IUPAP Commission 20

Computational Physics

Working Group on Nanoscience

Risto M. Nieminen
COMP/Laboratory of Physics
Helsinki University of Technology
02150 Espoo, Finland

rni@fyslab.hut.fi
http://www.fyslab.hut.fi/

Courtesy of The Archives, California Institute of Technology.

"There Is Plenty of Room at the Bottom"

Richard P. Feynman
December 1959

- How do we write small?
- Information on a small scale
- Better electron microscopes
- The marvellous biological system
- Miniaturizing the computer
- Miniaturization by evaporation
- Problems of lubrication
- A hundred tiny hands
- Rearranging the atoms
- Atoms in a small world

10^{-9} m

Three pillars of nanosciences

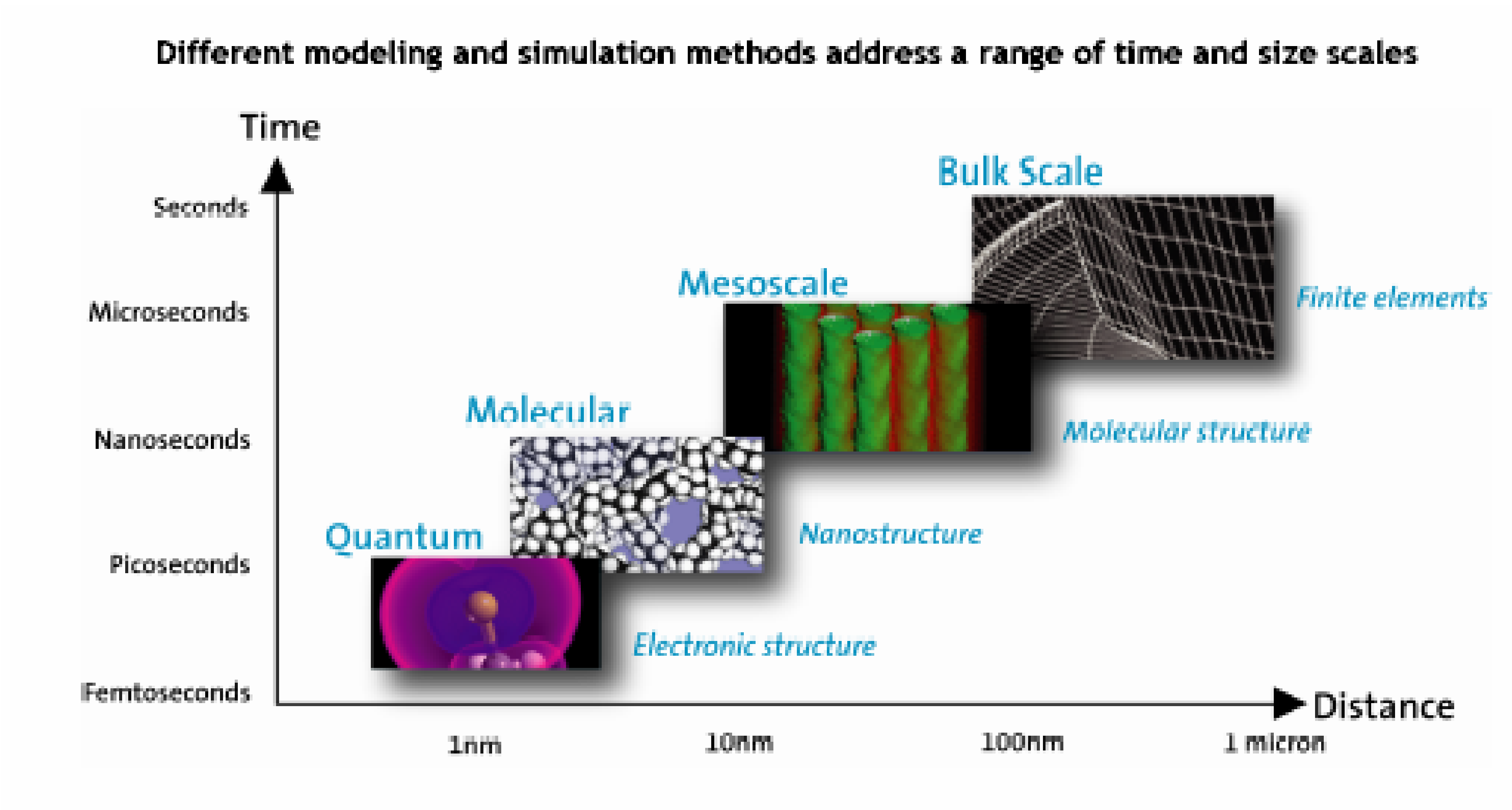
Manufacture and processing of nanometer-scale structures
- •"top-down": lithography
- •"bottom-up": self-assembly

