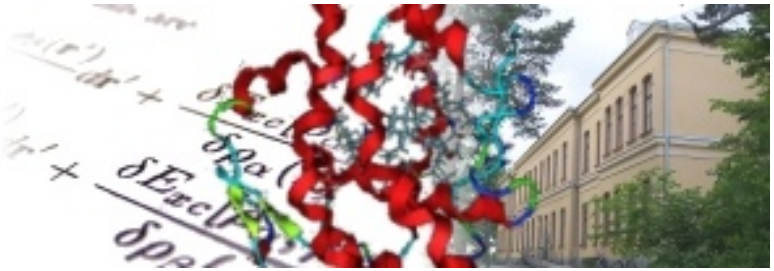
Royal Institute of Technology
School of Biotechnology
Theoretical Chemistry and Biology



E-science development of quantum, quantum-relativistic and quantum-classical computer modeling

Inauguration of Beskow

2015-01-27

Ab Initio Quantum Mechanics:

Keep system operators intact

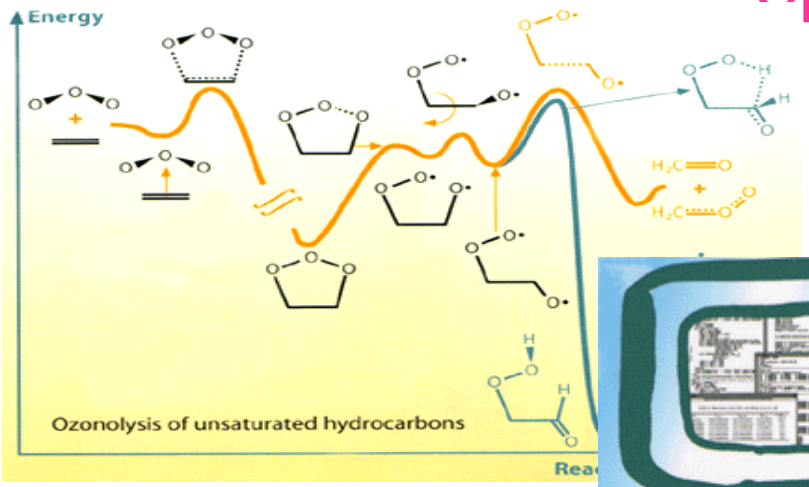
Project them on a basis

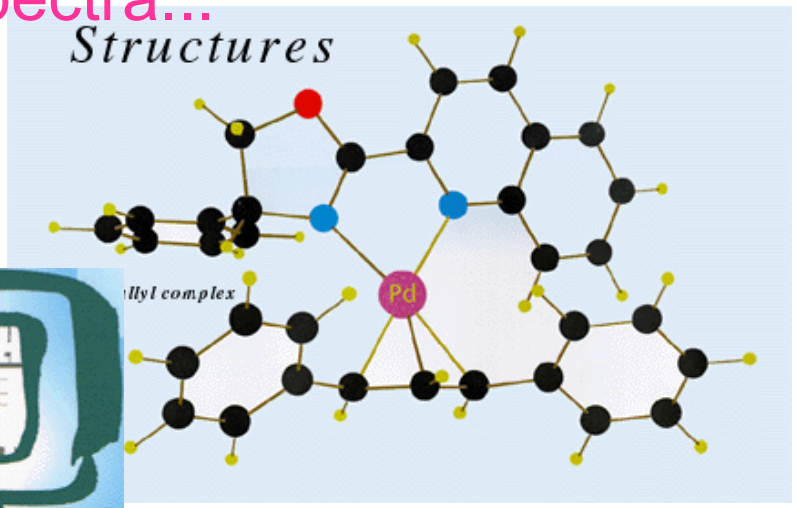
Solve projected problem exactly

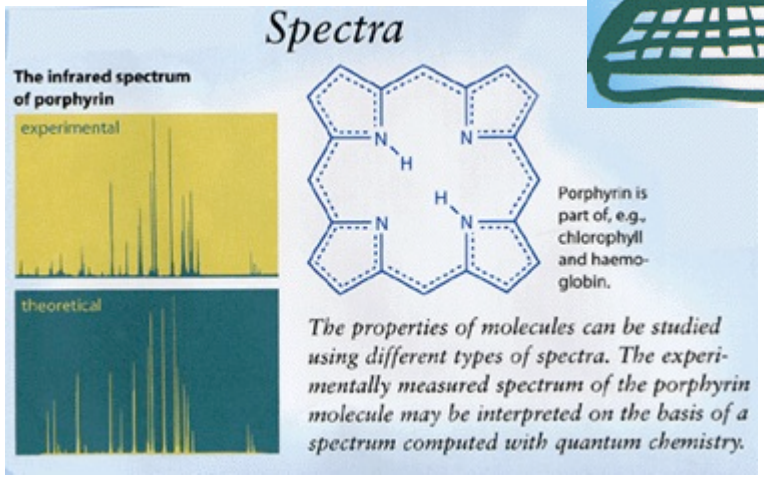
Hierarchical projection → Theory develops independently from Experiment

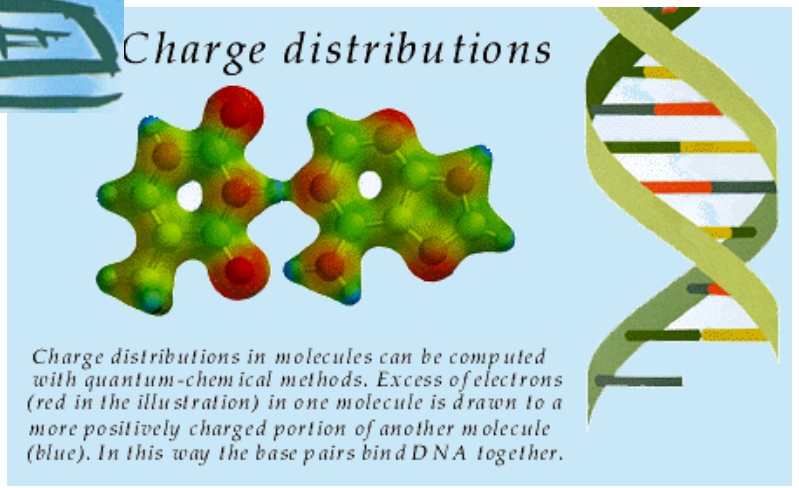
Find out about ….

