QuantumWise

www.quantumwise.com

Atomic-scale modeling platform for nanoelectronics

Anders Blom

QuantumWise at a glance

- Founded in December 2008
- Standing on the shoulders of Atomistix (2003)
- Profitable every quarter from day 1
- World-leading competence in electron transport in nanostructures, electron structure, atomic-scale modeling software development
- Services and solutions for industrial and other customers in the area of atomic-scale modeling
- Main office in Copenhagen, Denmark
  Sales offices in USA, Singapore, Japan
- Worldwide distribution and marketing partners
- >100 customers in leading electronics companies and universities around the world

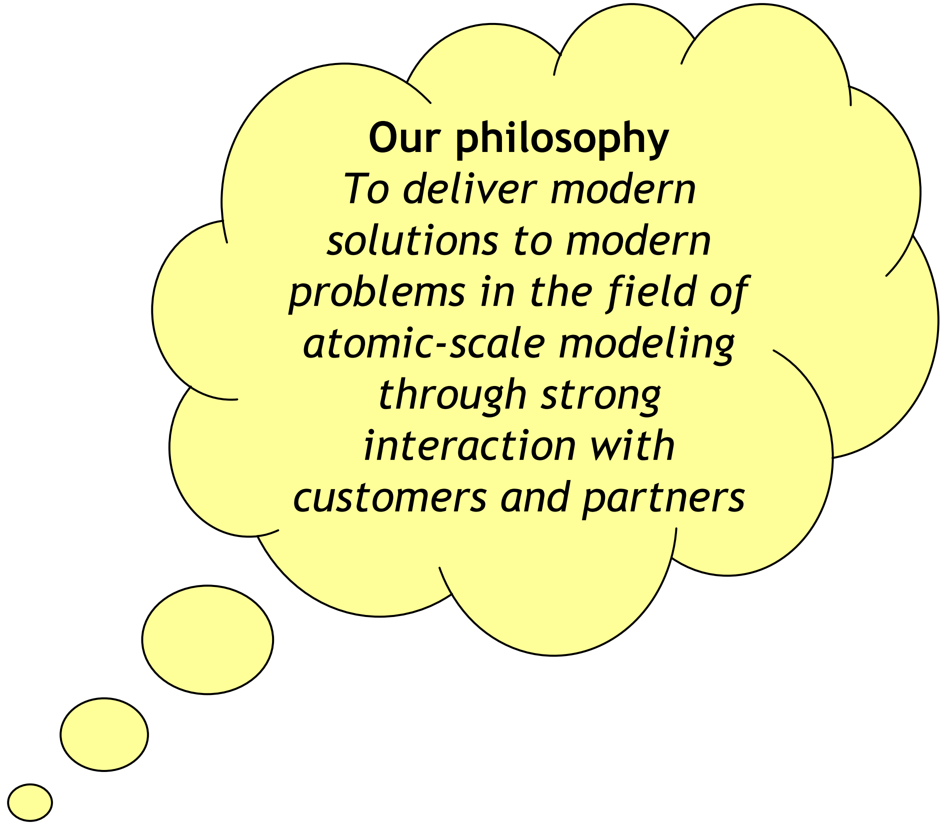
Quantum Wise

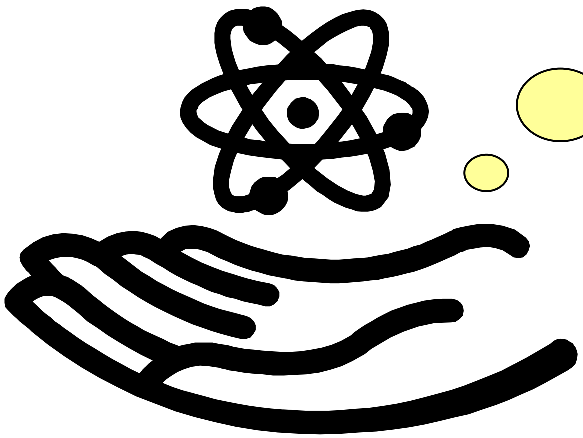
atomistix

Commercially engineered atomic-scale software
Atomistix ToolKit

What we do

Help industrial companies extract the most value possible from atomic-scale modeling

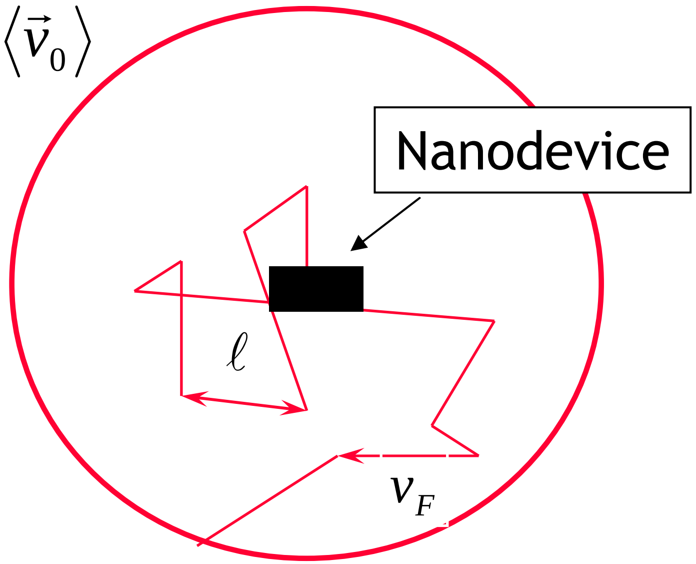




Quantum limit for electrical currents

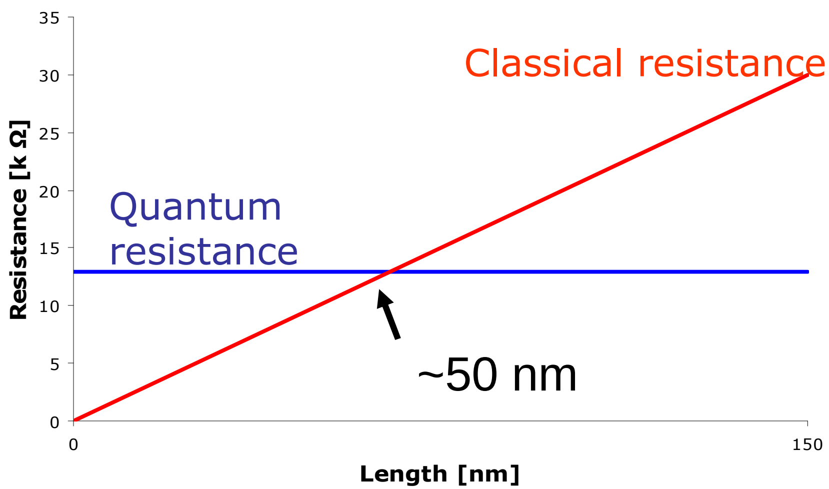
Electrons move around randomly with some average velocity

$$v_F = \langle \vec{v}_0 \rangle$$

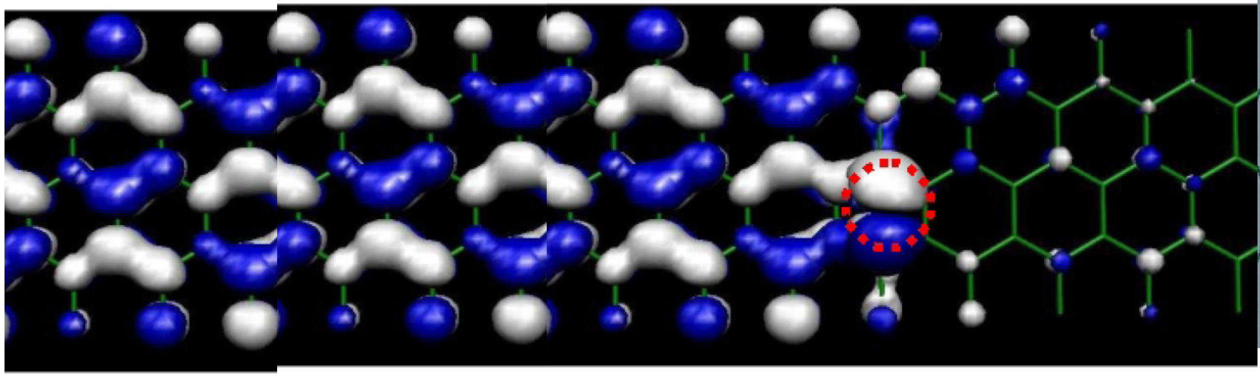


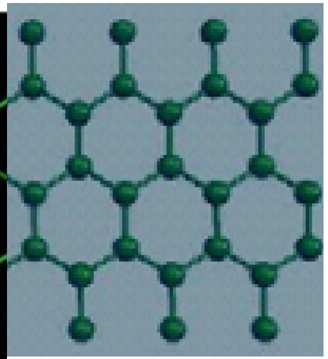
This picture breaks down when the device dimensions are smaller than the mean free path ℓ

For metals like Cu, the mean free path is about 50 nm!



