with published data

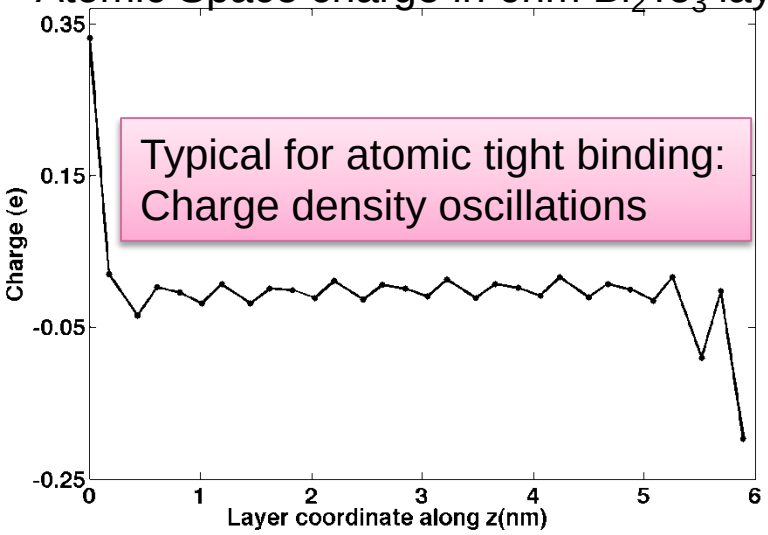
NEMO5: 2 different charge models

Motivation:
Most semiconductor devices allow to distinguish electrons from holes
but
Broken-gap nanodevices and topological insulators have no band gap and do not allow to distinguish

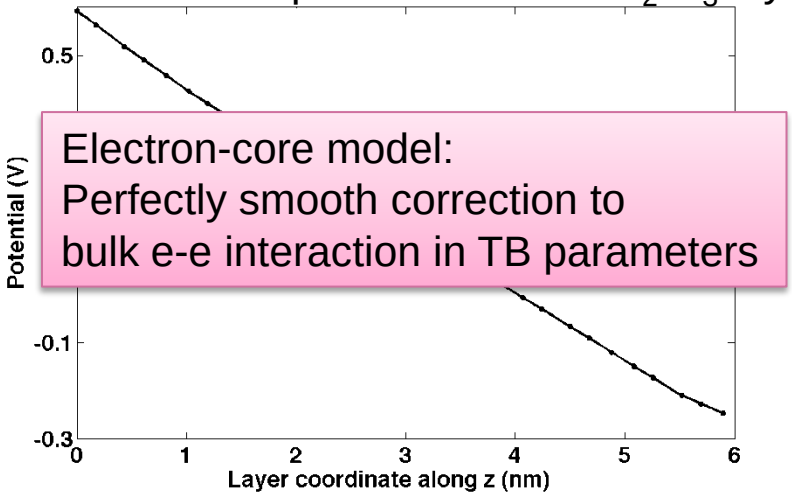
NEMO5:
- Charge self-consistent tight-binding Schrödinger/Poisson
- Standard electron-hole model
- Novel "electron-core" model: All states are electronic
- Every atom core contains intrinsic ion charge (parameterization and material dependent)

Results of electron-core model:
Self-consistent Poisson potential = smooth correction to empirical TB Hamiltonian

Atomic Space charge in 6nm Bi_2Te_3 layer



Atomic Poisson potential in 6nm Bi_2Te_3 layer



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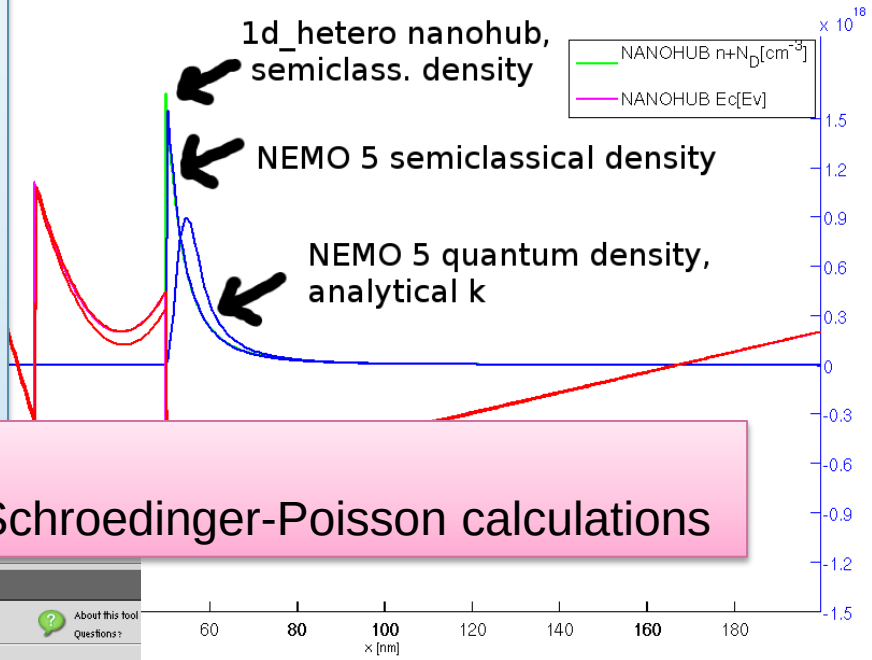
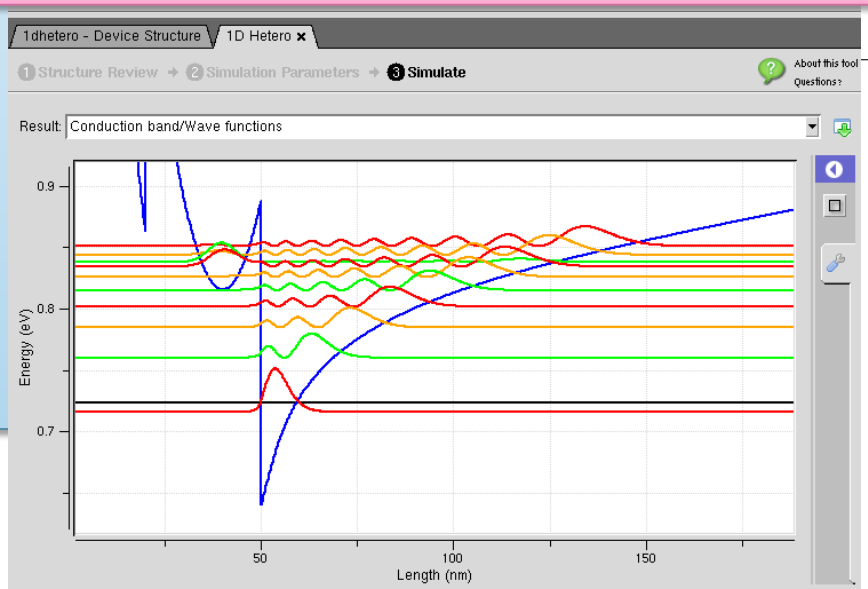
NEMO5: Schrödinger-Poisson calculations

Electron-hole example of 1d_hetero nanohub tool

- » semiclassical density
- » quantum density, numerical k-space
- » quantum density, analytical k-space (assuming a parabolic dispersion)



Tutorial 4A Topological Insulators
Learn how to use NEMO5 to perform Schroedinger-Poisson calculations



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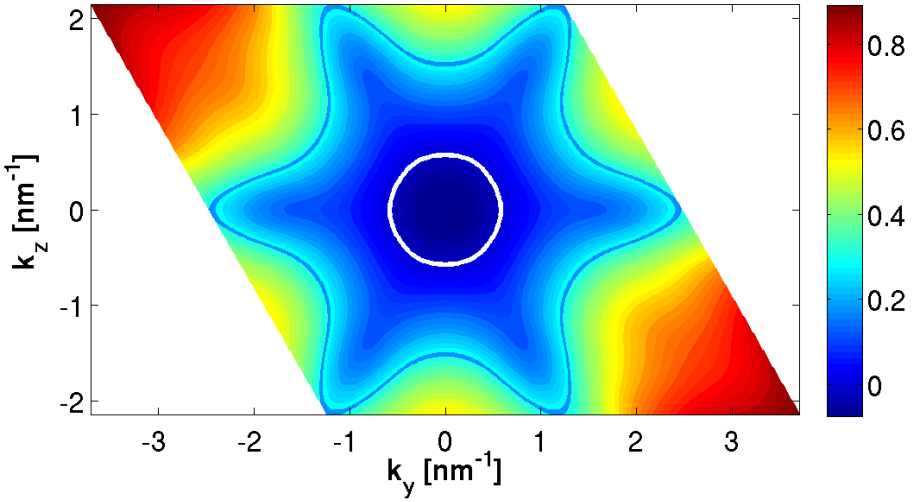
Topological insulators in NEMO5

Motivation:
Unique transport features of topological insulators (ballistic surface transport expected)
Question: surface conductance tunable?

