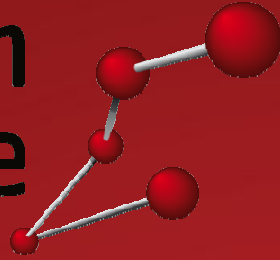


Quantum  
Wise



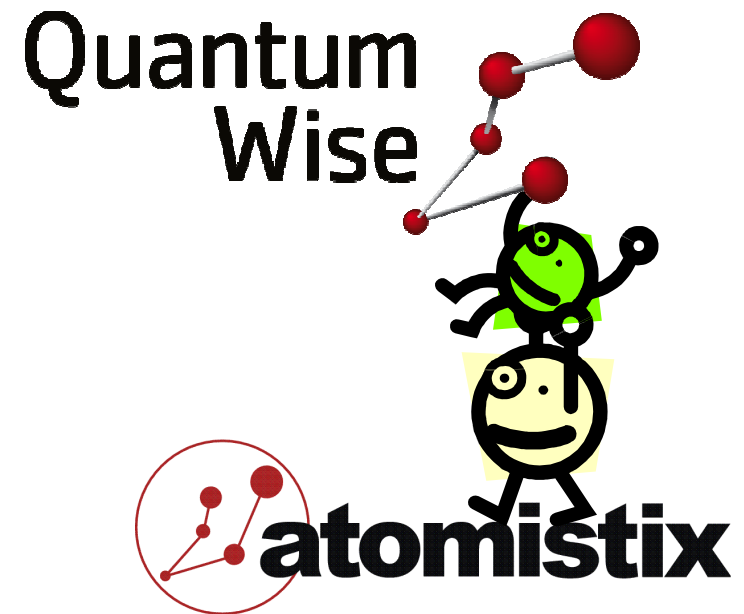
[www.quantumwise.com](http://www.quantumwise.com)

Atomic-scale modeling platform  
for nanoelectronics

Anders Blom

# QuantumWise at a glance

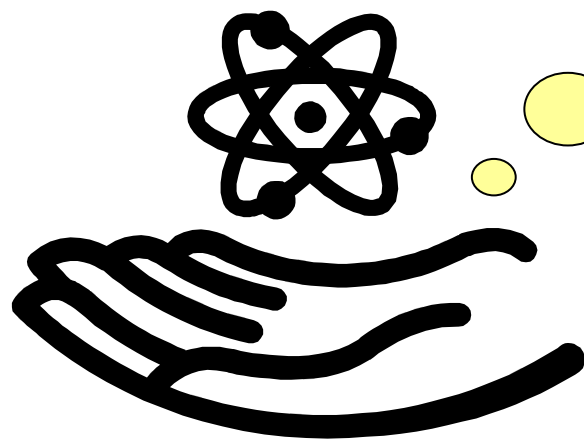
- ❖ Founded in December 2008
- ❖ Standing on the shoulders of Atomistix (2003)
- ❖ Profitable every quarter from day 1
- ❖ World-leading competence in electron transport in nanostructures, electron structure, atomic-scale modeling software development
- ❖ Services and solutions for industrial and other 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



**Commercially engineered  
atomic-scale software**  
Atomistix ToolKit

## What we do

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

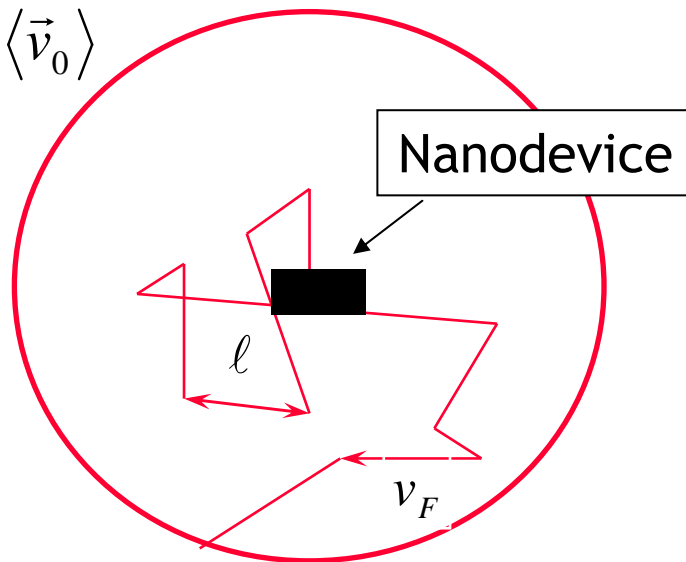


**Our philosophy**  
*To deliver modern solutions to modern problems in the field of atomic-scale modeling through strong interaction with customers and partners*

# Quantum limit for electrical currents

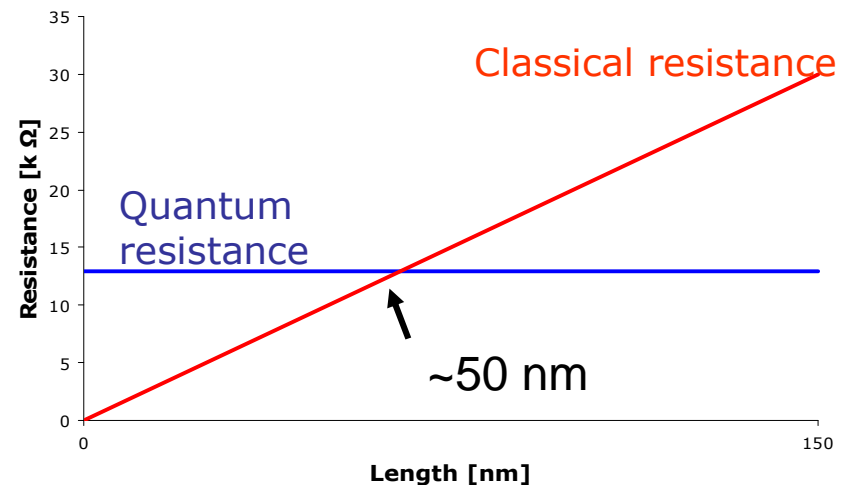
Electrons move around randomly with some average velocity

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

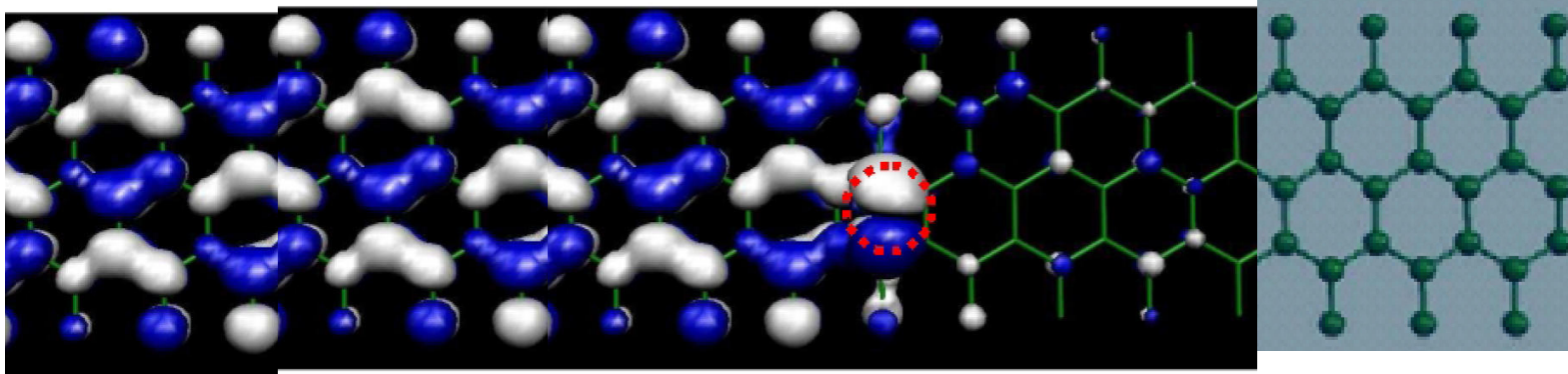


*This picture breaks down when the device dimensions are smaller than the mean free path  $\ell$*

