NEMO5 on Blue Waters - A Flexible Package for Nanoelectronics Modeling Problems

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Network for Computational Nanotechnology

PRAC - Accelerating Nano-scale Transistor Innovation

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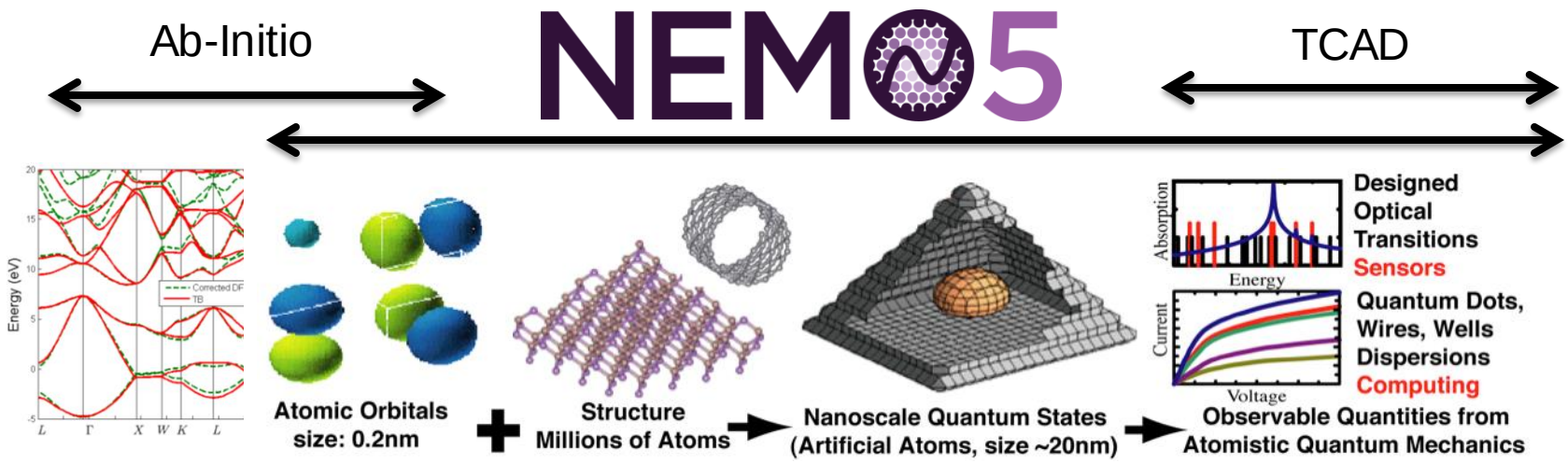
Blue Waters Symposium

May 2015

PURDUE UNIVERSITY

NEMO5 - Bridging the Scales From Ab-Initio to Realistic Devices



Goal:

- Device performance with realistic extent, heterostructures, fields, etc. for new / unknown materials

Problems:

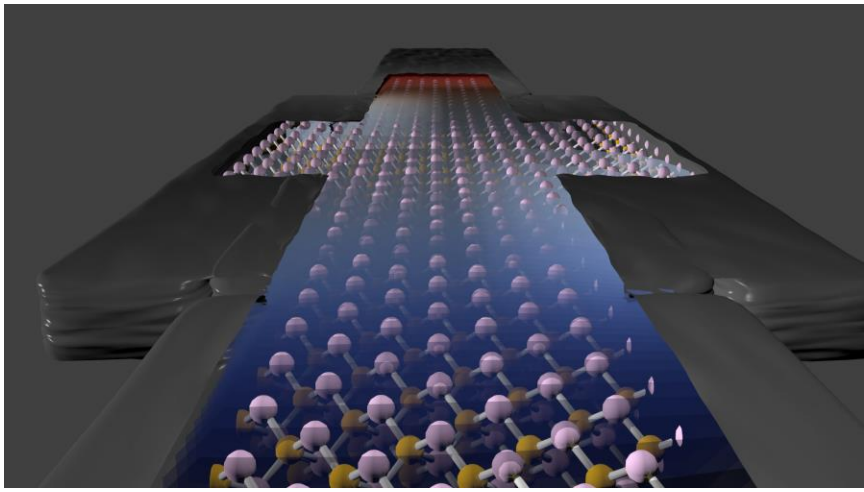
- Need ab-initio to explore new material properties
- Ab-initio cannot model non-equilibrium.
- TCAD uses quantum corrections

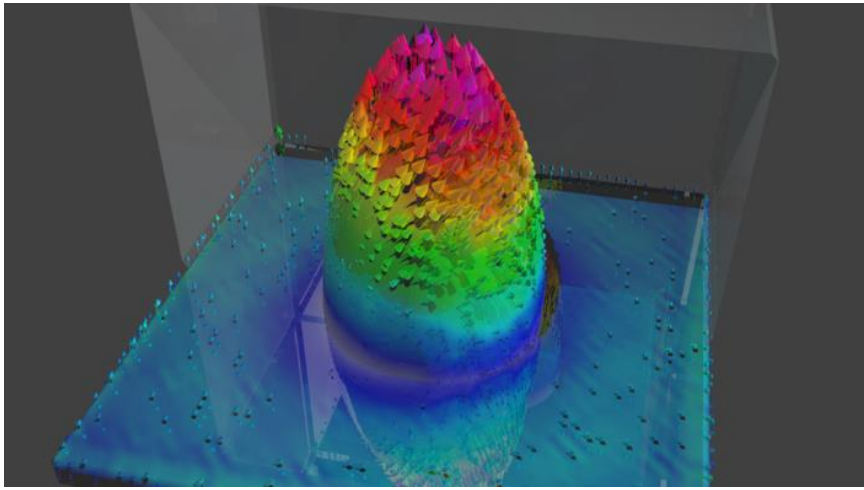
Approach:

- Ab-initio:
  - Bulk constituents
  - Small ideal superlattices
- Map ab-initio to tight binding (binaries and superlattices)
- Current flow in ideal structures
- Study devices perturbed by:
  - Large applied biases
  - Disorder
  - Phonons

NEMO5 – A multiscale simulation tool for nanoelectronic modelling

- **Multiscale/multiphysics**
  - Empirical tight binding
  - NEGF, DD, QTBM, EM
  - Electron core, k.p, mode space
  - Ohmic and Schottky contacts
  - Scattering optical and acoustic
  - Phonons
  - Strain models-VFF, Keating, Lazarenkova
  - External magnetic fields
- **Solves**
  - Atomistic strain
  - Electronic band structures
  - Charge density
  - Potential
  - Current
- **4-level MPI parallelization**
  - bias, energy, momentum, space

