

Materials Simulation Center presents:

Introduction to
***Computational Chemistry
Programs***

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Course contents

- Overview: What is ***Computational Chemistry***
- 1: *ab initio* method
- 2: Density Functional Theory
- 3: Molecular mechanics method
- 4: Introduction to some programs

Overview: What is ***Computational Chemistry***

Computational Chemistry uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids.

Computational chemistry methods range from highly accurate (i.e. *Ab initio* methods and DFT) to less accurate, (i.e. semi-empirical method), to very approximate (i.e. Molecular Mechanics, Coarse-Grain model).

It can deal with system of a single molecule, a group of molecules, a liquid or solid.

It calculates properties such as properties are structure, relative energies, charge distributions, dipoles and multipole moments, vibrational frequencies, reactivity and other spectroscopic quantities, etc.

Simulation method for length and time scale

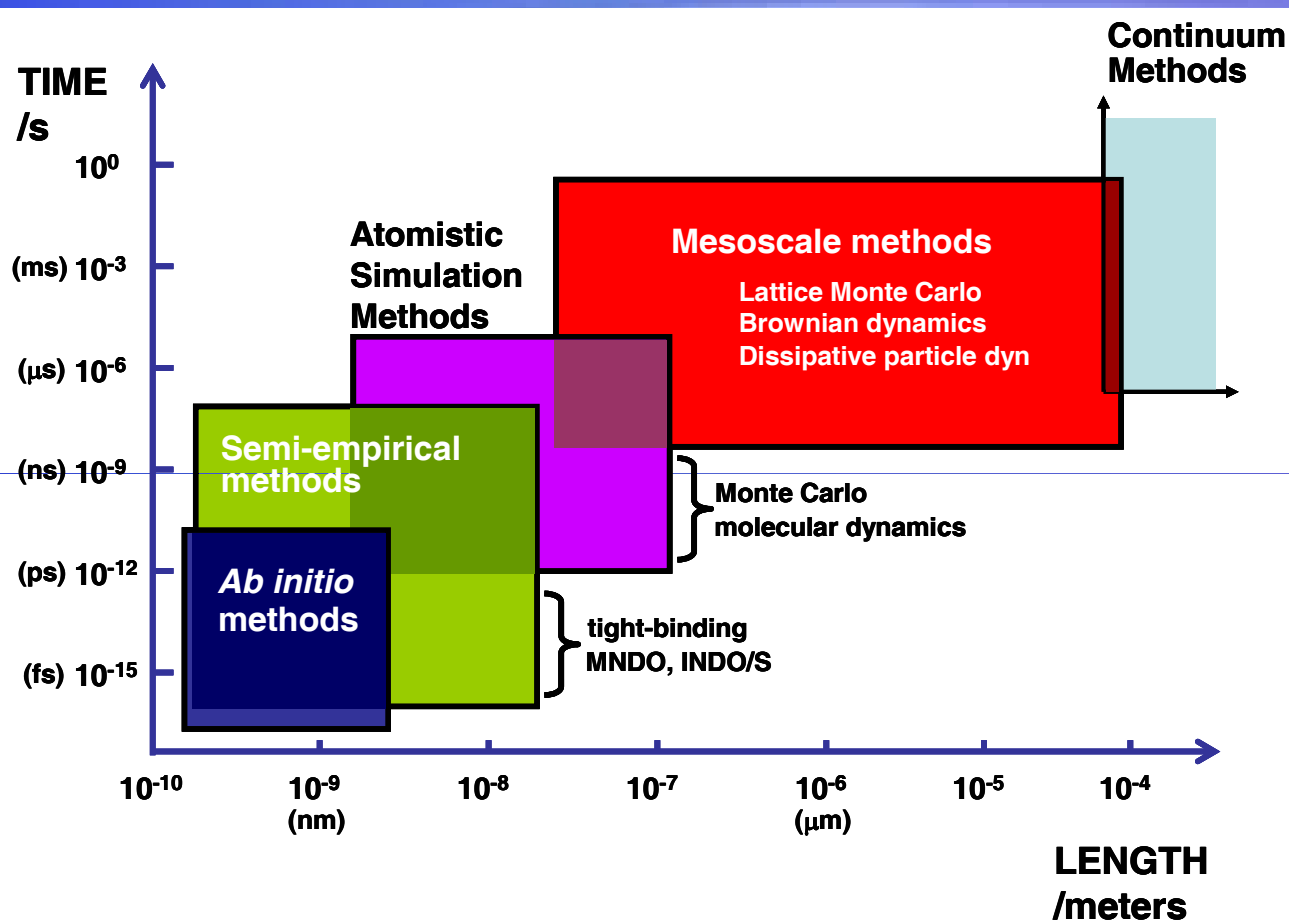


Figure 1. Schematic illustration of the simulation methods for different length and time scales

Methods

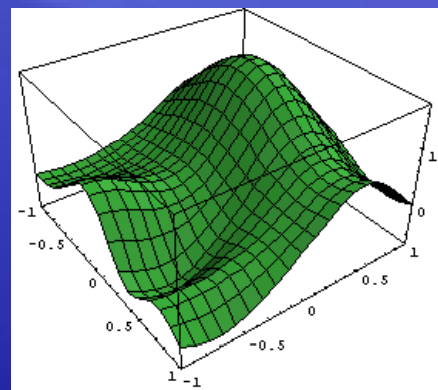
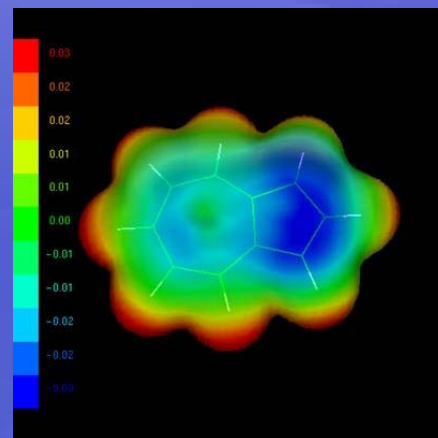
- *Ab initio* quantum chemistry methods
- Density functional theory (DFT) methods
- Semi-empirical quantum chemistry method
- Molecular mechanics method
- Specially treatment for periodic boundary condition
 - Plane waves implementation
 - Ewald summation for long-range interaction
- Molecular dynamics and Monte Carlo simulation
- Hybrid quantum mechanics/molecular mechanics method

Ab initio quantum chemistry methods

Ab initio quantum chemistry solves electronic Schrödinger equation from mathematical principles. The term *ab initio* indicates that the calculation is derived from first principles and does not rely on any empirical data.

$$\begin{aligned}\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots) &= E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots) \\ \hat{H} &= \sum_i \hat{h}_i + \frac{e^2}{4\pi\epsilon_0} \sum_i \sum_{j>i} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \\ \hat{h}_i &= -\frac{\hbar^2}{2m_e} \nabla_i^2 - \frac{e^2}{4\pi\epsilon_0} \sum_{\alpha} \frac{1}{|\mathbf{r}_i - \mathbf{R}_{\alpha}|}\end{aligned}$$

$$E(\mathbf{R}_{\alpha}, \mathbf{R}_{\beta}, \dots) = E_{\text{elec}} + \frac{e^2}{4\pi\epsilon_0} \sum_{\alpha} \sum_{\beta>\alpha} \frac{Z_{\alpha}Z_{\beta}}{|\mathbf{R}_{\alpha} - \mathbf{R}_{\beta}|}$$



Commonly used methods

□ Hartree-Fock methods

- Hartree-Fock (HF)
- Restricted Open-shell Hartree-Fock (ROHF)
- Unrestricted Hartree-Fock (UHF)