Current from transmission





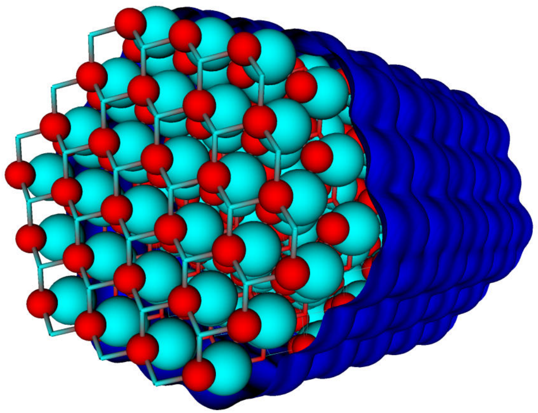
Current = propagation of wave function

Landauer-Büttiker formalism

$$I = \frac{2e^2}{h} \int dE (f_R(E) - f_L(E)) T_{\text{tot}}(E)$$

$T_{\text{tot}}(E)$: Total Quantum Transmission

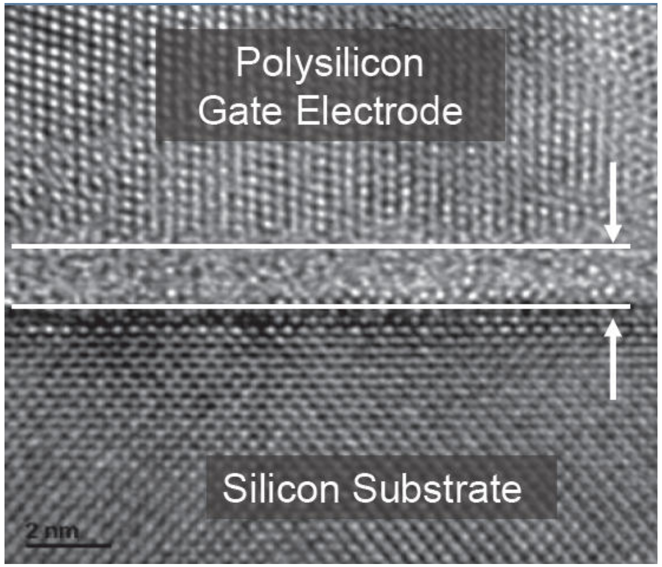
$$T_{\text{tot}}(E) = \text{Tr}[\mathbf{t}^\dagger \mathbf{t}](E)$$



Motivation

International Technology Roadmap for Semiconductors

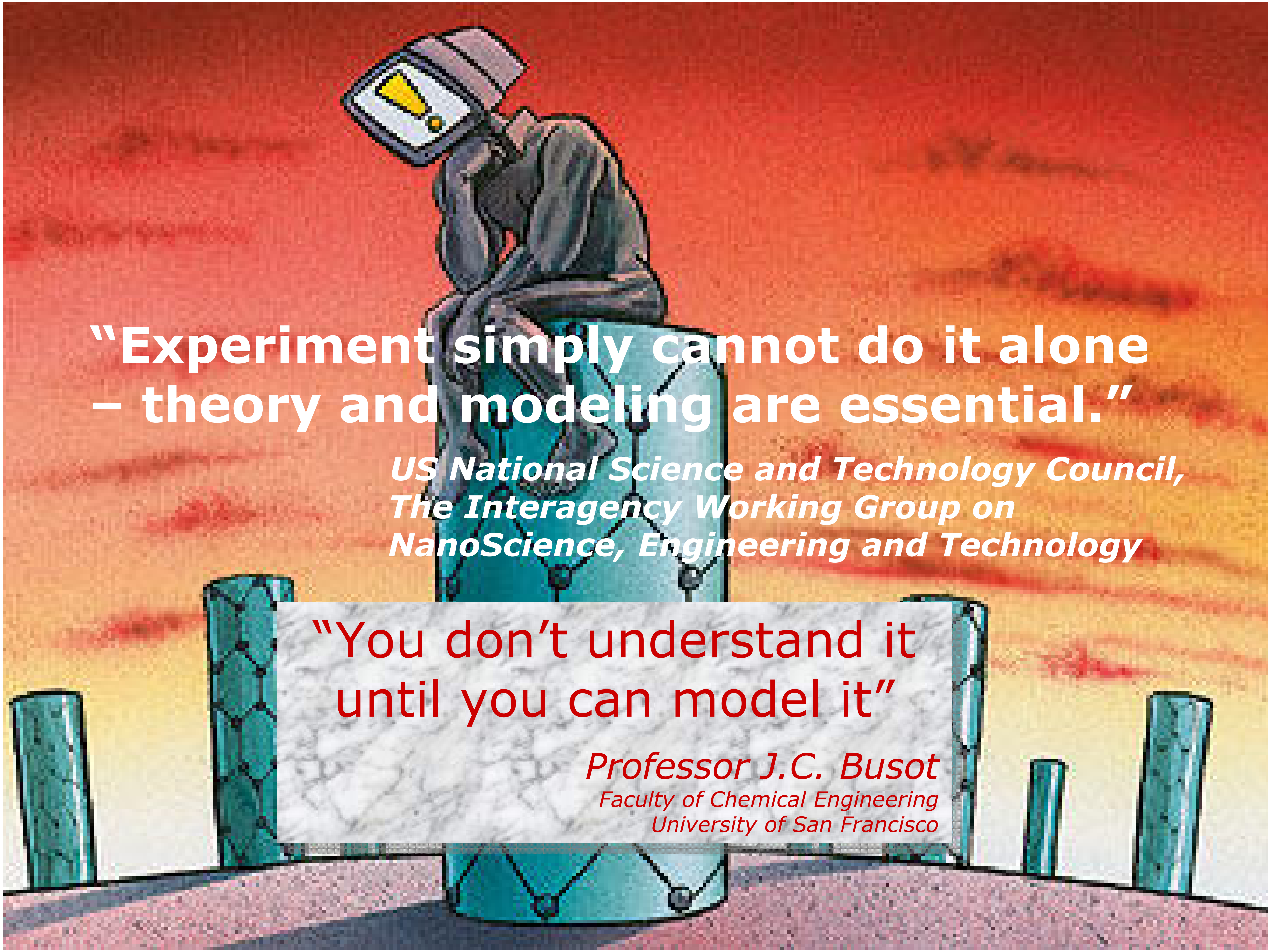
- “Atomistic” – 18 times
- “Ab initio” – 11 times (+11 “first principles”)
- “Multi-scale” – 3 times



1.2 nm SiO_2

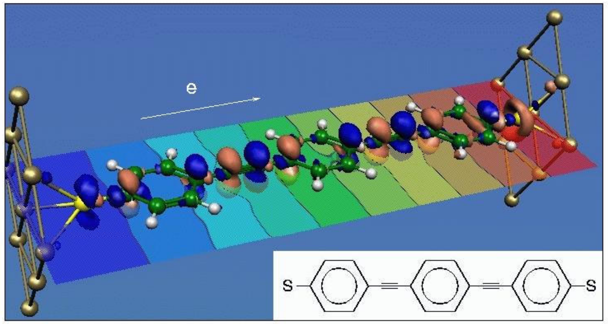
”We are running out of atoms”
Paula Goldschmidt, Intel
(2007)

“Feature size is approaching mean free path of electrons in Cu”
(P. Gargini, Intel, Semicon West 2007)

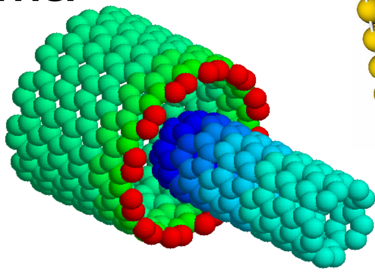

"Experiment simply cannot do it alone
– theory and modeling are essential."
US National Science and Technology Council,
The Interagency Working Group on
NanoScience, Engineering and Technology
"You don't understand it
until you can model it"
Professor J.C. Busot
Faculty of Chemical Engineering
University of San Francisco

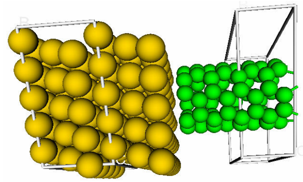
Application areas (1/2)

Molecular junctions and tunneling devices (rectification, NDR)

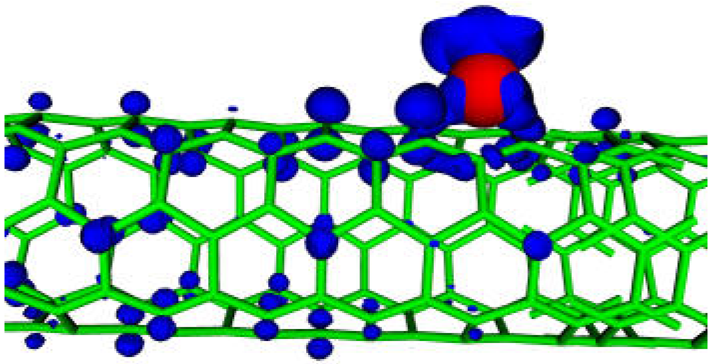


Contact resistance and capacitance of metal-nanotube and nanotube-nanotube contacts; Schottky barrier