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



# Current from transmission



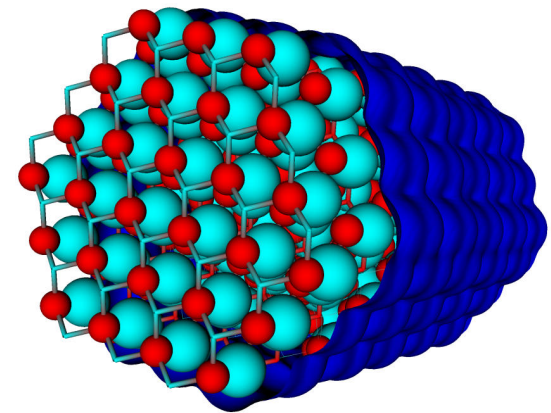
Current = propagation of wave function

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

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

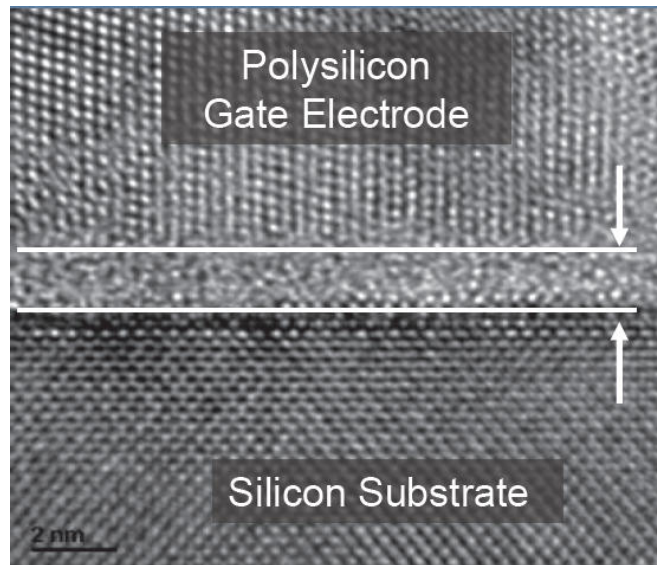


# Motivation



International Technology Roadmap for Semiconductors

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



“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.”**

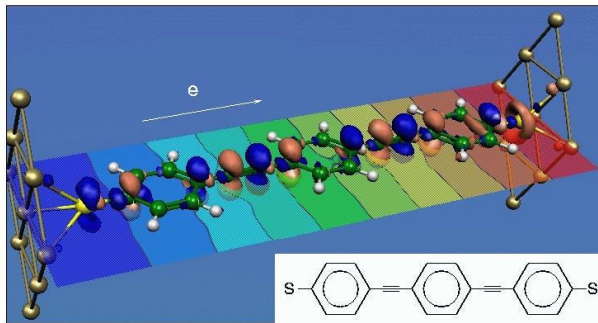
*US National Science and Technology Council,  
The Interagency Working Group on  
NanoScience, Engineering and Technology*

**“You don’t understand it  
until you can model it”**

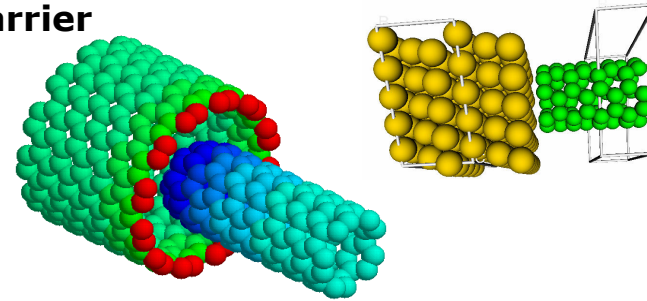
*Professor J.C. Busot  
Faculty of Chemical Engineering  
University of San Francisco*

# Application areas (1/2)

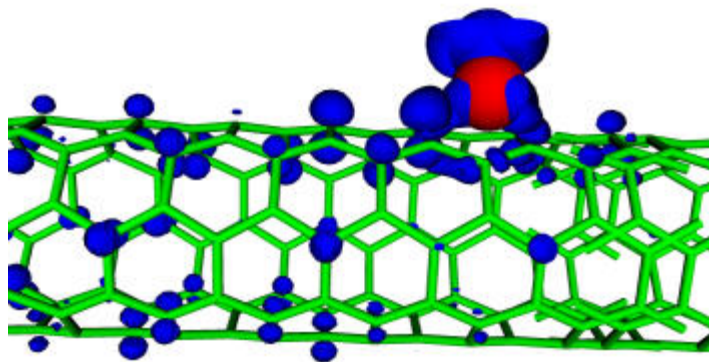
## Molecular junctions and tunneling devices (rectification, NDR)



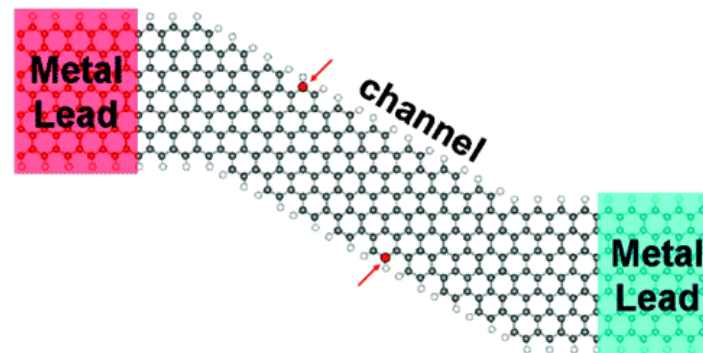
## Contact resistance and capacitance of metal-nanotube and nanotube-nanotube contacts; Schottky barrier



## Functionalized carbon nanotubes



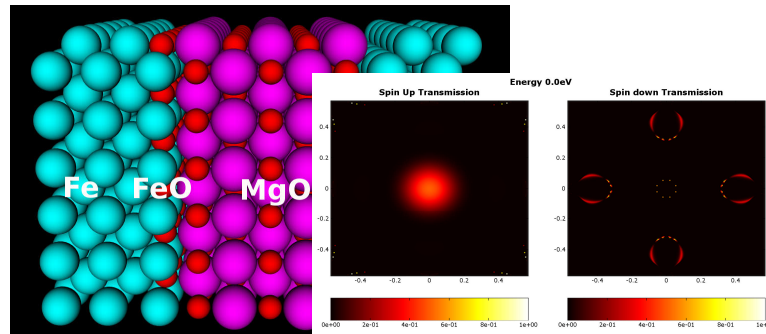
## Graphene devices



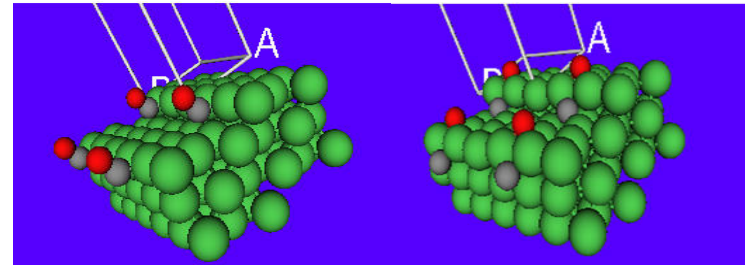


# Application areas (2/2)

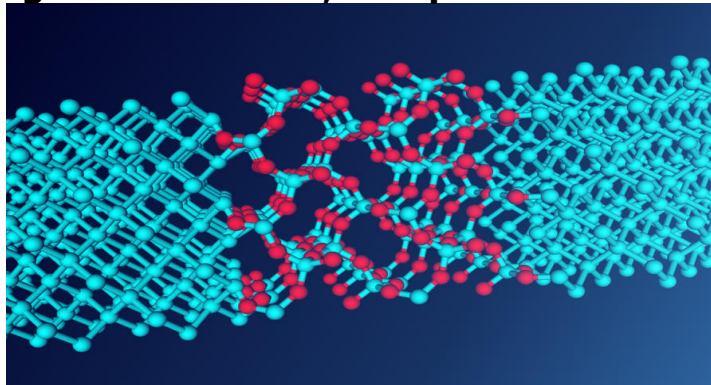
## Spin-dependent transport across crystalline magnetotunnel junctions



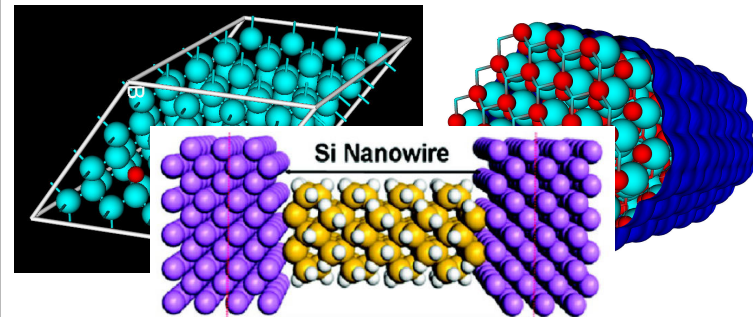
## Reaction paths on surfaces for catalysis