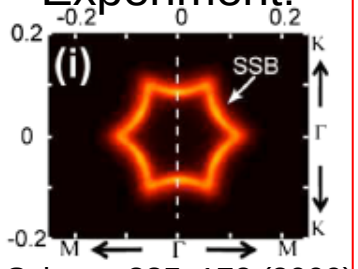
Method :
Charge self-consistent tight-binding (sp3d5s*) Schrödinger/Poisson (electron-core model)
Spin analysis and scattering rates

Results:
Agreement with experiment:
- ✓warping of Fermi surface
- ✓spin polarized surface states
- ✓Dirac hyperbolas in thin Bi_2Te_3 layers

NEMO5: Warping of the Fermi surface



Experiment:



Science **325**, 178 (2009)

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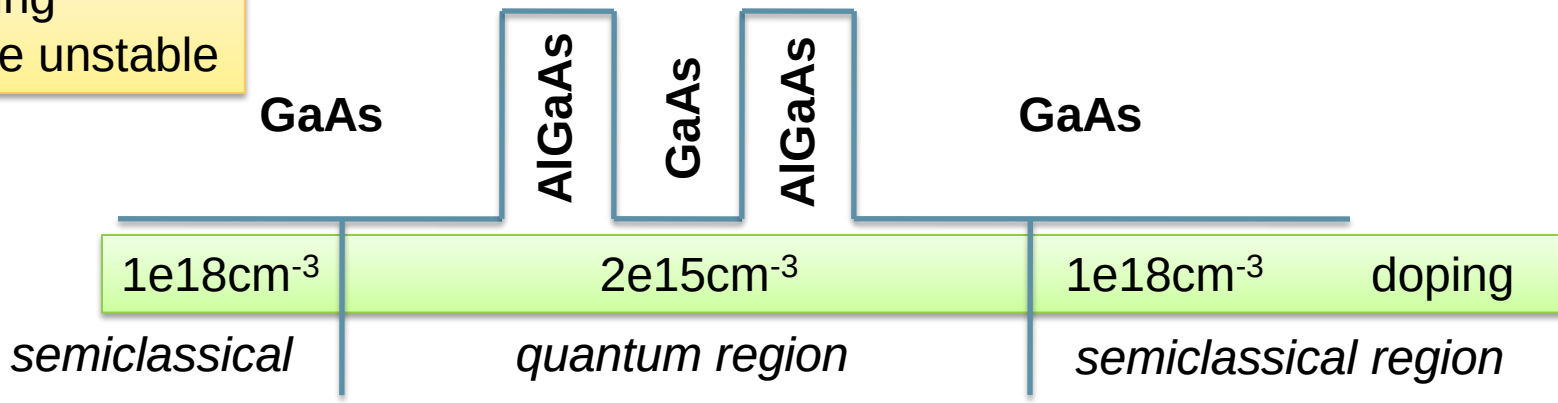
Transport capabilities of NEMO5

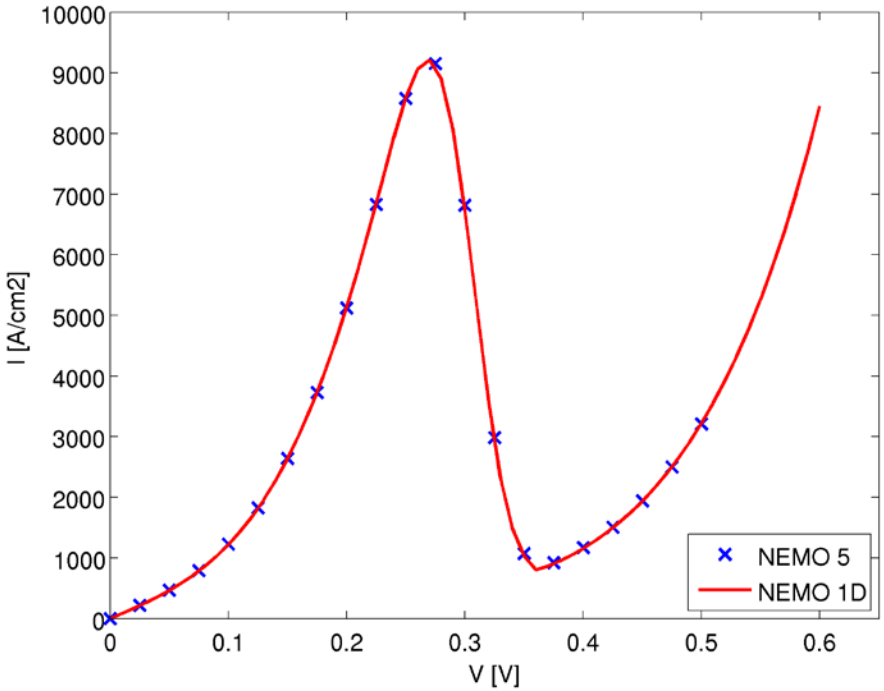
- **Quantum transport models**
  - Nonequilibrium Green's function (NEGF) formalism
  - Open-boundary transfer matrix method ("wavefunction" formalism)
  - Top of the barrier transport model
- **Various physical models**
  - Ohmic and Schottky contacts
  - Simple and fast phonon scattering model
  - *Strain under test*
  - *Magnetic field under test*
- **General simulation structures**
  - 1D, 2D, 3D structures
  - Heterostructures, arbitrary shapes, multiple contacts
- **4-level MPI parallelization**
  - bias, energy, momentum, space
- **Quantum and semi-classical hybrid simulation**

NEMO5: Transport in layered Structures

NEGF calculations:
- time consuming
- can be charge unstable

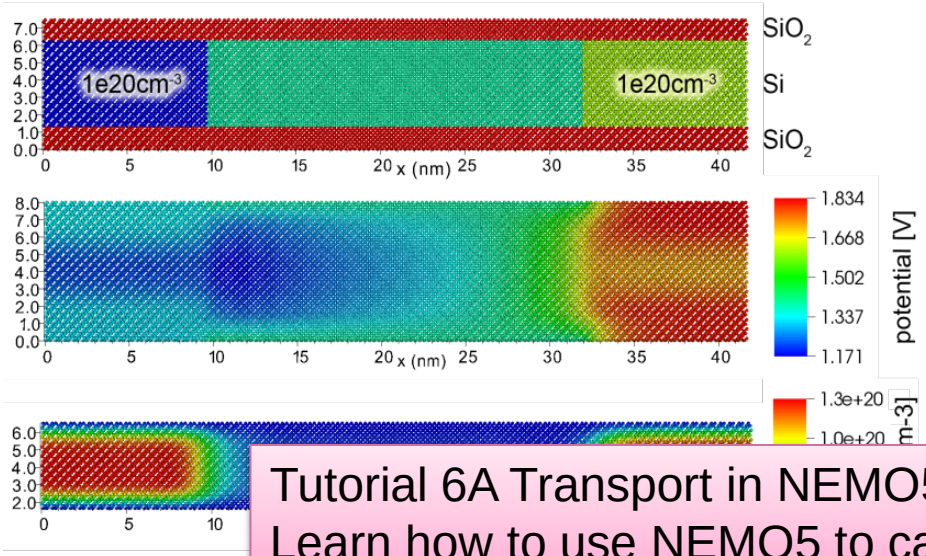


NEMO5: User may…
- limit quantum region to relevant device regions
- apply approximations to other device regions