Structure, Dynamics, Reactions, Properties, Spectra…







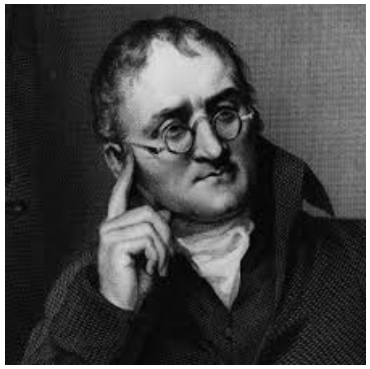


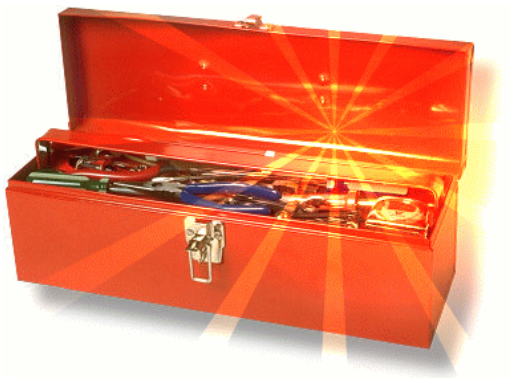
DALTON program

"3rd dimension of Quantum Chemistry": Properties

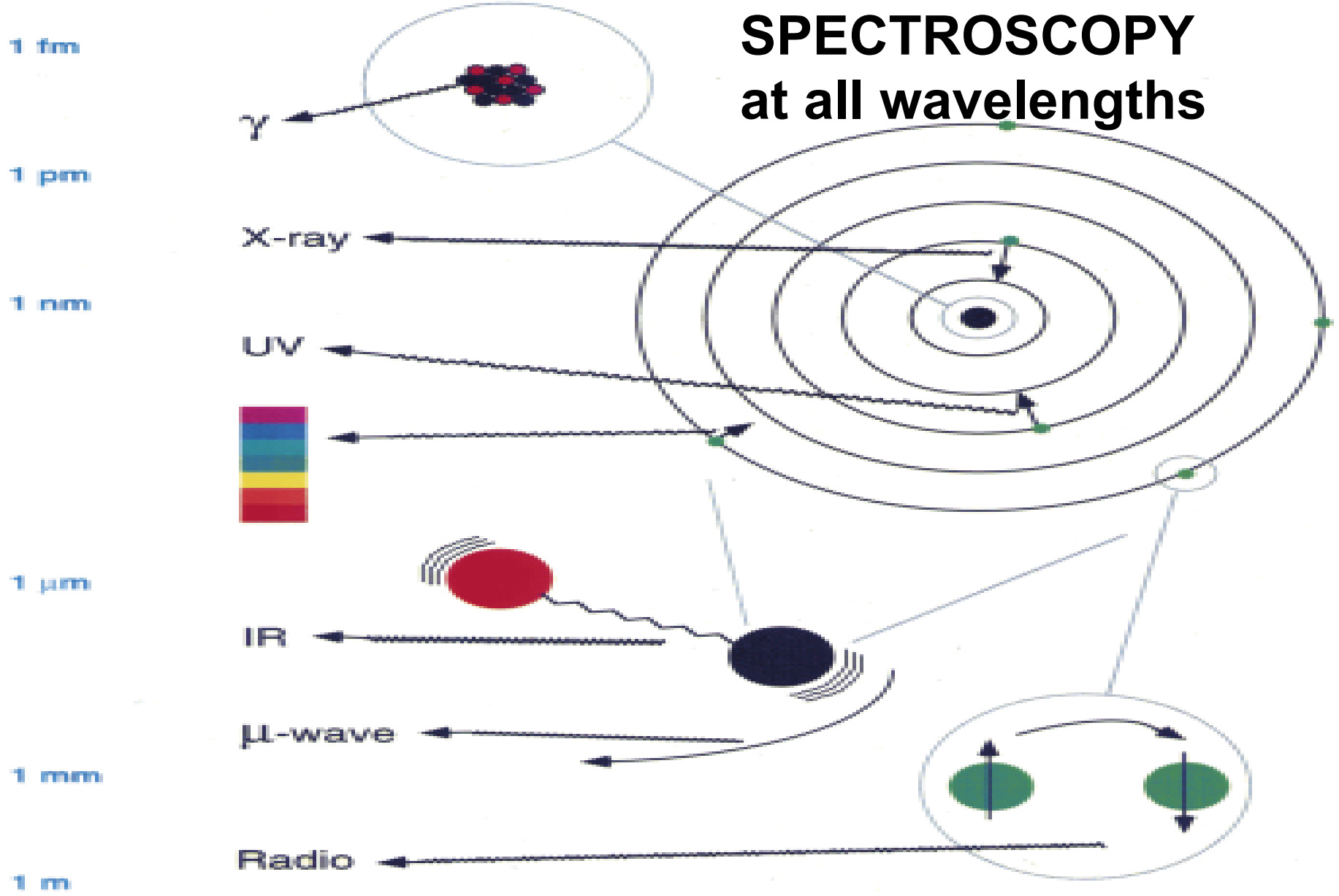
- Hartree-Fock Self Consistent Field (HF)
- Multiconfigurational Self Consistent Field (MCSCF)
- Coupled Cluster (CC)
- Density Functional Theory (DFT)
- Quantum Mechanics-Molecular Mechanics (QMMM)

$$\langle\langle A;B\rangle\rangle_{\omega_1} \quad \langle\langle A;B,C\rangle\rangle_{\omega_1,\omega_2} \quad \langle\langle A;B,C,D\rangle\rangle_{\omega_1,\omega_2,\omega_3}$$



