NanoElectronic Modeling with the NEMO toolkit on nanoHUB

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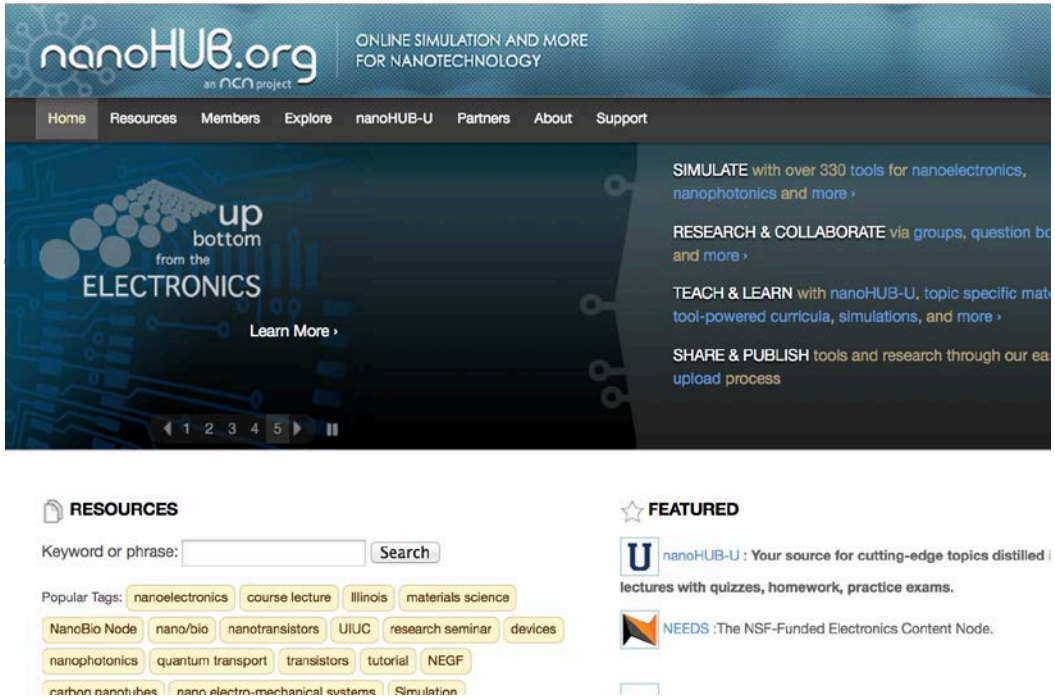
Overview

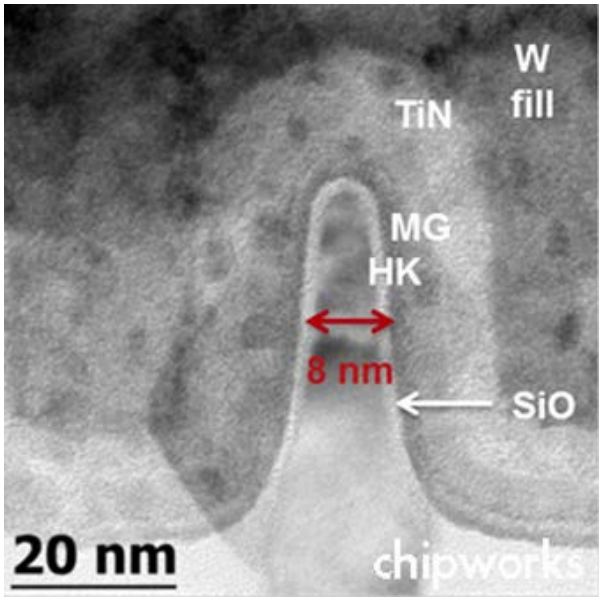
- nanoHUB
- Nanoelectronics modeling
- NEMO5 engine
- NEMO-powered nanoHUB tools
- Best practices

- 330,000 annual users
- 330 simulation tools
  - » Nanoelectronics, nanophotonics, materials science, molecular electronics, carbon-based systems Microelectromechanical systems
- 4,200 resources (video lectures, presentations, tutorials, etc.)