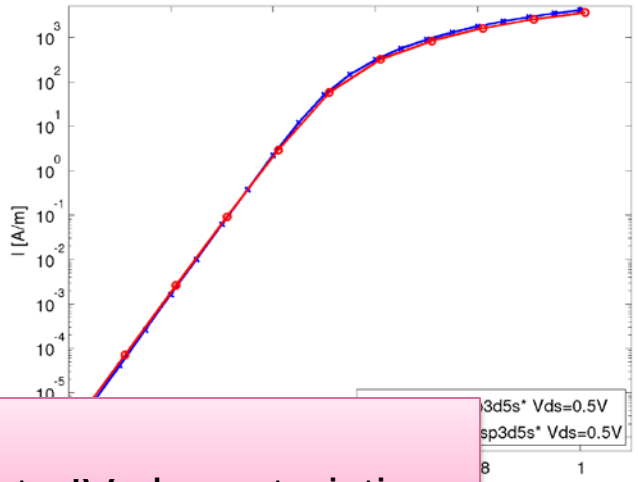


NEMO5: Transport in Nonplanar Structures

Potential and density in ultra thin body

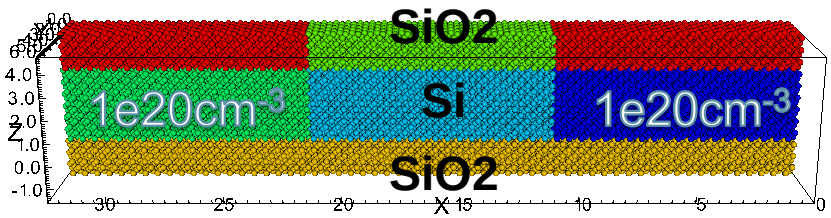


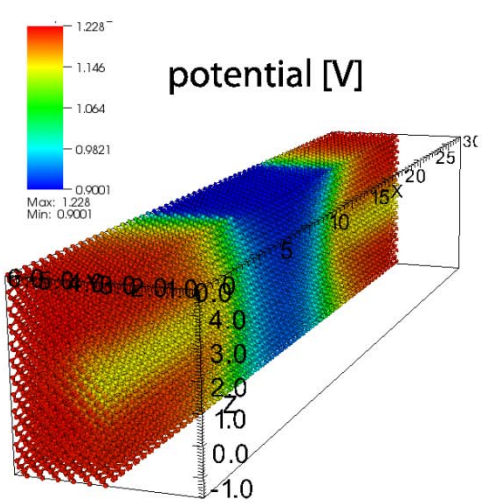
IV-characteristics of ultra thin body

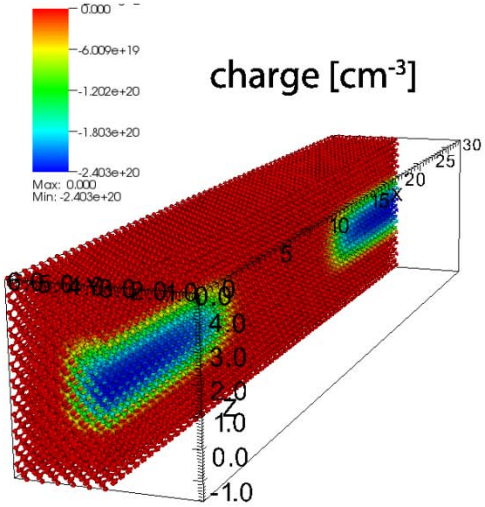


Tutorial 6A Transport in NEMO5
Learn how to use NEMO5 to calculate IV characteristics

Potential and density in nanowires







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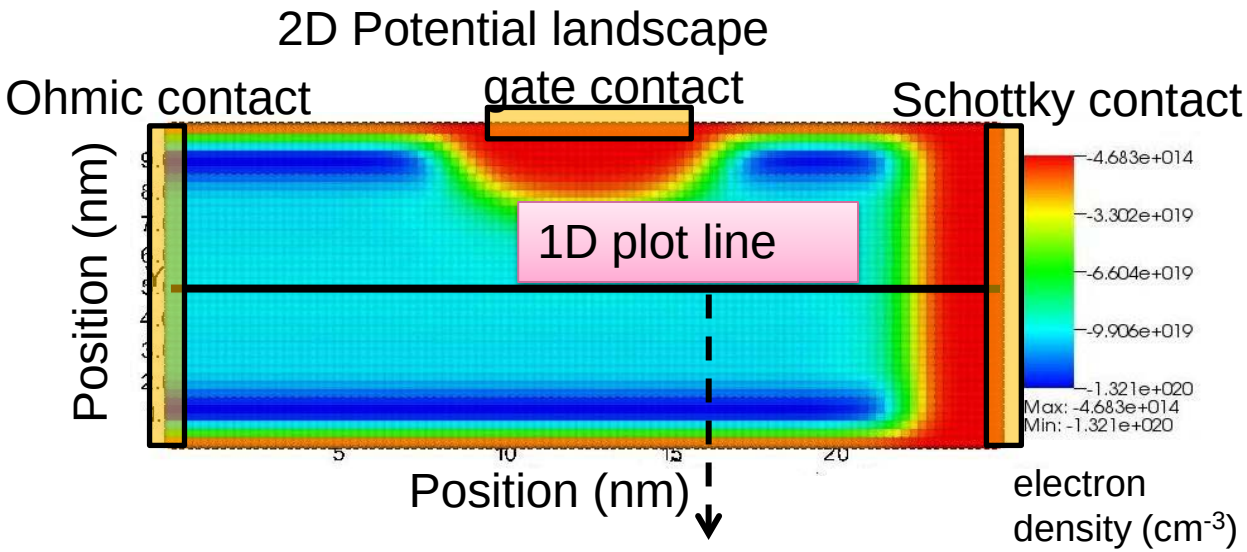
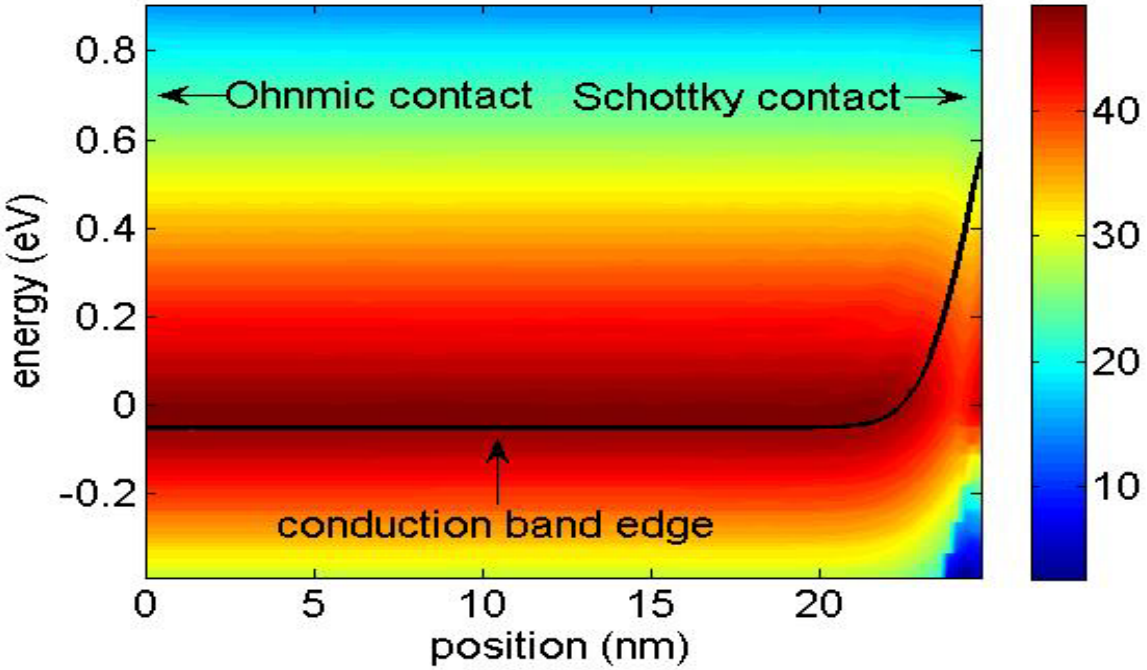
NEMO5: Multidimensional graphs