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

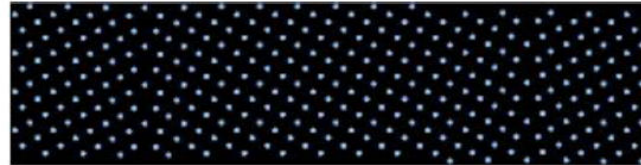


## Defect states in semiconductors, nanowires, nanotubes

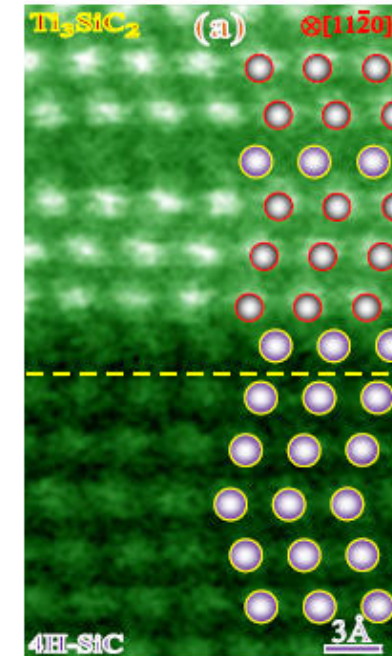
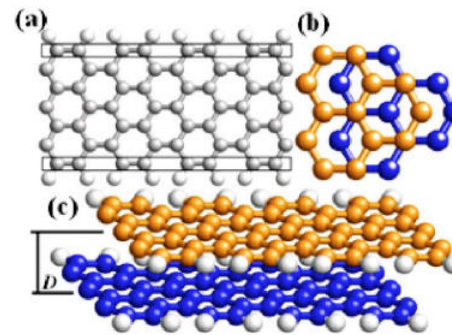
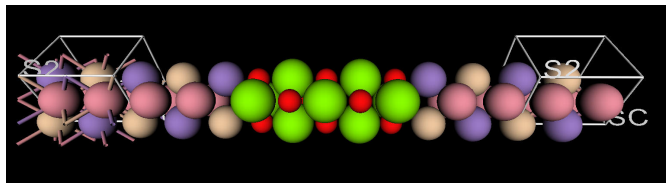


# Essential points of atomic-scale device modeling

- ❖ Atomistic models
  - » Defects, vacancies
  - » Random alloys?

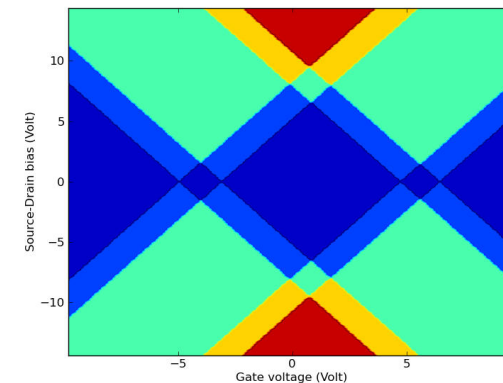


- ❖ Quantum models
  - » New physics governs nanoscale conduction mechanisms



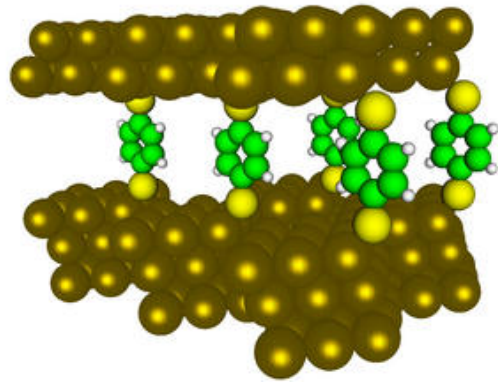
- » Features smaller than mean-free path
- » ... but not always

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

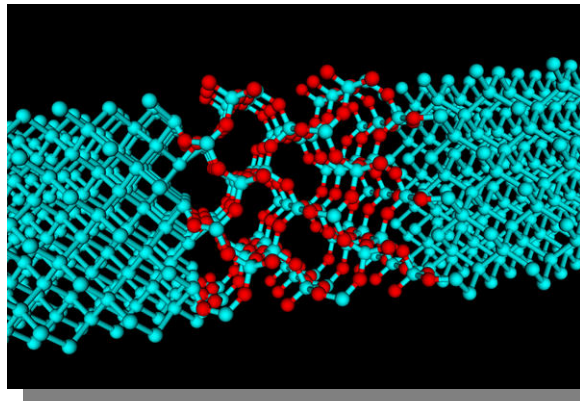


# Complex boundary conditions

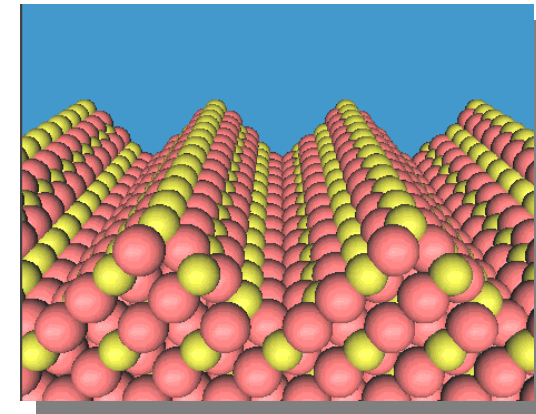
The main application areas in nanotechnology are related to effects occurring at



Junctions

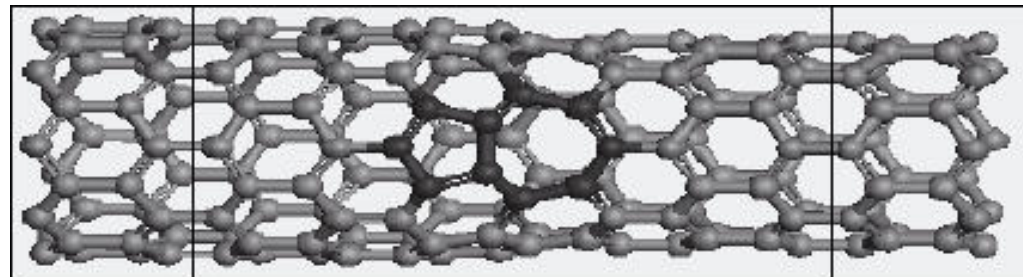


Interfaces



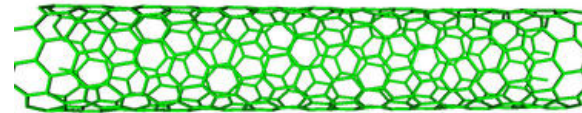
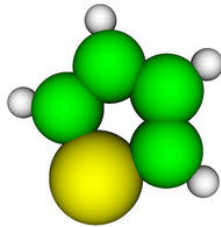
Surfaces

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

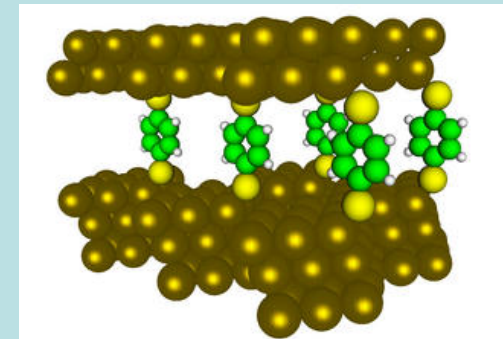
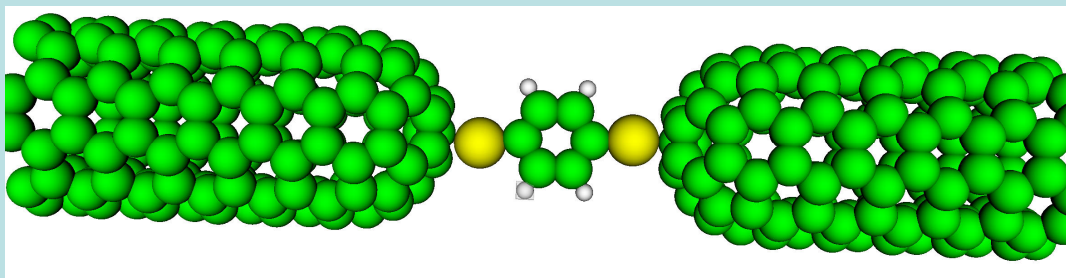


# Electronic transport in nanostructures

Traditional quantum-based software can model either  
isolated molecules or periodic systems