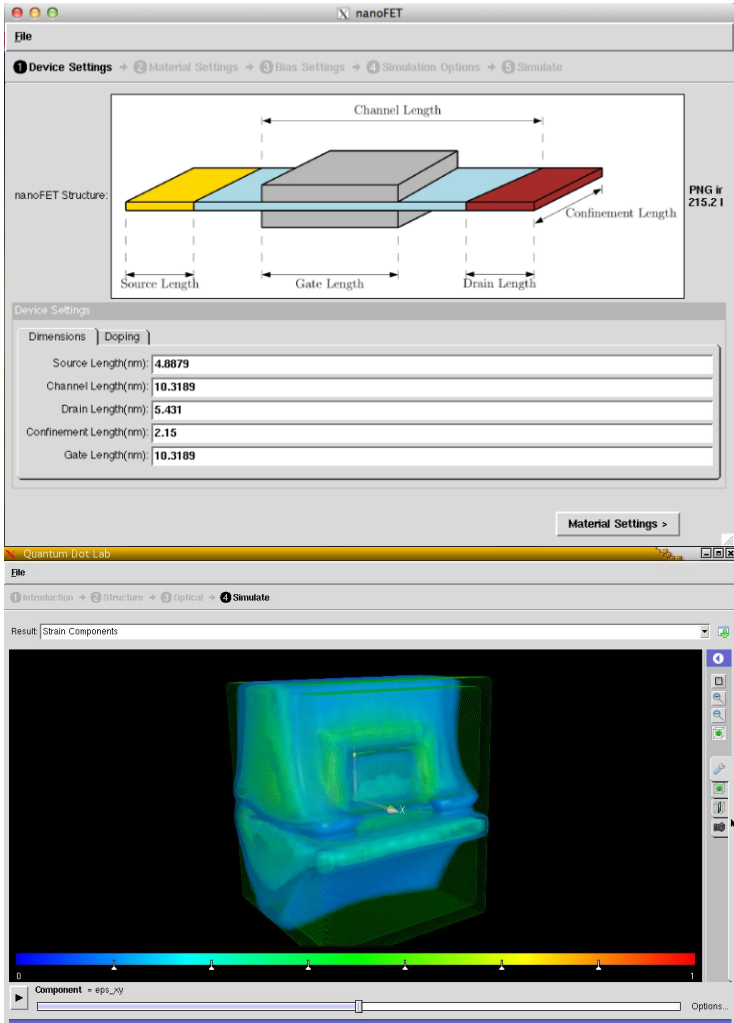




NEMO5 and nanoHUB

- Distribution and Support Group on nanoHUB.org
  - » https://nanohub.org/groups/nemo5distribution
  - » Source code, example, discussion forum, run NEMO5 on Purdue Resources

- nanoHUB.org
  - » 330,000 annual users
  - » 4,200 resources (video lectures, presentations, tutorials, etc.)
  - » 330 simulation tools
  - » Nanoelectronics, nanophotonics, materials science, molecular electronics, carbon-based systems, Microelectromechanical systems
  - » 4,200 resources (video lectures, presentations, tutorials, etc.)
  - » NEMO5 Tools
    - ✓ Quantum Dot Lab
    - ✓ Crystal Viewer
    - ✓ Bandstructure Lab
    - ✓ …



Non-equilibrium Green's functions method: Non-trivial and disordered leads

Yu He, Yu Wang, Tillmann Kubis,
Gerhard Klimeck

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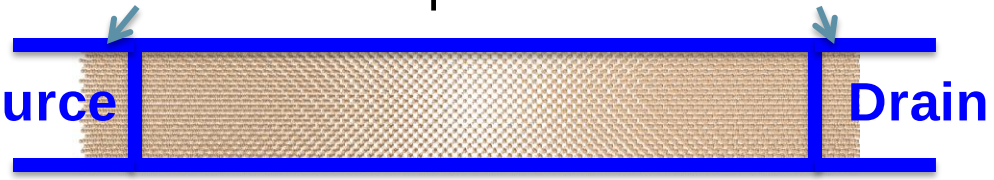
Problem: assumption of periodic contacts in NEGF contradicts experiment

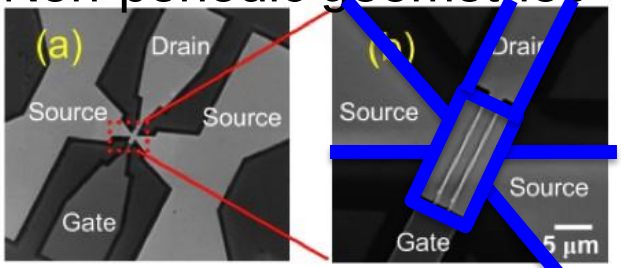
Common self-energy methods Sancho Rubio, transfer matrix

semi-infinite periodic contacts.



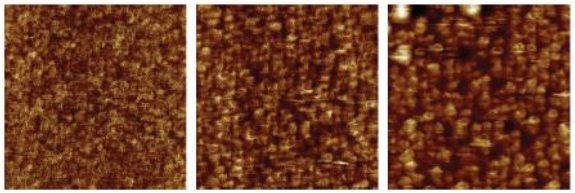
But in the real world…

Non-periodic geometries



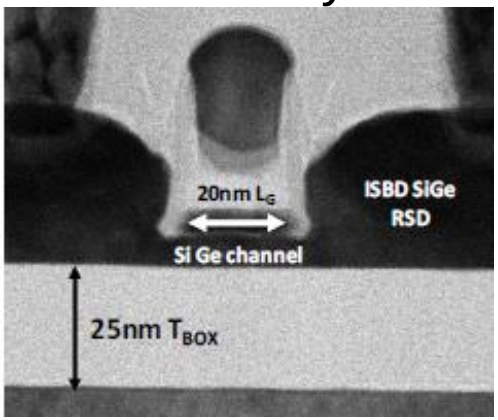
http://www.electroiq.com/articles/sst/2010/12/iedm-reflections_.html

Roughness



S. Koenig et al, Appl. Phys. Lett, Vol. 104, pp. 103106, 2014

Random alloy



Q. Liu, et al, IEDM p.229 2013

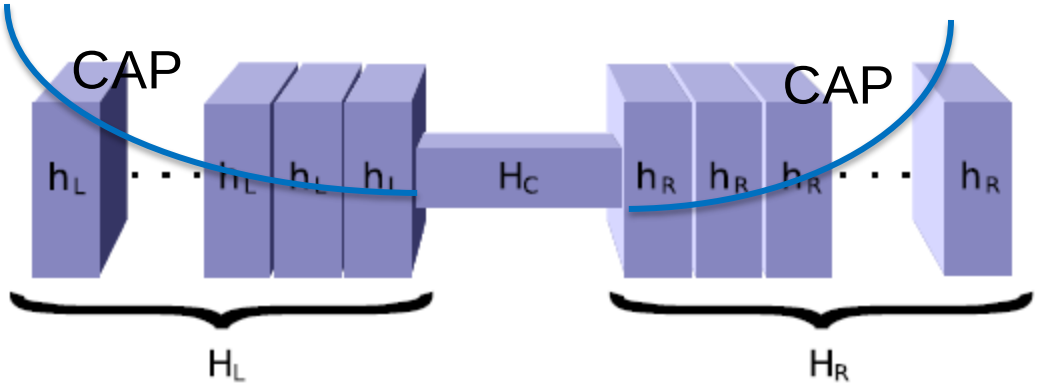
Periodic assumption contradicts realistic contacts

How to solve non-periodic contacts?