Silicon n-type UTB
$n = 10^{20}/cm^3$
V_{source} = 0 V (Schottky)
V_{drain} = 0 V (Ohmic)
V_{gate} = 0.5 V (Gate)

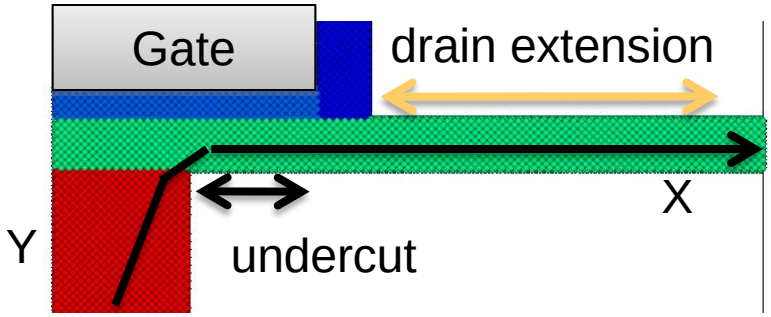
Charge self-consistent simulation with phonon scattering

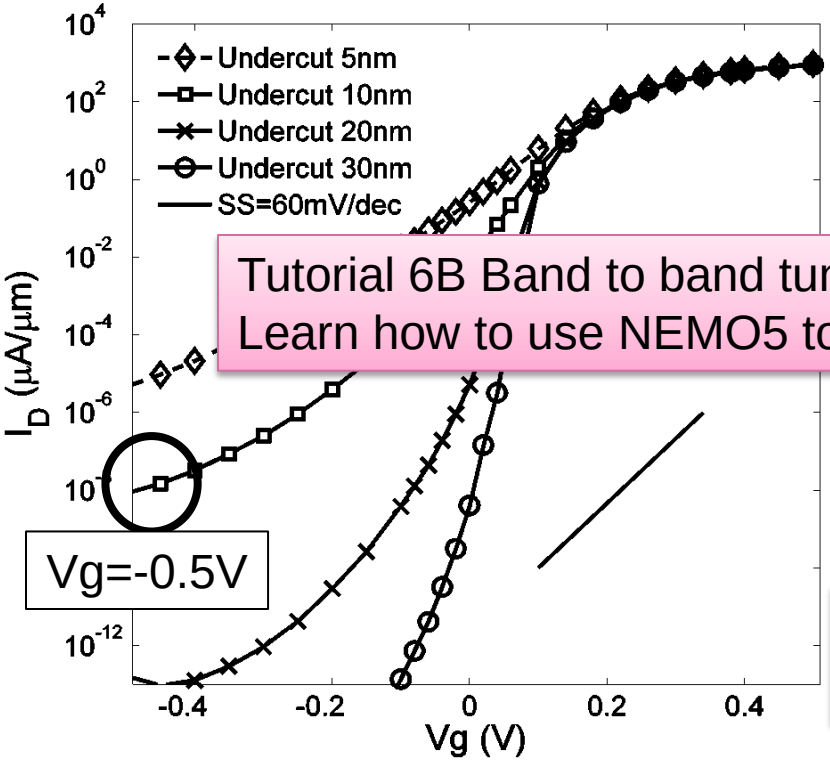


Devices with different types of contacts
3D, 2D, and 1D output along a line

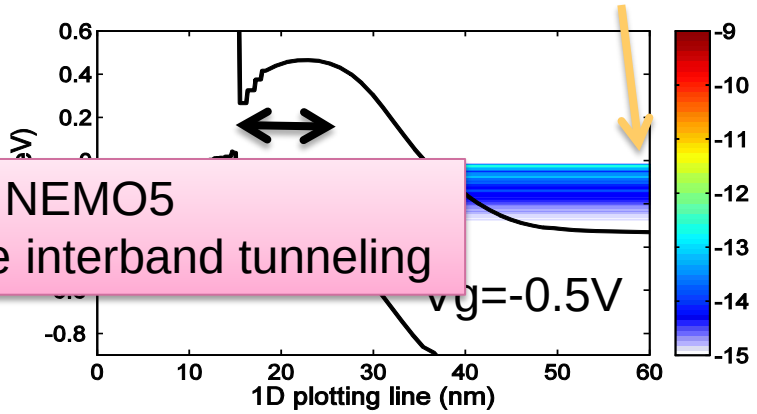
NEMO5: tunneling field effect transistor

NEMO5:
Transport in band-to-band tunneling devices
Geometry affects the device performance





Energy and spatially resolved current



Tutorial 6B Band to band tunneling in NEMO5
Learn how to use NEMO5 to calculate interband tunneling

Tunneling between valence and conduction band tunable via gate geometry

NEMO5: features for transport

Electron models: effective mass, 1st and 2nd NN tight binding

Inhomogeneous, self adaptive energy grid

Simplified inelastic scattering on phonons

Under testing:

Transport in strained systems

Nonlocal inelastic scattering

LRA method (efficiency improvement)

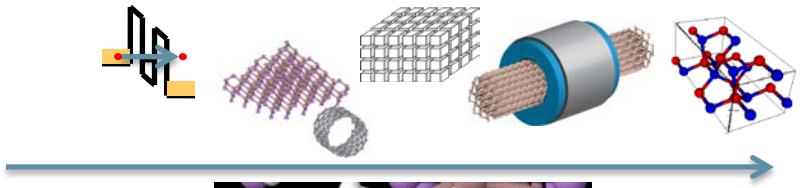
Under development/implementation:

Spatial parallelization perpendicular to transport

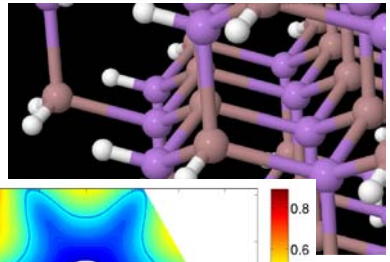
Phonon transport

NEMO5 lecture - overview

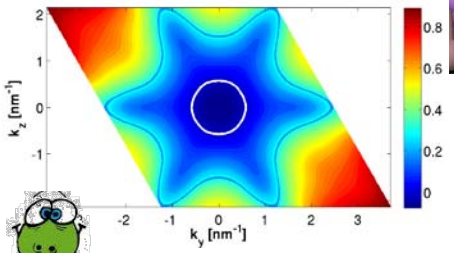
NEMO5 origins + history



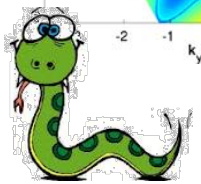
NEMO5 and atomic representations



NEMO5 solvers + physics



NEMO5 expandability + flexibility



NEMO5 on supercomputers (scalability and compatibility)

NEMO5 support (for output and users)

NEMO5 – an expandable code library

"What if I want to implement my own model?"

NEMO5 supports & welcomes that!