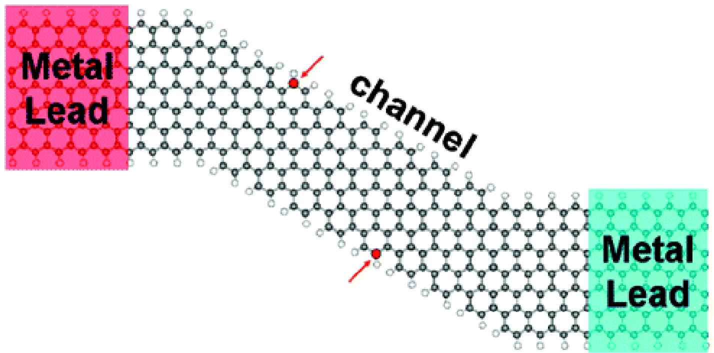




Functionalized carbon nanotubes

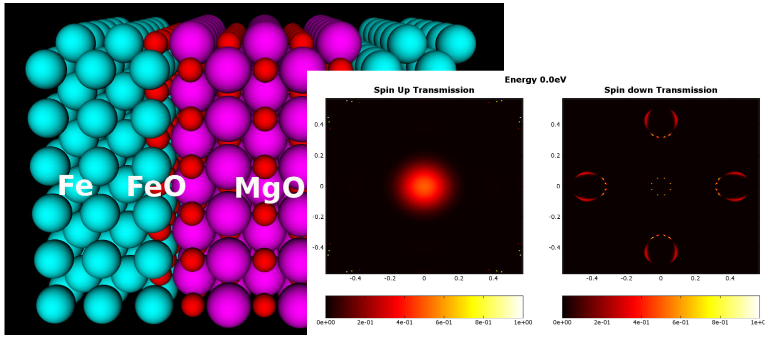


Graphene devices

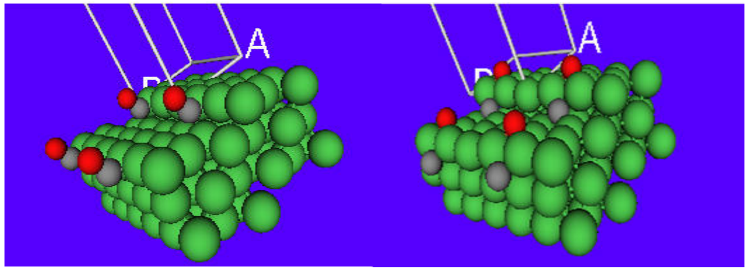


Application areas (2/2)

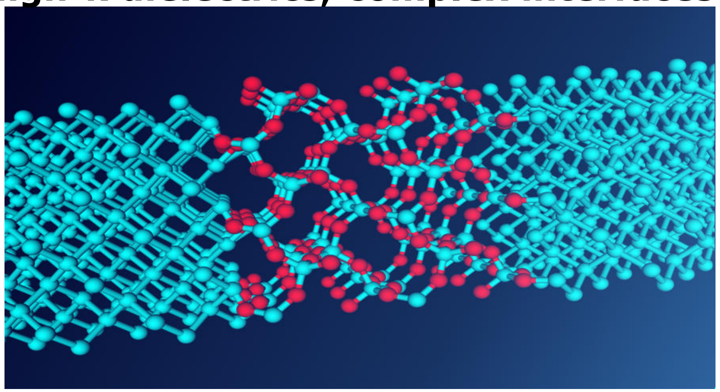
Spin-dependent transport across crystalline magnetotunnel junctions



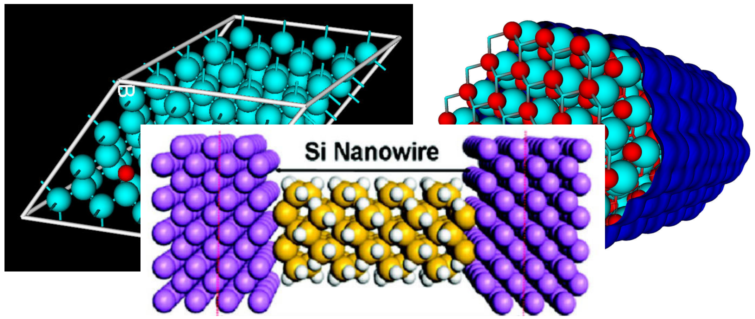
Reaction paths on surfaces for catalysis



Leakage currents in MOS structures High-k dielectrics, complex interfaces

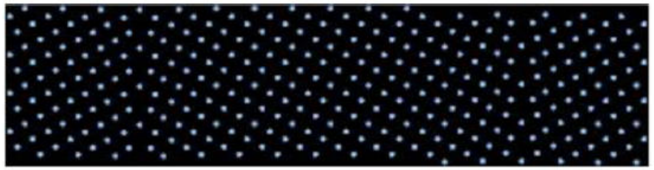


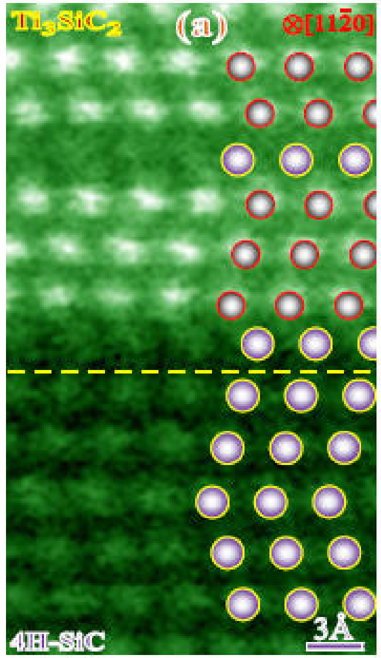
Defect states in semiconductors, nanowires, nanotubes



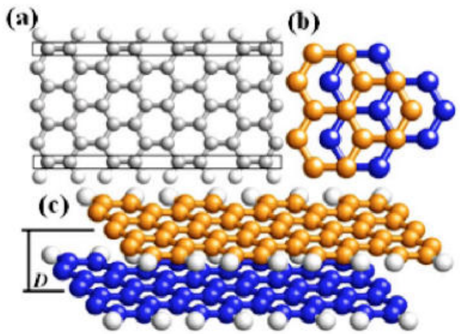
Essential points of atomic-scale device modeling

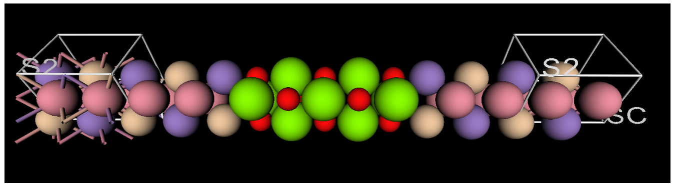
- Atomistic models
  - Defects, vacancies
  - Random alloys?





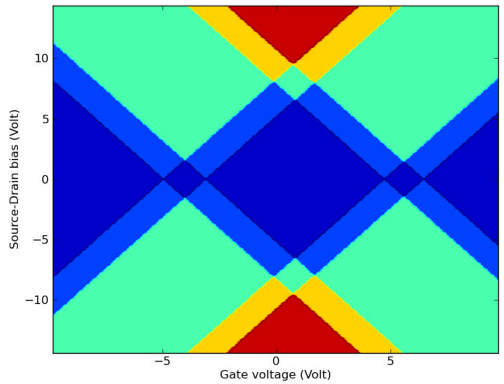
- Quantum models
  - New physics governs nanoscale conduction mechanisms





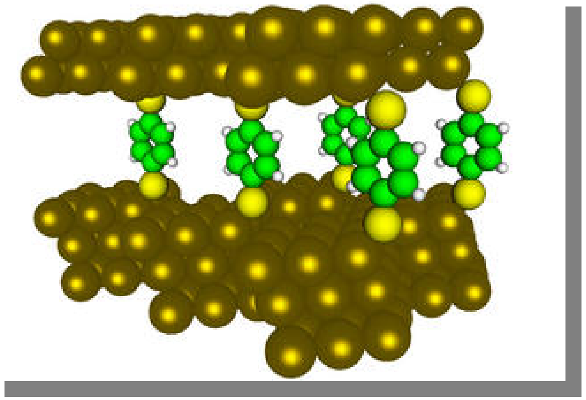
  - Features smaller than mean-free path
  - … but not always

- Accurate electronic structure
- Proper boundary conditions
- Non-linear response

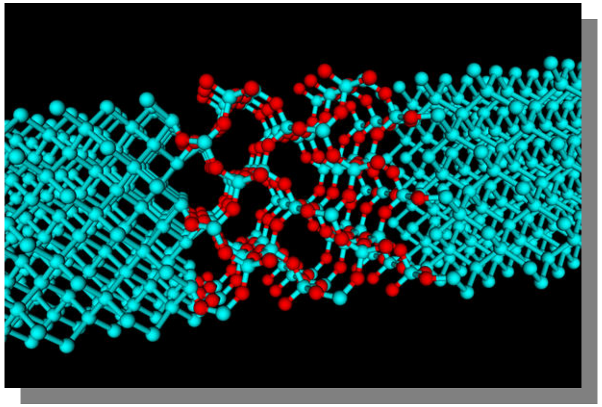


Complex boundary conditions

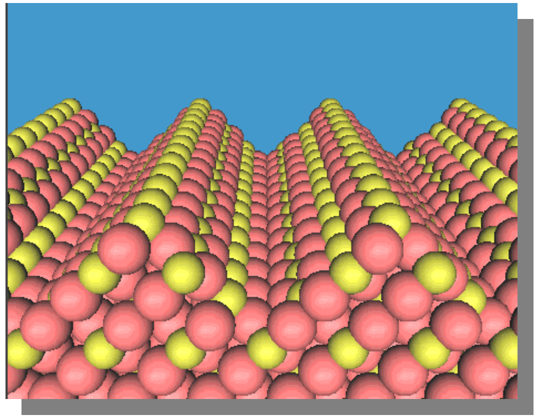
The main application areas in nanotechnology are related to effects occurring at



Junctions

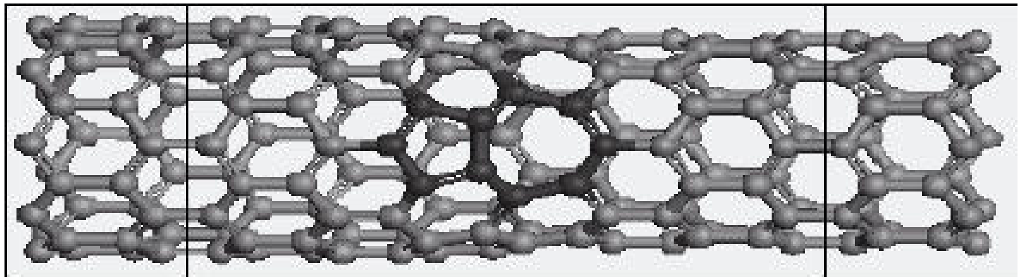


Interfaces



Surfaces

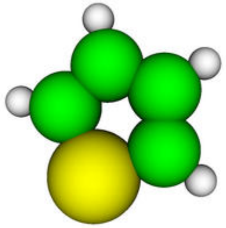
It is critical to be able to accurately model systems with complex boundary conditions from quantum theory