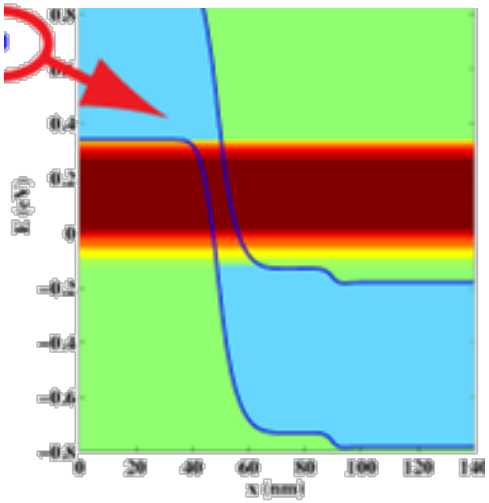
- nanoHUB-U (online courses)
  - » Nanoscale transistors (Prof. Mark Lundstrom)
  - » Fundamentals of Nanoelectronics (Prof. Supriyo Datta)
  - » From Atoms to Materials: Predictive Theory and Simulations (Prof. Alejandro Strachan)
  - » Principles of Electronic Nanobiosensors (Prof. Ashraf Alam)

Nanoelectronics Today



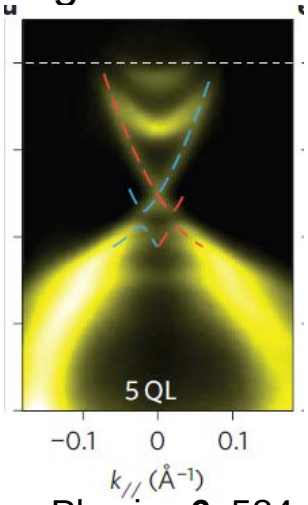
- $300 billion semiconductor industry
- International Technology Roadmap for Semiconductors (ITRS)
- Moore's Law
- Countable number of atoms
- Quantum effects
- Devices (transistors)
  - Smaller, faster, more energy efficient
  - Designs, materials

Band-to-band tunneling



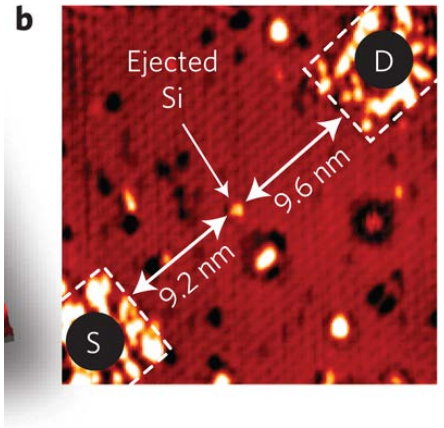
IEEE Elec. Dev. Lett. **30,** 602 (2009)

Topological insulators



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

Single atom transistors

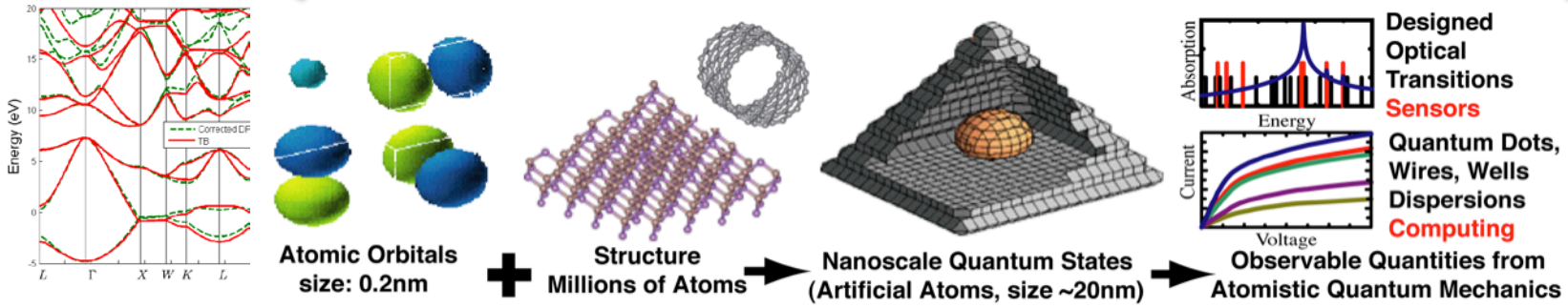


Nature Nanotechnology **7**, 242 (2012)