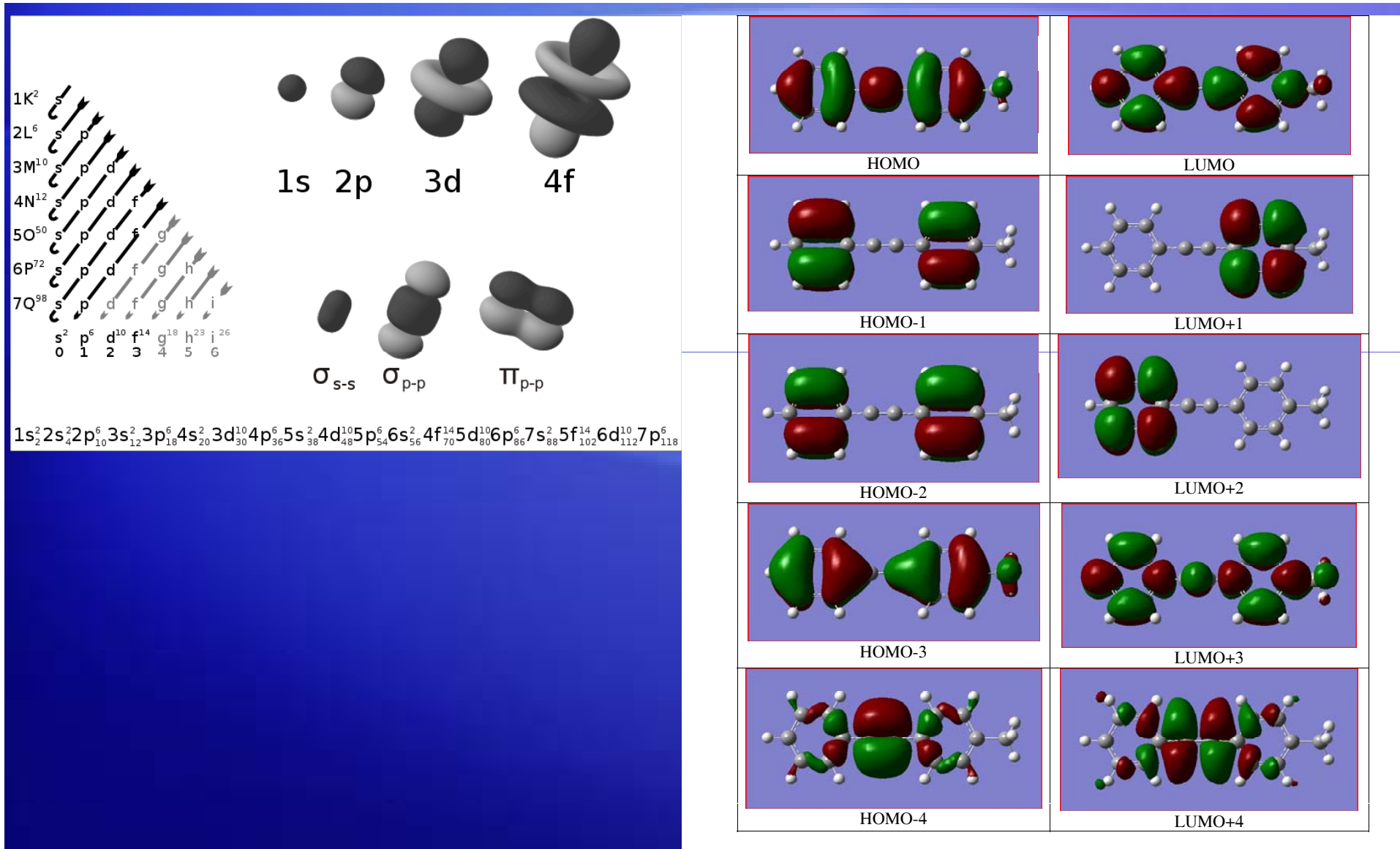
□ Post-Hartree-Fock methods

- Møller-Plesset perturbation theory (MPn)
- Configuration interaction (CI)
- Coupled cluster (CC)
- Quadratic configuration interaction (QCI)
- Quantum chemistry composite methods (G1, G2, CBS)

□ Multi-reference methods

- Multi-configurational self-consistent field (MCSCF)
- Multi-reference configuration interaction (MRCI)
- Complete Active Space Perturbation Theory (CASPTn)

Electron atomic and molecular orbitals



Molecular Orbital Theory & Hartree-Fock Method

Total wave function as a Slater Determinant

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1) & \phi_2(1) & \cdots & \phi_N(1) \\ \phi_1(2) & \phi_2(2) & \cdots & \phi_N(2) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_1(N) & \phi_2(N) & \cdots & \phi_N(N) \end{vmatrix}$$

$$\phi_i = \sum_{\mu=1}^N c_{\mu i} \chi_{\mu}$$

LCAO: Linear Combination of Atomic Orbitals

$$\phi_i = \sum_{\mu=1}^N c_{\mu i} \chi_{\mu}$$

Variation Principle \longrightarrow Hartree-Fock (HF)

$$F\phi_i = \varepsilon_i \phi_i$$

F = Fock operator = $h_i + \sum_j (2J_{ij} - K_{ij})$ for closed shells

Post-Hartree-Fock Method

Perturbation Theory Methods

$$\mathcal{H}_e = \mathcal{H}_0 + \lambda \mathcal{H}_1$$

$$\Psi = \Psi_0 + \lambda \Psi_1 + \lambda^2 \Psi_2 + \dots$$



MP2

MP3

MP4

...

Coupled Cluster Methods

$$\Psi = e^T \Phi_0$$

$$T = T_1 + T_2 + T_3 + \dots$$

$$\begin{array}{c} T_2 \\ T_1 + T_2 \\ T_1 + T_2 + T_3 \\ \dots \end{array}$$



CCD

CCSD

CCSDT

...

Variational Methods

$$\Psi = \Phi_0 + \sum_{\{ai\}} C_a^i \Phi_a^i + \sum_{\{ab\}} \sum_{\{ij\}} C_{ab}^{ij} \Phi_{ab}^{ij} + \dots$$



SDCI

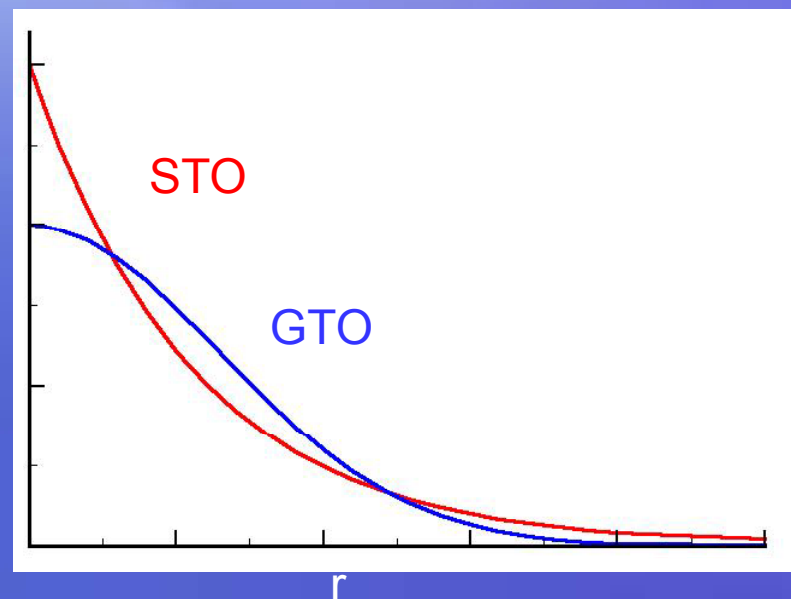
SDTCI

...

MRCI

Basis Set

$$\phi_i = \sum_{\mu=1}^N c_{\mu i} \chi_{\mu}$$



- **Minimal basis sets:** STO-3G
- **Split-valence basis sets:** 3-21G, 6-31G
- **Polarisation functions** are denoted with * (3-21G*, 6-31G*)
- **Diffuse functions** are denoted by + (6-31+G*)

* The selection of basis set is a key factor to the accuracy of the numeric solution.

Level of Theory

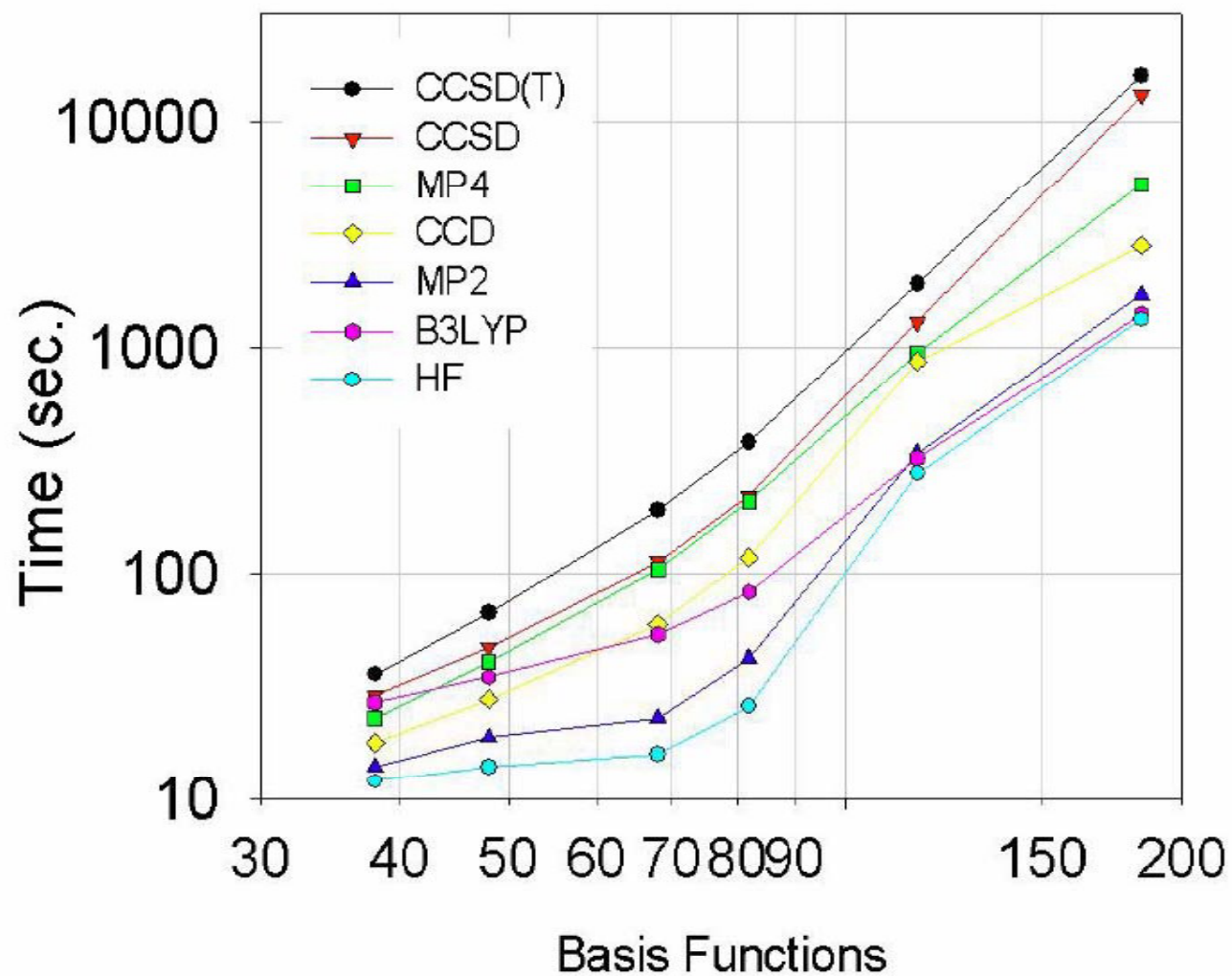
Methods

- AM1, PM3
- HF, ROHF
- MP2(full), MP2(frozen core), MP4
- BLYP, B3LYP, B3PW91, MPW1PW91, PBE
- CID, CISD
- QCISD, QCISD(T)
- CCD, CCSD, CCSD(T)
- G1, G2, G2MP2, CBS-Q

Basis Sets

- 3-21G, 3-21G*
- 6-31G, 6-31G*
- 6-311G*
- 6-31G**
- 6-31+G**
- cc-pVDZ
- cc-pVTZ
- ECPs