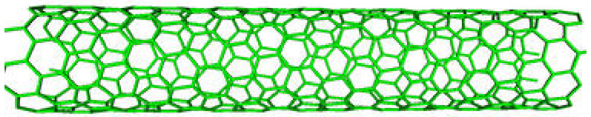


Electronic transport in nanostructures

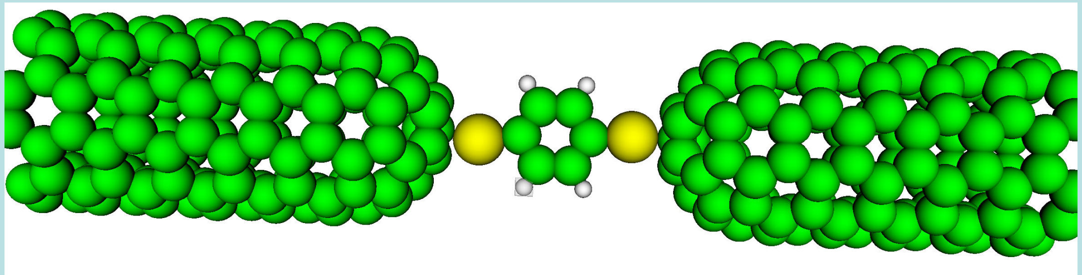
Traditional quantum-based software can model either

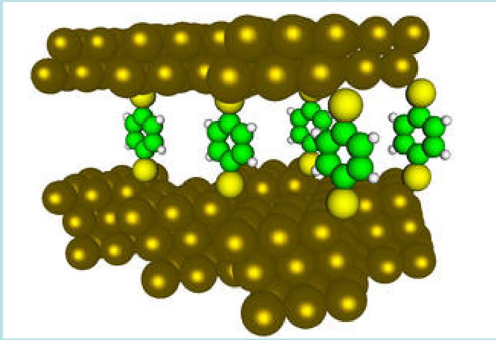
isolated molecules or periodic systems





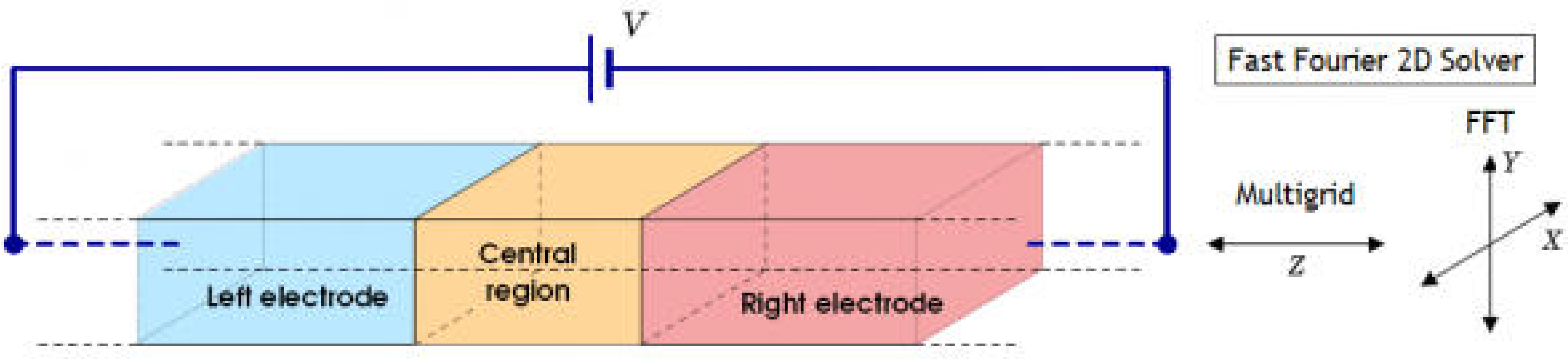
Devices are more complex; need to model nanostructures combining molecules with periodic systems and macroscopic elements

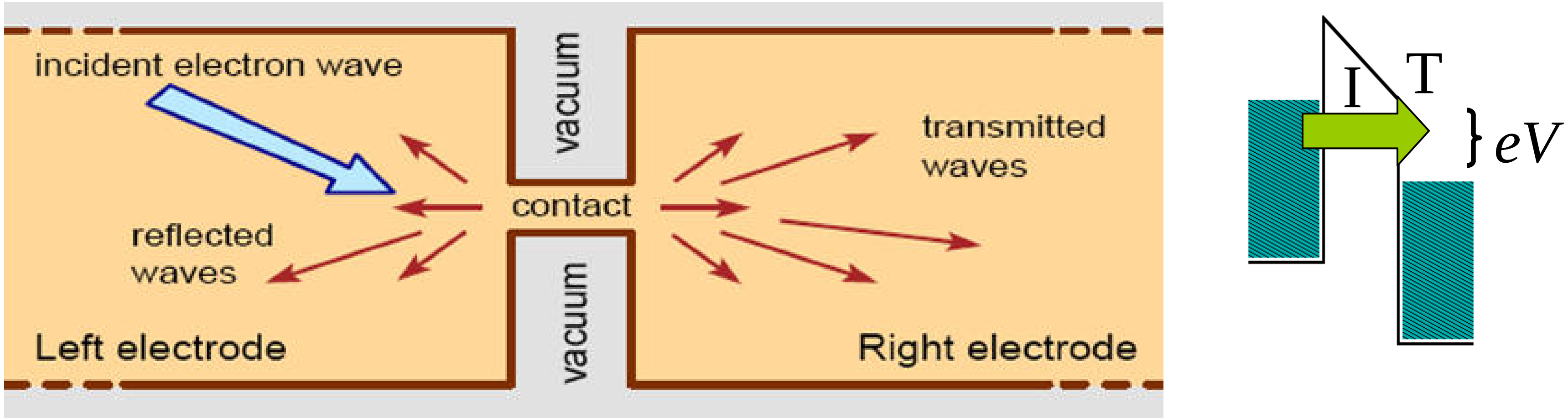




This enables simulations of electrical properties of complex nanoscale components and systems like transistors or gate stacks

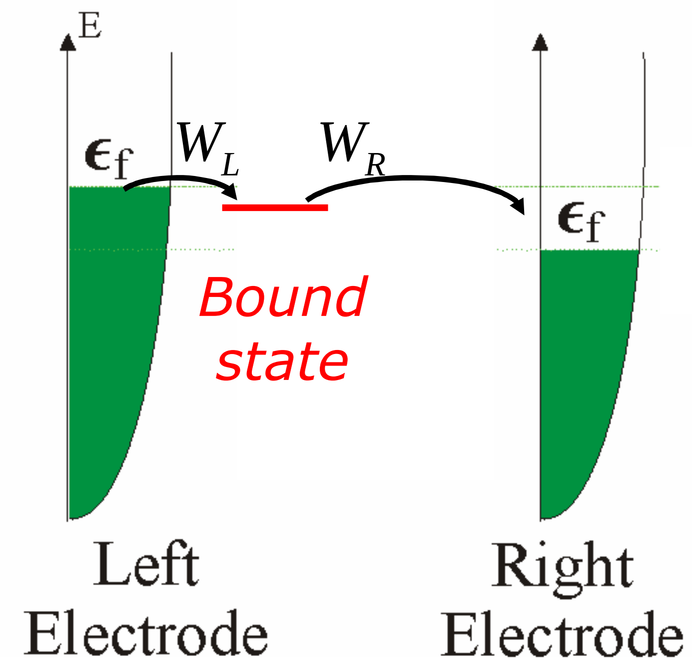
Open boundary conditions

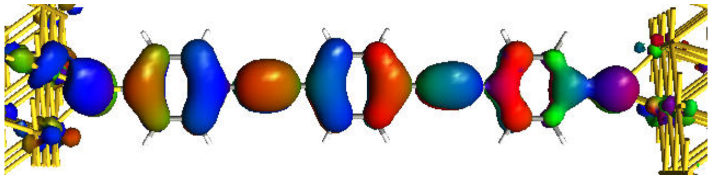


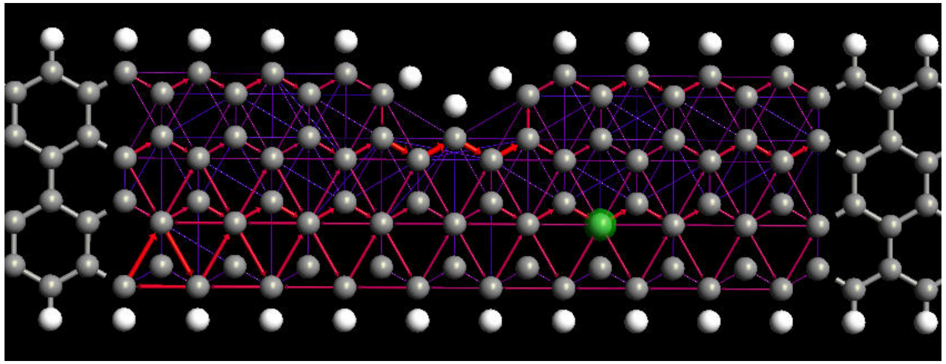


Details

- Double contour NEGF
- Include ALL matrix elements
- Complex band structure
- LDA/GGA+U, meta-GGA
- Vacuum basis sets (ghost atoms)
- Transmission for bulk systems
- Transmission pathways / eigenstates
- Krylov subspace matrix inversion