http://www.chipworks.com/media/wpmu/uploads/blogs.dir/2/files/2012/08/Intel22nmPMOSfin.jpg

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

Ab-Initio ⟷ NEMO5 ⟷ TCAD



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 lacks real material physics

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

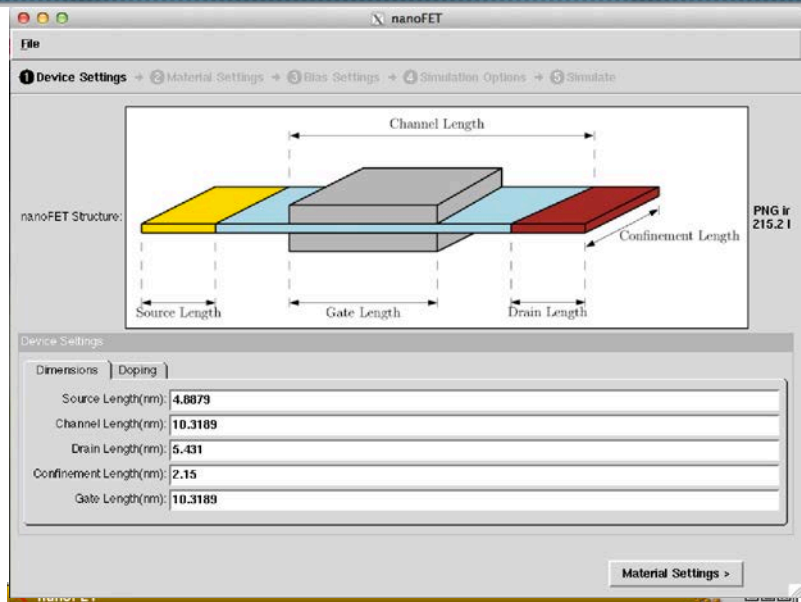
NEMO5 (on nanoHUB)

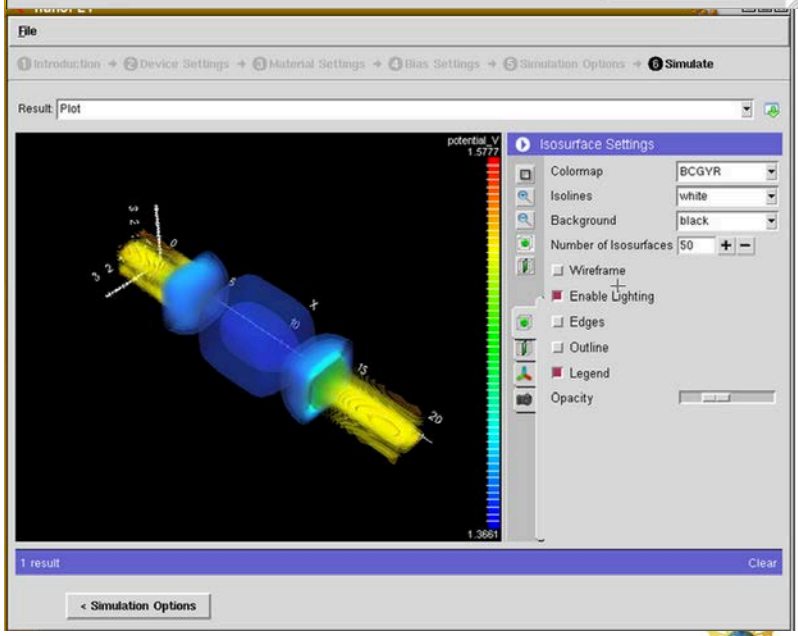
- NEMO5
  - » Academic and industrial use
  - » Free for academic use
  - » ~30 developers currently
  - » 500,000 lines of code
    - ✓ C++, python
    - ✓ 3rd party libraries
  - » Input files 100s to 1000s of lines
  - » 3 ways to use NEMO5
    - ✓ Distribution and support group on nanoHUB
      - – Source code available
      - – nanoHUB workspace → Purdue's RCAC clusters
    - ✓ nanoHUB tools

```
                    ...
solver {
    name = QTBM:bands_source_mode_contact
    type = Schroedinger
    iterator {
      set {
        active_regions = (1,2,3)
        allow_reinit_k_points = true
        automatic_threshold = true
        charge_model = electron_hole
        convergence_limit = 1.e-10
        cutoff_distance_to_bandedge = 0.05
        domain = source_mode_contact
        eigen_values_solver = krylovschur
        job_list = (assemble_H,passivate_H,
calculate_band_structure)
        k_degeneracy = 1
                    ...
      }
    }
  }
  solver {
    name = QTBM:bands_drain_mode_contact
    type = Schroedinger
                    ...
```