Characterisation, imaging and probing

Theory, modelling and simulation
- Predictive computation of physical, chemical and biological functions
- Process design
- Interpretation of characterisation and imaging

"Mimicking Nature"

COMPUTATIONAL PHYSICS


Different modeling and simulation methods address a range of time and size scales
Time
Seconds
Microseconds
Nanoseconds
Picoseconds
Femtoseconds
Bulk Scale
Finite elements
Mesoscale
Molecular structure
Molecular
Nanostructure
Quantum
Electronic structure
Distance
1nm
10nm
100nm
1 micron

Multiple length and time scales

m

10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2}

Atomic-scale **Nano-scale** **Meso-scale** **Macro-scale**

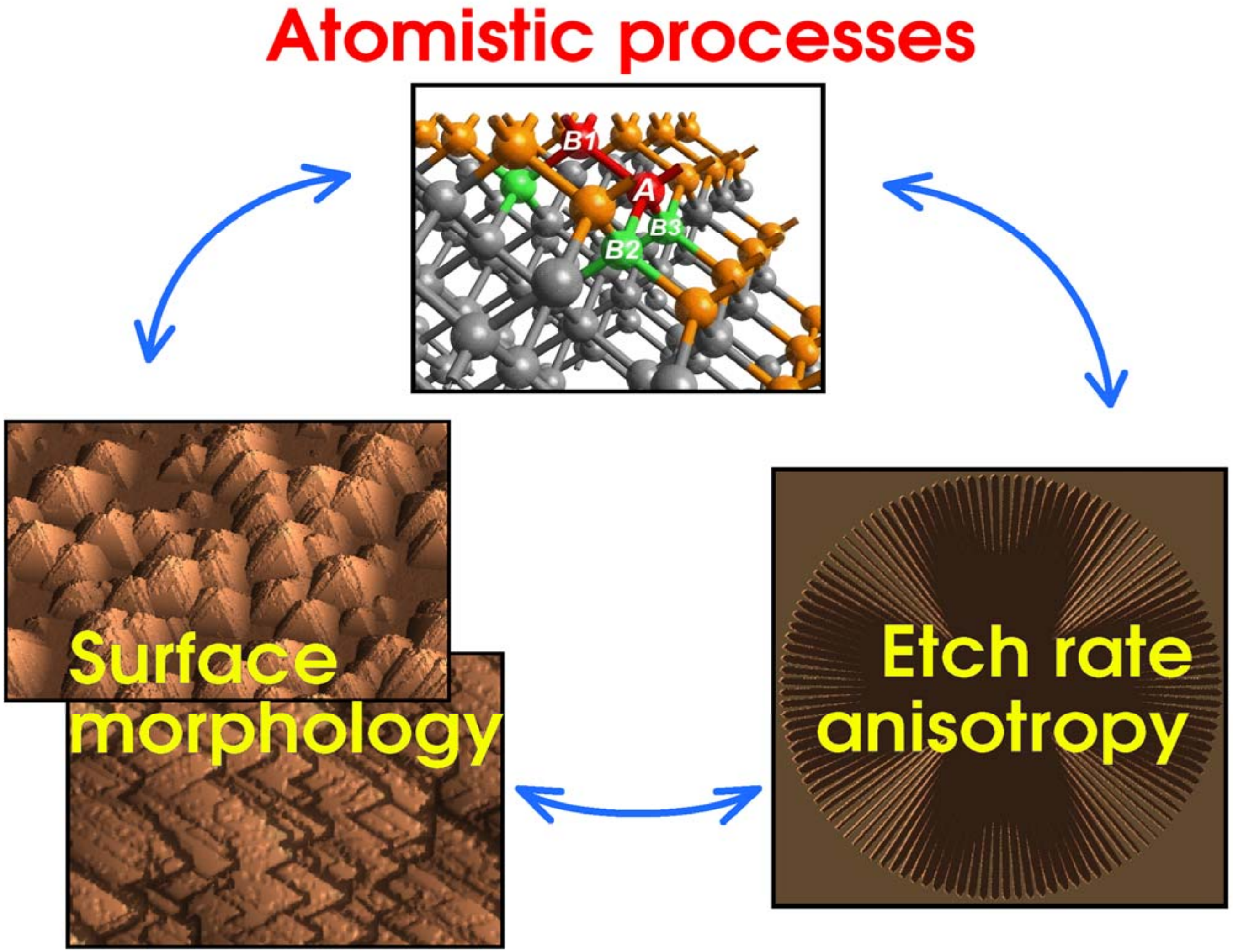
Quantum theory, DFT → **Statistical physics, MC, MD** → **Finite-elements, finite-differences**