Transmission is bias-dependent

- Non-equilibrium, non-linear models needed for accurate description of transport properties
  - » NEGF
  - » Finite bias (transport boundary conditions)

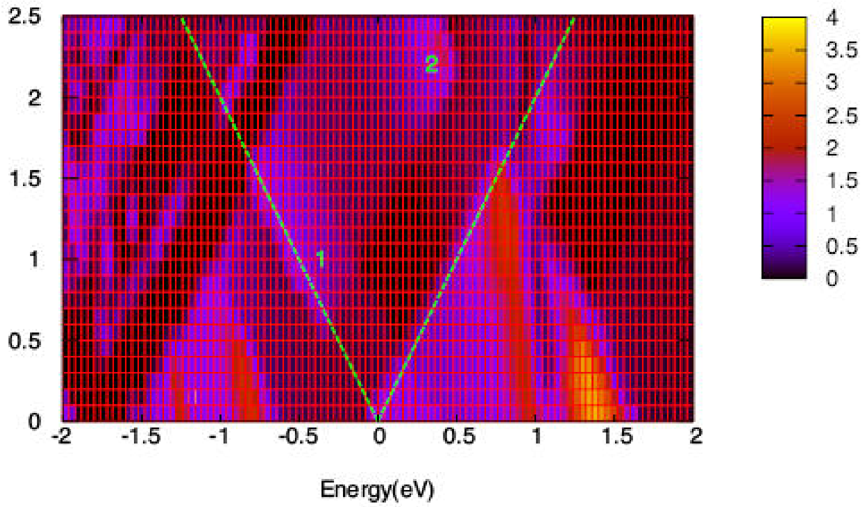
Conductance (Landauer-Büttiker)

$$I = \frac{2e^2}{h} \int dE (f_R(E) - f_L(E)) T_{\text{tot}}(E)$$

$T_{\text{tot}}(E)$: Total Quantum Transmission

$$T_{\text{tot}}(E) = \mathrm{Tr}[\mathbf{t}^\dagger \mathbf{t}](E)$$

$$\mathbf{t}(E) = (\mathrm{Im}\,[\Sigma_{\mathrm{R}}]\,(E))^{1/2}\,\mathbf{G}(E)\,(\mathrm{Im}\,[\Sigma_{\mathrm{L}}]\,(E))^{1/2}$$



Two models for the electronic structure

DFT

- Linear combination of numerical atomic orbitals (LCAO)
  - SIESTA method (own implementation)
- Finite range basis functions
  - Sparse matrices (+)
  - Non-variational (–)
- Pseudopotentials
  - Normconserving
  - Ultrasoft / PAW coming
- Hubbard U model
- Meta-GGA (coming)

J. M. Soler *et al.*,
J. Phys. Condens. Matter **14**, 2745 (2002)

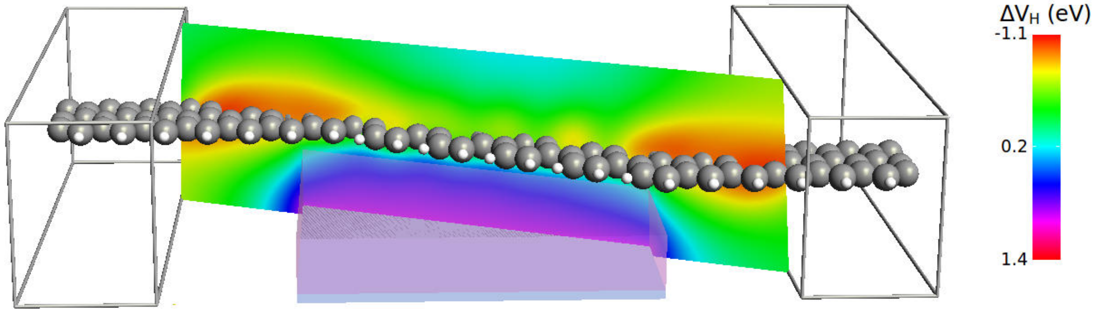
Extended Hückel

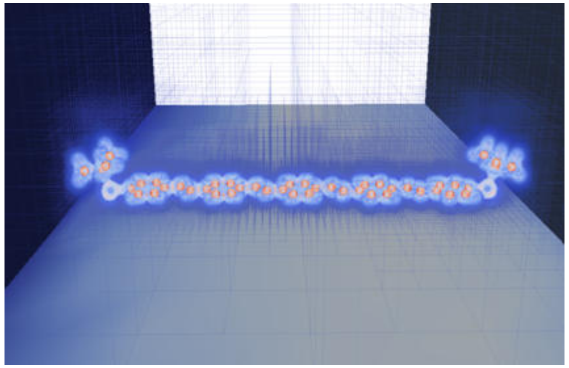
- Robust model, popular in molecular physics
- Several benefits over DFT
  - Faster
  - Larger systems
  - Tunable
- Less transferable than DFT
  - But more transferable than tight-binding
- Self-consistent Hartree term for coupling to electrostatic environment

More tight-binding models coming soon!
DFTB
User-defined TB models

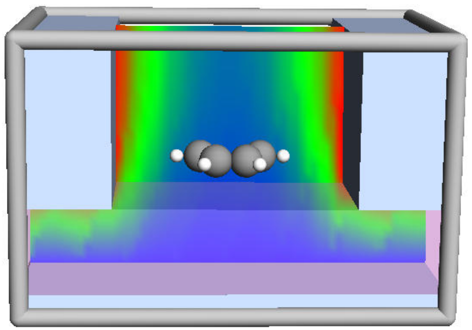
Advanced electrostatic models

- Transistor: gates & dielectric regions
  Phys. Rev. B **82**, 075420 (2010)





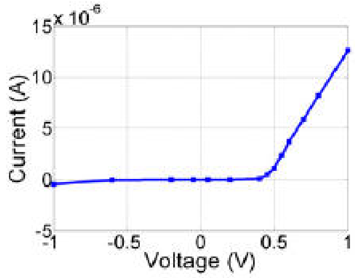
- Single-electron transistors
  J Phys Chem C **114**, 20461 (2010)

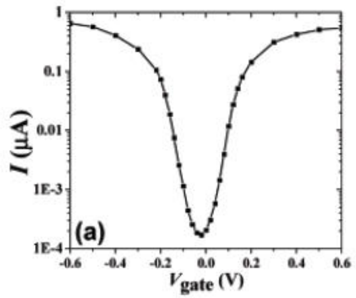


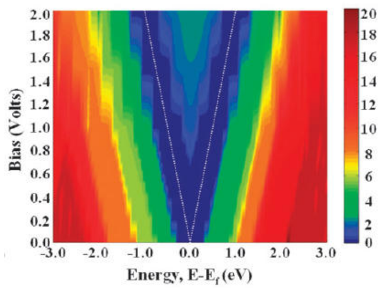
- Lots of vacuum…
  J. Avery, Ph.D. thesis (2011)

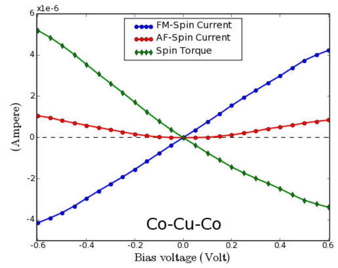
Finite bias calculations

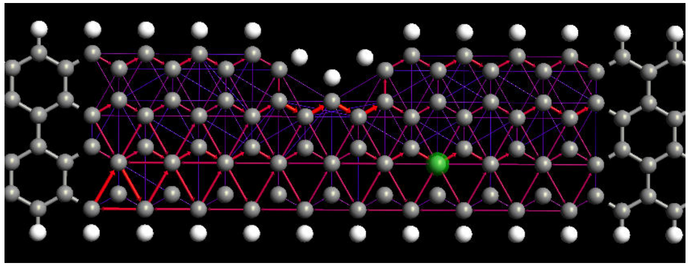
- Source-drain bias
  - Non-equillibrium electron distribution
  - Charge flows (steady-state)
- Calculate I–V characteristics
  - Schottky barrier height
  - Leakage current
  - Charge transfer
  - NDR, rectification, switching
  - Conductance
  - Tunnel magneto-resistance
  - Spin current
  - Contact resistance
- Advanced electrostatics
  - Transistor characteristics via explicit metallic gates and dielectric screening regions
  - Implicit solvent model
- Analyze transmission properties
  - Transmission coefficients/channels, pathways
  - Projections (DOS, molecular levels)