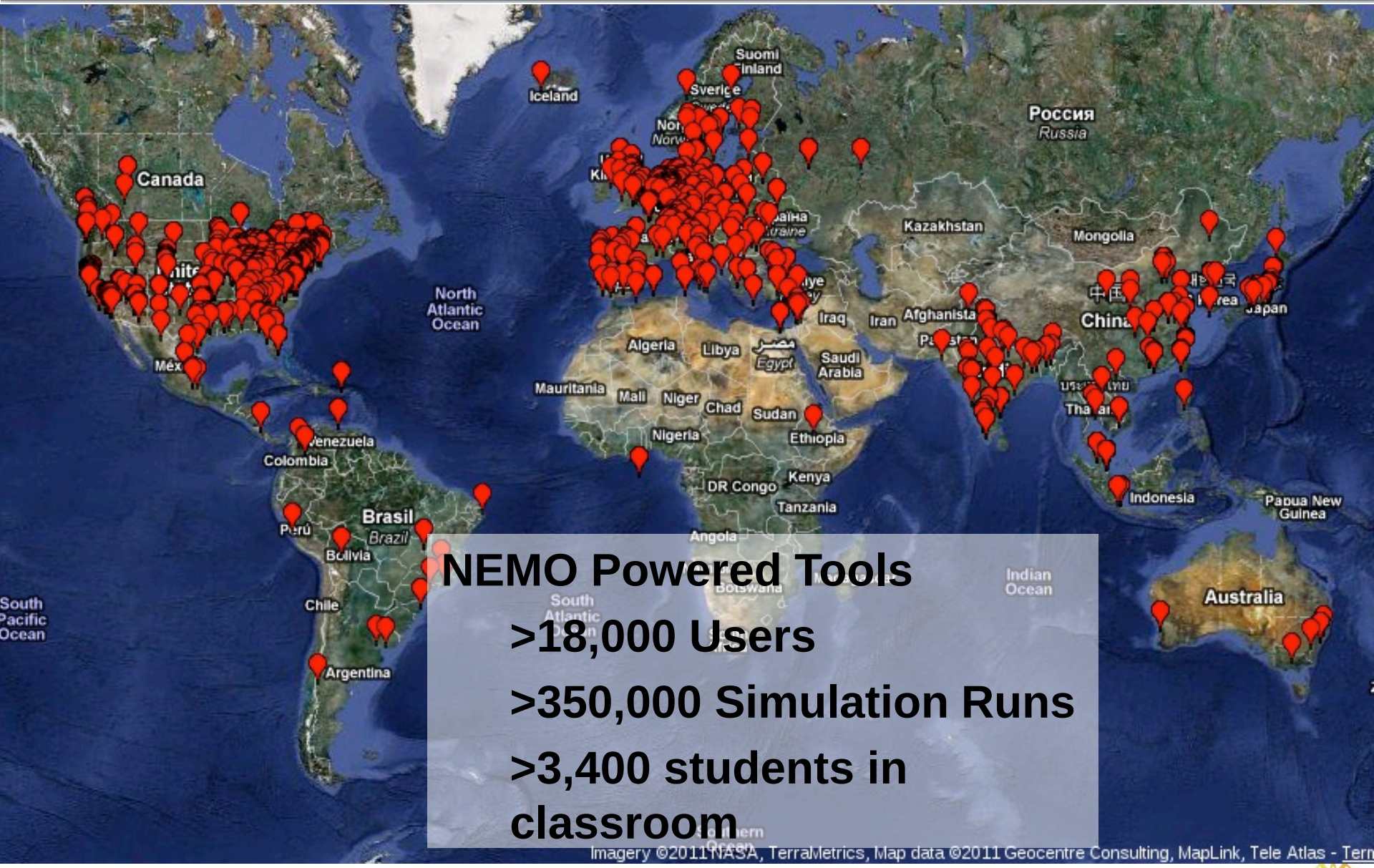
NEMO5 on nanoHUB.org

- OMEN/NEMO5-based nanoHUB tools
  - » Brillouin Zone Viewer
    - ✓ Crystal theory
  - » Crystal Viewer
    - ✓ Visualize crystals, design your own
  - » Bandstructure Lab
    - ✓ Semiconductor fundamentals
  - » 1dhetero
    - ✓ Poisson-Schroedinger Solver for 1 dimensional heterostructures
  - » RTDNEGF –
    - ✓ Calculate current through resonant tunneling diodes
  - » Quantum Dot Lab
    - ✓ Eigenstates (energy levels) of particle in a box system
  - » nanoFET
    - ✓ Calculate transport properties of transistors
    - ✓ NEMO5 powered version of OMENwire, OMEN_FET
  - » ITRS tool OMEN/PADRE/NEMO5 powered - (coming soon)