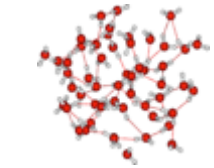


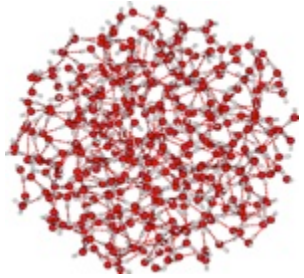
Electromagnetic radiation emitted from microscopic processes

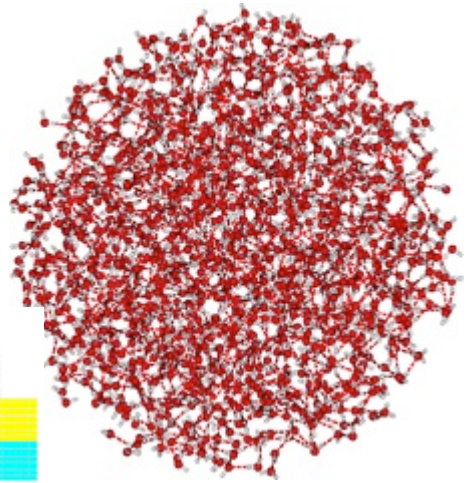


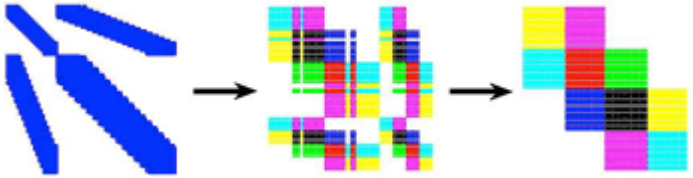
SPECTROSCOPY
at all wavelengths

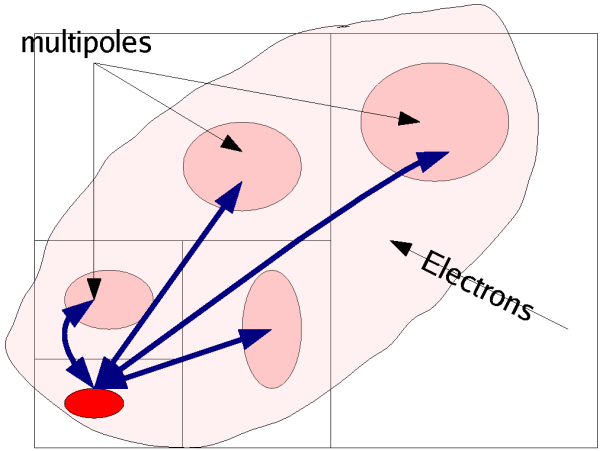
Linear Scaling Quantum Mechanics

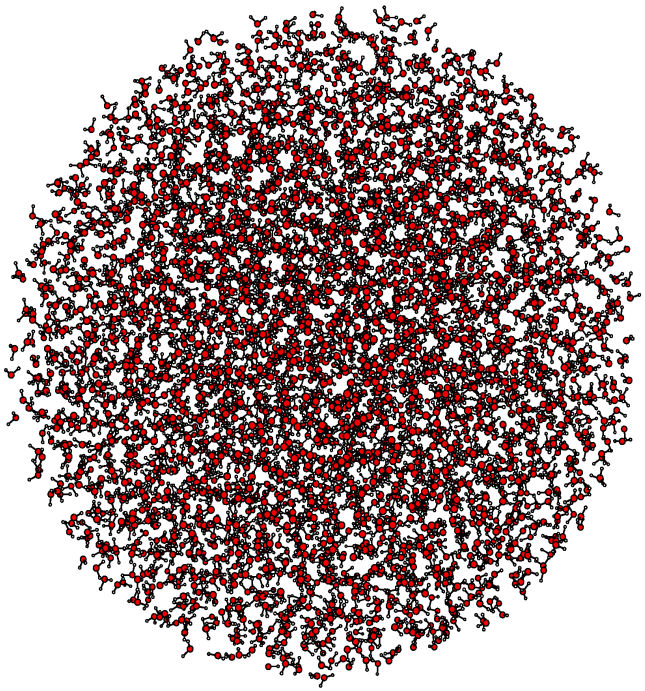