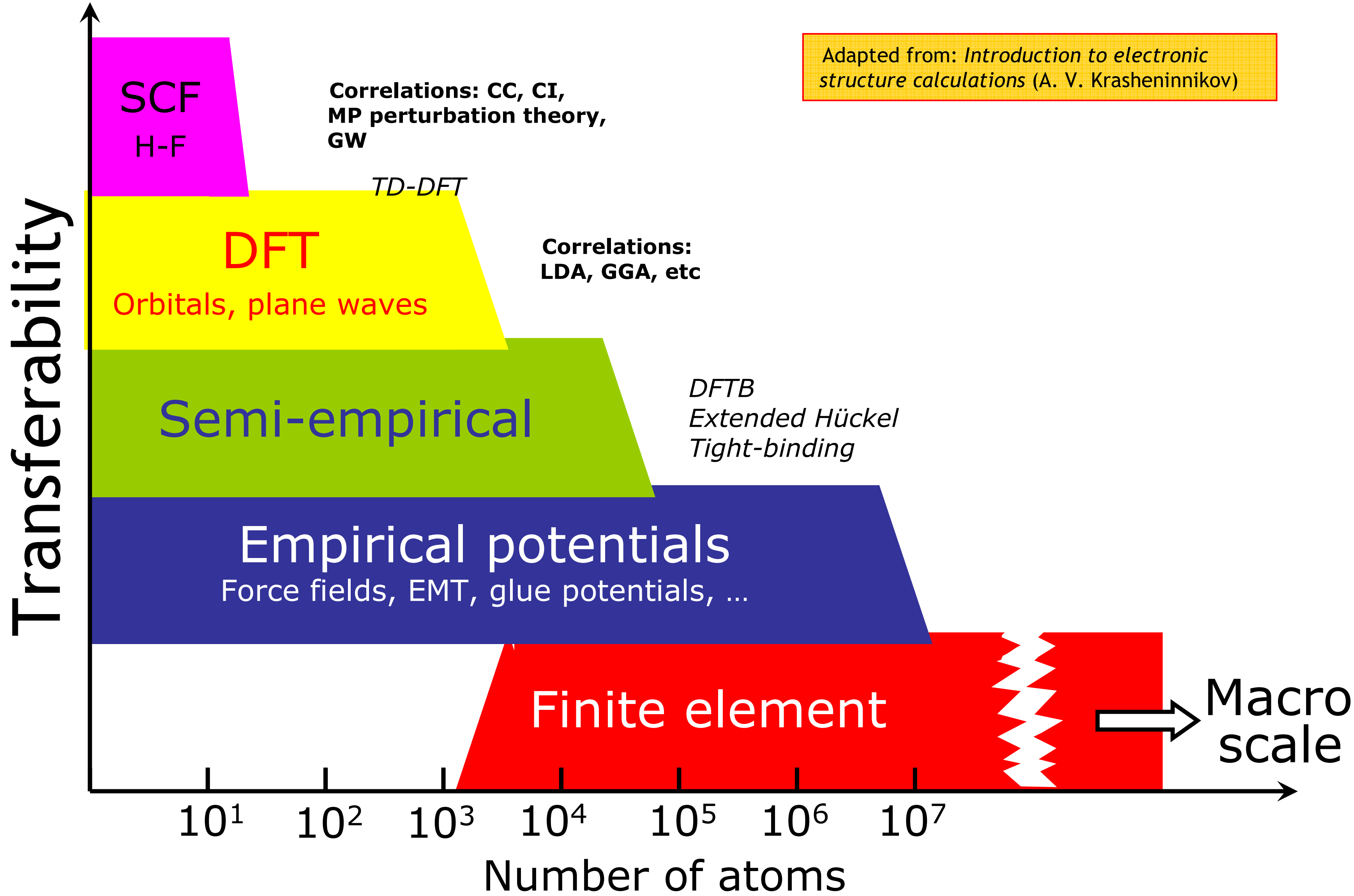








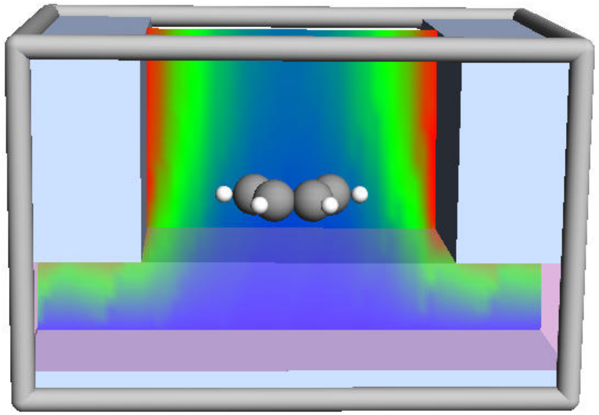
Multi-scale across length and time scales



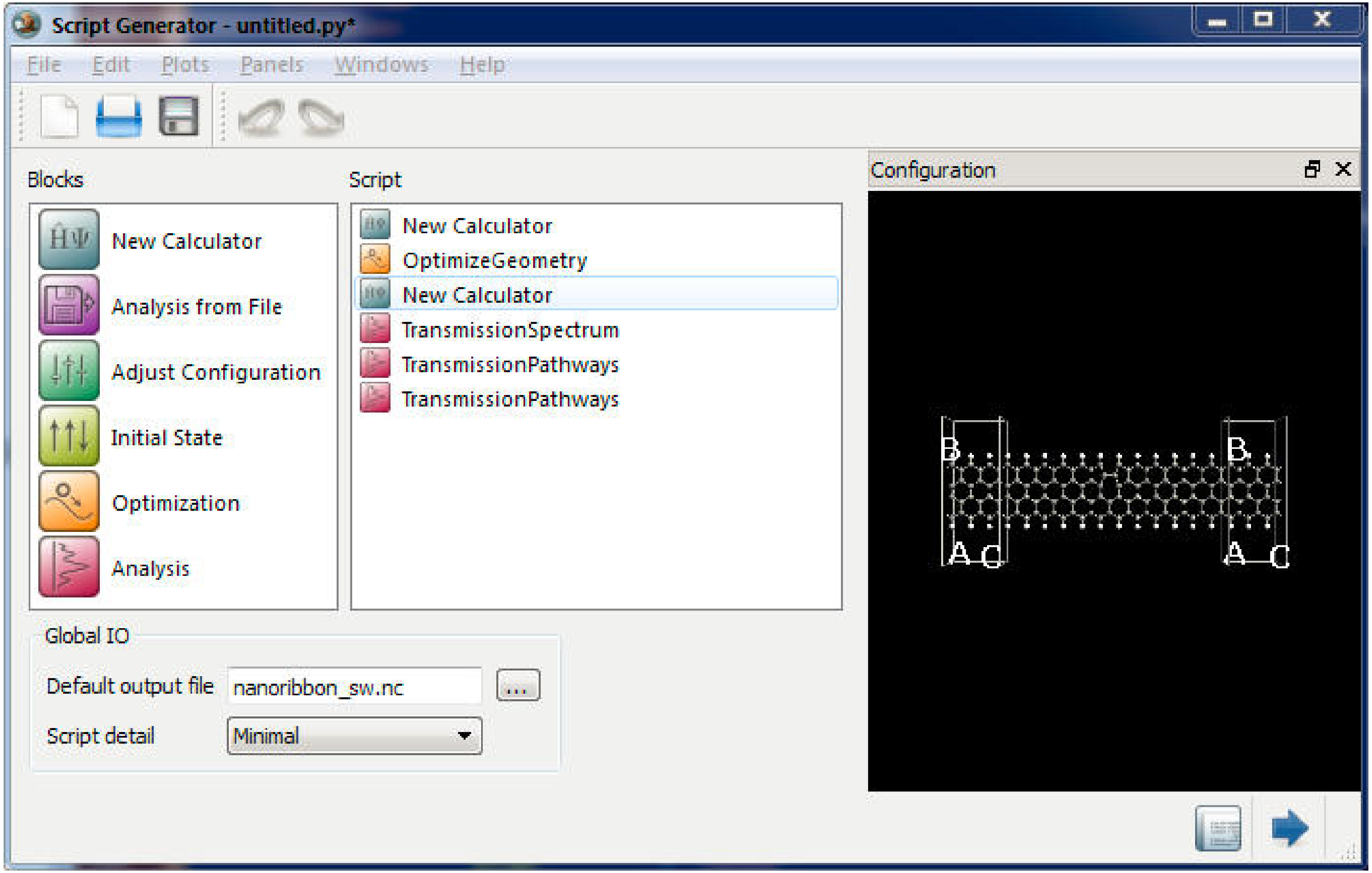
Adapted from: *Introduction to electronic structure calculations* (A. V. Krasheninnikov)

Multi-scale

- Models feeding models
  - » Parameter food chain
  - » Surrogate modeling
- Integrate models
  - » Quantum atomic
  - » Classical atomic
  - » Continuum



Combining different simulation engines




Every user and
every problem is different

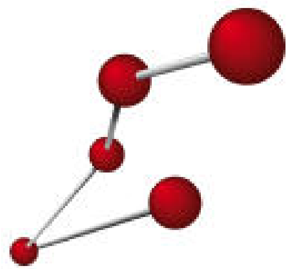
Don’t reinvent the wheel

- Large amount of commonality among codes and methods
  - Matrix storage
  - Self-consistent loop
  - I/O – reading parameters, writing data files
  - Poisson equation
  - Computing standard quantities – band structure routes etc
  - Plotting
  - Etc, etc