General Lead Method: problem & idea

Problem:

- No exact solution for semi-infinite systems unless periodicity assumed
- Approximate solution
  - ✓ Physically correct
  - ✓ Numerically solvable for arbitrary contact structures

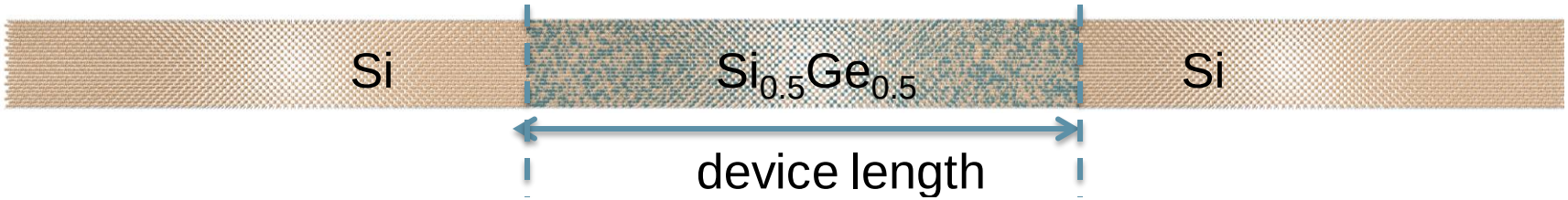


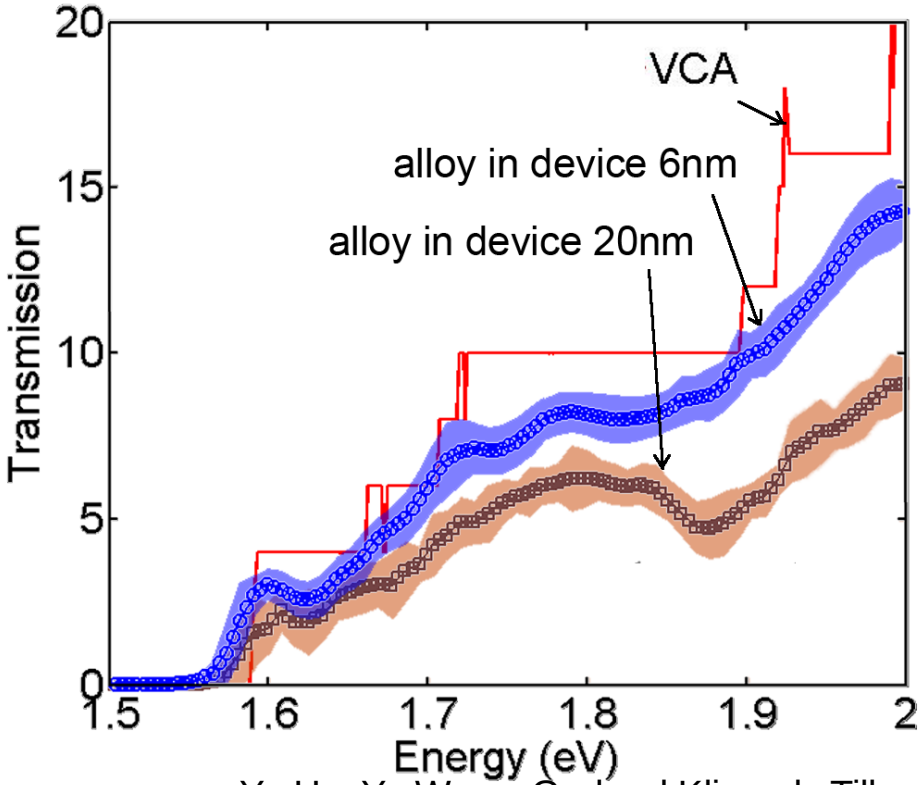
J. Driscoll et al, Phys. Rev. B. Vol. 78, pp. 245118, 2008

Idea: extend complex absorbing potential (CAP) method

- **Non-periodic contact** : Hamiltonian for explicit contact segments;
- **CAP serves as scattering** : physical assumption of contacts;
- **Efficient, memory thin** : converge within finite iterations;

Example: SiGe random alloy



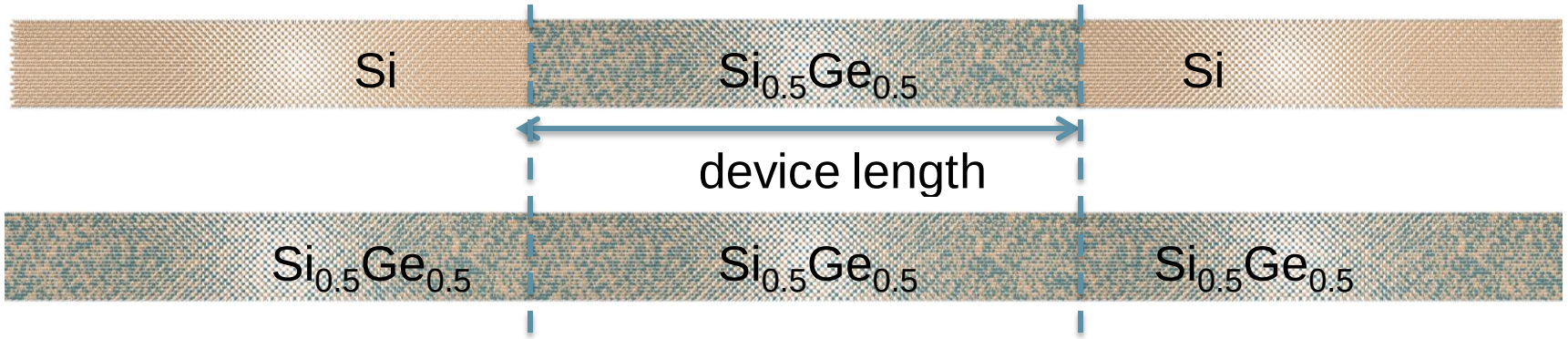


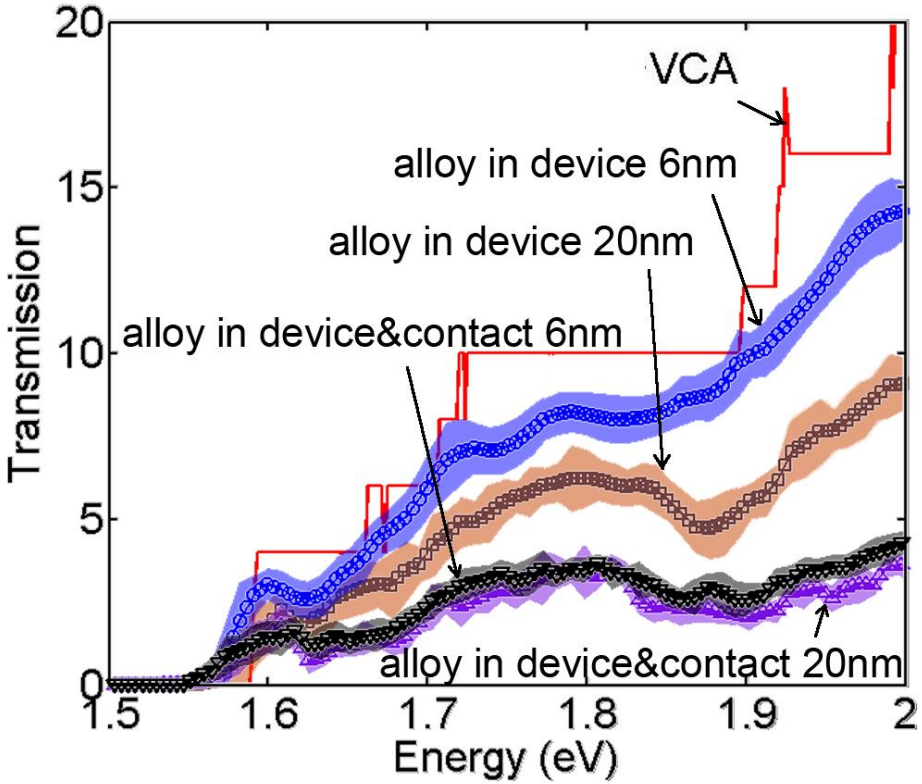
Example:
3x3nm $Si_{0.5}Ge_{0.5}$ nanowire in sp3d5s* tight binding
Device length 20nm and 6nm
Results averaged over 50 samples