Cost vs. Accuracy



Methods

- *Ab initio* quantum chemistry methods
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Density functional theory methods

- Hohenberg-Kohn Theorem (1964)
 - All properties of the many-body system are determined by the ground state density $n_0(r)$
 - Each property is a functional of the ground state density $n_0(r)$ which is written as $f[n_0]$
 - A functional $f[n_0]$ maps a function to a result: $n_0(r) \rightarrow f$
- Kohn-Sham ansatz (1965)
 - Replace original many-body problem with an independent electron problem – that can be solved!
 - The ground state density is required to be the same as the exact density

Exchange-Correlation Functional

$$n_0(\mathbf{r}) = \sum_{\sigma} \sum_{i=1} |\psi_i^{\sigma}(\mathbf{r})|^2,$$

$$E_{KS} = \frac{1}{2} \sum_{\sigma} \sum_{i=1} |\nabla \psi_i^{\sigma}|^2 + \int d\mathbf{r} V_{ext}(\mathbf{r}) n(\mathbf{r}) + E_{Hartree}[n] + E_{II} + E_{xc}[n].$$

- Local Density Approximation - LDA

$$E_{XC}[n_{\uparrow}, n_{\downarrow}] = \int \epsilon_{XC}(n_{\uparrow}, n_{\downarrow}) n(\vec{r}) d^3r$$

Exc can be determined using homogeneous electron gas model or using quantum Monte Carlo methods

- Gradient approximations - GGA

$$E_{XC}[n_{\uparrow}, n_{\downarrow}] = \int \epsilon_{XC}(n_{\uparrow}, n_{\downarrow}, \vec{\nabla} n_{\uparrow}, \vec{\nabla} n_{\downarrow}) n(\vec{r}) d^3r$$

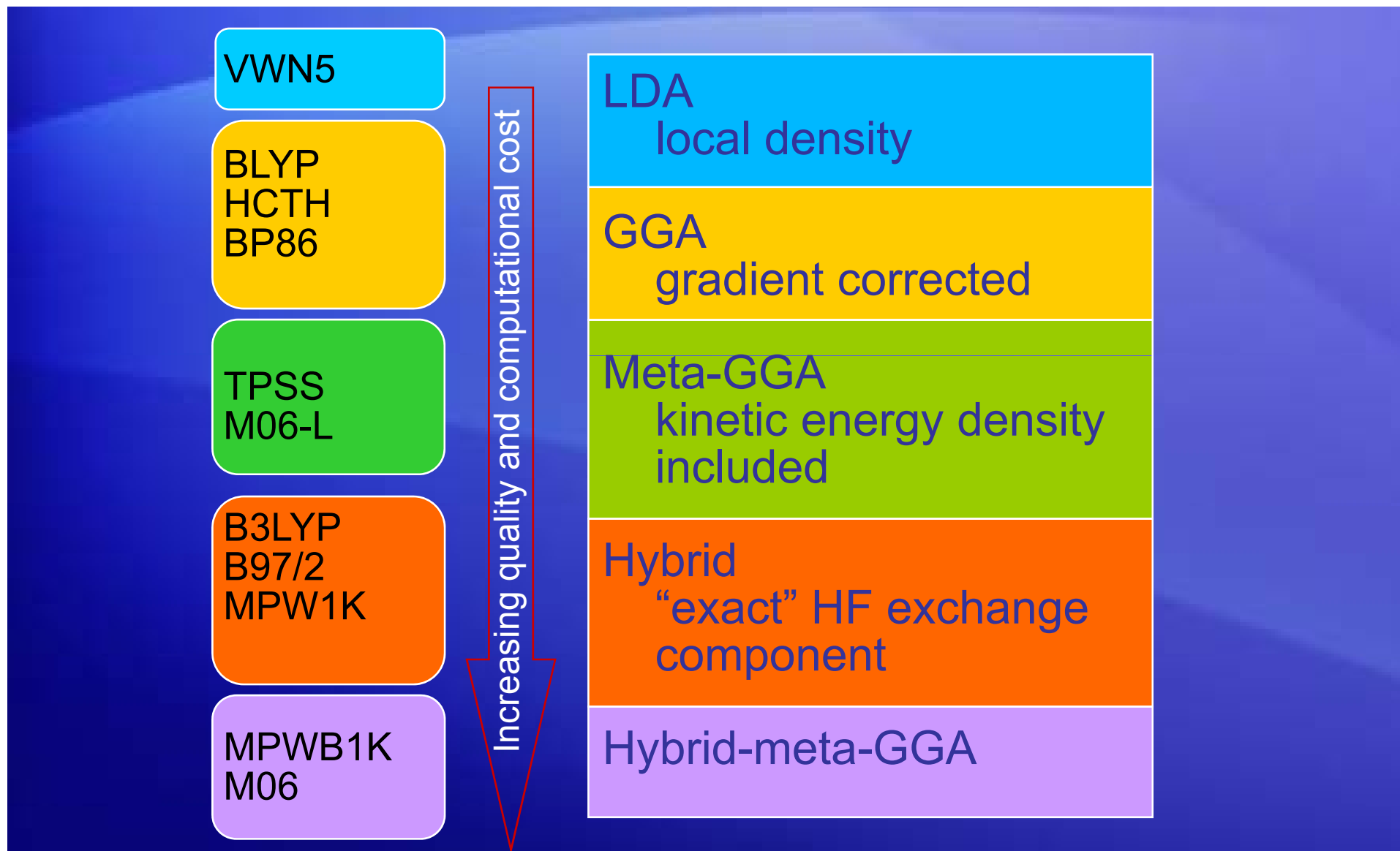
$$\frac{\delta E_{KS}}{\delta \psi_i^{\sigma*}(\mathbf{r})} = 0, \quad (1)$$

$$\langle \psi_i^{\sigma} | \psi_j^{\sigma'} \rangle = \delta_{i,j} \delta_{\sigma,\sigma'}. \quad (2)$$

$$(-\frac{1}{2} \nabla^2 + V_{KS}^{\sigma}(\mathbf{r}), -\epsilon_i^{\sigma}) \psi_i^{\sigma}(\mathbf{r}) = 0 \quad (3)$$

$$\begin{aligned} V_{KS}^{\sigma}(\mathbf{r}) &= V_{ext}(\mathbf{r}) + \frac{\delta E_{Hartree}}{\delta n(\mathbf{r}, \sigma)} + \frac{\delta E_{xc}}{\delta n(\mathbf{r}, \sigma)} \\ &= V_{ext}(\mathbf{r}) + V_{Hartree}(\mathbf{r}) + V_{xc}^{\sigma}(\mathbf{r}) \end{aligned} \quad (4)$$

Correlation-Exchange Functional



Software supporting DFT

Software supporting DFT

- | | | |
|---|---|-----------------------------|
| ■ Abinit | ■ HiLAPW ↗ | ■ SPR-KKR ↗ |
| ■ ADF | ■ JAGUAR | ■ TURBOMOLE |
| ■ AIMPRO ↗ | ■ MOLCAS | ■ VASP |
| ■ Ascalaph Quantum ↗ | ■ MOLPRO | ■ WIEN2k ↗ |
| ■ Atomistix Toolkit | ■ MPQC | |
| ■ Atompaw/PWPAW | ■ NRLMOL | |
| ■ CADPAC | ■ NWChem | |
| ■ CASTEP | ■ OCTOPUS | |
| ■ CP2K ↗ | ■ OpenMX ↗ | |
| ■ CPMD ↗ | ■ ORCA ↗ | |
| ■ CRYSTAL06 ↗ | ■ ParaGauss [1] ↗ | |
| ■ DACAPO | ■ PARATEC [2] ↗ | |
| ■ DALTON | ■ PARSEC | |
| ■ deMon2K ↗ | ■ PC GAMESS | |
| ■ DFT++ ↗ | ■ PLATO | |
| ■ DMol3 ↗ | ■ Petot ↗ | |
| ■ EXCITING | ■ Parallel Quantum Solutions | |
| ■ Fireball ↗ | ■ Priroda | |
| ■ FLEUR ↗ | ■ PWscf (Quantum-ESPRESSO ↗) | |
| ■ FSatom, dozens of free and proprietary DFT programs ↗ | ■ Q-Chem | |
| ■ GAMESS (UK) | ■ SIESTA | |
| ■ GAMESS (US) | ■ Socorro | |
| ■ GAUSSIAN | ■ Spartan | |
| ■ GPAW | ■ S/PHI/nX ↗ | |

http://en.wikipedia.org/wiki/Density_functional_theory

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Semi-empirical quantum chemistry method

- CNDO (1965, Pople et al)
- MINDO (1975, Dewar)
- MNDO (1977, Thiel)
- INDO (1967, Pople et al)
- ZINDO
- SINDO1
- STO-basis (/S-spectra,/2 d-orbitals)
- /1/2/3, organics
- /d, organics, transition metals
- Organics
- Electronic spectra, transition metals
- 1-3 row binding energies, photochemistry and transition metals

Further improvement

■ AM1

- Modified nuclear repulsion terms model to account for H-bonding (1985, Dewar et al)
- Widely used today (transition metals, inorganics)

■ PM3 (1989, Stewart)

- Larger data set for parameterization compared to AM1
- Widely used today (transition metals, inorganics)

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Molecular mechanics method

Interactions between atoms (Potential Energy Function) are represented by functions of distance, angle or dihedral

Collection of empirical parameters and potential functions is known as a *force field*.

i.e. AMBER
force field:

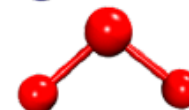
$$U(\mathbf{R}) = \sum_{bonds} K_r (r - r_{eq})^2$$

bond



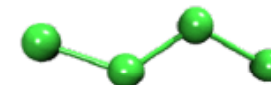
$$+ \sum_{angles} K_{\theta} (\theta - \theta_{eq})^2$$

angle



$$+ \sum_{dihedrals} \frac{V_n}{2} (1 + \cos[n\phi - \gamma])$$

dihedral



$$+ \sum_{i < j}^{atoms} \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^6}$$

van der Waals

$$+ \sum_{i < j}^{atoms} \frac{q_i q_j}{\epsilon R_{ij}}$$

electrostatic



- ▶ Improper term

$$+ \sum_{Improper} K_{\omega}(\omega - \omega_0)^2$$

Improvers

amino types	142964 dnc 18k, 53M and proteins with T1P1 bases, 0.02 MCMC-1.2 in energy groups $\begin{matrix} \text{C} & 11.1\% & \text{epg 1: overdesign group} \\ \text{W} & 11.1\% & \text{epg 2: alternative C} \\ \text{W} & 11.1\% & \text{epg 3: alternative C} \\ \text{W} & 11.1\% & \text{epg 4: nitrogen in waste groups} \end{matrix}$		
cond mismatch	three quartal	equilibrium	
	$\begin{matrix} \text{C-G} & 217.5 & 1.126 & \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{C-G} & 227.5 & 1.444 & \text{TCGTC} & 700.7 & 1096.0 & 230.0 & \text{AA} \\ \text{C} & 605.0 & 1.255 & \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$		
single bending	CT-C	$\begin{matrix} \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$	AA general
sequence frequency	CT-C	$\begin{matrix} \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$	$\begin{matrix} \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$
van der Waals term	$\begin{matrix} \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$	$\begin{matrix} \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$	$\begin{matrix} \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \\ \text{TCGTC} & 1096.0 & 230.0 & \text{AA} \end{matrix}$

Commonly used force field

Amber	DNA,proteins and lipids. Generalized Amber Force Field (GAFF) covers most organic space.
OPLS	Organic molecules in the liquid phase.Available as all-atom (AA) or united-atom (UA) form.
CHARMM	DNA,proteins,lipids, sugars.
GROMOS	General purpose.Organic and biochemical space.
Dreiding	General purpose.Includes some parameters for metals and main group elements.
MM2/MM3	General purpose.MM2 used for hydrocarbons.MM3 includes most of organic space plus some other main group and metal atom types.
Water	Rigid and flexible models available. TIP3P widely used in biological simulation.

Commonly used softwares

AMBER	General Molecular Simulation Package
BOSS	OPLS
CHARMM	General Molecular Simulation Package
GROMACS	High performance MD
GROMOS	Geared towards <u>biomolecules</u>
LAMMPS	Has potentials for soft and solid-state materials and coarse-grain systems
<u>MacroModel</u>	OPLS-AA, GBSA solvent model, conformational sampling, minimization, MD
Materials Studio	Materials Studio is a software environment that brings the materials simulation technology to desktop computing, solving key problems throughout the R&D process.
<u>MCCCS</u> Towhee	Originally designed for the prediction of fluid phase <u>equilibria</u>
MOE	Molecular Operating Environment
Prime	Homology modeling, loop and side chain optimization, minimization, OPLS-AA, SGB solvent model, <u>parallalized</u>
TINKER	Software Tools for Molecular Design
VMD + NAMD	Fast, parallel MD

Common tasks

- Sampling conformational spaces (Structure and dynamics)
- Free energy calculation (Binding energy)
- Structural refinement (based on NMR data)
- Reaction path (Transition Path Sampling)
- Molecular interaction (Ligand-Protein)
- Investigate mutational effects
- etc.

Applications

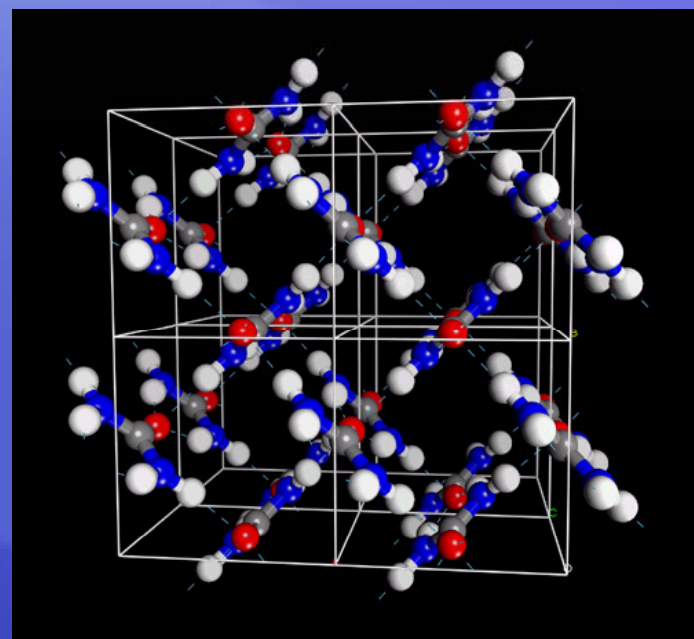
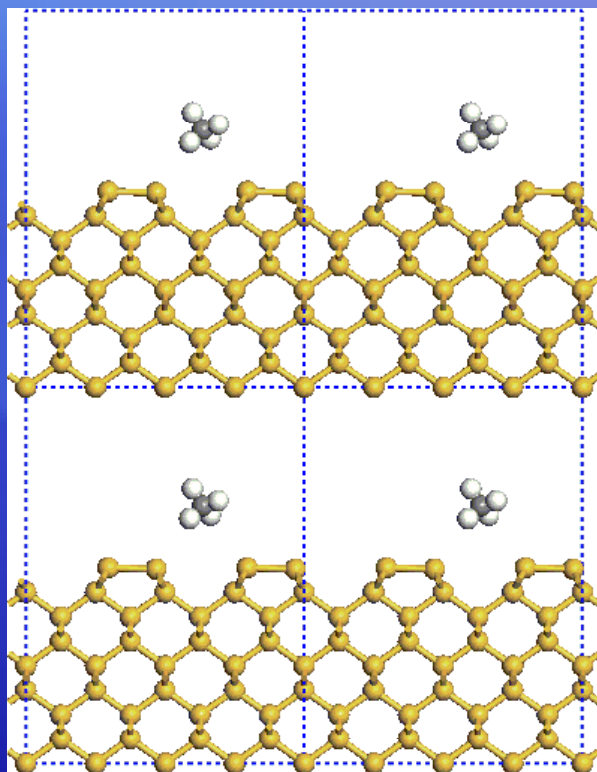
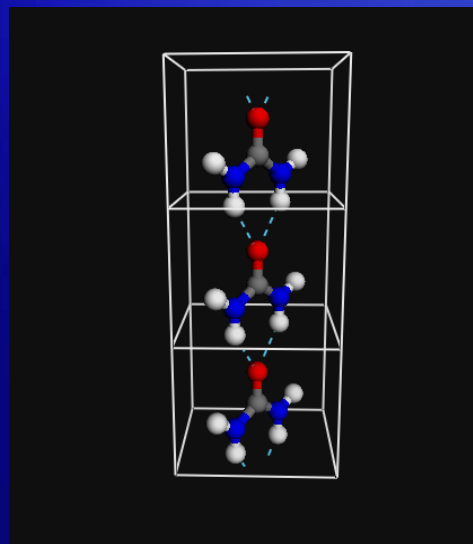
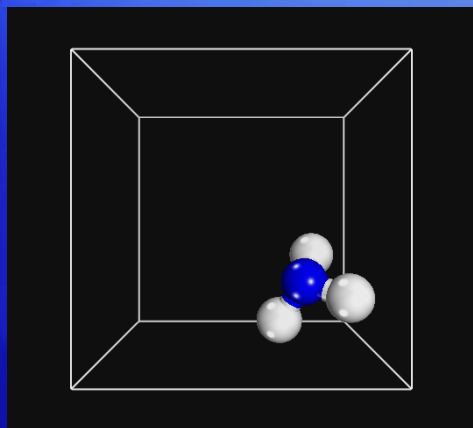
- Speed of method opens up a wide range of systems
 - Amorphous condensed phase – liquids, liquid crystals, glasses
 - Biological systems – Biopolymers, membranes
 - Nanotubes and molecular machines
- Fast calculations allow large numbers of conformers to be screened
 - Drug docking analysis
 - Global minimum searches
- Statistical data can be collected
 - Access to bulk properties (via statistical mechanics)
 - Simulation of finite temperature behaviour and phase changes

Methods

- *Ab initio* quantum chemistry methods
- Density functional theory (DFT) methods
- Semi-empirical quantum chemistry method
- Molecular mechanics method
- Specially treatment for periodic boundary condition
 - Periodic Electronic Structure Calculations
 - Ewald summation for long-range interaction
- Molecular dynamics and Monte Carlo simulation
- Hybrid quantum mechanics/molecular mechanics method

Systems with periodic boundary condition

- 0 to 3 Dimension system (3D (condense phase), 2D (surfaces), 1D (polymers) and 0D (molecule))