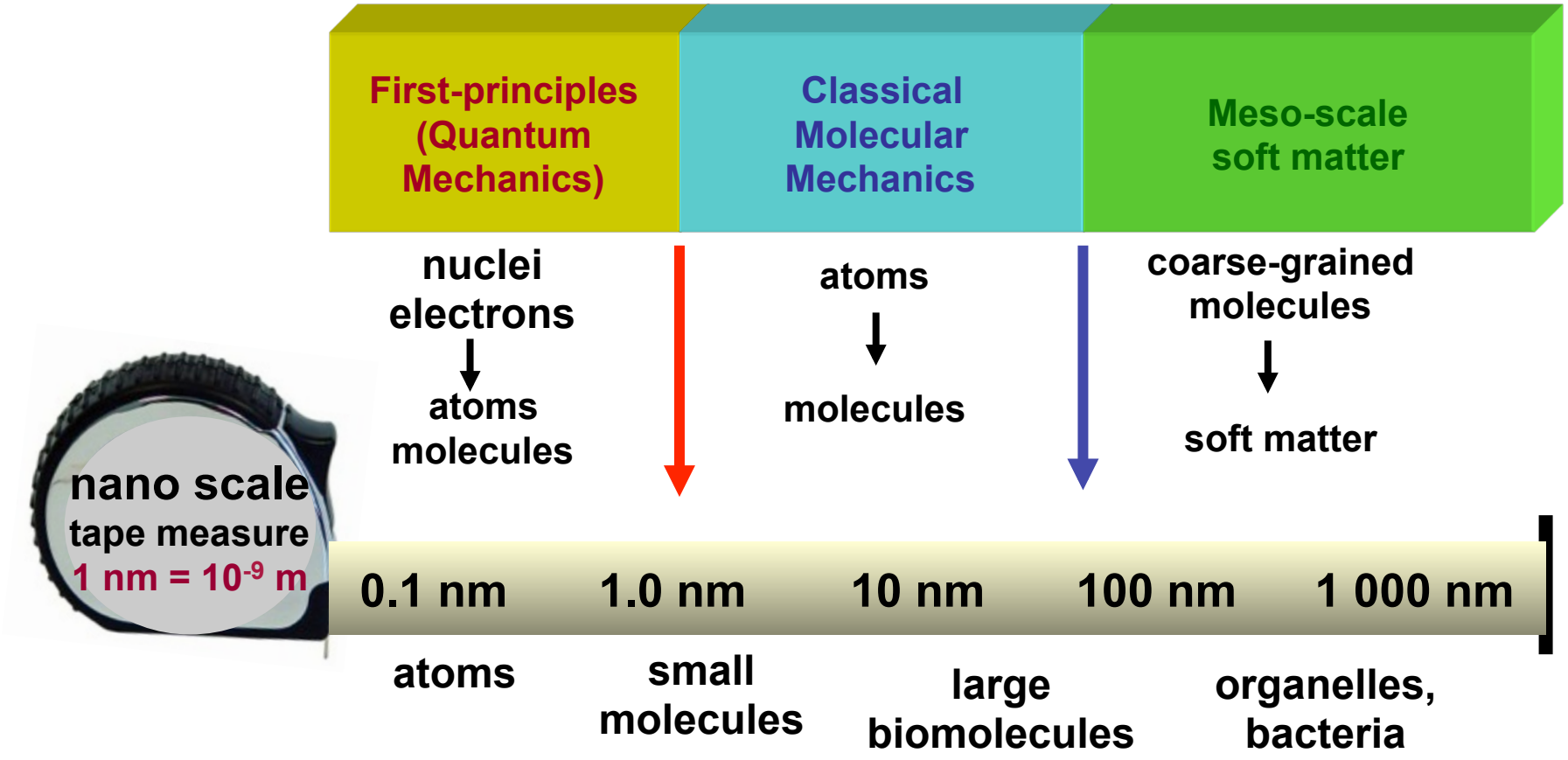




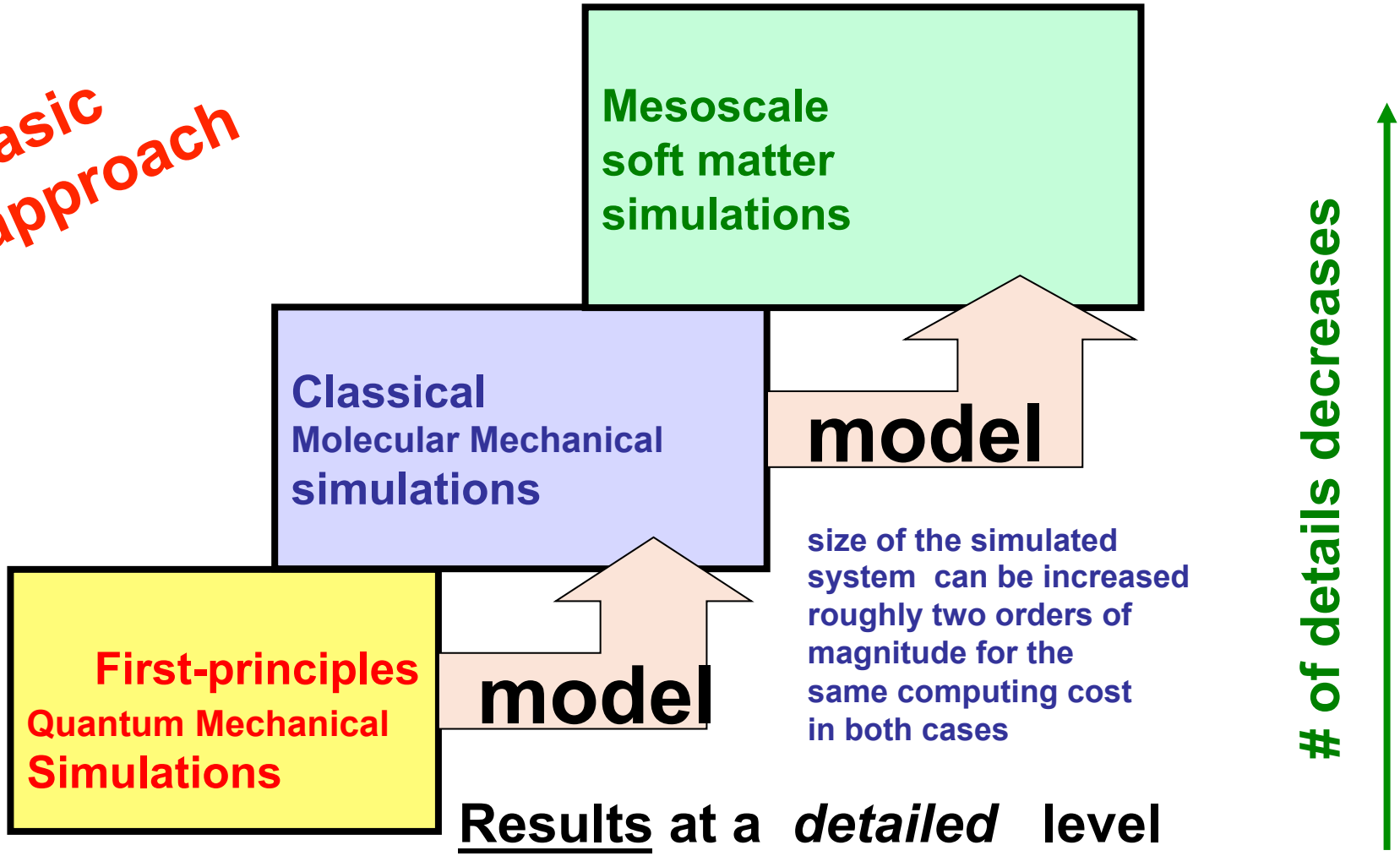







First-principles (Quantum Mechanics)
Classical Molecular Mechanics
Meso-scale soft matter
nuclei
electrons
atoms
molecules
atoms
molecules
coarse-grained molecules
soft matter
nano scale
tape measure
1 nm = 10-9 m
0.1 nm
1.0 nm
10 nm
100 nm
1 000 nm
atoms
small molecules
large biomolecules
organelles, bacteria