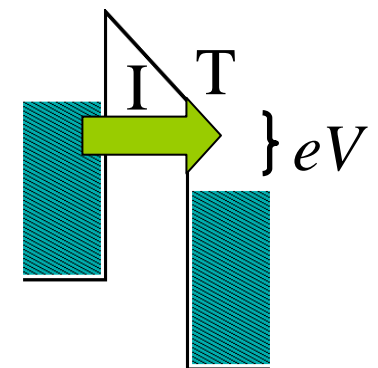
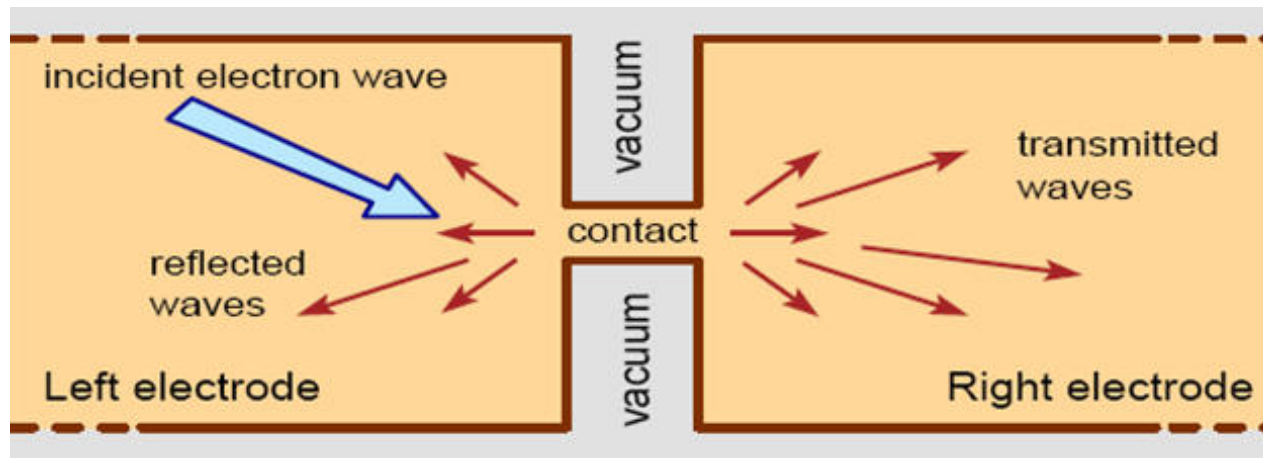
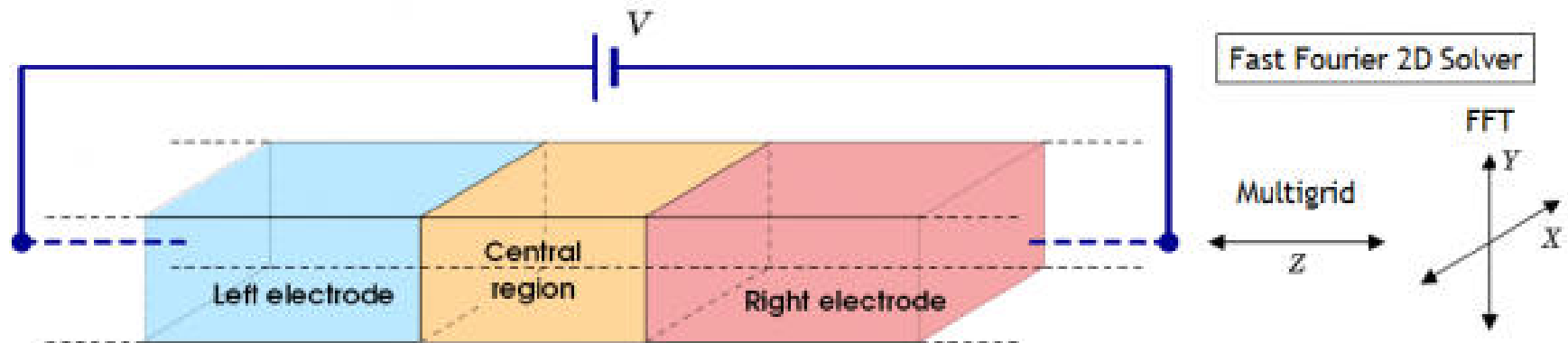


Devices are more complex; need to model nanostructures combining  
molecules with periodic systems and macroscopic elements



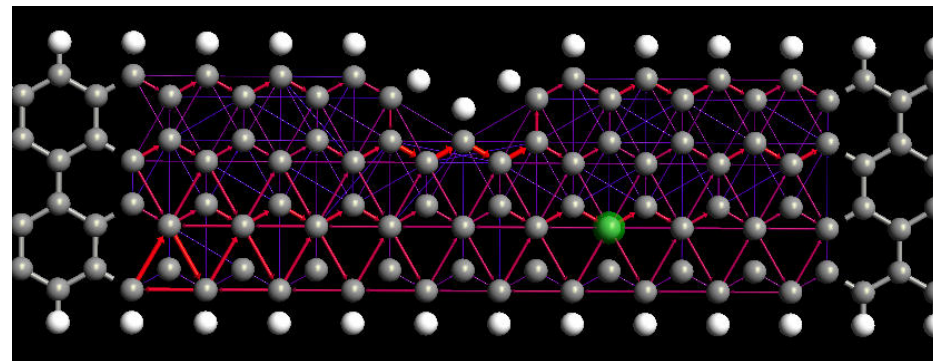
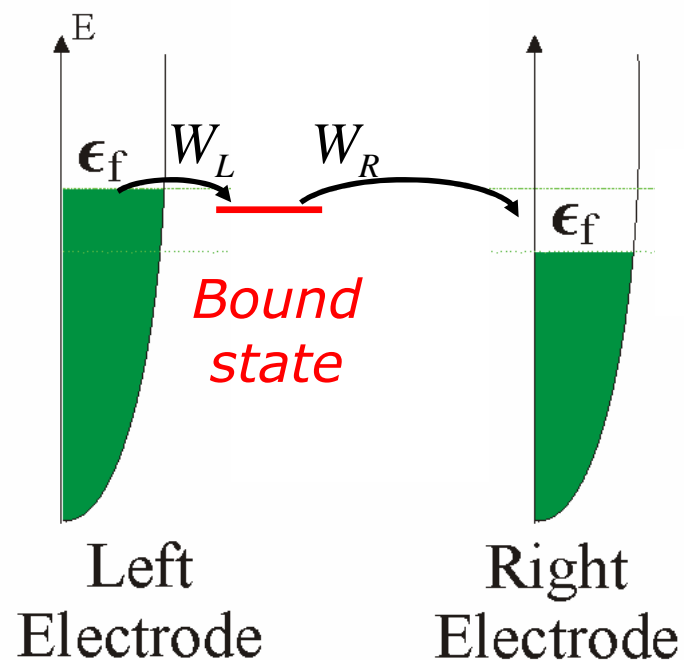
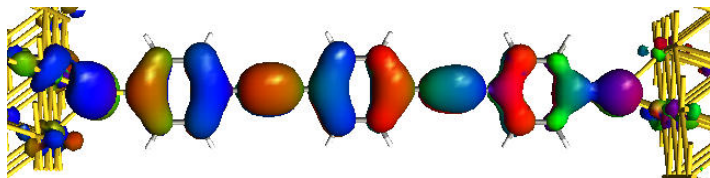
This enables simulations of electrical properties of complex  
nanoscale components and systems like **transistors or gate stacks**

# 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)

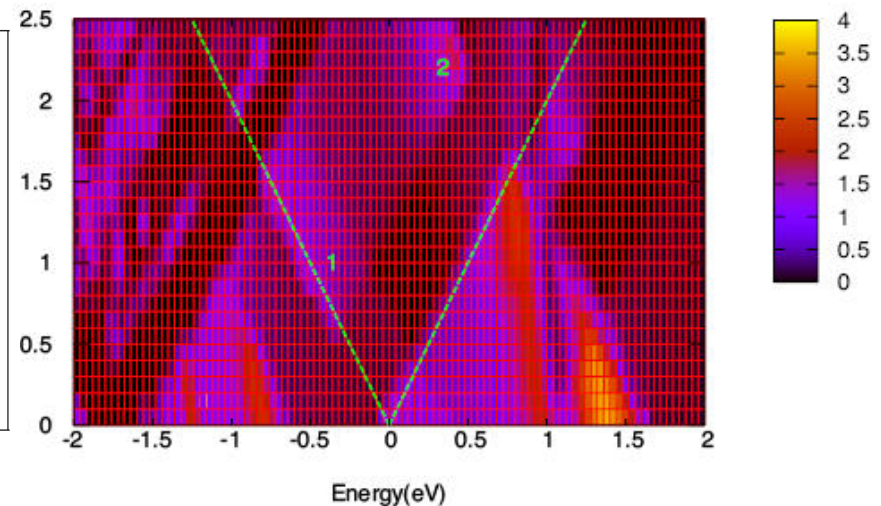
## Conductance (Landauer-Büttiker)