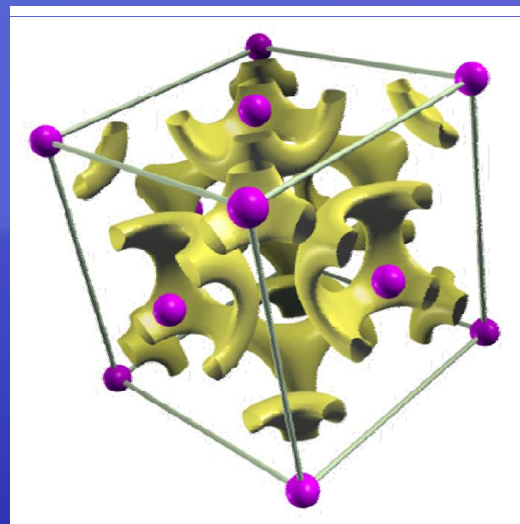
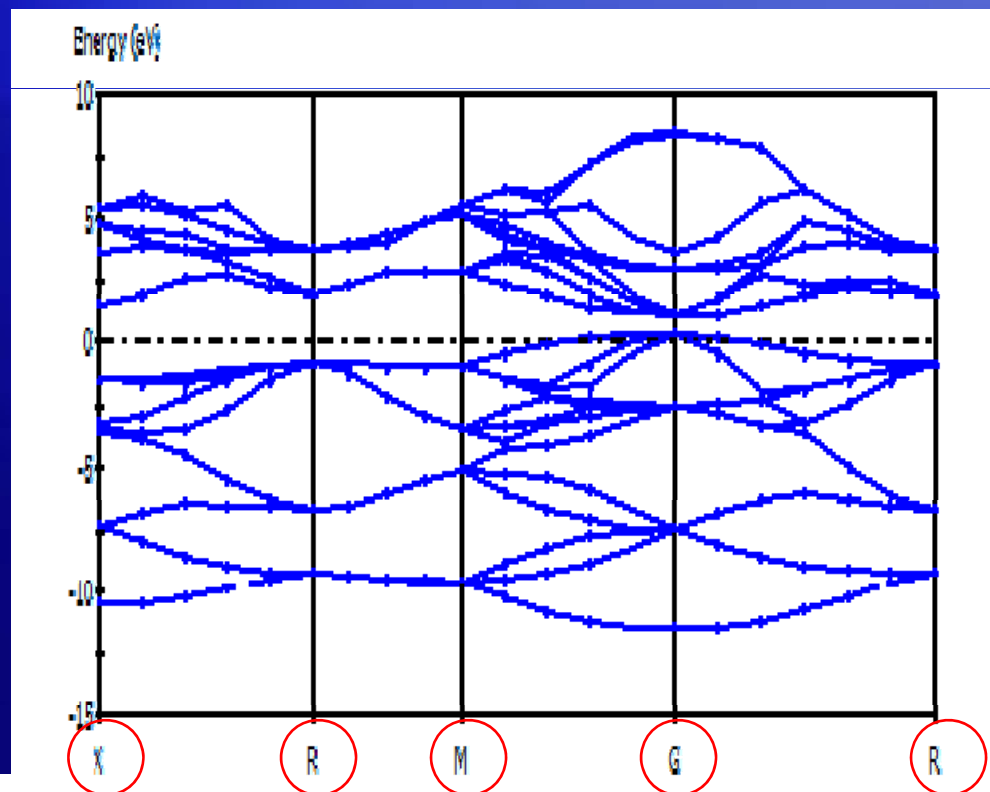


Bloch's Theorem

The electronic wave function in a periodic potential $u_{nk}(r)$ can be expressed as

$$\Psi_{nk}(r) = \sum_k c_{ik} \exp(ik \cdot r) \phi_{nk}(r)$$

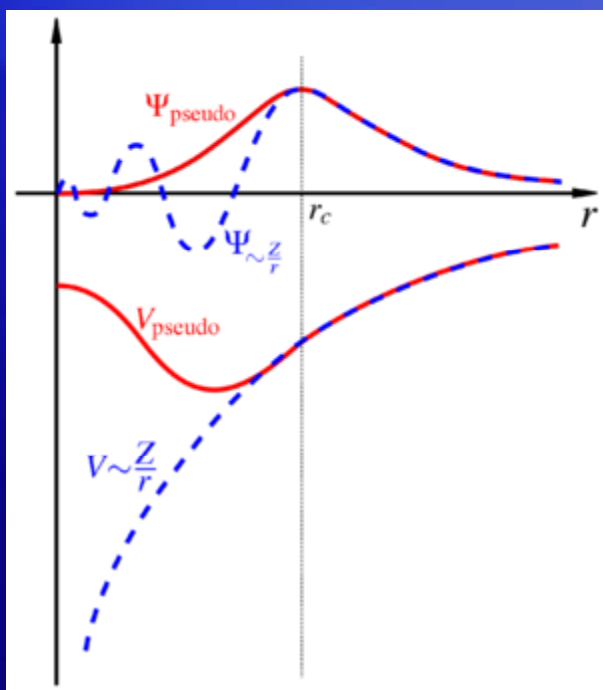
k is wavevector within the first Brillouin zone



Plane wave and pseudopotential

Plane wave basis set is a natural choice for the periodic electronic wave function due to its periodicity and its mathematical and computational convenience.

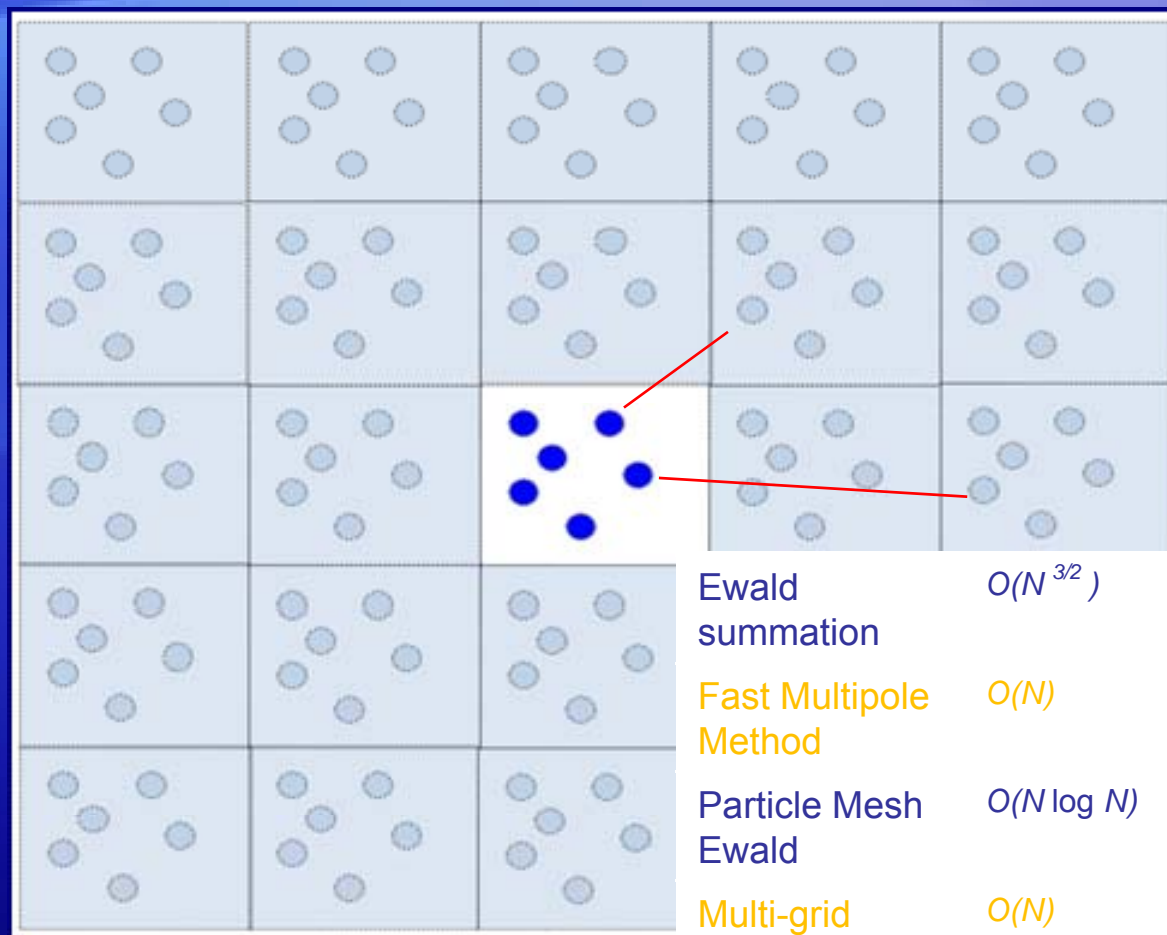
$$\Psi_i(r) = \sum_k c_{ik} \exp(ik \cdot r)$$



Application of **pseudopotential** can effectively:

- *reduce the size of basis set ;*
- *reduce the size of the system (less electrons)*
- *take into account of the relativistic and other effects*

Long-range interaction in Molecular Mechanics



Ewald
summation

$O(N^{3/2})$

Ewald, 1921

Fast Multipole
Method

$O(N)$

Greengard, 1987

Particle Mesh
Ewald

$O(N \log N)$

Darden, 1993

Multi-grid
summation

$O(N)$

Brandt et al., 1990
Skeel et al., 2002
Izaguirre et al., 2003

Computational Chemistry Codes on Clusters

- Quantum Chemistry package for molecular systems

— GAMESS	— NWCHEM	— SPARTAN
— GAUSSIAN	— ORCA	— TURBOMOLE
— Jaguar	— QCHEM	

- Quantum chemistry package for solids/surface

— ABINIT	— CASTEP	— VASP
— CPMD	— NWCHEM	

- Molecular Mechanics Packages

— AMBER	— GROMACS	— XPLOR
— CHARMM	— LAMMPS	
— DL_POLY	— NAMD	

- Others

— 3D-DOCK	— Molden	— VMD
— AUTODOCK	— Pymol	
— HADDOCK	— Rosetta	

Molecular Quantum Chemistry Packages

[ACES](#)

[CADPAC](#)

[COLUMBUS](#)

[DALTON](#)

[GAMESS \(UK\)](#)

[GAMESS \(US\)](#)

[GAUSSIAN](#)

[JAGUAR](#)

[Materials Studio \(DMol3\)](#)

[MOLCAS](#)

[MOLPRO](#)

[MPQC](#)

[NWChem](#)

[PSI](#)

[Q-Chem](#)

[SPARTAN](#)

[TURBOMOLE](#)

Quantum Chemistry package on clusters

- GAMESS (US)
- GAUSSIAN
- NWCHEM
- ORCA
- QCHEM
- SPARTAN
- TURBOMOLE

GAMESS

- General Atomic and Molecular Electronic Structure System
 - Primary focus is on ab initio quantum chemistry calculations
 - Also includes DFT, semi-empirical (AM1, PM3) and QM/MM capabilities
- Early version of GAMESS is available under /usr/global/gamess
 - scripts need to execute the program

GAMESS Input file

```
!  
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE COORD=CART  
  NZVAR=0 MULT=1 ICHARG=0 $END  
$SYSTEM TIMLIM=20000 MEMORY=10000000 $END  
$STATPT NSTEP=1000 $END  
$BASIS GBASIS=STO NGAUSS=3 $END  
$GUESS GUESS=HUCKEL $END  
$DATA  
Test...HCHO molecule - RHF/STO-3G (a comment line)  
Cn 1  
  
C      6.0      0.6084782705      -0.0000011694      0.000000000000  
O      8.0     -0.6082418894      -0.0000002093      0.000000000000  
H      1.0      1.2040919862     -0.9264398115      0.000000000000  
H      1.0      1.2040973125      0.9264340484      0.000000000000  
$END
```

GAUSSIAN

Gaussian 03 is a general electronic structure programs. Gaussian 03 is used by chemists, chemical engineers, biochemists, physicists and others for research in established and emerging areas of chemical interest.