Justification:
With same effective alloyed disorder in contacts, expected transmission has weak dependence of device length

Yu He, Yu Wang, Gerhard Klimeck, Tillmann Kubis, "Non-equilibrium Green's functions method: Non-trivial and disordered leads" Appl. Phys. Lett. 105, 213502 (2014)

Example: SiGe random alloy

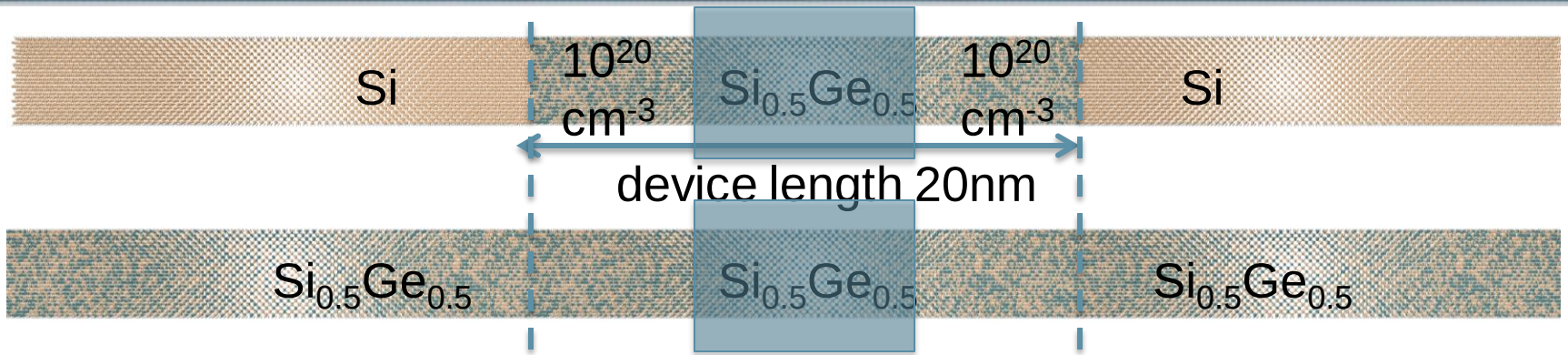


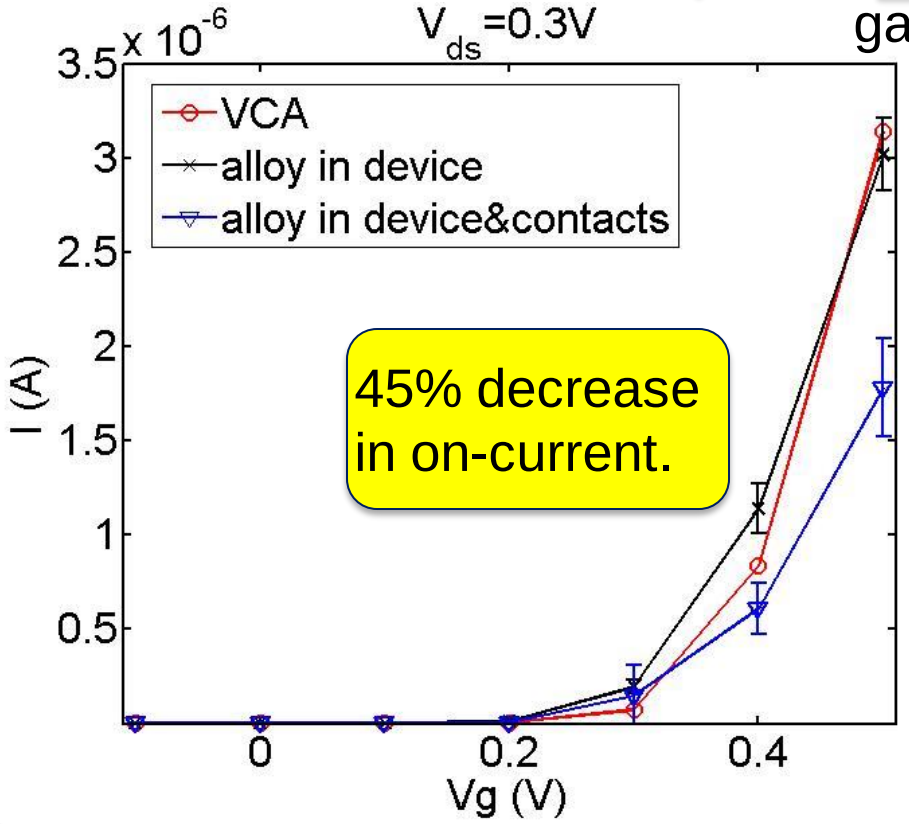


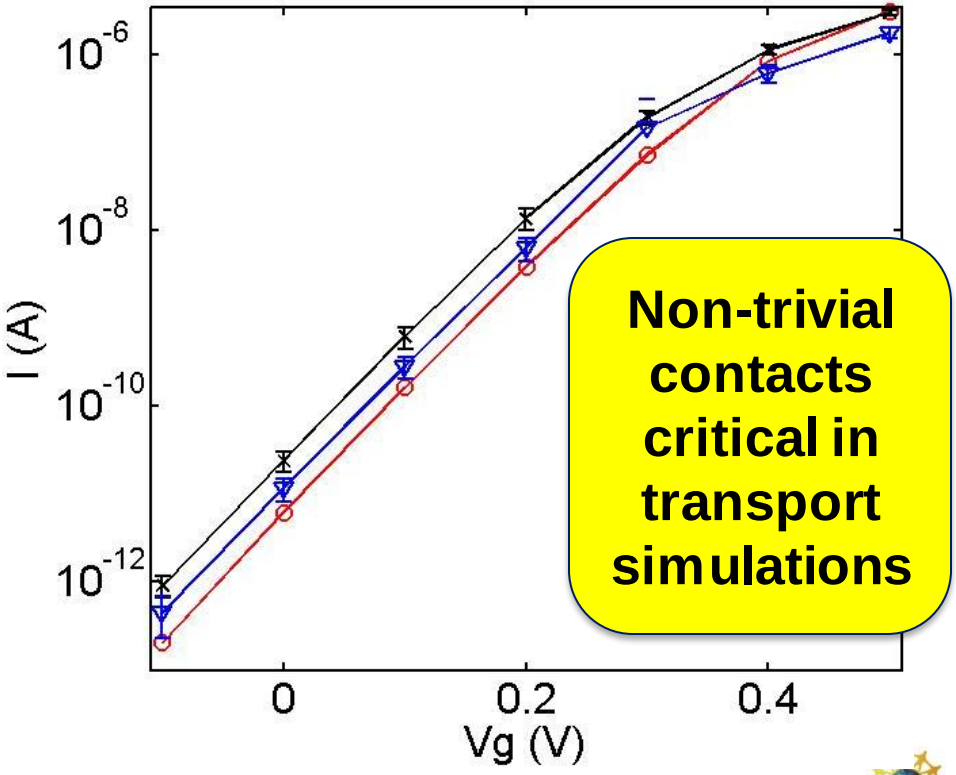
- ✓ Alloyed contact yield virtually device length independent transmission;
- ✓ DOS of contacts match device better → less reflections of electrons;

General lead approach works well for contacts with alloy randomness.