MULTISCALE MODELLING

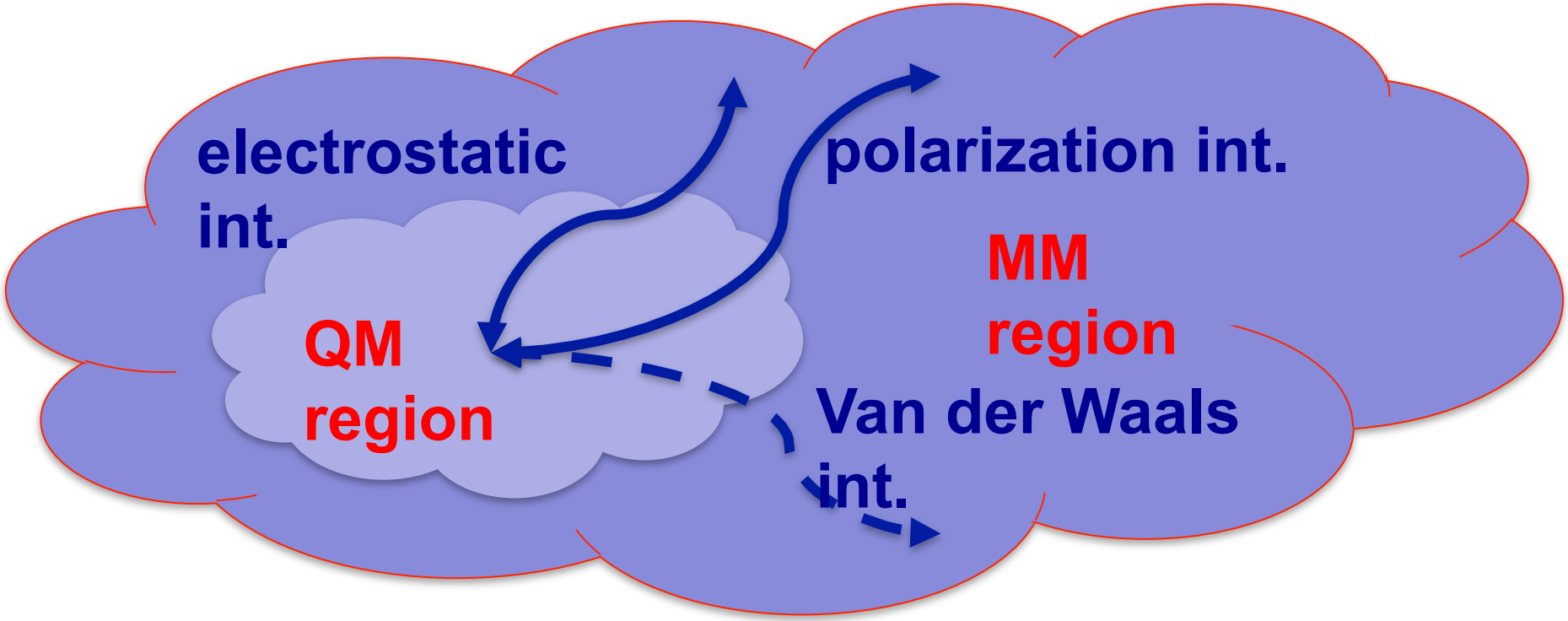


Results at a *detailed* level

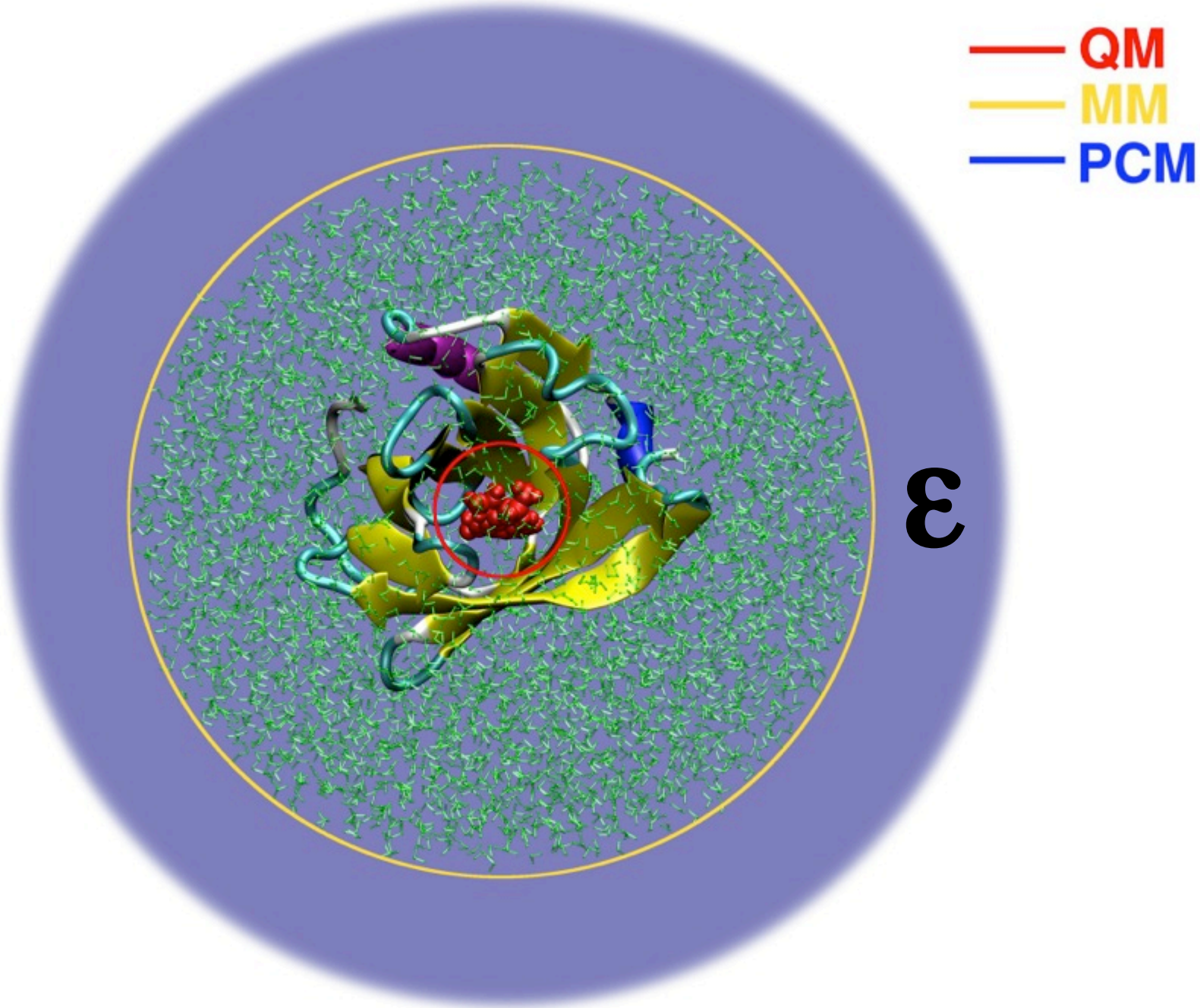
⇓

give **model** to a *less detailed* level !

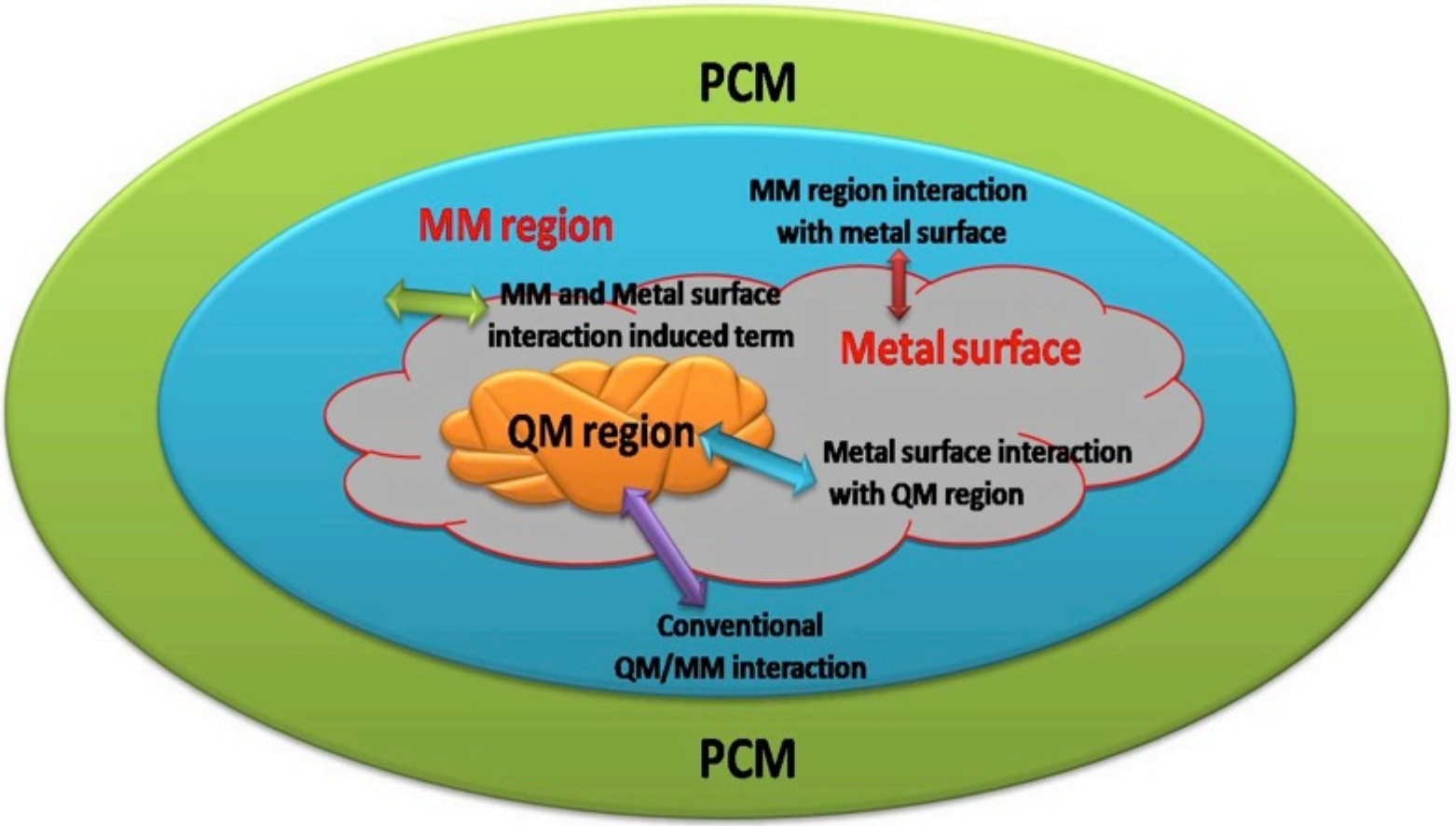
QM/MM Philosophy



- Electrostatic (QM region - electron density : MM region –chargers, dipoles, quadrupoles, octupoles)
- Polarization (QM region - molecular polarization : MM region –distributed anisotropic polarizabity)
- Van der Waals (QM and MM regions empircal LJ or opther similar potential)