NEMO5 nanoHUB Usage



NEMO Powered Tools

>18,000 Users

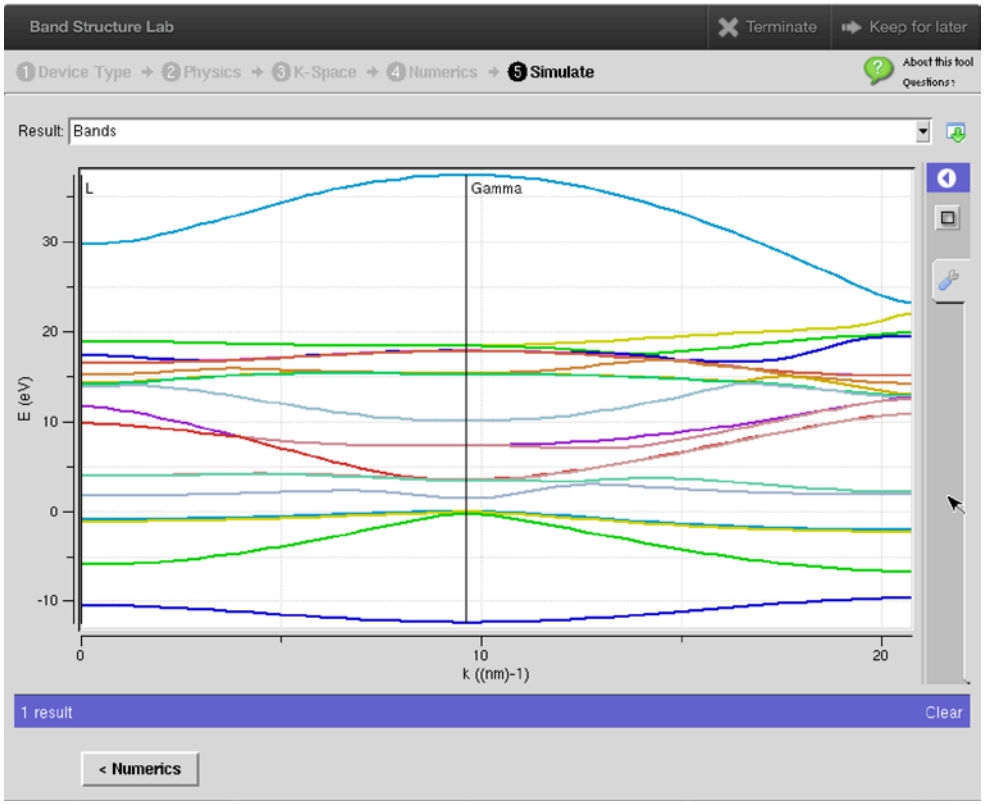
>350,000 Simulation Runs

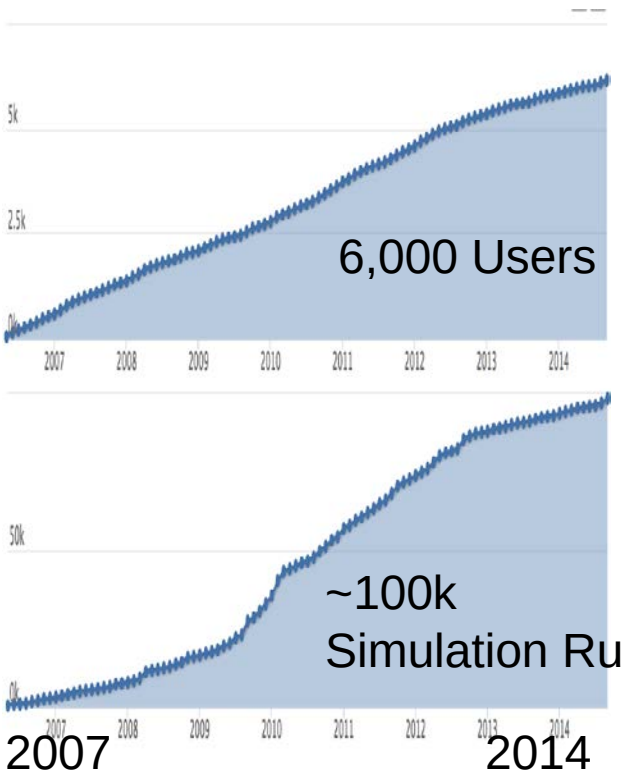
>3,400 students in classroom

Bandstructure Lab