s

10^{-14} 10^{-11} 10^{-8} 10^{-5} 10^{-3} 10^{0} 10^{3}

First-principles MD, TD-DFT → **MD, Kinetic Monte Carlo** → **Continuum equations**

Bridging the different length scales



Interrelation between microscopic, mesoscopic and macroscopic features of the etching process

Multiscale computational methods

Method	Type of information	Time scale	Length scale
Quantum Monte Carlo/ED	Microscopic	-	~100 atoms
Density-functional theory	Microscopic	-	~ 1000 atoms
Ab initio molecular dynamics	Microscopic	t < 10 psec	~ 100 atoms
Semi-empirical molecular dynamics	Microscopic	t < 1 nsec	~ 100000 atoms
Kinetic Monte Carlo	Microscopic to mesoscopic	1 psec< t< 1 hour	~1 micrometer
Rate equations	Averaged	0.1 sec < t <∞	All
Continuum equations	Macroscopic	1 sec < t < ∞	> 10 nm

Commission conferences (C20)

International Conference in Computational Physics (CCP*XXXX*)

- CCP2003 Xian, China
- CCP2004 Genoa, Italy
- CCP2005 Los Angeles, USA

CCP2003

Postponed to 2004 due to the SARS epidemic;
difficulties in scheduling

CCP2004

1. Nanoscience in plenary talks

- electron transport and dissipation in nanoscale devices (R. Car)
- optical, electrical and mechanical properties of nanostructures (S. Louie)
- resonating valence-bond wave functions: from lattice models to realistic simulations (S. Sorella)

2. Nanoscience in invited talks

- molecular nanostructures
- semiconductor/metal interfaces
- carbon nanotubes
- large molecules at metal interfaces

- partially folded states of proteins
- from nanodiamonds to nanotube growth
- wave function optimisation for accurate quantum Monte Carlo
- doped helium clusters
- multiscale alorithms

….

<u>Three major themes:</u>

- condensed-matter and materials physics, especially nano (including soft and biological matter) (50 %)

- statistical physics and complexity (30 %)

- particle physics, astrophysics and cosmology (20 %)

CCP2005

1. Nanoscience in plenary talks

- physics and chemistry in the non-scalable and emergent regimes (Landman)
- soft matter and biomaterials (Klein)
- dielectric response and polarization (Vanderbilt)

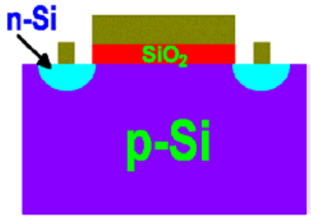
2. Nanoscience in invited talks

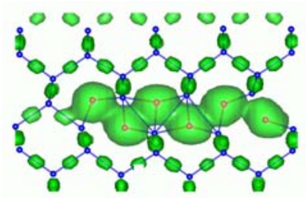
- carbon nanotubes (several talks)
- quantum dots
- semiconductor nanoparticles
- nanowires and nanocorrals
- metallic nanoparticles
- future directions in the simulation of nanomaterials