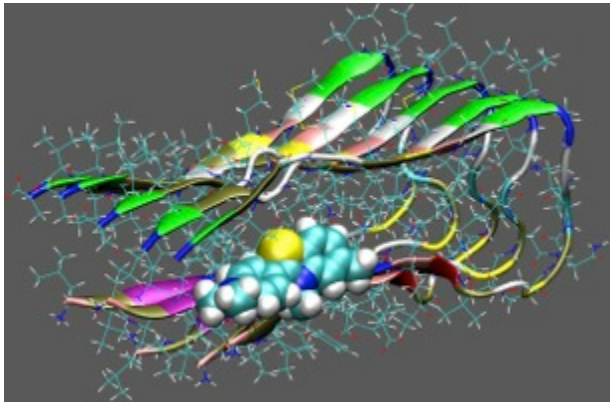

QM
MM
PCM
ε

Quantum Mechanics
Capacitance Molecular Mechanics

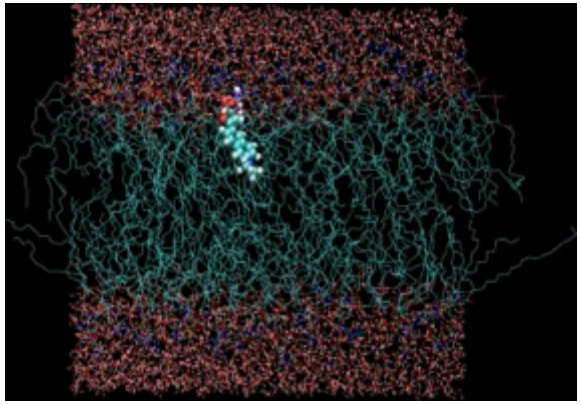


TheoChemBio

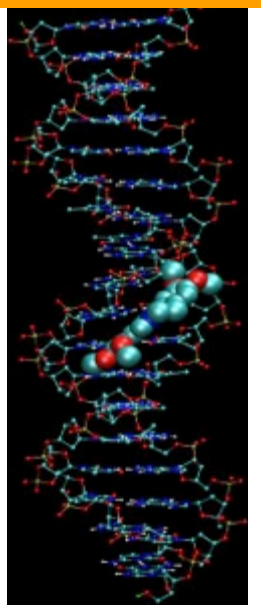
QMMM-Virtual Laboratory for Molecular Probes



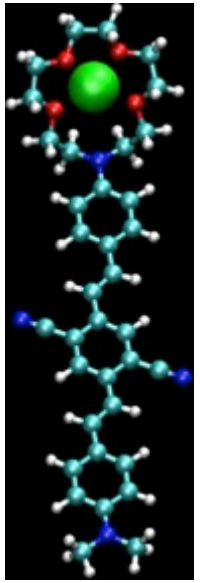
Fibril-probe



Membrane-probe

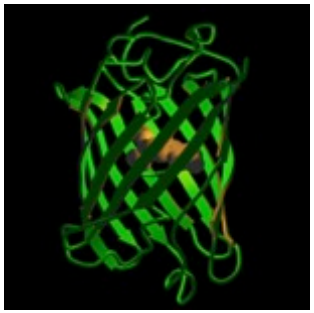


DNA-probe

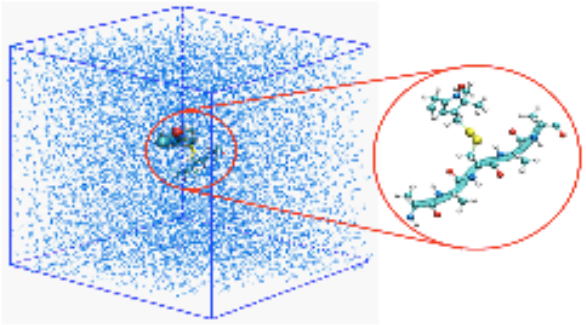


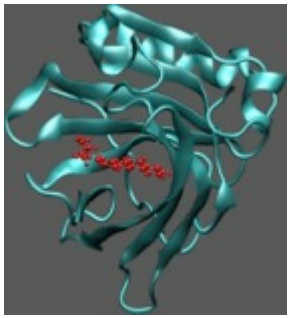
Metal probe

Intrinsic Biomarkers and GFPs



pH-probe





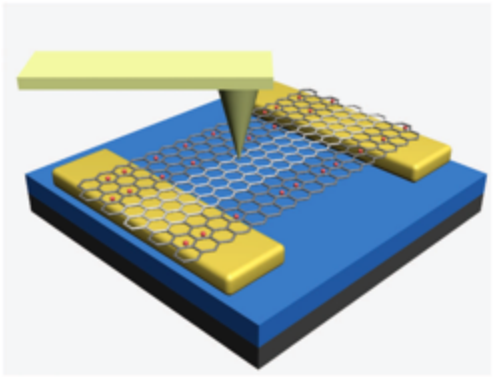
Protein probe

TheoChemBio

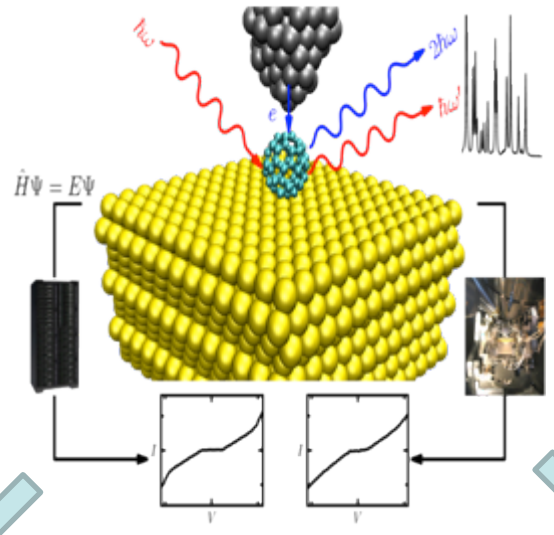
Single Molecular Electronics and Photonics

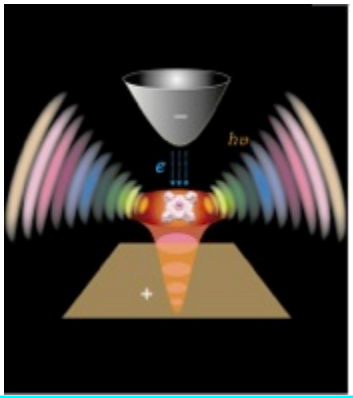
To Join one of the world's leading research groups and to make the difference!