Example: SiGe random alloy







Bilayer Graphene: a Good candidate for Transistors?

Fan Chen, Hesameddin Ilatikhameneh,
Rajib Rahman, Gerhard Klimeck

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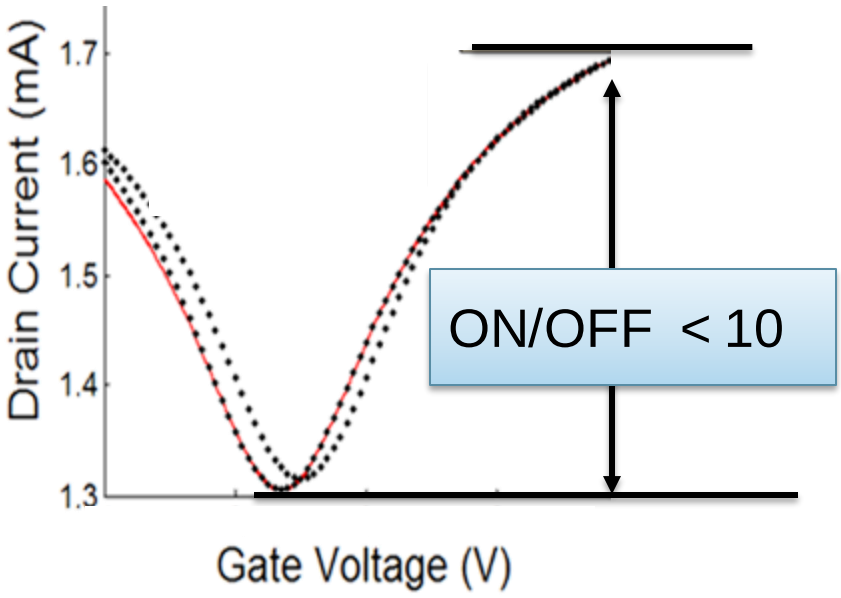
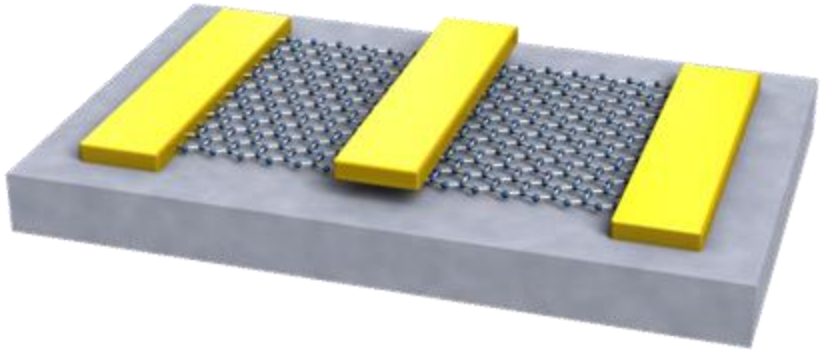
Graphene Transistor





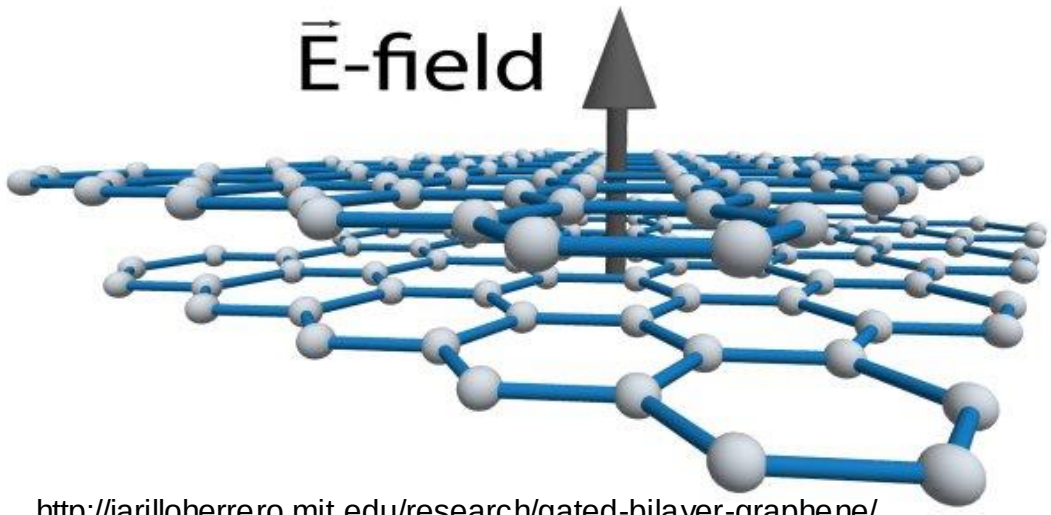
- Graphene has a zero band gap
- It has a good high ON current, but it can't be turned off

We need to achieve:

- Large ON/OFF ratio needed in transistors (~10^5)
- Small OFF current -> Low power consumption

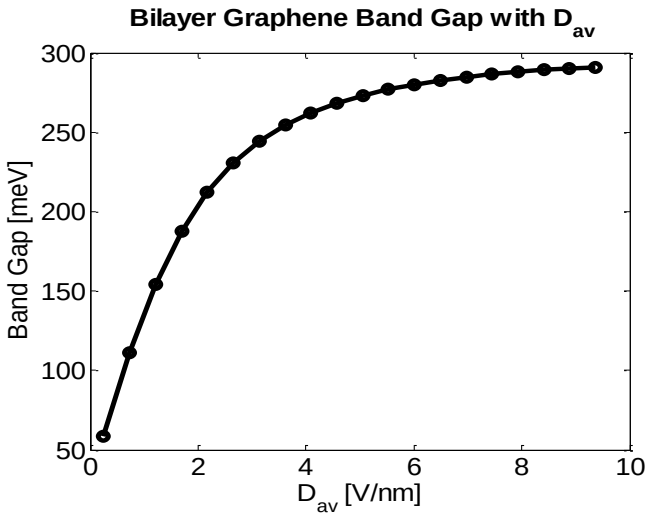
http://www.jameshedberg.com/img/samples/
https://www.kth.se/en/ict/forskning/ickretsar/