Gaussian Input File Structures

Link 0 Commands (% lines): System specific parameter

Route section (# lines): Specify calculation type, model chemistry and other options

Title section: Brief description of the calculation

Molecule specification: Specify molecular system to be studied

Optional additional sections: Additional input needed for specific job types

```
%NProcShared=2
```

Link 0 section (#of processors for SMP)

```
%MEM=64MW
```

(amount of memory)

```
%chk=h2o_opt.chk
```

(checkpoint file name and location)

```
# RHF/6-31g** OPT
```

Route section

```
H2O RHF/6-31g** optimization
```

Title section

```
0 1
```

Molecule Specification section (charge, multiplicity)

```
O
```

Structure representation in Z-matrix format

```
H 1 r1
```

```
H 1 r1 2 tha1
```

```
r1 1.000
```

```
tha1 105.0
```

Route Section: Keywords

<u>#</u>	<u>Dreiding</u>	<u>LSDA</u>	<u>Scale</u>
<u>ADMP</u>	<u>ExtendedHuckel</u>	<u>MaxDisk</u>	<u>Scan</u>
<u>AM1</u>	<u>External</u>	<u>MINDO3</u>	<u>SCF</u>
<u>Amber</u>	<u>ExtraBasis</u>	<u>MM</u>	<u>SCRF</u>
<u>Archive</u>	<u>Frozen Core Options</u>	<u>MNDO</u>	<u>SP</u>
<u>B3LYP</u>	<u>Field</u>	<u>MP* Keywords</u>	<u>Sparse</u>
<u>BD</u>	<u>FMM</u>	<u>Name</u>	<u>Stable</u>
<u>BOMD</u>	<u>Force</u>	<u>NMR</u>	<u>Symmetry</u>
<u>CASSCF</u>	<u>Frequency</u>	<u>ONIOM</u>	<u>TD</u>
<u>CBS Keywords</u>	<u>G* Keywords</u>	<u>Opt</u>	<u>Temperature</u>
<u>CBSExtrapolate</u>	<u>Gen</u>	<u>Output</u>	<u>Test</u>
<u>CCD</u>	<u>Geom</u>	<u>OVGF</u>	<u>TestMO</u>
<u>Charge</u>	<u>GFInput</u>	<u>PBC</u>	<u>TrackIO</u>
<u>ChkBasis</u>	<u>GFPrint</u>	<u>PM3</u>	<u>Transformation</u>
<u>CID</u>	<u>Guess</u>	<u>Polar</u>	<u>UFF</u>
<u>CIS</u>	<u>GVB</u>	<u>Population</u>	<u>Units</u>
<u>CNDO</u>	<u>Hartree-Fock</u>	<u>Pressure</u>	<u>Volume</u>
<u>Complex</u>	<u>Huckel</u>	<u>Prop</u>	<u>W1U</u>
<u>Constants</u>	<u>INDO</u>	<u>Pseudo</u>	<u>Zindo</u>
<u>Counterpoise</u>	<u>Integral</u>	<u>Punch</u>	<u>Link 0 Commands</u>
<u>CPHF</u>	<u>IOp</u>	<u>QCISD</u>	<u>Non-Standard Routes</u>
<u>Density</u>	<u>IRC</u>	<u>ReArchive</u>	<u>Program Development Keywords</u>
<u>DensityFit</u>	<u>IRCMaX</u>	<u>SAC-CI</u>	<u>Density Functional Methods</u>

Keywords (Job types)

- SP Single point energy.
- Opt Geometry optimization.
- Freq Frequency and thermochemical analysis.
- IRC Reaction path following.
- IRCMax Find the maximum energy along a specific reaction path.
- Scan Potential energy surface scan.
- Polar Polarizabilities and hyperpolarizabilities.
- ADMP and BOMD Direct dynamics trajectory calculation.
- Force Compute forces on the nuclei.
- Volume Compute molecular volume.

Keywords (Molecular properties)

- Atomic charges, Dipole moment, Multipole moments : Pop
- Electron affinities and ionization potentials via propagator methods: OVGF
- Electron density: cubegen
- Electronic circular dichroism: TD
- Electrostatic potential: cubegen, Prop
- Electrostatic-potential derived charges: Pop=**Chelp**, **ChelpG** or **MK**
- Frequency-dependent polarizabilities/hyperpolarizabilities: Polar **CPHF=RdFreq**
- High accuracy energies: CBS-QB3, G2, G3, W1U
- Hyperfine coupling constants (anisotropic): Prop
- Hyperfine spectra tensors (incl. *g* tensors): Freq=(**VCD**, **VibRot**[, **Anharmonic**])
- Hyperpolarizabilities: Freq, Polar
- IR and Raman spectra: Freq
- Molecular orbitals: Pop=**Regular**
- NMR shielding and chemical shifts: NMR
- NMR spin-spin coupling constants: NMR=**SpinSpin**
- Optical rotations: Polar=**OptRot** **CPHF=RdFreq**
- Polarizabilities: Freq, Polar
- Thermochemical analysis: Freq
- UV/Visible spectra: CIS, Zindo, TD
- Vibration-rotation coupling: Freq=**VibRot**
- Vibrational circular dichroism: Freq=**VCD**

Available model calculations

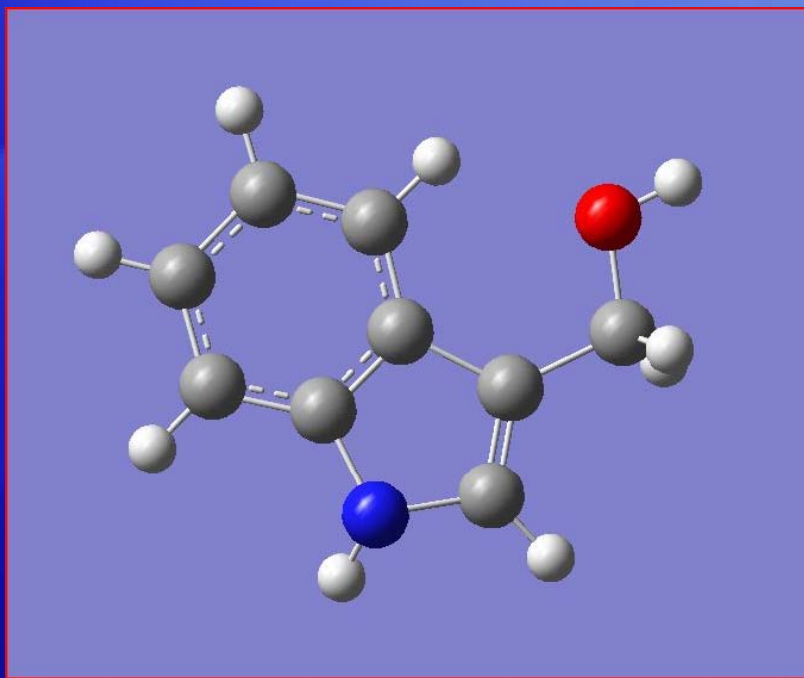
Method Availabilities in *Gaussian 03*

	SP, Scan	Opt, Force, BOMD	Freq	IRC	ADMP	Polar	Stable	ONIOM	SCRIF	PBC
Molecular Mechanics	*	*	*					*		
AM1, PM3 (etc.)	*	*	num.	*				*		
HF	*	*	*	*	*	*	*	*	*	*
DFT methods	*	*	*	*	*	*	*	*	*	*
CASSCF	*	*	*	*		*		*	*	
MP2	*	*	*	*		*		*		
MP3, MP4(SDQ)	*	*		*				*		
MP4(SDTQ), MP5	*							*		
QCISD, CCD, CCSD	*	*		*				*		
QCISD(T) or (TQ)	*							*		
BD	*							*		
OVGF	*									
CBS, G _n , W1 methods	*									
CIS	*	*	*	*		*		*	*	
TD	*							*	*	
ZINDO	*							*		
CI	*	*		*				*		
GVB	*	*		*				*		

Keyword (Basis set)

Basis Set	Applies to	Polarization Functions	Diffuse Functions
STO-3G	H-Xe	*	
3-21G	H-Xe	* or **	+
6-21G	H-Cl	(d)	
4-31G	H-Ne	(d) or (d,p)	
6-31G , 6-311G	H-Kr	(3df,3pd)	++
D95	H-Cl except Na and Mg	(3df,3pd)	++
D95V	H-Ne	(d) or (d,p)	++
SHC	H-Cl	*	
CEP-4G , CEP-31G, CEP121G	H-Rn	* (Li-Ar only)	
LanL2MB	H-Ba, La-Bi		
LanL2DZ	H, Li-Ba, La-Bi		
SDD, SDDAll	all but Fr and Ra		
cc-pV(DTQ5)Z	H-He, B-Ne, Al-Ar, Ga-Kr	included in definition	added via AUG- prefix
cc-pV6Z	H, B-Ne	included in definition	added via AUG- prefix
SV , SVP	H-Kr	in SVP	
TZV and TZVP	H-Kr	included in definition	
MidiX	H, C-F, S-Cl, I, Br	included in definition	
EPR-II, EPR-III	H, B, C, N, O, F	included in definition	
UGBS	H-Lr	UGBS(1,2,3)P	
MTSmall	H-Ar		
DGDZVP	H-Xe		
DGDZVP2	H-F, Al-Ar, Sc-Zn		
DGTZVP	H, C-F, Al-Ar		

Molecular Specification



Molecules can be specified by Z-matrix or Cartesian coordinate.