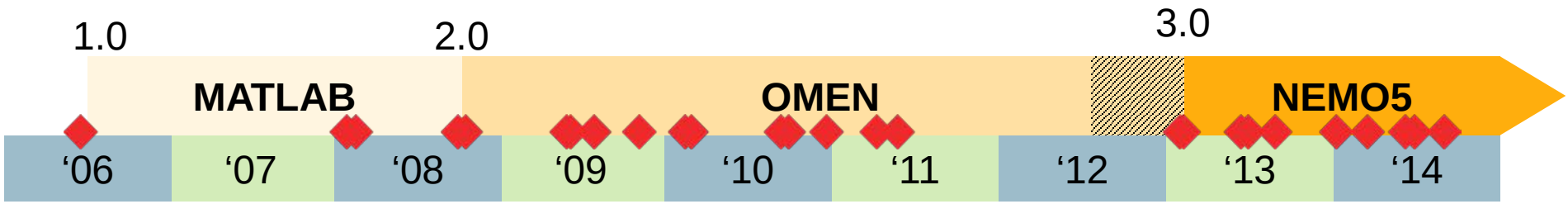
- Computes the electronic and phonon structure of various materials in the spatial configuration of bulk, quantum wells, and wires
- Various materials (Si, Ge, GaAs, etc.)