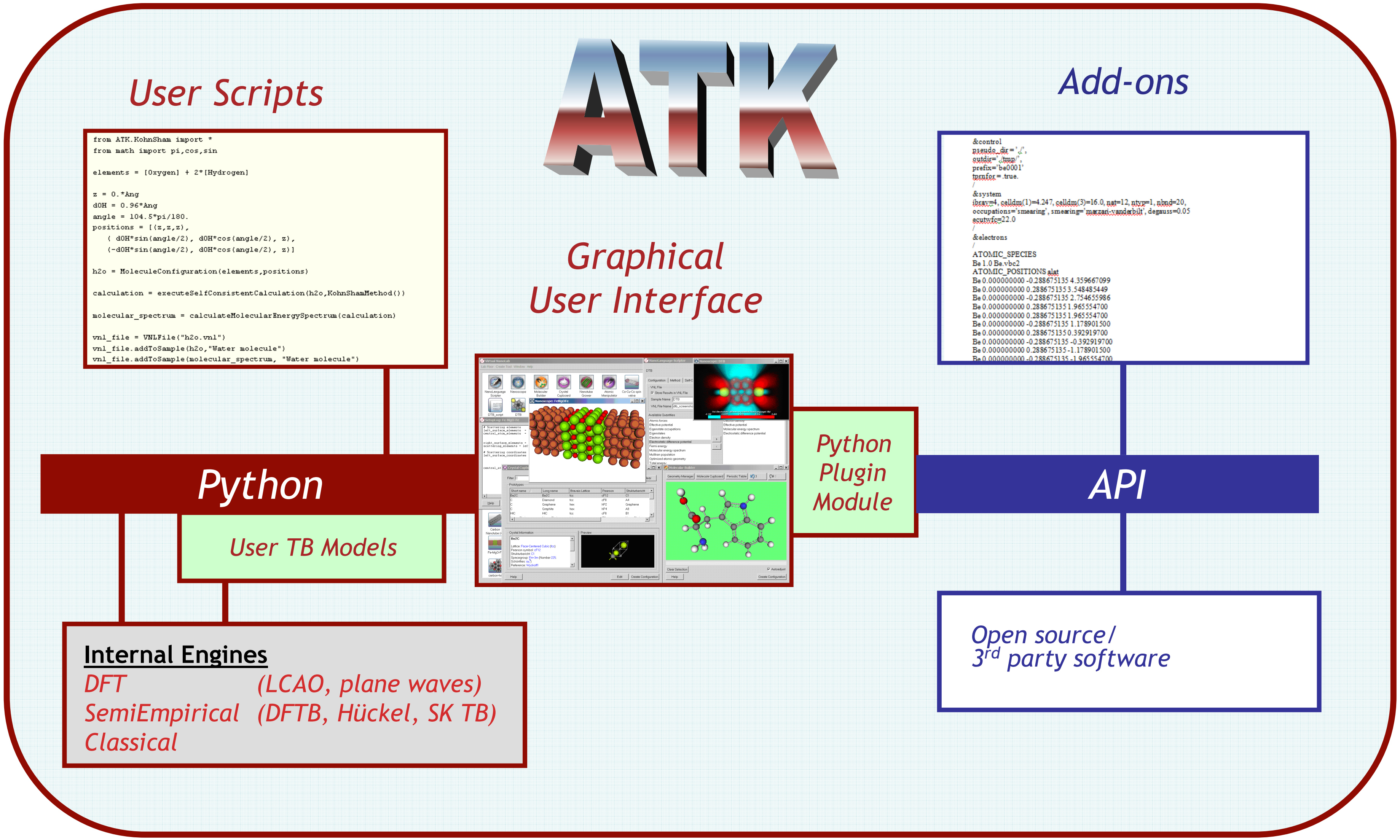
The solution?

- This is not a unique problem to atomic-scale modeling. Look around!

- Let’s make an open platform, with “apps”/plug-ins, for atomic-scale modeling

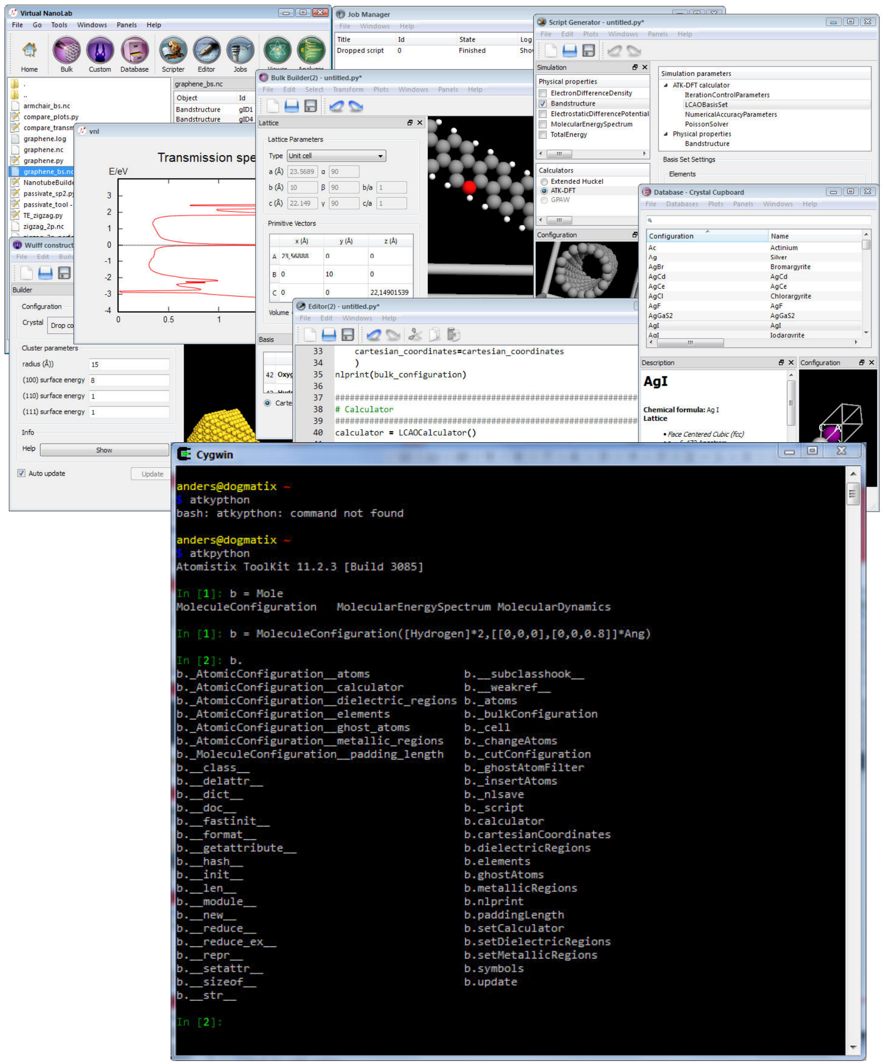


Software platform

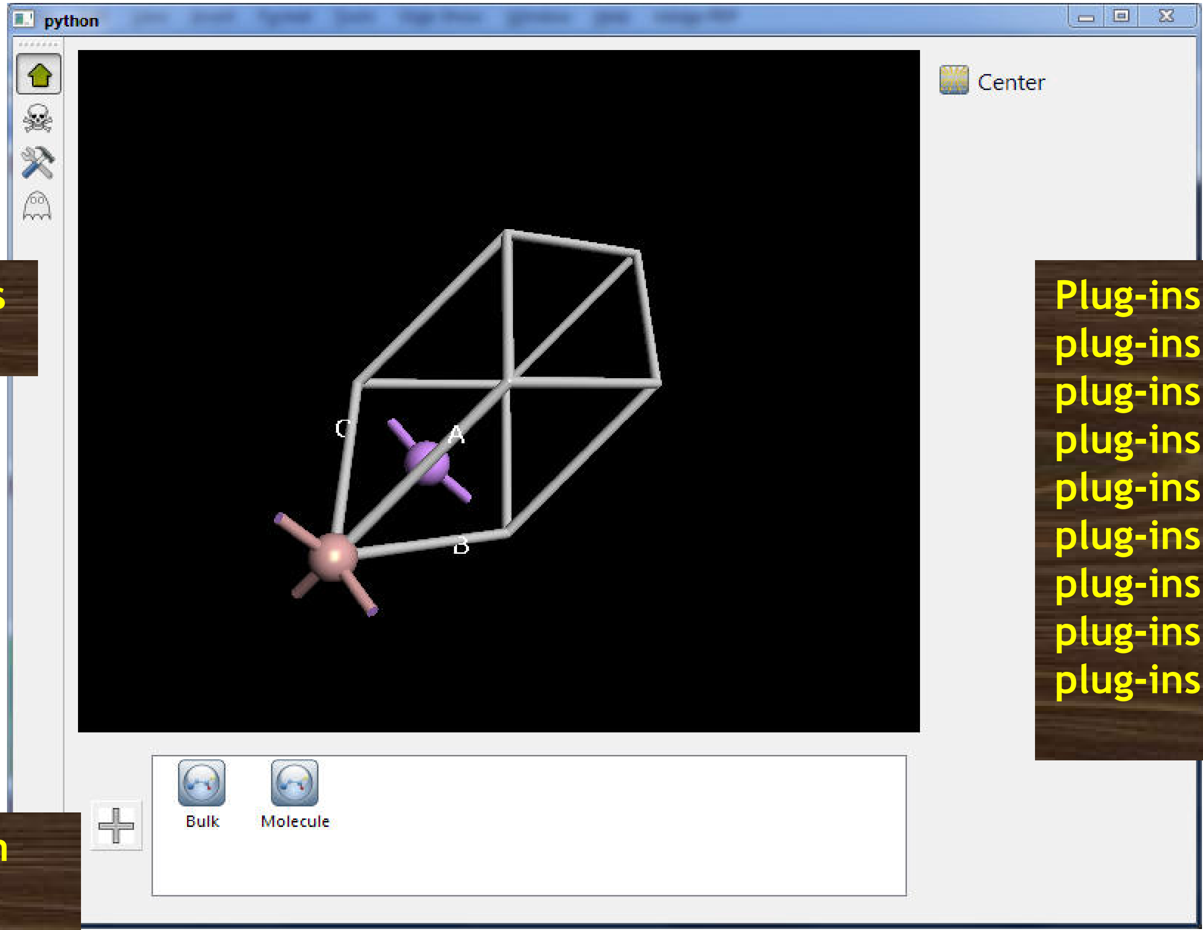


Programmable

- GUI is a thin API with direct Python bindings
- User can implement and share plug-ins for everything
  - » Building structures
  - » Wrapping external codes
    - Setting up parameters and models)
    - Running external codes
    - Importing result files
  - » Operations on computed data
    - Calculations
    - Plotting
- Command-line ATK interface is a fully programmable Python engine
  - » Interactive
  - » GUI is too, with PyQt for buttons, menus, windows, etc