Bilayer Graphene



http://jarilloherrero.mit.edu/research/gated-bilayer-graphene/

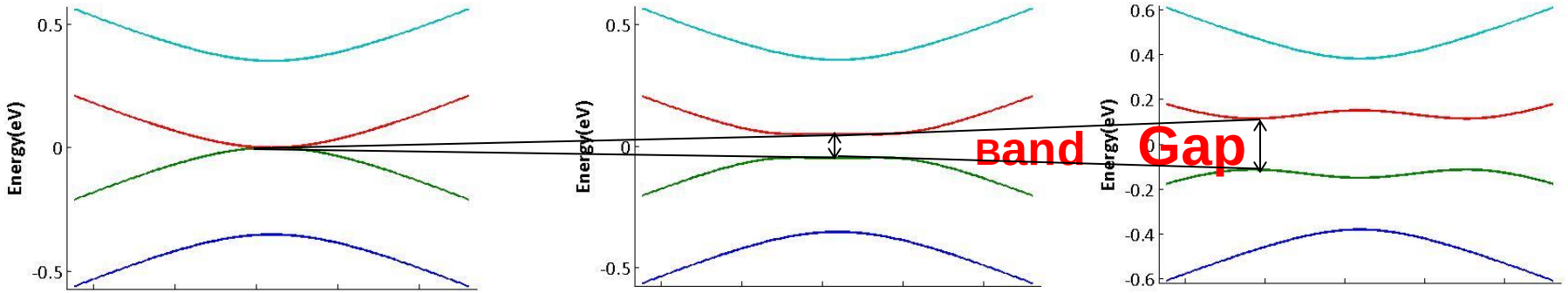
Bandgap vs. E-Field



Bandstructure

Small field

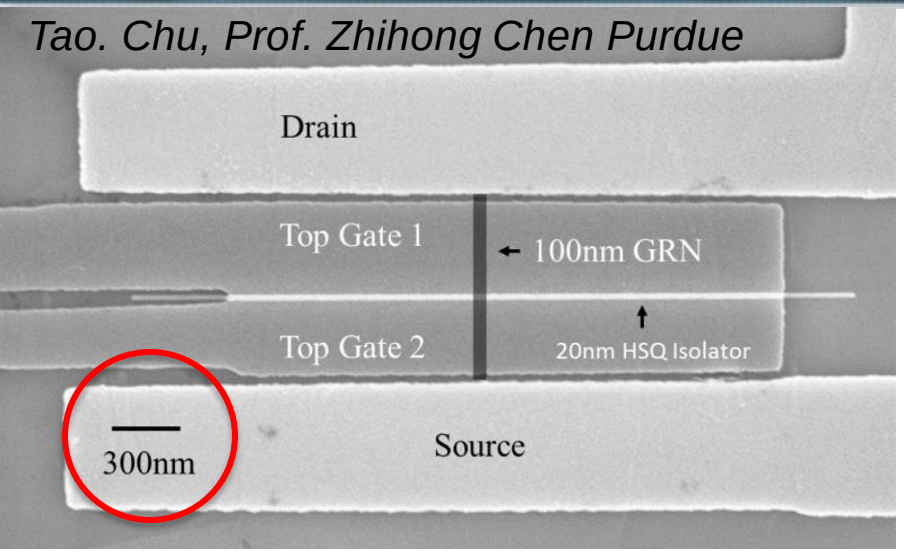
Large field



Bilayer Graphene: Create a Band-Gap by Electric Field

- Control band-gap by applying vertical electric field

NEMO5 - realistic atomic approach

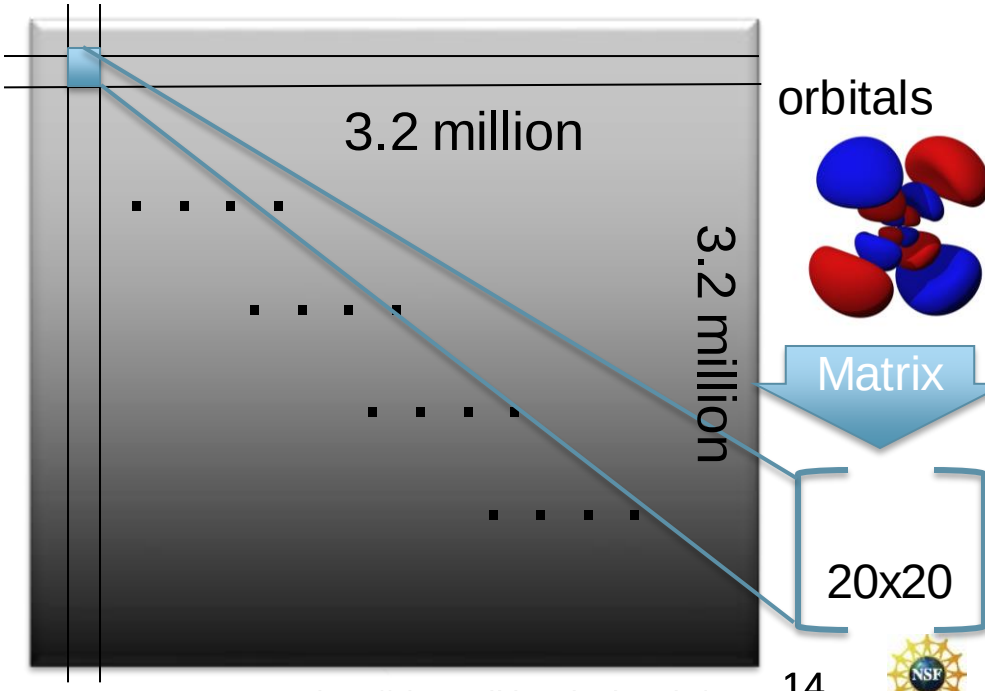


Daniel Mejia

Challenge:
- Matrix size ~ 64 million
- Inverse, Eigenvalues

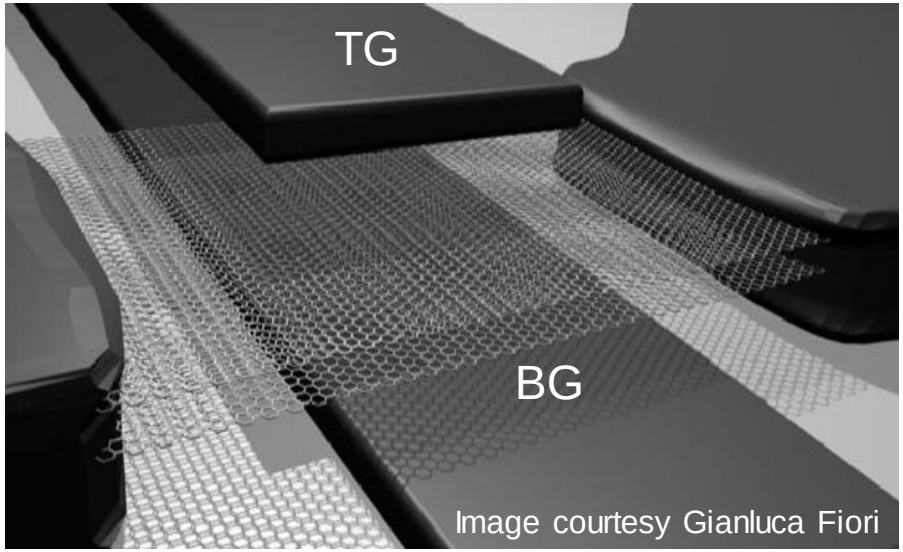
① Limitation from fabrication technique, short channel effect, gate leakage …
② Device size is typically 100nm (thick) x 200nm (long) x 20nm (wide)