NEMO5 development -- Samik Mukherjee

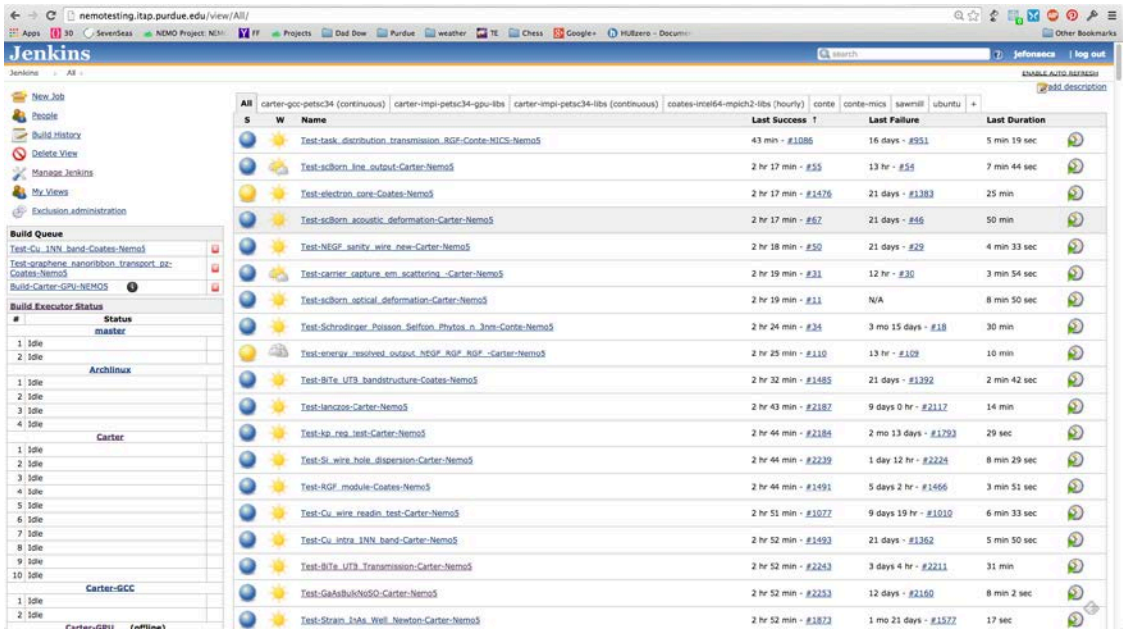




Tool Development Timeline and Testing



- ~100 svn commits of Bandstructure Lab
- ~9200 commits of NEMO5 during development
- Jenkins
  - » http://jenkins-ci.org/
  - » Continuous integration and testing system
  - » Alerts developers / owners
    - ✓ Validity
    - ✓ performance
- 12 bandstructure lab regression tests



Best Practices

- Multiple, noncurrent developers
  - » Testing
  - » activation Energy
- Development Guide and Resources
  - » Linux
  - » SVN
  - » NEMO5
  - » nanoHUB
  - » Rappture
  - » Wrapper code
    - ✓ Tcl, C
  - » HPC systems