VNL 11.8 Builder



Add custom buttons to toolbar

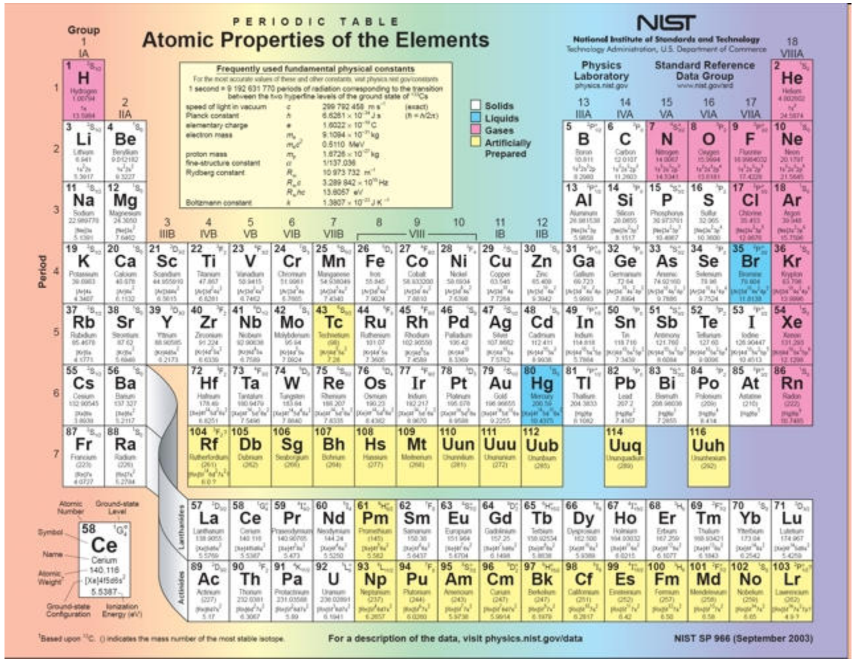
Plug-ins, plug-ins, plug-ins, plug-ins, plug-ins, plug-ins, plug-ins, plug-ins, plug-ins,

Add structures from
- File
- Database
- Template generator

Manipulate and combine several structures

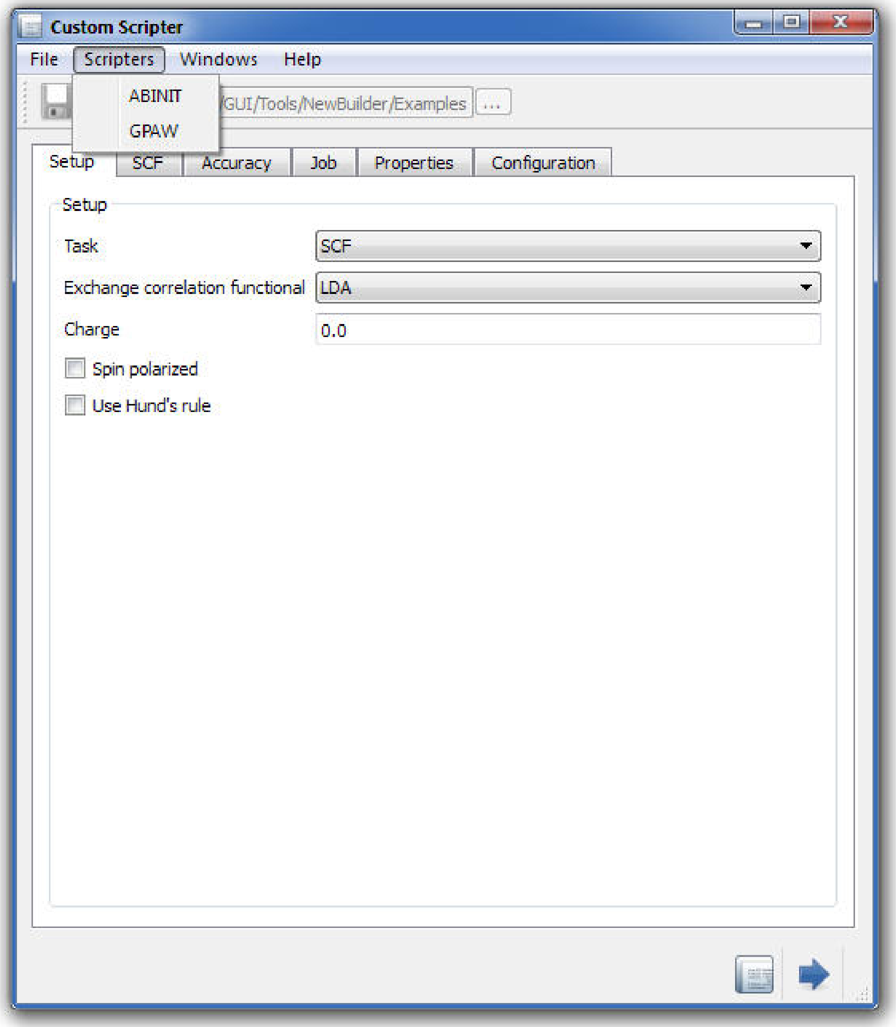
BYO (Bring Your Own) Method

- Integrate your own Slater-Koster tight-binding model in our framework
- Automatic addition of spin polarization
- Pair potentials for geometry optimization
- NEGF transport
- Sparse matrix format – minimize memory footprint
- GUI with advanced tools for geometry setup
- Python scripting, data handling, plotting, etc



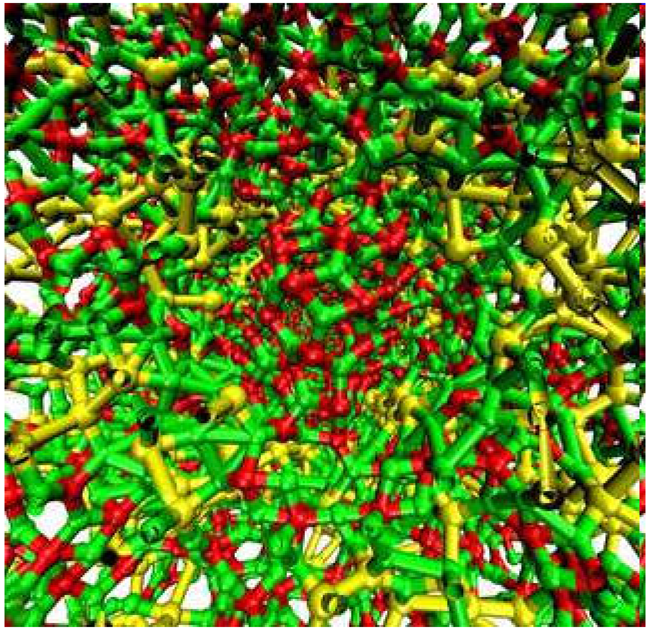
Integrate your own code

- Use our platform to generate input files for your own code
- GUI with advanced tools for model setup
- GUI widgets for setting parameters
  - API allows any PyQt code
- Push a button to generate all input files
- Convert datafiles to our open NetCDF format, and we can also visualize the data
- Plans also include "runner wrappers" so VNL can launch the job



Thermal / mechanical

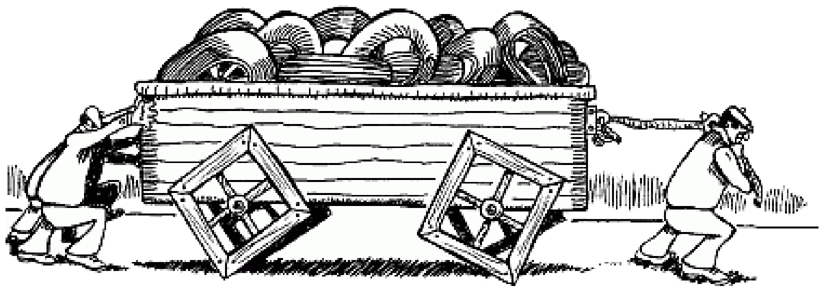
- Large systems – classical models needed
- Materials – parameters?
  - Gaussian Approximation Potentials
    A. Bartok-Partay, Ph.D. thesis, University of Cambridge, 2009
- Phonon transport
- Electron-phonon coupling



Courtesy of M. Griebel group, Fraunhofer-SCAI

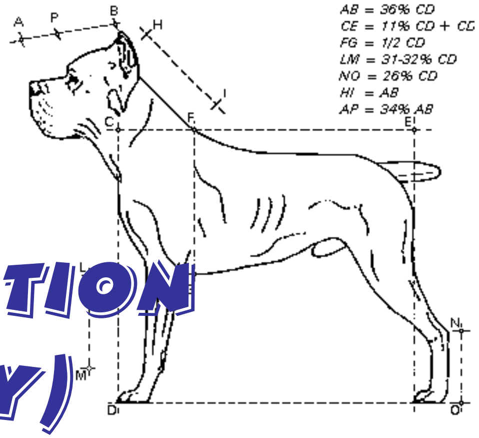
Summary

- Leverage commonality
  - Don't reinvent the wheel)
  - Open platform
- Multi-scale – in practice
- Focus on the problem, not the method
  - Multiple methods in one package
  - It's ok to approximate
- Europe is strong on software – US (and Japan) on applications



Discussion points

❖ Do we agree on what the terms mean – and which implications they have?



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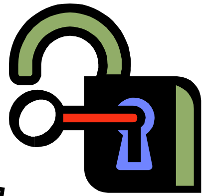

STANDARDIZATION (LEGITIMACY)

PLATFORM

COMMERCIAL ⇔ COMMUNITY

Thank you

for your attention!