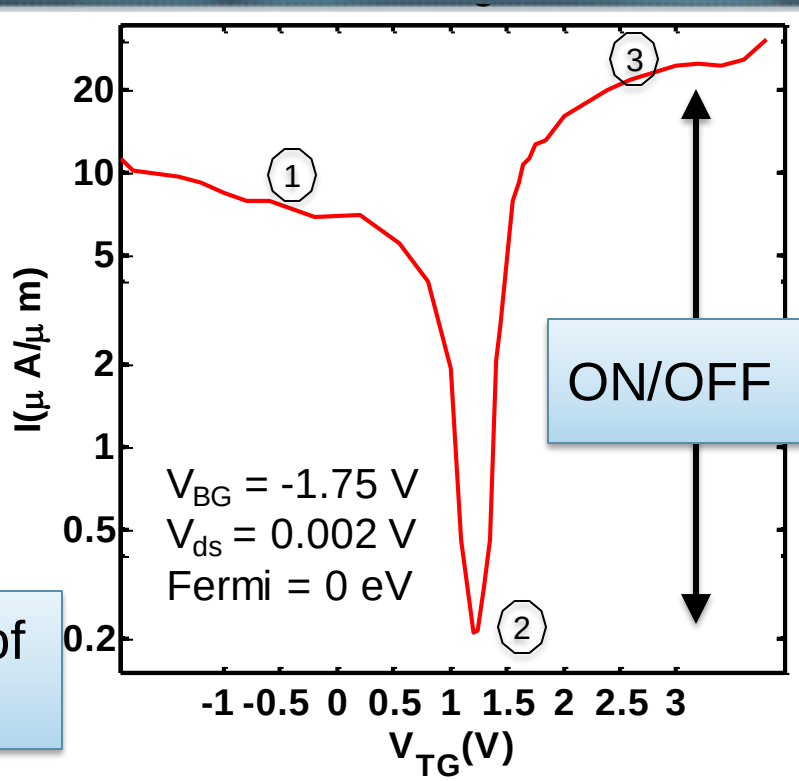
- 3.2 million atoms in simulation



http://chemwiki.ucdavis.edu/

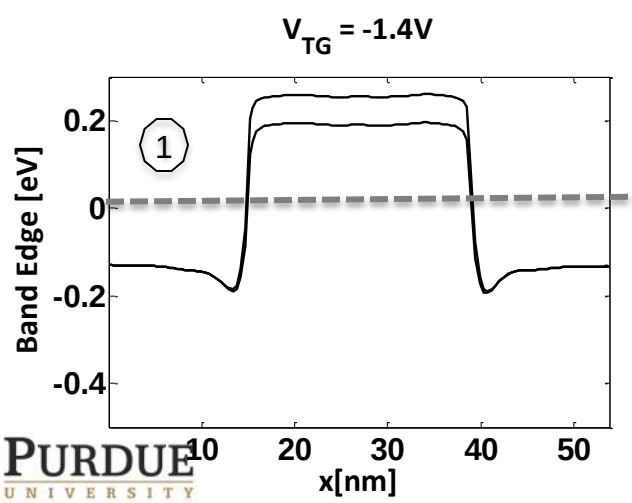
Bilayer Graphene: Open band gap

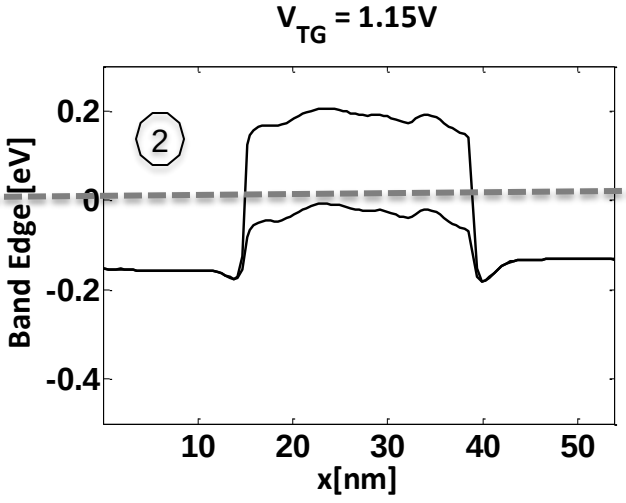


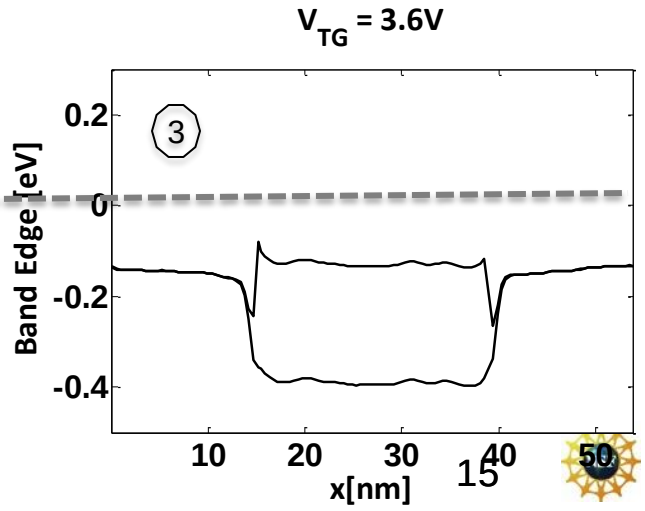


ON/OFF = 100

Band Gap opens through the change of Top Gate

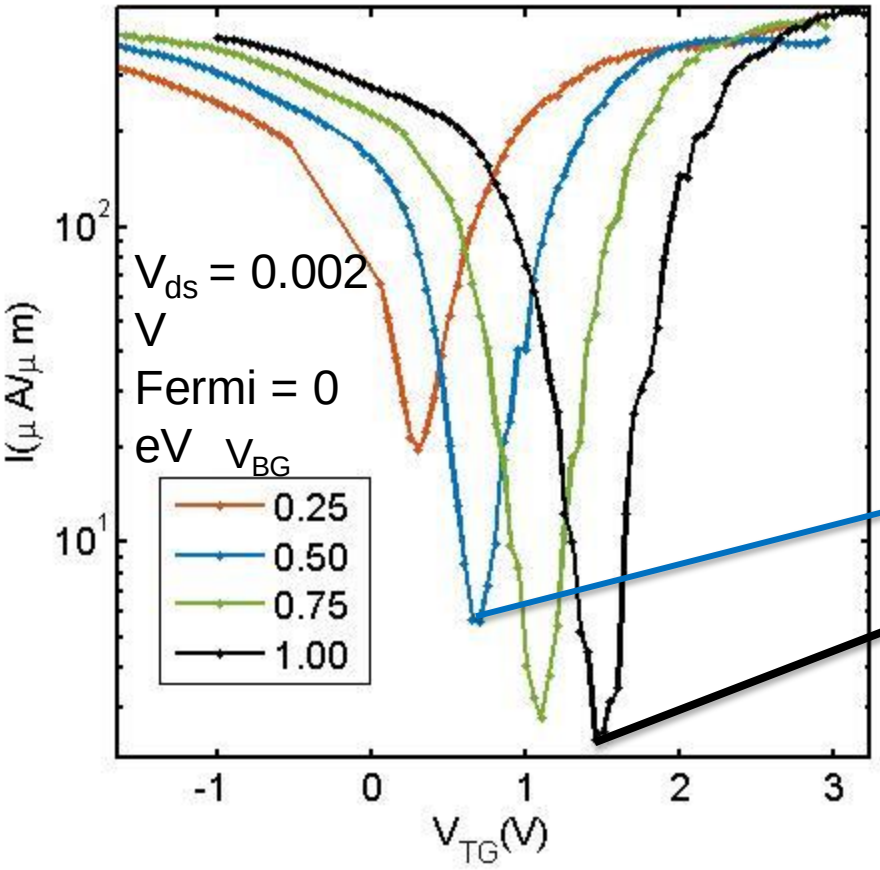




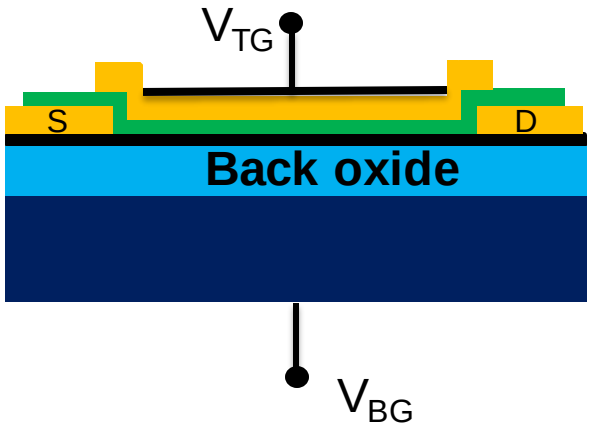


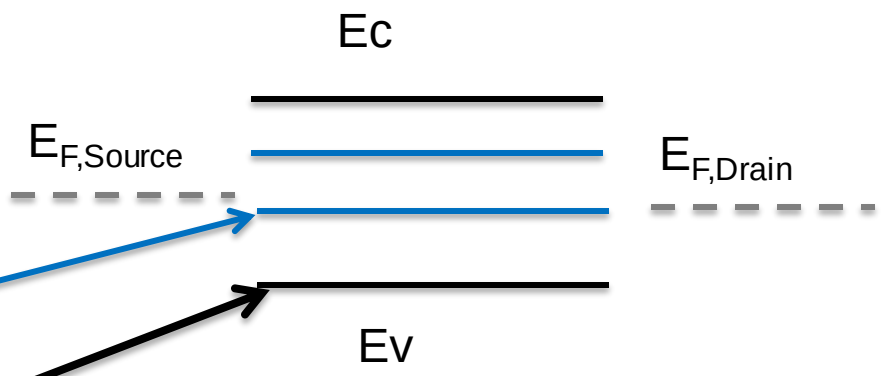
Dynamic Band gap

Dynamic band gap:
$|V_{BG}| \uparrow \Rightarrow E \uparrow \Rightarrow E_g \uparrow \Rightarrow I_{ON}/I_{OFF} \uparrow$



Physical structure





Band Gap modulated by back gate

NEMO5 - self consistent simulation

Construct Hamiltonian

64 million x 64 million matrix

Add Potential

Determine energy grid

64 M x 64 M Eigenvalue

Calculate charge density