NEMO Agenda, Funding, and Leverage

Industrial Use

Intel Samsung
TSMC Philips

Industrial Development

Tunneling Transistors GaN, MoS_2

18,000 users

NEMO5

FCRP

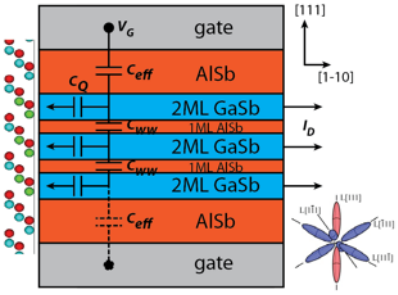
NRI

FAME

Contacts, HEMTs

NSF-NCN NSF-OCI

NSF-NEB



Peta-Scale Computing

Quantum Computing

nature nanotechnology

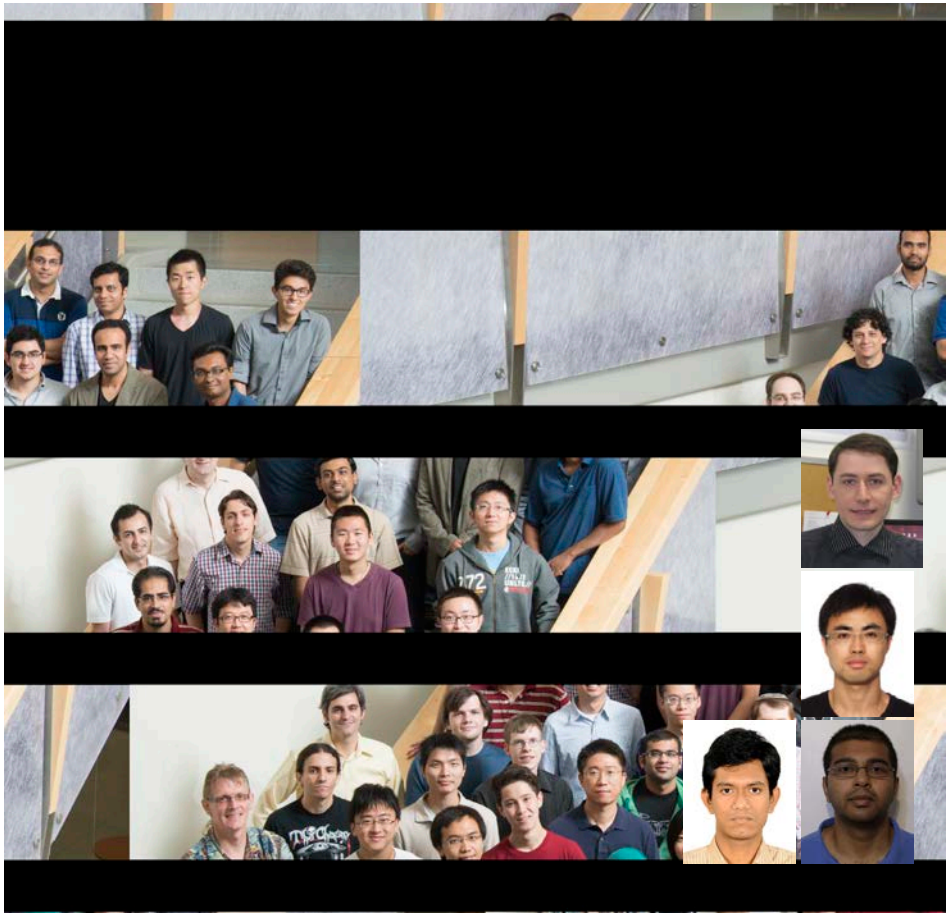
A single-atom transis

Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard

The ability to control matter at the atomic scale and build

iNEMO Group

- PI: Gerhard Klimeck
- 3 Research Faculty: Tillmann Kubis, Michael Povolotskyi, Rajib Rahman
- Research Scientist: Jim Fonseca
- 2 Postdocs: Bozidar Novakovic, Jun Huang
- Students: Kyle Aitken, **Tarek Ameen**, Yamini Bansal, James Charles, Chin-Yi Chen, **Fan Chen**, **Yuanchu (Fabio) Chen**, Rifat Ferdous, Jun Zhe Geng, Yu He, Yuling Hsueh, Jun Huang, Hesameddin Ilatikhameneh, **Zhengping Jiang**, Daniel Lemus, Pengyu Long, **Daniel Mejia Padilla**, Kai Miao, **Samik Mukherjee**, Ahmed kamal Reza, **Santiago Rubiano**, Harshad Sahasrabudhe, **Mehdi Salmani Jelodar**, **Prasad Sarangapani**, Saima Sharmin, Yaohua Tan, Yui Hong Tan, **Archana Tankasala**, **Daniel Valencia Hoyos**, KuangChung Wang, Yu Wang, **Evan Wilson**
- SURF Students: **Josef Borga, Woody Gilbertson, Kevin Margatan**, **Vincent Ntarugera**, **Travis Shepherd, Zach Schaffter**



PURDUE UNIVERSITY NEMO5