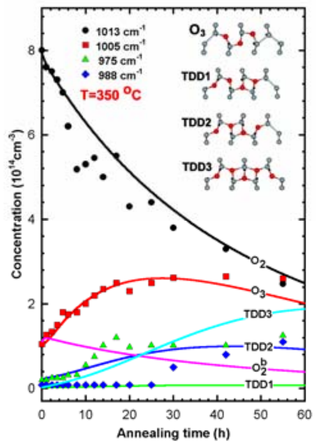
Major themes:

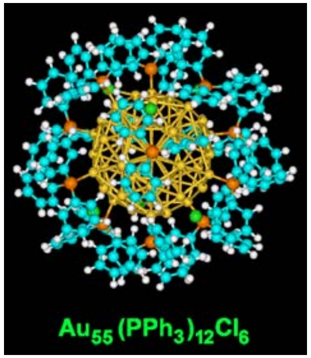
- condensed matter and materials, including nano (50 %)
- biological physics (15 %)
- statistical physics and complexity (15 %)
- quantum information and computing (15 %)
- algorithms (5 %)

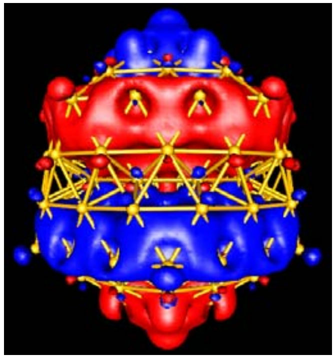
Some recent research areas

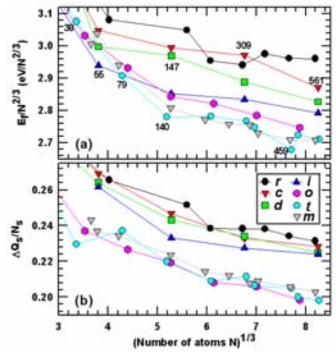


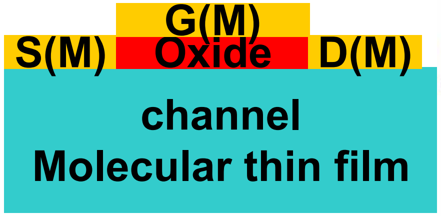


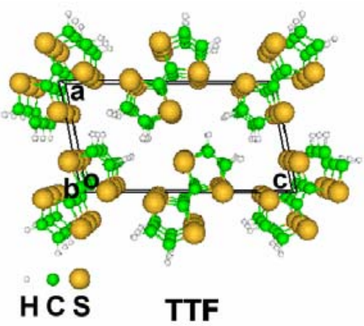


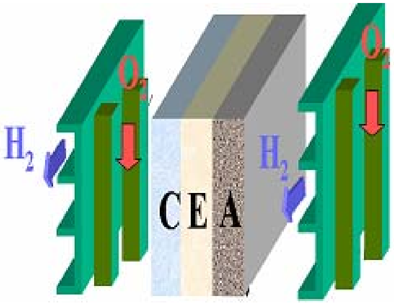


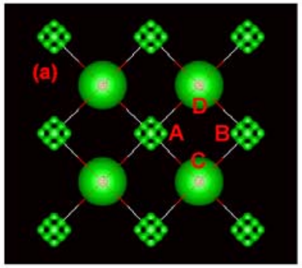


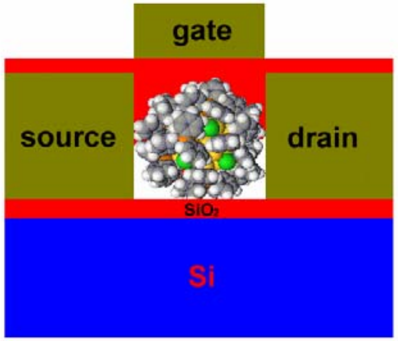


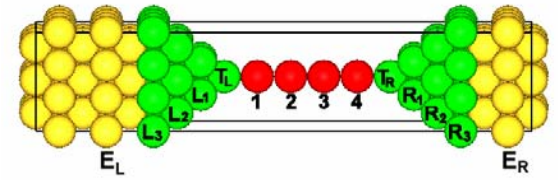


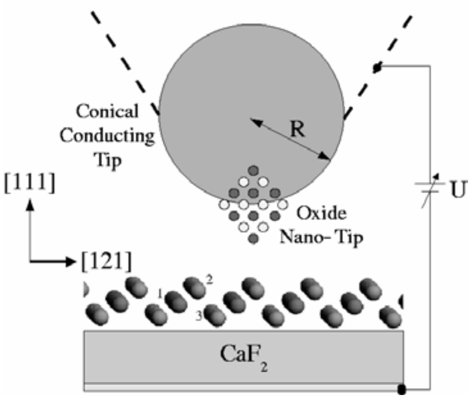


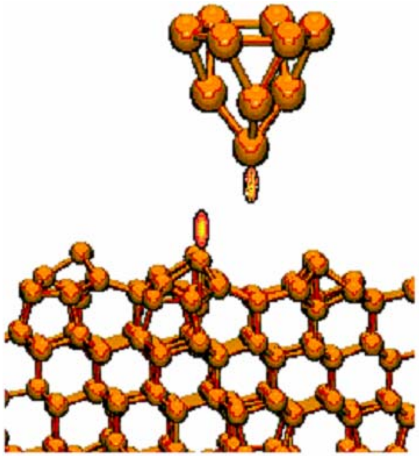












"The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

P.A.M. Dirac, 1929

1902-1984

Physics Nobel Prize 1933 (with E. Schrödinger)

"It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."

*P.A.M. Dirac, Proc. Royal Soc. London A **123**, 714 (1929)*

Density-Functional Theory (DFT)

$$E_{ks}[\{\psi_i(\mathbf{r})\}] = -\frac{1}{2}\sum_i f_i \int \psi_i \nabla^2 \psi_i d\mathbf{r} + \frac{1}{2}\sum_{i\neq j} \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r} d\mathbf{r}'$$
$$+ \int V_{ion}(\mathrm{r})\rho(\mathrm{r})d(\mathrm{r}) + E_{xc}[\rho(\mathrm{r})] + E_{ion}(\{\mathrm{R}_I\})$$

Kohn-Sham Eqs. self-consistently solved