The Z-matrix is a way to represent a system built of atoms. It provides a description of each atom in a molecule in terms of its atomic number, bond length, bond angle, and dihedral angle, the so-called **internal**

Molecular builders

- ① Some softwares provide sketcher ease, i.e. GaussView, Accelrys's **Discovery Studio** Molecular Editor, HyperChem, Gallop
- ② Some softwares provide interface coordinates, i.e. Molden

#	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							-6.722681	-0.505425	0.577958
2	C	1			1.359414			-7.546196	-0.102287	1.581606
3	C	1	2		1.519296	106.636397		-6.629638	0.653302	-0.400282
4	H	2	1	3	1.070000	124.601181	170.004847	-7.933013	-0.744400	2.345126
5	N	2	1	3	1.492105	110.780216	-9.725129	-7.842439	1.355839	1.469867
6	C	5	2	1	1.480139	102.645563	14.326477	-7.389792	1.674183	0.097067
7	C	3	1	2	1.390206	129.847972	-177.898052	-5.951045	0.745392	-1.610119
8	H	5	2	1	1.000000	113.263529	136.706967	-8.804844	1.576600	1.628106
9	C	6	5	2	1.392313	128.383959	166.502774	-7.646571	2.817723	-0.654544
10	C	7	3	1	1.409831	117.429306	174.077911	-6.146247	1.912146	-2.377063
11	H	7	3	1	1.070000	121.287108	-5.466034	-5.311137	-0.042090	-1.949661
12	H	9	6	5	1.070000	121.099591	-4.470662	-8.297125	3.584676	-0.289220
13	C	10	7	3	1.420340	120.170334	-0.234787	-7.012493	2.936478	-1.910451
14	H	10	7	3	1.070000	119.914184	-179.991658	-5.643539	2.024559	-3.314905
15	H	13	10	7	1.070000	119.819212	-177.895492	-7.182855	3.804448	-2.512534
16	C	1	2	5	1.540000	126.599592	166.961898	-5.965707	-1.843849	0.493033
17	H	16	1	2	1.070000	109.471221	61.979295	-6.668631	-2.650164	0.467462
18	H	16	1	2	1.070000	109.471221	-58.020705	-5.332008	-1.950118	1.348623
19	O	16	1	2	1.430000	109.471221	-178.020705	-5.170284	-1.867048	-0.695102
20	H	19	16	1	0.960000	109.471221	180.000000	-4.698404	-2.701390	-0.748042

NWCHEM

NWChem is a computational chemistry package with many capabilities, including:

- Molecular electronic structure calculations
- Pseudopotential plane-wave electronic structure calculations
- Ab initio and classical molecular dynamics
- and more

NWCHEM Input file format

```
start water

Title "H2o energy"

geometry units au
O 0.00000 0.000000 0.000000
H 0.00000 1.43042809 -1.10715266
H 0.00000 -1.43042809 -1.10715266
End

Basis
* library 3-21G
End

MP2; freeze atomic; END
Task mp2 energy
```

- Job name determines names for temporary files
- <module> ... end blocks change settings for future calculations
- task directive triggers calculation
- input is handled strictly top-to-bottom (only settings above a task have an impact)
- Python procedures for more complicated structures

Quantum chemistry package for solids/surface

— ABINIT

— ADF/Band

— CPMD

— CASTEP

— NWCHEM

— VASP

VASP (Vienna Ab-initio Simulation Package)

VASP is a complex package for performing ab-initio quantum-mechanical molecular dynamics (MD) simulations using pseudopotentials or the projector-augmented wave method and a plane wave basis set.

- The approach implemented in VASP is based on the (finite-temperature) local-density approximation with the free energy as variational quantity and an exact evaluation of the instantaneous electronic ground state at each MD time step. VASP uses efficient matrix diagonalisation schemes and an efficient Pulay/Broyden charge density mixing.
- The interaction between ions and electrons is described by ultra-soft Vanderbilt pseudopotentials (US-PP) or by the projector-augmented wave (PAW) method.
- Forces and the full stress tensor can be calculated with VASP and used to relax atoms into their instantaneous ground-state.

VASP Input

INPUT Files

POSCAR
POTCAR
KPOINTS
INCAR

STOPCAR is used to
signal stopping VASP
execution

OUTPUT Files

OUTCAR
OSZICAR
CONTCAR
CHGCAR
WAVECAR
EIGENVAL
PROCAR
XDATCAR
LOCPOT
DOSCAR
CHG

Structure Input File

POSCAR

P.8

BCC Fe(100) - 3

2.8224

1.00000000 0.00000000 0.00000000

0.00000000 1.00000000 0.00000000

0.00000000 0.00000000 4.54308390

3

Direct

.5000000000000000 .5000000000000000 .1100573995562793

.0000000000000000 .0000000000000000 .0000000000000000

.5000000000000000 .5000000000000000 -.1100573995562793

ascale (A°)

$\vec{a}_1, \vec{a}_2, \vec{a}_3$

natom

Direct (other)

$x_1(i)\vec{a}_1 + x_2(i)\vec{a}_2 + x_3(i)\vec{a}_3$

Cartesian (C, c, K, k)

$\text{ascale} \times (x_1\vec{i} + x_2\vec{j} + x_3\vec{k})$

Example

3.12383080835807814

.9999999999999999 .0000000000000000 .0000000000000000

.0000000000000000 .9999999999999999 .0000000000000000

.0000000000000000 .0000000000000000 13.2902443002697161

3 2

Selective dynamics

Direct

.5000000000000000 .5000000000000000 .0376786968277952 T T T

.0000000000000000 .0000000000000000 .0000000000000000 F F F

.5000000000000000 .5000000000000000 .9623213031722048 T T T

.0000000000000000 .0000000000000000 .9247419794041822 T T T

.0000000000000000 .0000000000000000 .0752580205958178 T T T

n_1, n_2

The ordering must be consistent with the POTCAR

fixed

Pseudopotential File

P.9

POTCAR

PAW W 19Jan2001

6.000000000000000000

parameters from PSCTR are:

VRHFIN =W: 5p6s5d

LEXCH = CA

EATOM = 206.5370 eV, 15.1800 Ry

TITEL = PAW W 19Jan2001

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.330 partial core radius

POMASS = 183.850; ZVAL = 6.000 mass and valenz

RCORE = 2.750 outmost cutoff radius

RWIGS = 2.750; RWIGS = 1.455 wigner-seitz radius (au A)

ENMAX = 223.126; ENMIN = 167.344 eV

RCLOC = 2.147 cutoff for local pot

.....

Description

	E	TYP	RCUT	TYP	RCUT
1	E				
2	.000	23	2.500		

.....

$$E_{cut} = \frac{\hbar^2 G_{max}^2}{2m}$$

$$|\vec{G} + \vec{k}| \leq G_{max}$$

E_{cut}
 PREC = Low
 Medium (default)
 High
 (High : ENMAX + 30%)

KPOINT Sampling

P.10

KPOINTS

10x10x10

0

Monkhorst-pack

10 10 10

0 0 0

Automatic mesh

Shift of the mesh

10x10x10

0

Gama

10 10 10

0 0 0

Gama centered grid

Example

3

Cartesian

0.0 0.0 0.0 1.0

0.0 0.0 0.1 1.0

0.0 0.0 0.2 1.0

Only the first character of the third line is significant.
(C, c, K, k) for Cartesian coordinates
Any other character will switch to reciprocal coordinates

KPOINTS for band structure

k-points along high symmetry lines

10 ! 10 intersections

Line-mode

cart

0 0 0 ! gamma

0 0 1 ! X

0 0 1 ! X

0.5 0 1 ! W

0.5 0 1 ! W

0 0 1 ! gamma

CONTROL File

P.12

INCAR

System = bcc W(100) – 5 layers

ISMEAR = 1

SIGMA = 0.2

RWIGS = 1.455

ISIF = 2

NSW = 50

IBRION = 2

How to get the partial occupancies

Wigner Seitz radius (for PROCAR)

Which degrees of freedom to move

ISIF = 2 (default) relax ions only

Number of ionic steps

How the ions are moved

IBRION = 2 (conjugate-gradient)

System = bcc Fe(001) – 3 layers

ISMEAR = 1

SIGMA = 0.2

ISIF = 2

NSW = 50

IBRION = 2

RWIGS = 1.302

ISPIN = 2

MAGMOM = 3*3

LVTOT = .TRUE.