Object oriented C++ code:

Encapsulation

Write code without interfering with the rest of NEMO5

Polymorphism & Abstraction

Most NEMO5 code is flexible and handles also new models

Avoid rewriting code "just" because of a new model/crystal structure

Inheritance

NEMO5 code is written efficiently avoiding "copy&paste"

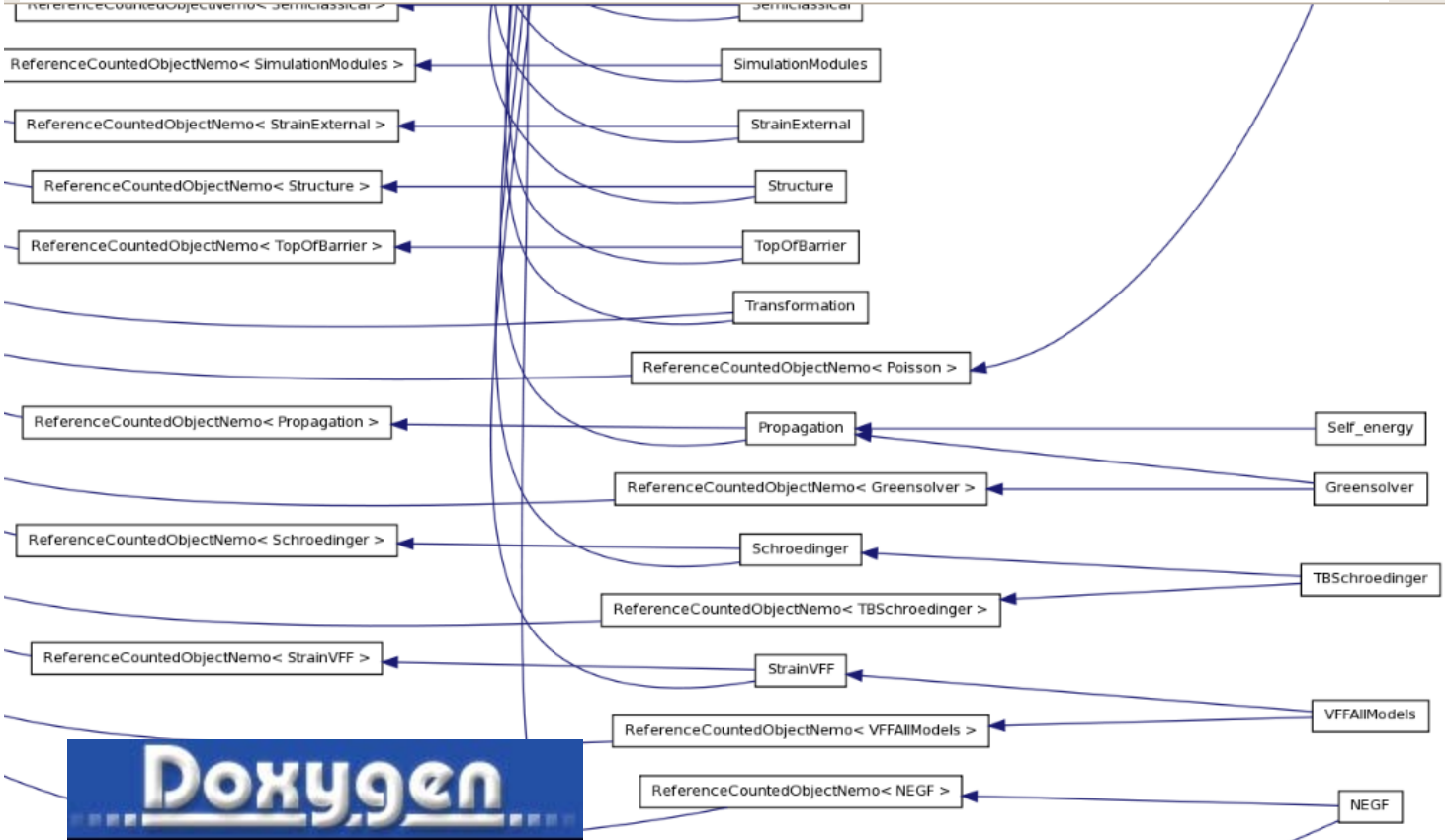
Zhengping Jiang (Graduate student of Klimeck group):
"Learning NEMO5, implementing and testing a new Hamiltonian took me 2 weeks. After that, it worked with all NEMO5 features."

NEMO5: Automated documentation with Doxygen

Browsing large source code can be cumbersome (even with Visual Studio or Eclipse)

NEMO5:
NEMO5 code is compatible with Doxygen
Doxygen documentation requires only a web browser
(NEMO/prototype/doc/html/index.html)

Snapshot of Doxygen's "Graphical Class Hierarchy" of NEMO5



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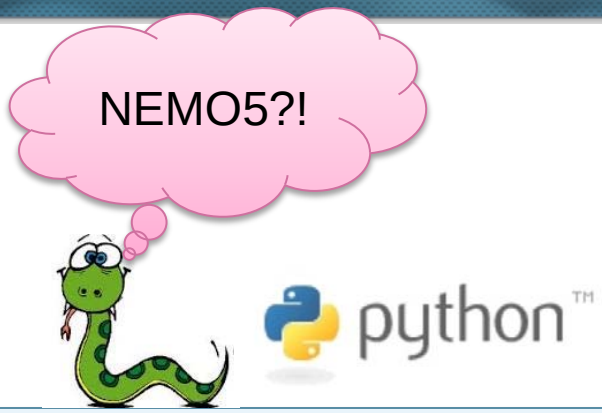
NEMO5: easy prototyping new code in Python



"What if I want to quickly test a new idea?"

Prototype in Python:

- Python is linked to NEMO5
  usage with "nemo python_file.py"
  (python_file.py needs to be compatible)
- The linked Python version supports NumPy and SciPy
- NEMO5 can load Python scripts and Python solvers
- Write python code and embed NEMO5 routines within your Python script
  (similar to matlab toolbox)

NEMO5 & Python: Python solver

NEMO5 solvers have a common API (to set up, to solve, to communicate, …)
Your own new solvers have to stick to this API

C++ Solver	Python Solver
void MyNewSolver::do_solve()	def do_solve(self):
void MyNewSolver::do_init(){}	def do_init (self):
void MyNewSolver::do_reinit(){}	def do_reinit (self):
void Simulation::do_output(){}	def do_output (self):
void MyNewSolver::get_data(string v, type&) get_data(vector<complex<double> >)	def get_data_type(v) get_data_list_complex()
void MyNewSolver::get_data(string v, type1, type2&, .) get_data(unsigned int, vector<double>, .)	def get_type1_data_type2_.(v) get_uint_data_list_double (v)

```
    [Simulation] initializing boundary conditions...  boundary conditions a
 initialized.
[PythonSolver] printer found file: ./python/printer.py
[PythonSolver] printer init was executed
[Simulation] printer is initialized.
[Nemo] simulations were created and initialized in 0.02475 seconds.

============================================================
[Nemo] Running Simulation "printer"...
============================================================
[PythonSolver] printer solve was executed
[Simulation] setting active regions for "printer"...
```

NEMO5 & Python: Metasolver

```
    density_solver = density_solver
    potential_solver = potential_solver

    contacts = (source_contact, drain_contact)

    source_contact = (0.0, 0.0)
    drain_contact =  (0.0, 0.1)
  }
  solver
  {
    name = density_solver
    type = WF
    domain = device
    active_regions = (1, 2, 3)
```

Standard NEMO5 situation:

Several solve… …settings in
Some options…
(obsolete for specific tasks)
Some option names are “developer style”

Long and complex inputdeck

Tutorial 4D Python & NEMO5
Learn how to prototype in Python and use NEMO5 with it

```
Solvers
{
  solver
  {
    name = Transport
    type = MetaTransport
    transport_type = NEGF
    domain = device
    active_regions = (1, 2, 3)
    output_name = SNWT
    contact_domains = (source_contact, drain_contact) //names
    source_contact_voltages = (0.0, 0.0)     //list of voltages
    drain_contact_voltages = (0.0, 0.05)      //list of voltage
    use_Poisson_potential = true            //if true, Poisson
```

Solution: Metasolver

NEMO5 inputdeck: only relevant options are visible
Option names are convertible

Short inputdeck (1 Solver only)

```
    //Knum = 10

    ramper_name = ramper

    self_consistent  = true

    potential_criteria          = 0.001
```