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

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

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

$$t(E) = (\text{Im} [\Sigma_R](E))^{1/2} \mathbf{G}(E) (\text{Im} [\Sigma_L](E))^{1/2}$$



# 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

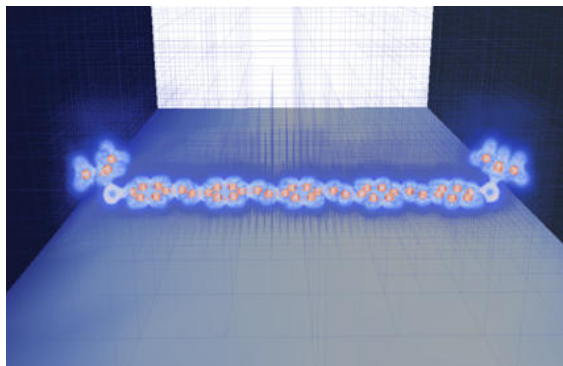
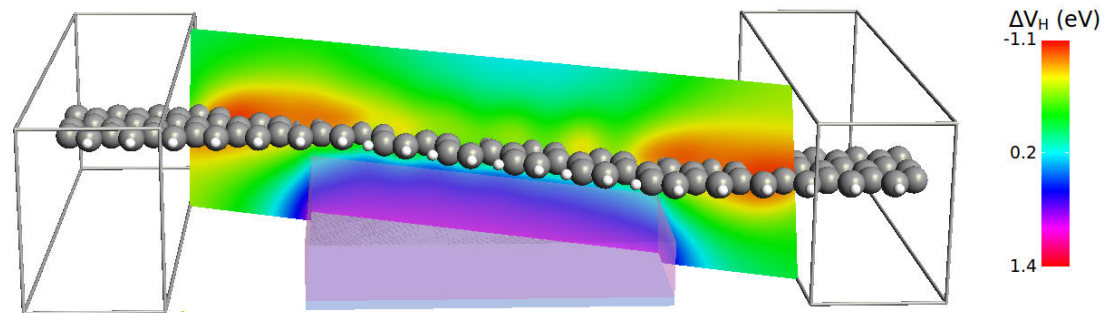
*More tight-binding models coming soon!*  
**DFTB**  
*User-defined TB models*



# Advanced electrostatic models

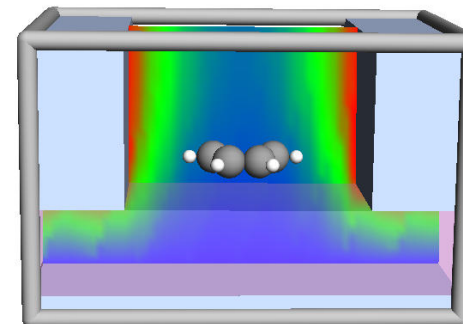
## ❖ Transistor: gates & dielectric regions

Phys. Rev. B 82, 075420 (2010)



## ❖ Single-electron transistors

J Phys Chem C 114, 20461 (2010)

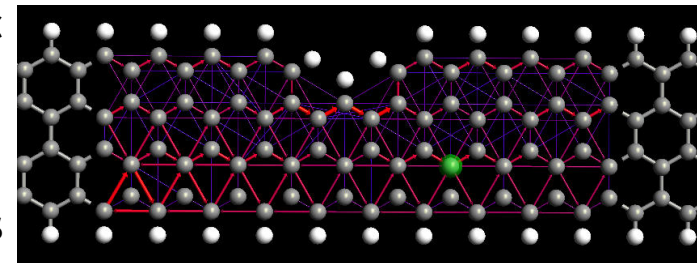
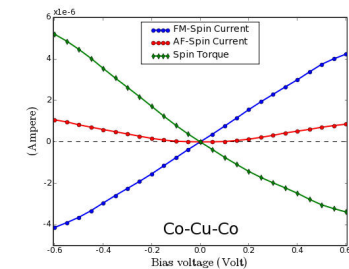
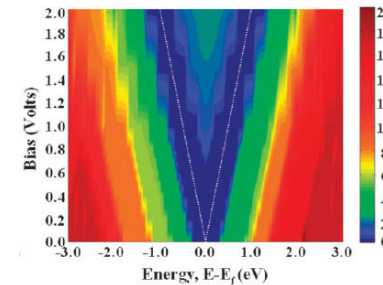
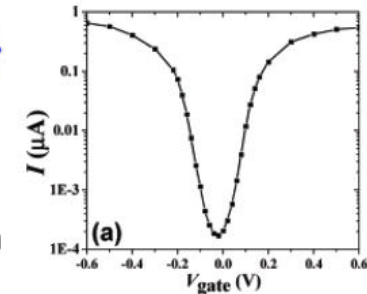
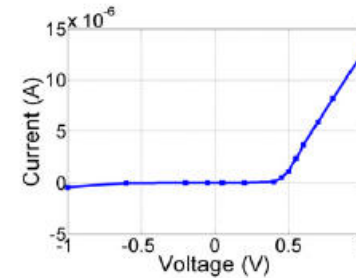


## ❖ Lots of vacuum...

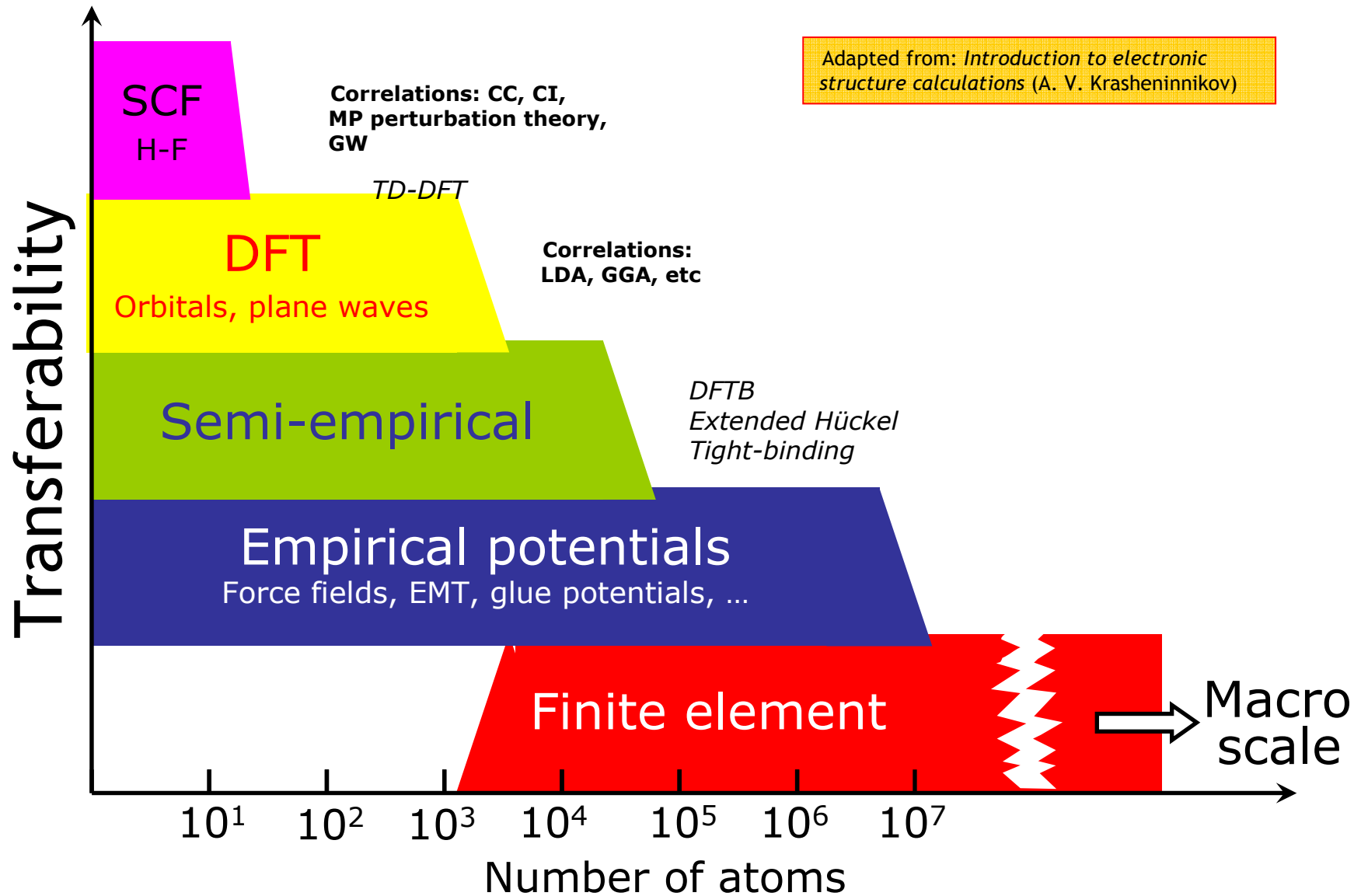
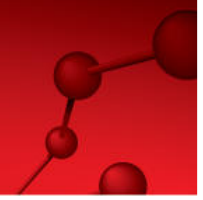
J. Avery, Ph.D. thesis (2011)