$$\left(-\frac{1}{2}\nabla^2 + V_{ion}(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r})$$
$$\rho(\mathrm{r}) = \sum_i \left|\psi_i \psi_i\right|^2$$

First-principles Molecular Dynamics

$$F_I = -\frac{dEks}{d\mathbf{R}_I} = -\frac{\partial E_{ks}}{\partial \mathbf{R}_I} - \sum_i \frac{\partial E_{ks}}{\partial \psi_i}\cdot\frac{d\psi_i}{d\mathbf{R}_I} - \sum_i \frac{\partial E_{ks}}{\partial \psi_i}\cdot\frac{d\psi_i^*}{d\mathbf{R}_I}$$

Density functional theory provides a very efficient way for the application to both solids and molecules, with higher accuracy than Hartree-Fock.

DFT Methods

all-electron full potential
all-electron muffin-tin
pseudopotential
jellium

beyond LDA
- GW
- time-dependent DFT
- LDA+U
- self-interaction corr. (SIC)
- sx-LDA

GGA
LDA

$$\left(-\frac{1}{2}\nabla^2 + V_{ion}(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\,\psi_i(\mathbf{r})$$

fully-relativistic
scalar-relativistic
non-relativistic

periodic
non-periodic

spin-polarized
collinear spin
non-collinear spin
spin-nonpolarized

plane waves
atomic orbitals
GTO, STO, numerical
augmented waves
FLAPW, PAW, LMTO, ASW
fully numerical

Scientific software used at COMP

QUANTUM SCALE

QMC — Quantum Monte Carlo

FINGER VASP
CASTEP WIEN2k
FLEUR MIKA
SIESTA

Density-functional theory

ATOMISTIC SCALE

TB-MOLDY MOLDY

Molecular dynamics

MESOSCOPIC SCALE

KMC — Kinetic Monte Carlo
TAPAS — Cellular automata

CONTINUUM SCALE

ELMER — Finite-element methods