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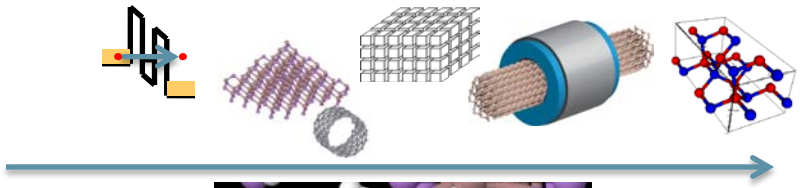
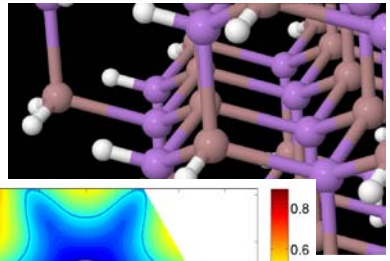
NEMO5 lecture – overview

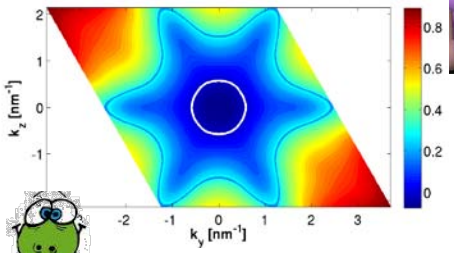
NEMO5 origins + history



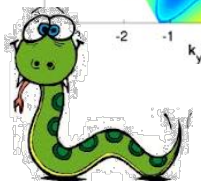
NEMO5 and atomic representations



NEMO5 solvers + physics



NEMO5 expandability + flexibility



NEMO5 on supercomputers (scalability and compatibility)

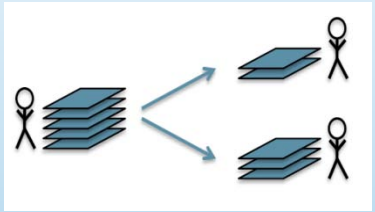
NEMO5 support (for output and users)

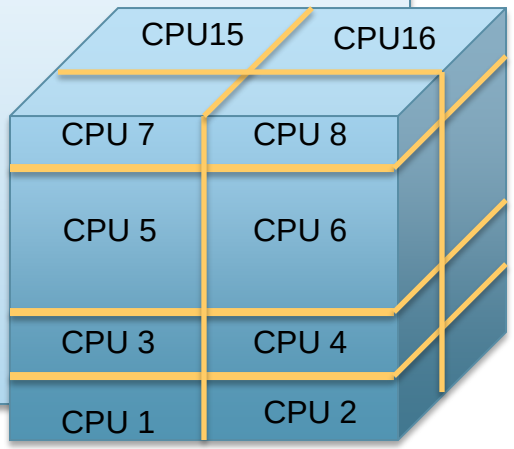
NEMO5: MPI parallelization

Device calculations are typically very time consuming:
10x10x10 nm Si gives ~ 64k atoms ~ 1.3 million degrees of freedom
Many matrix operations scale like N^2 – N^3

NEMO5 is MPI parallelized:

- **k**-space and **x**-space parallelization for Schrödinger-Poisson
- **x**-space parallelization for Strain
- **V**, **k**, **E** and **slab** parallelization for NEGF-Poisson and WF-Poisson

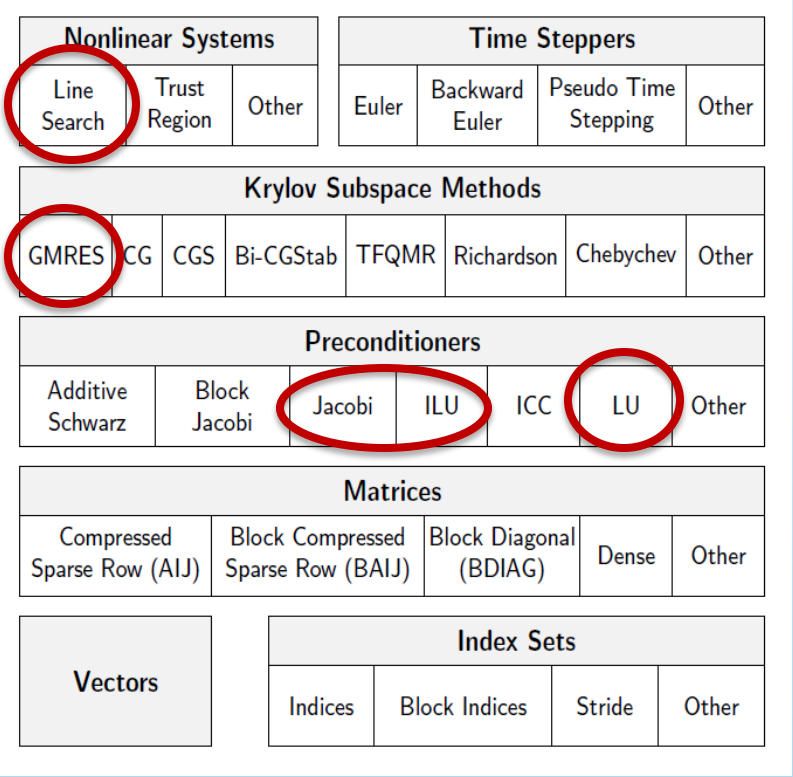




within NEMO5: Linear Solvers and Eigensolvers

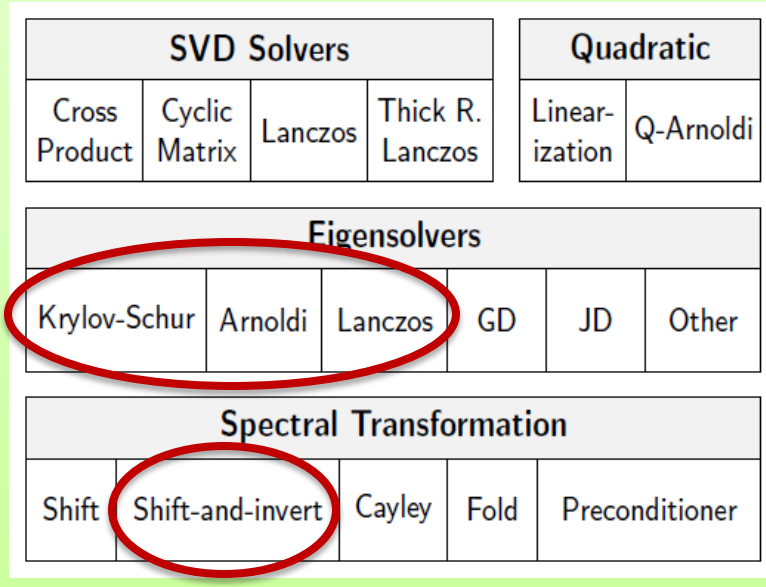
Linear and Newton solvers: **PETSc**

- lots of parallel direct & iterative solvers
- interface to LAPACK, MUMPS, SuperLU, HYPRE



Eigensolvers: **SLEPc**

- Uses PETSc for linear solvers, parallelism
- interface to PARPACK (problem in RCAC installation)



NEMO5: MPI scalability

MPI status in NEMO5

- Massively parallel numerical solvers implemented
  - » Externally developed libraries SLEPc, PETSc and Libmesh
- Scaling reached up to 100k CPUs
- Efficient parallel writing of data to disk implemented in NEMO5
- Fast initialization for NEMO5 on up to 100k CPUs

NEMO5:
Very good scaling shown
up to 100k CPUs

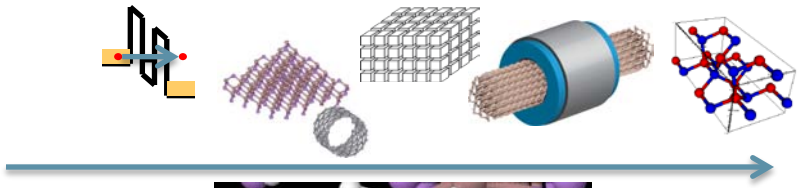
NEMO5: platform compatibility

Architectures where NEMO5 can be compiled and run:

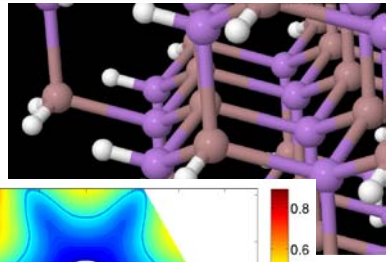
- RCAC machines coates, steele, rossmann, hansen, … (GCC & Intel)
- Ubuntu (GCC)
- nanoHUB.org workspace (Intel)
- jaguar.ccs.ornl.gov (GCC)
- ranger.tacc.utexas.edu (GCC)
- kraken.ccs.ornl.gov (GCC)
- Your Linux system…

NEMO5 lecture – overview

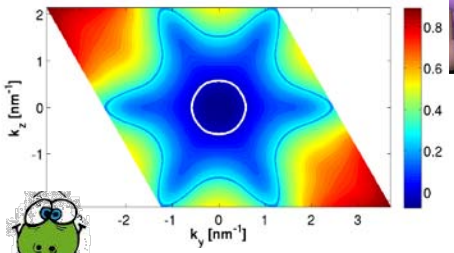
NEMO5 origins + history



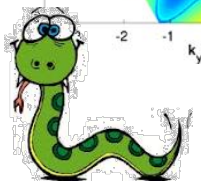
NEMO5 and atomic representations



NEMO5 solvers + physics



NEMO5 expandability + flexibility



NEMO5 on supercomputers (scalability and compatibility)

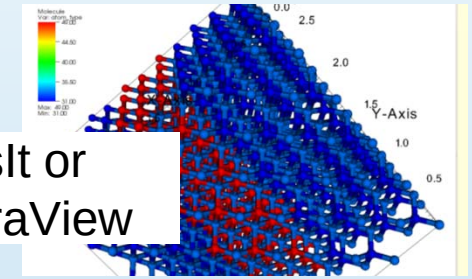
NEMO5 support (for output and users)

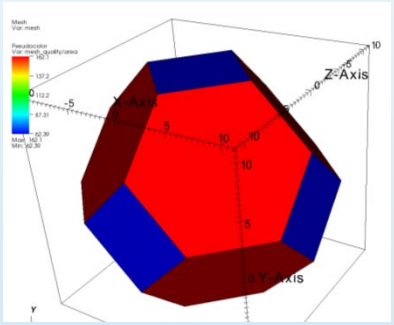
Input and Output

Different purposes and visualization software require different output format

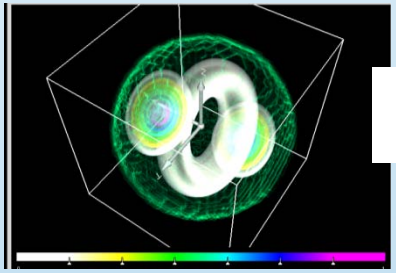
- **NEMO5 supported formats:**
  - VTK

    VisIt or ParaView





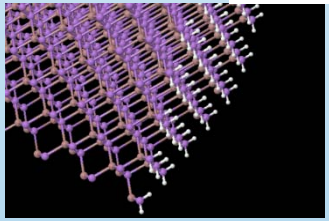
  - DX (simple-cubic)



NanoViz

  - XYZ

jmol



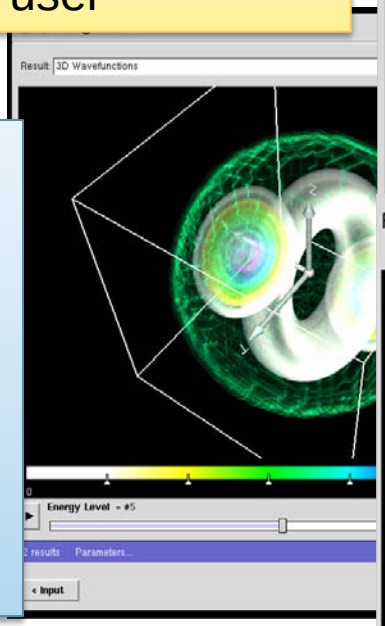
  - PDB (zincblende struct. only)
  - Text files (eigenvalues, 1D graphs)

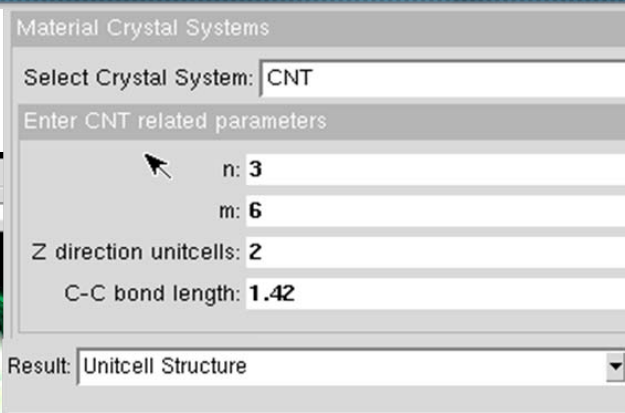
NEMO5: on nanoHUB

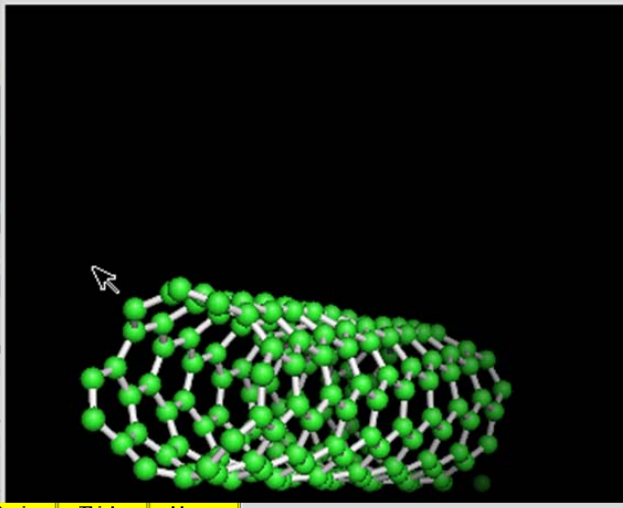
Specific purposes typically require a small set of options
Full flexibility of NEMO5 burdens the fast user

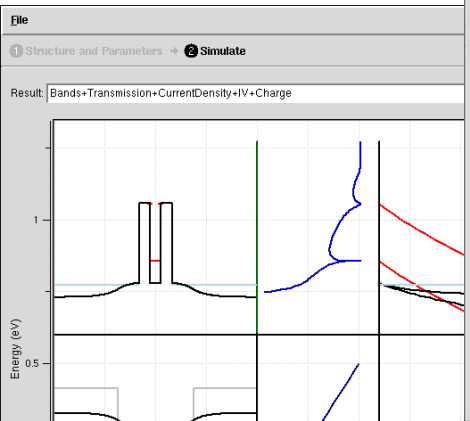
nanoHUB.org offers GUI controlled tools powered by NEMO5:

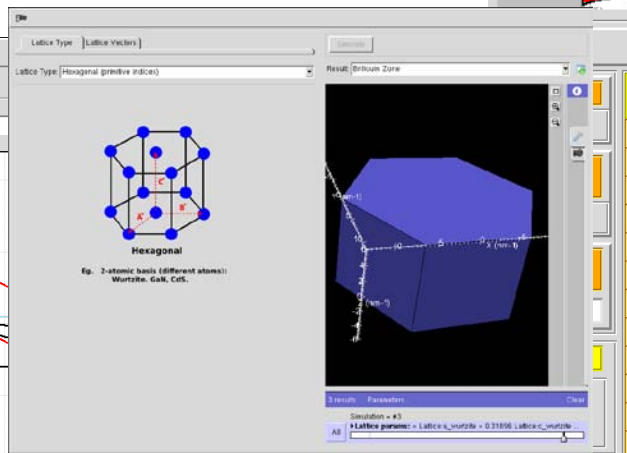
- Quantum Dot Lab
- 1d Heterostructure Design Tool
- Crystal Viewer
- RTD Simulation with NEGF
- Brillouin Zone Viewer