# Finite bias calculations

- ❖ Source-drain bias
  - » Non-equilibrium 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)

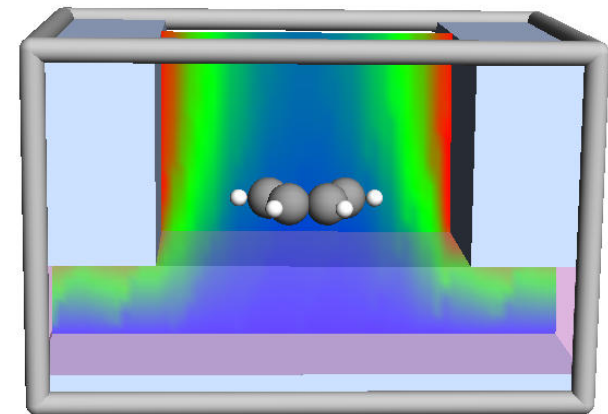
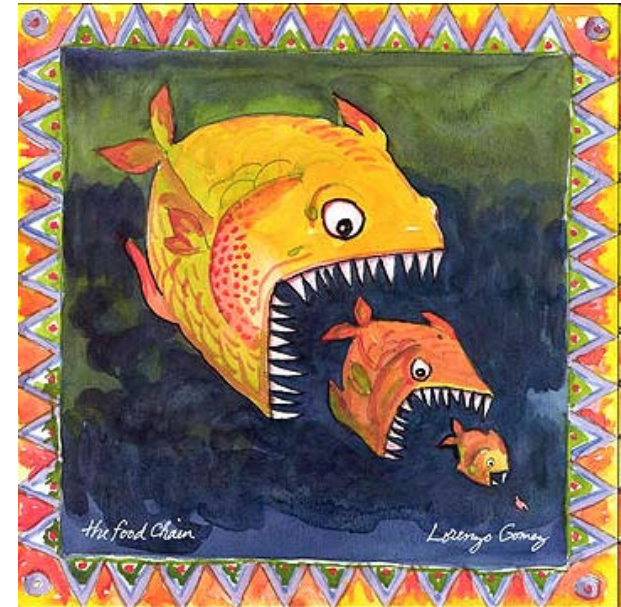


# Multi-scale across length and time scales

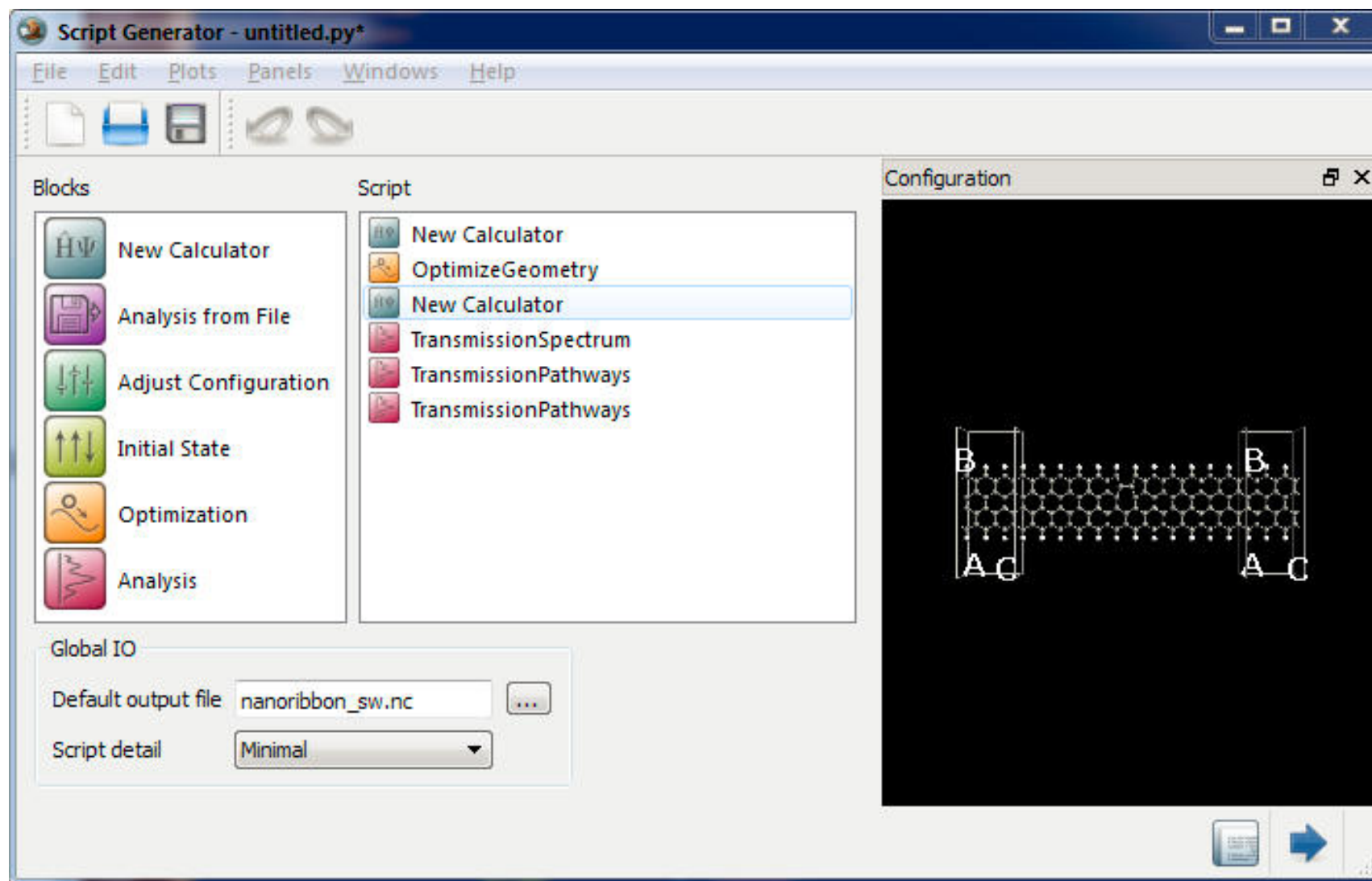


# Multi-scale

- ❖ 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

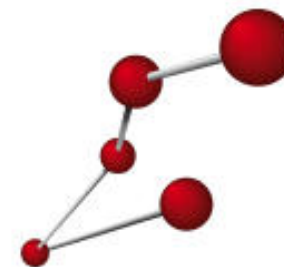


# The solution?

- ❖ 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



## User Scripts

```
from ATK.KohnSham import *
from math import pi,cos,sin

elements = [Oxygen] + 2*[Hydrogen]

z = 0.*Ang
dOH = 0.96*Ang
angle = 104.5*pi/180.
positions = [(z,z,z),
             (dOH*sin(angle/2), dOH*cos(angle/2), z),
             (-dOH*sin(angle/2), dOH*cos(angle/2), z)]

h2o = MoleculeConfiguration(elements,positions)

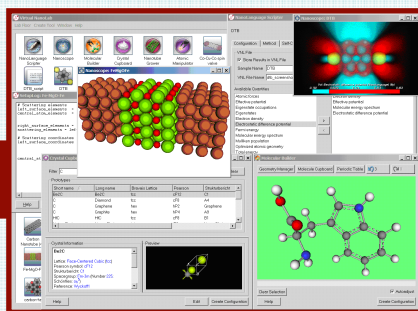
calculation = executeSelfConsistentCalculation(h2o,KohnShamMethod())

molecular_spectrum = calculateMolecularEnergySpectrum(calculation)

vml_file = VMLFile("h2o.vml")
vml_file.addToSample(h2o,"Water molecule")
vml_file.addToSample(molecular_spectrum, "Water molecule")
```