Invent new Concepts w and design new devices for future information technology and biotechnology

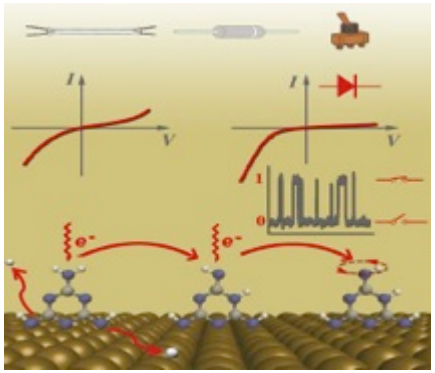


Direct writing of nanodevices
Nature Communications, 2012



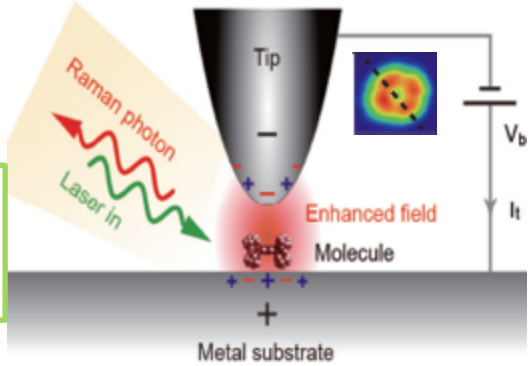


Tuning the color of molecules
Nature Photonics, 2010
Phys. Rev. Lett., 2011



The first dual functional single molecular device
PNAS, 2009

Sub-nm resolution of Raman imaging
Nature, 2013



Software Crisis in Quantum Chemistry

Most quantum chemistry programs are based on legacy code developed in 1980-1990 and thus can not take full advantage of latest hardware featured in modern HPC systems

New software developments in quantum chemistry are needed…

Modern HPC Systems

- Homogeneous & heterogeneous systems

CPU ACCELERATORS GPGPU

Modern HPC Systems

- **Main trends in computer architectures**
  - Large number of cores:
    - Up to 18 cores in CPU
    - Up to 61 cores in Xeon Phi
    - 2600+ CUDA cores in GPGPUs
  - Support of vector instructions:
    - AVX (256) in current CPUs
    - Extended AVX (512) current Xeon Phi and future CPUs
  - Heterogeneous execution environment

New Quantum Chemistry Software

- **Main requirements for new QM software**
  - Modern programing languages/practices
  - Code portability and transferability
  - Multilevel parallelism (shared and distributed memory)
  - Ability to scale is more important than single core performance
  - Development of new or revision of old algorithms with emphasis on massive parallelism

Our Development Efforts

- **Two-electron integrals evaluation library**
  - written in C++ with extensive usage of code autogeneration
  - implements our K4MIRROR algorithm for two-electron integrals calculations
  - supports OpenMP and hybrid MPI/OpenMP execution mode
- **GPUnCH program**
  - new code targets heterogeneous HPC systems

written in C++ and CUDA

EFS Library Performance

K4MIRROR Performance

DALTON 2013/ECHIDNA: openMP 24

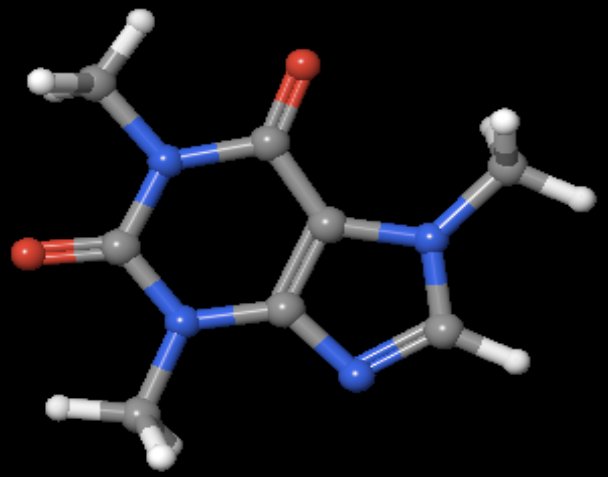
8 min. 44 sec. **Speed Up: 19.6 X**

DALTON 2013/ECHIDNA: MPI 2 openMP 12

8 min. 53 sec. **Speed Up: 19.3 X**

DALTON 2013: MPI 24

- **2 h 51 min. 29 sec.**



General Contraction Basis Set
- [14s9p4d/4s3p2d] for C, N, O
- [8s4p/3s2p] for H

GPUnCH Code Performance on CPU

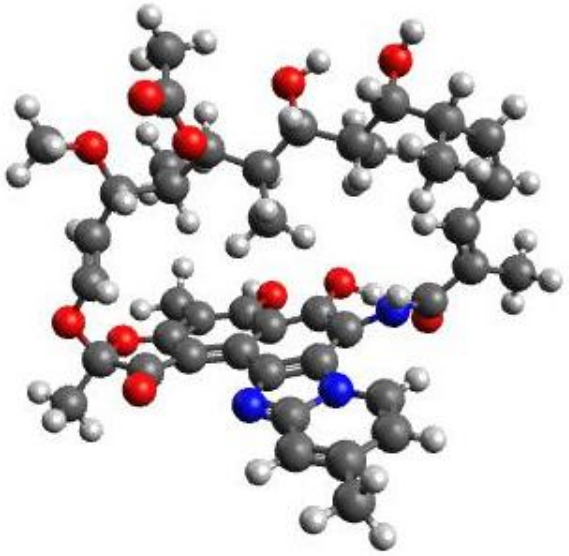
- **Rifamycin (Def2-SVP basis)***

DALTON-2013

1169 s

GPUnCH

203 s **x5.7 times**



* Dual Intel Xeon E5-2620 (12 cores @2.0 GHz), hyper-threading disabled.

Where We Go?

Current scientific computations/modeling perhaps should be re-evaluated

and

more resources invested in development and maintenance of software for modern HPC systems