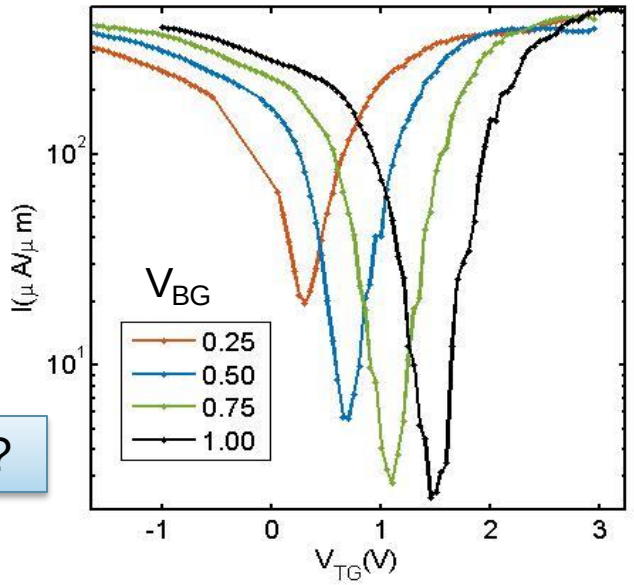
64 M x 64 M Inverse

Calculate Potential

Convergence?

Hundreds of data points

One I-V data point



iNEMO Group

iNEMO

- PI: Gerhard Klimeck
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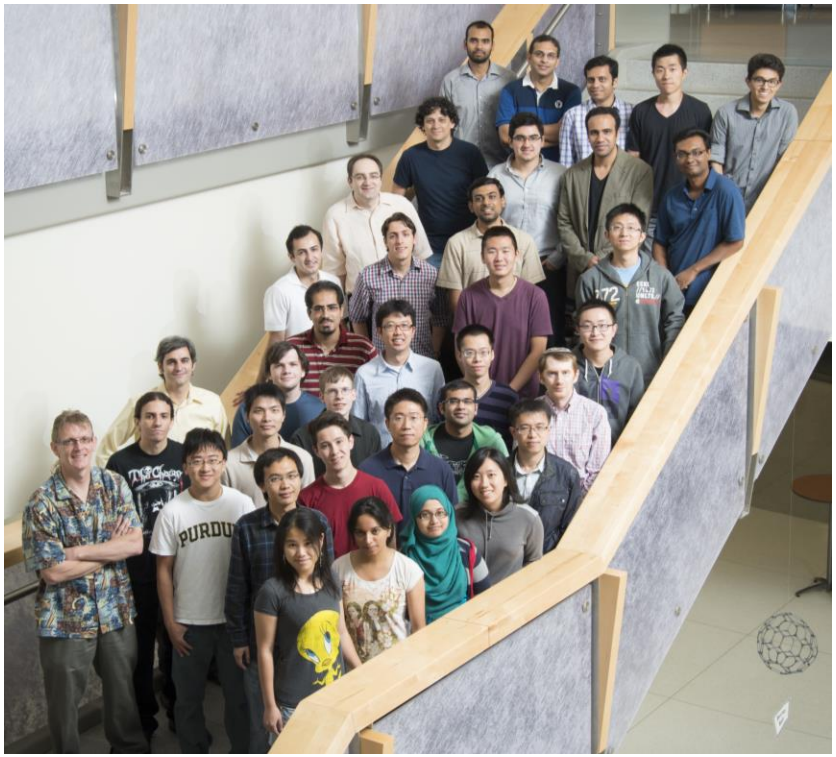
- Research Scientist: Jim Fonseca
- 2 Postdocs: Bozidar Novakovic, Jun Huang
- Students: Tarek Ameen, Robert Andrawis, James Charles, Chin-Yi Chen, **Fan Chen**, Yuanchu (Fabio) Chen, Rifat Ferdous, Jun Zhe Geng, **Yu He**, Yuling Hsueh, **Hesameddin Ilatikhameneh**, Zhengping Jiang, Daniel Lemus, Pengyu Long, Daniel Mejia Padilla, Kai Miao, Samik Mukherjee, **Harshad Sahasrabudhe**, Prasad Sarangapani, Saima Sharmin, Yaohua Tan, Yui Hong (Matthias) Tan, **Archana Tankasala**, Daniel Valencia Hoyos, Kuang Wang, **Yu Wang**, Evan Wilson



- Ryan Mokos
- Intel, Samsung, Philips, TSMC