# ATK

## Graphical User Interface



## Add-ons

```
&control
  pseudo_dir = "."
  suffix = ".tmp"
  prefix = "atkv001"
  prefixes = true
/
&system
  lbray=4, cellm(1)=247, cellm(3)=16.0, nat=12, ntyp=1, nbe=20,
  occupations='smearing', smearing='mulliken', dgauss=0.05
  scutoff=22.0
/
&electrons
  ATOMIC_SPECIES
  Be 1.0 Be.vb2
  ATOMIC_POSITIONS alat
  Be 0.00000000 0.28867135 4.359667099
  Be 0.00000000 0.28867135 5.48485449
  Be 0.00000000 -0.28867135 2.754655986
  Be 0.00000000 0.28867135 1.96554700
  Be 0.00000000 0.28867135 1.96554700
  Be 0.00000000 -0.28867135 1.178901500
  Be 0.00000000 0.28867135 0.392919700
  Be 0.00000000 -0.28867135 -0.392919700
  Be 0.00000000 0.28867135 -1.178901500
  Be 0.00000000 -0.28867135 -1.96554700
```

## Python

User TB Models

**Internal Engines**  
DFT (LCAO, plane waves)  
SemiEmpirical (DFTB, Hückel, SK TB)  
Classical

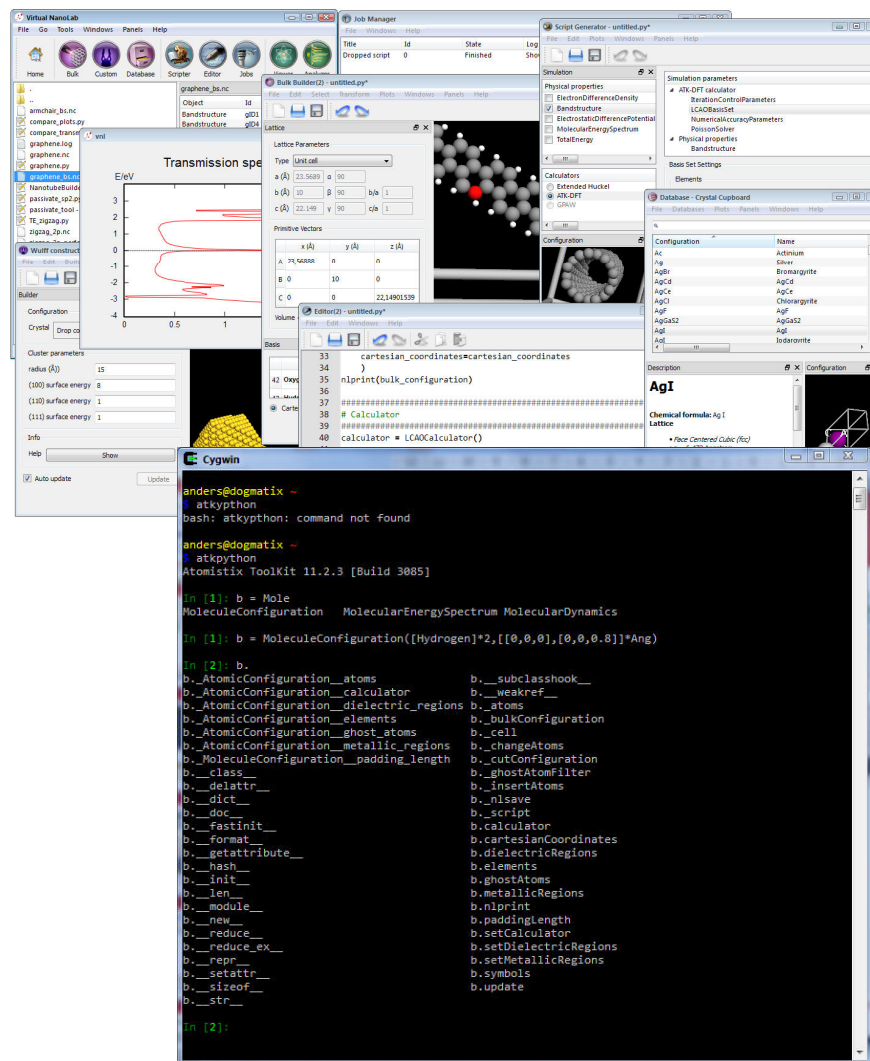
Python Plugin Module

## API

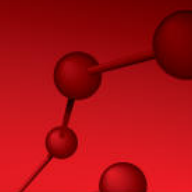
Open source/  
3<sup>rd</sup> party software

# Programmable

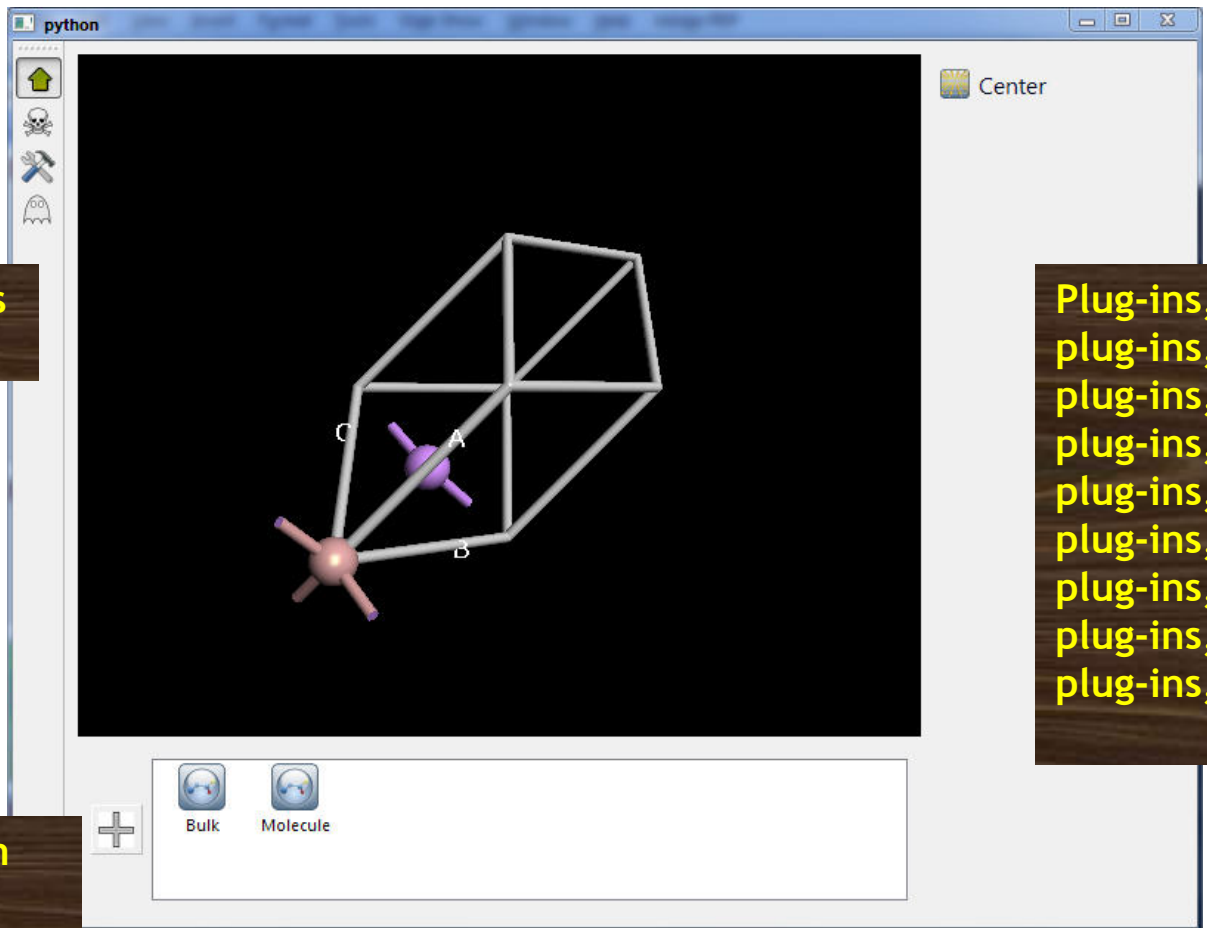
- ❖ GUI is a thin API with direct Python bindings
- ❖ User can implement and share plug-ins for everything
  - » Building structures
  - » Wrapping external codes
    - Setting up parameters and models)
    - Running external codes
    - Importing result files
  - » Operations on computed data
    - 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,

- 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

**PERIODIC TABLE**  
Atomic Properties of the Elements

NIST  
National Institute of Standards and Technology  
Technology Administration, U.S. Department of Commerce  
www.nist.gov