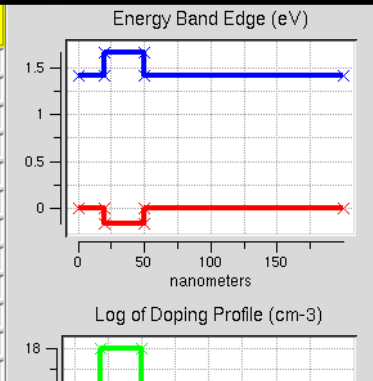








Layer	Material System	n-Doping (cm-3)	Thick. (nm)	Mono-layers
Substr.	GaAs	1.e+14	1000.06	3538
L01	GaAs	1.e+14	149.81	530
L02	AlGaAs	1.e+18	29.96	106
L03	GaAs	1.e+14	19.79	70
L04				
L05				
L06				
L07				
L08				
L09				
L10				
L11				



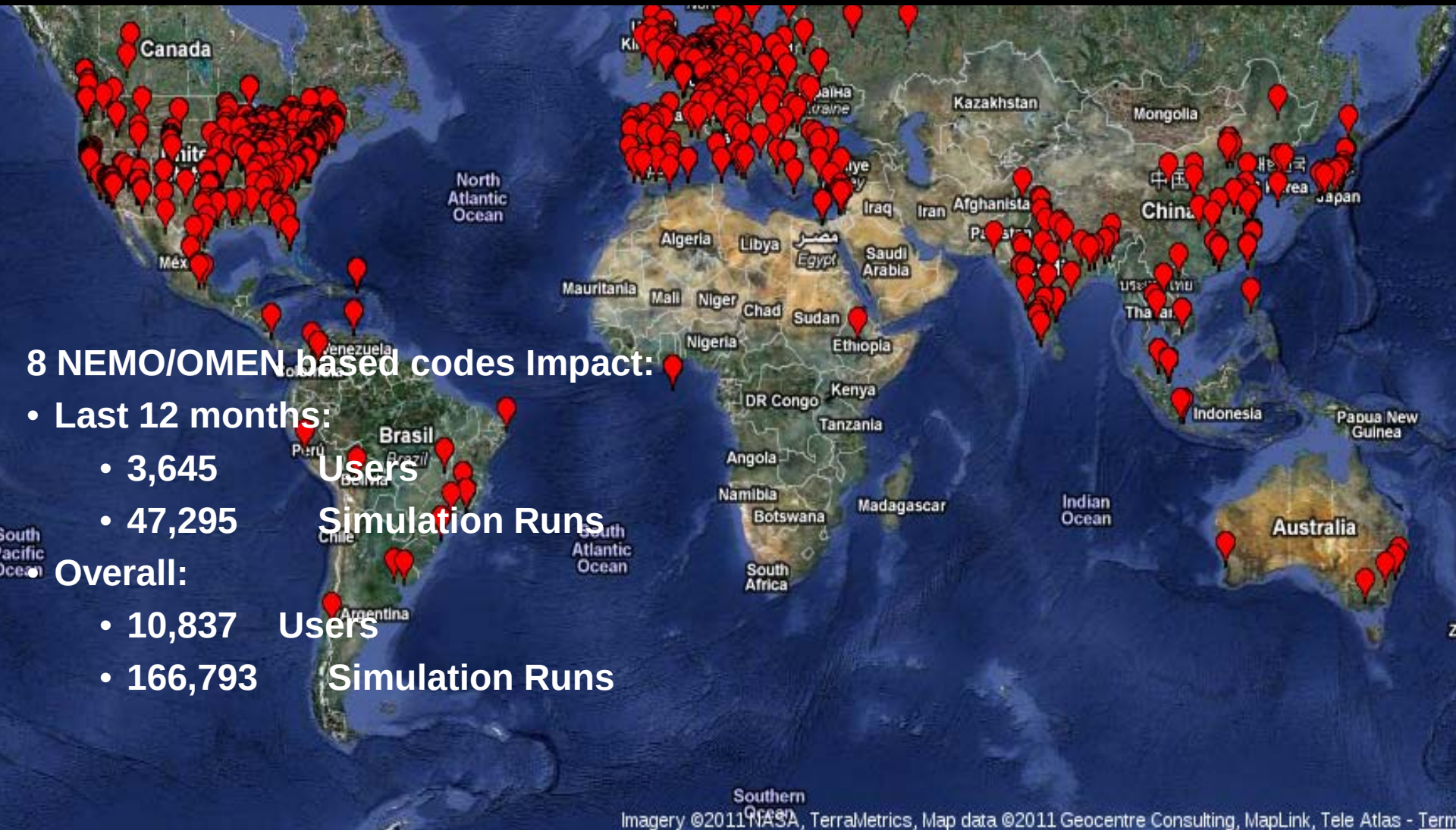
35 Klimeck tools:

- **22,000 users**
- **>820,000 simulations**

Systemic Education:

>5,700 students, 461 courses

>60 universities



8 NEMO/OMEN based codes Impact:

- **Last 12 months:**
  - **3,645 Users**
  - **47,295 Simulation Runs**
- **Overall:**
  - **10,837 Users**
  - **166,793 Simulation Runs**

NEMO5: support and discussion forum

NEMO5 distribution and support group on nanohub

Thanks, Jim

Mahesh R Neupane @ 01:20 PM on 26 Apr, 2012

Hi Jim!

I need one help. If you could, please run the following input deck in parallel using the command:

submit -v coates -i ./all.mat -

I would like to see, if there is

For me, the simulation never

Si_NW_3nm.in

James Fonseca @ 02:51 P

What output do you get?

when I submit the request su

the stderr file gives me qsub: Job exceeds queue and/or server resource limits

Tillmann Christoph Kubis @ 03:02 PM on 26 Apr, 2012

Hi, checking the resources on coates it seems there are only 64 CPUs reserved for ncn-hub. So please, try to run your command with e.g. … -n 30 first and see what happens.

Thanks, Tillmann

Samiran Ganguly @ 03:15 PM on 26 Apr, 2012

a quick question…is there anyway to check on the status of the job (equivalent of qstat of pbs) from the nanoHUB workspace?

Post questions and look for answers in the NEMO5 discussion forum

Any feedback/suggestions are very welcome

You can contribute to the code, too

Schedule for the NEMO5 tutorial

Device Modeling with NEMO5
10:00 Break
10:30 Lecture 14 (NEMO5 Team): “NEMO5 Introduction”
12:00 LUNCH
1:30 Tutorial 1 (NEMO5 Team): “NEMO5 Technical Overview”
3:00 Break
3:30 Tutorial 2 (NEMO5 Team): “NEMO5 Input and Visualization”
4:30 Tutorial 3 first part (NEMO5 Team): “Models”
5:00 Adjourn

Schedule for the NEMO5 tutorial

Friday, July 20

8:00 Coffee and rolls

8:30 Tutorial 3 second part (NEMO5 Team): “NEMO5 Models”

9:00 Tutorial 4 first part (NEMO5 Team): “Device Simulation – Graphene”

10:00 Break

10:30 Tutorial 4 second part (NEMO5 Team): “Device Simulation – Graphene”

- 4A Topological Insulators
- 4B Metals
- 4C Graphene
- 4D Python+NEMO5

12:00 LUNCH

1:30 Tutorial 5 (NEMO5 Team): “Device Simulation – Quantum Dots”

- 5A Quantum Dots Introduction
- 5B Strain
- 5C Quantum Dots

3:00 Break

3:30 Tutorial 6 (NEMO5 Team) : “Device Simulation – Transistor”

- 6A Transport (DG MOSFETs)
- 6B Transport (BTBT)

5:00 2012 Summer School Adjourns

This time schedule is flexible adjusting to your needs and interests

Conclusion

NEMO5:
Multipurpose, multiscale highly parallelized nanodevice simulation tool
Compatible with many external software (both for output and input)
Can be used as a tool or as a library

NEMO5 is under constant development
Your feedback is very valuable to us!

Thank you!

Sponsors:
SRC, GRC, NSF,
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Intel, Samsung,
Global foundries,
IBM, Lockheed Martin