**Frequently used fundamental physical constants**  
For the most accurate values of these and other constants, visit physics.nist.gov  
1 second = 8 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of <sup>133</sup>Cs  
speed of light in vacuum  $c = 299\,792\,458\text{ m s}^{-1}$  (exact)  
Planck constant  $h = 6.626\,070\,15 \times 10^{-34}\text{ J s}$  (exact)  
elementary charge  $e = 1.602\,176\,634 \times 10^{-19}\text{ C}$  (exact)  
proton mass  $m_p = 1.672\,621\,923 \times 10^{-27}\text{ kg}$   
 $m_p/c^2 = 1.875\,612\,124 \times 10^{-36}\text{ kg}$   
neutron mass  $m_n = 1.674\,927\,282 \times 10^{-27}\text{ kg}$   
fine-structure constant  $\alpha = 1/137.035\,999\,074$   
Rydberg constant  $R_\infty = 109\,737\,315.685\,26 \times 10^6\text{ m}^{-1}$   
Bohrmann constant  $k_B = 1.380\,658\,4 \times 10^{-23}\text{ J K}^{-1}$

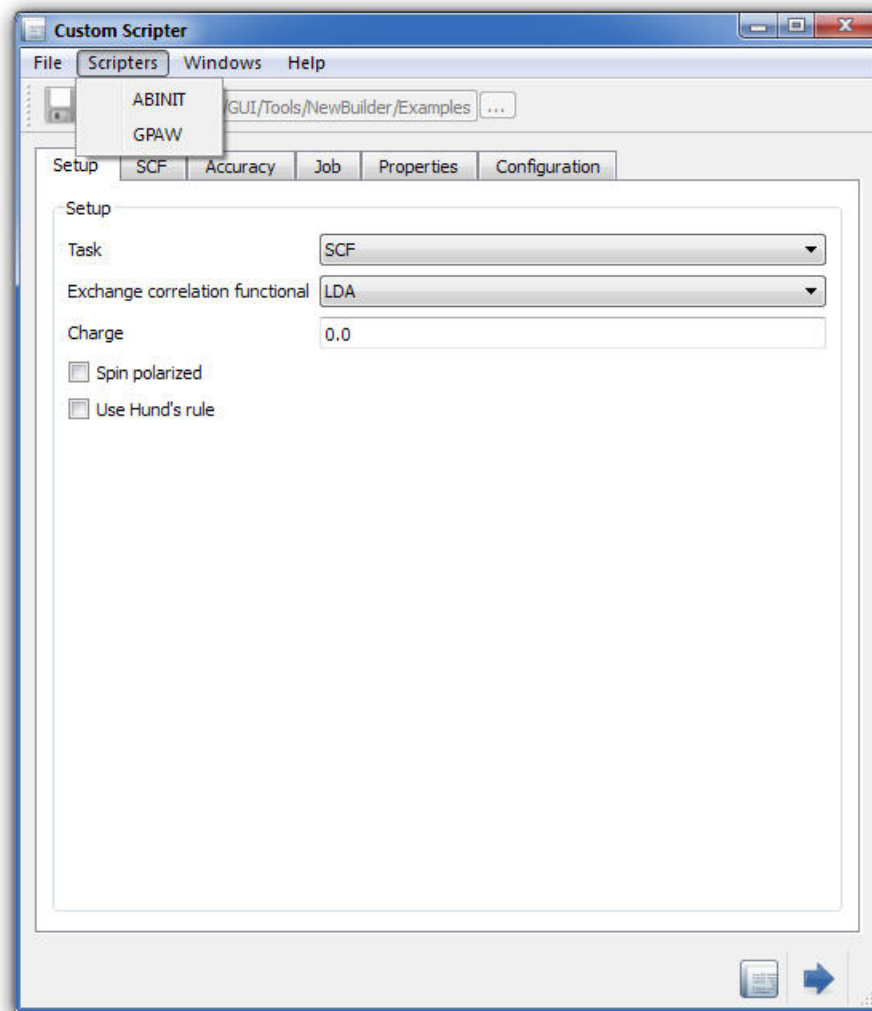
**Legend:**  
Solids (blue)  
Liquids (green)  
Gases (red)  
Artificially Prepared (yellow)

**Callout for Cerium (Ce):**  
Atomic Number: 58  
Ground-state Level:  $4f^1 5d^1 6s^2$   
Name: Cerium  
Symbol: Ce  
Atomic Weight: 140.118  
[X]4f15d1 6s2  
Ground-state Configuration: [Xe]4f15d1 6s2  
Ionization Energy (eV): 5.5387

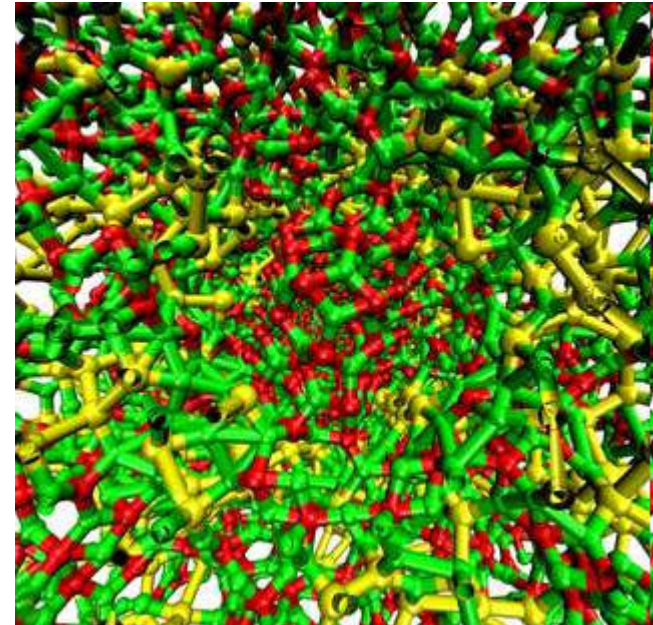
Based upon <sup>12</sup>C. ( ) indicates the mass number of the most stable isotope. For a description of the data, visit physics.nist.gov/data. NIST SP 966 (September 2003)

# 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



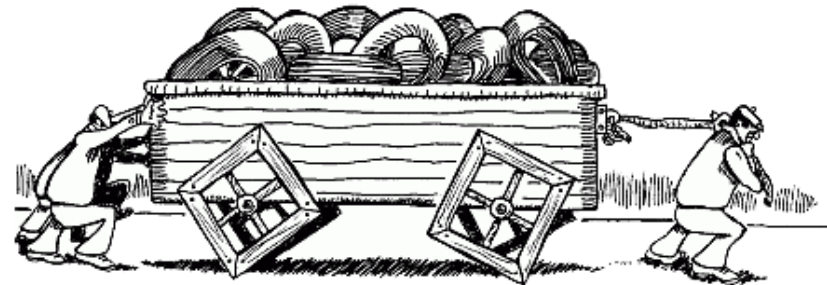
- ❖ Large systems - classical models needed
- ❖ Materials - parameters?
  - » Gaussian Approximation Potentials
- ❖ Phonon transport
- ❖ Electron-phonon coupling



*Courtesy of M. Griebel group, Fraunhofer-SCAI*

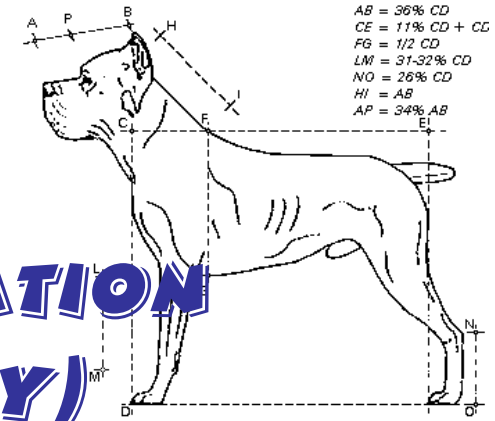
# Summary

- ❖ 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

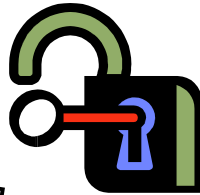


# Discussion points

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



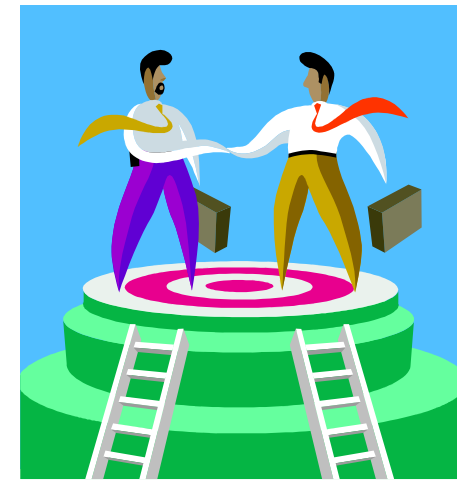
**OPEN**



**STANDARDIZATION  
(LEGITIMACY)**

**PLATFORM**

**COMMERCIAL ↔ COMMUNITY**





**Thank you**  
**for your attention!**