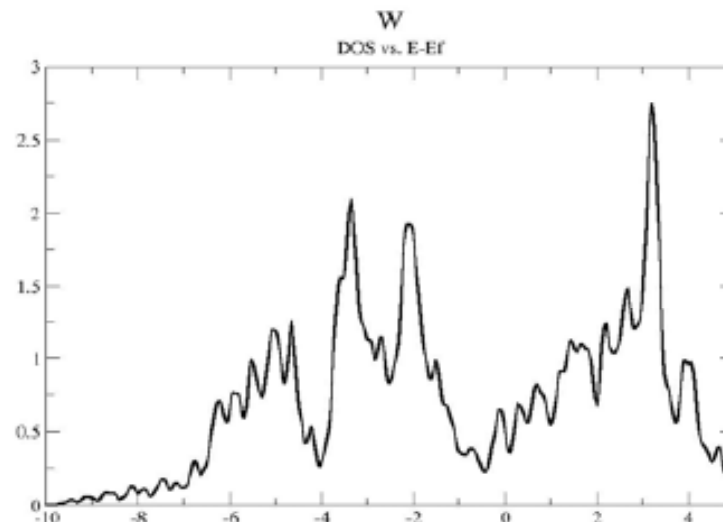
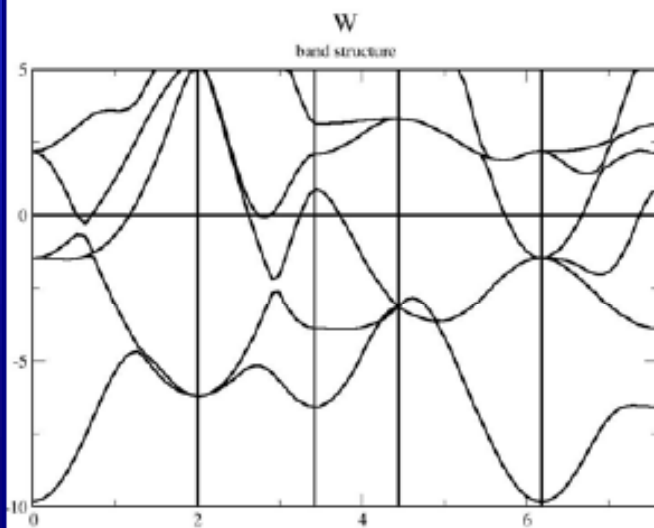
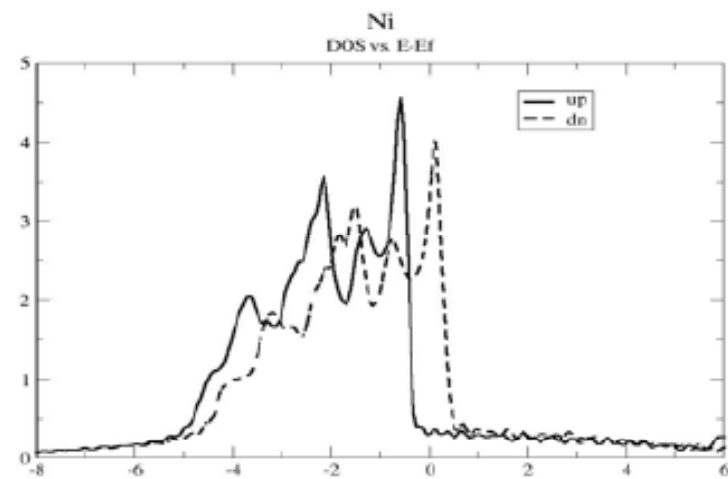
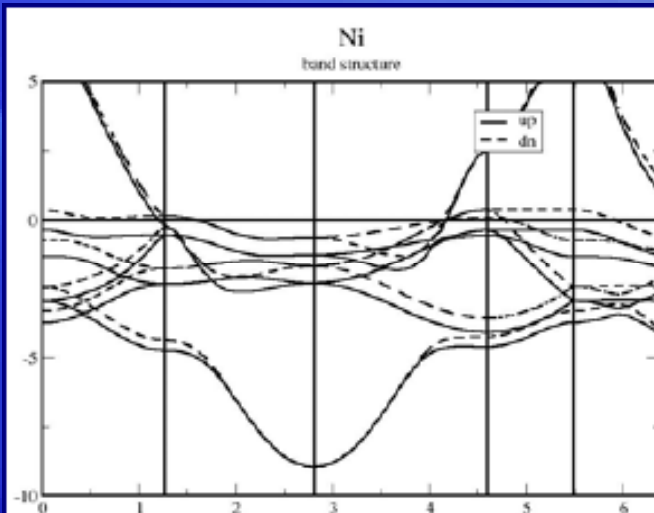
For spin polarized calculation

Initial magnetic moment

Nion * moment

Print out the local potential

Result analysis



CPMD

The CPMD code is a plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics.

- isolated systems and system with periodic boundary conditions; k-points
- molecular and crystal symmetry
- wavefunction optimization: direct minimization and diagonalization
- geometry optimization: local optimization and simulated annealing
- molecular dynamics: constant energy, constant temperature and constant pressure
- path integral MD
- response functions
- excited states
- many electronic properties
- time-dependent DFT (excitations, molecular dynamics in excited states)

CPMD Input file 1 (Wave Function)

```

&CPMD                                120.0                                0.998611043  1.609250000  7.210402167
OPTIMIZE WAVEFUNCTION                CHARGE
CONVERGENCE ORBITALS                0.0                                *O-q6.psp
1.0e-8                                &END                                LMAX=P
MAXSTEP                                20
200                                &ATOMS                                0.261992993  1.609250000  1.089966007
PRINT FORCES ON                                2.540193112  1.609250000 -0.147792007
RHOOUT                                *K-q9.psp                                1.769401965  1.609250000  2.032139989
ELECTROSTATIC POTENTIAL                LMAX=P                                3.428690989  1.609250000  3.491585919
ELF PARAMETERS                        4                                1.059363053  1.609250000  17.051501595
0.0 0.0                                3.014818112  1.609250000  14.986109219  1.636507007  4.827750000  10.326966007
STRUCTURE BONDS ANGLES DIHEDRALS        2.680681888  4.827750000  5.749109219  3.155306888  4.827750000  9.089207993
&END                                0.782181888  4.827750000  3.487890781  0.129098035  4.827750000  11.269139989
                                1.116318112  1.609250000  12.724890781  2.266809011  4.827750000  12.728585919

&DFT                                0.839136947  4.827750000  7.814501595
FUNCTIONAL LDA                        *Ti-q12.psp                                3.535007007  4.827750000  17.384033993
GC-CUTOFF                            LMAX=D                                1.256806888  4.827750000  18.621792007
5.0e-6                                4                                2.027598035  4.827750000  16.441860011
&END                                1.249212986  1.609250000  0.568999197  0.368309011  4.827750000  14.982414081
                                0.649287014  4.827750000  9.805999197  2.737636947  4.827750000  19.896498405

&SYSTEM                                2.547787014  4.827750000  17.905000803  2.160492993  1.609250000  8.147033993
SYMMETRY                            3.147712986  1.609250000  8.668000803  0.641693112  1.609250000  9.384792007
8                                3.667901965  1.609250000  7.204860011
POINT GROUP                        *Ta-q13.psp                                1.530190989  1.609250000  5.745414081
AUTO                            LMAX=D                                2.957863053  1.609250000  10.659498405
ANGSTROM                            4                                &END
CELL                                2.897111043  1.609250000  2.026597833
3.797 1.69528575 4.86542 0.0 0.0 0.0  2.798388957  4.827750000  11.263597833
CUTOFF                            0.899888957  4.827750000  16.447402167

```

CPMD Input file 2 (NMR Calculation)

&CPMD	&END				2.798388957	4.827750000	11.263597833
LINEAR RESPONSE					0.899888957	4.827750000	16.447402167
RESTART ALL LATEST	&ATOMS				0.998611043	1.609250000	7.210402167
CONVERGENCE ORBITALS	ISOTOPES						
1.0d-7	39.00				*O-q6.psp		
STRUCTURE BONDS ANGLES	48.00				LMAX=P		
&END	181.00				20		
	16.00				0.261992993	1.609250000	1.089966007
&RESP					2.540193112	1.609250000	-0.147792007
NMR	*K-q9.psp				1.769401965	1.609250000	2.032139989
FULL	LMAX=P				3.428690989	1.609250000	3.491585919
&END	4				1.059363053	1.609250000	17.051501595
	3.014818112	1.609250000	14.986109219		1.636507007	4.827750000	10.326966007
&DFT	2.680681888	4.827750000	5.749109219		3.155306888	4.827750000	9.089207993
FUNCTIONAL LDA	0.782181888	4.827750000	3.487890781		0.129098035	4.827750000	11.269139989
GC-CUTOFF	1.116318112	1.609250000	12.724890781		2.266809011	4.827750000	12.728585919
1.0e-6					0.839136947	4.827750000	7.814501595
&END	*Ti-q12.psp				3.535007007	4.827750000	17.384033993
	LMAX=D				1.256806888	4.827750000	18.621792007
&SYSTEM	4				2.027598035	4.827750000	16.441860011
SYMMETRY	1.249212986	1.609250000	0.568999197		0.368309011	4.827750000	14.982414081
8	0.649287014	4.827750000	9.805999197		2.737636947	4.827750000	19.896498405
ANGSTROM	2.547787014	4.827750000	17.905000803		2.160492993	1.609250000	8.147033993
CELL	3.147712986	1.609250000	8.668000803		0.641693112	1.609250000	9.384792007
3.797 1.69528575 4.86542 0.0 0.0 0.0					3.667901965	1.609250000	7.204860011
CUTOFF	*Ta-q13.psp				1.530190989	1.609250000	5.745414081
120.0	LMAX=D				2.957863053	1.609250000	10.659498405
CHARGE	4				&END		
0.0	2.897111043	1.609250000	2.026597833				

ABINIT

ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis.

ABINIT Input

To run abinis you need four things:

- (1) Access to the executable, abinis/abinip.
- (2) An input file.
- (3) A files file (list of file names in a file).
- (4) A pseudopotential input file for each kind of element in the unit cell.

Sample file of filelist

tparal_1.filelist

```
tparal_1.in  
tparal_1.out  
tparal_1i  
tparal_1o  
tparal_1  
82pb.4.hgh
```

- The main input filename
- The main output filename
- The root of input files
- The root of output files
- The root of temporary files
- The pseudopotential file name

Sample input control file

tparal_1.in

```
#                                kptopt 1                                typat 1
# Lead crystal                  nshiftk 4                                xred
#                                shiftk                                0.000 0.000 0.000
                                0.5 0.5 0.5                                nband 4
# Simulation parameters          0.5 0.0 0.0
ecut 30.0                        0.0 0.5 0.0                                # SCF procedure
acell 10.0 10.0 10.0            0.0 0.0 0.5                                nstep 3
rprim                            occopt 7                                tolvr 1.0d-10
    0.0 0.5 0.5                  tsmear 0.01                                # This line added when
    0.5 0.0 0.5                                                          defaults were changed
    0.5 0.5 0.0                                                          (v5.3) to keep the
                                # System description                      previous, old behaviour
                                ntypat 1                                iscf 5
# K-points                      znuc 82
ngkpt 8 8 8                    natom 1
```

Sample pseudopotential file

82pb.4.hgh

```
Hartwigsen-Goedecker-Hutter psp for Pb, from PRB58, 3641 (1998)
  82   4   010605 zatom,zion,pspdat
3 1    2 0 2001 0  pspcod,pspxc,lmax,lloc,mmax,r2well
0.617500    0.753143    0.000000    0.000000    0.000000 rloc, c1, c2, c3, c4
0.705259    1.979927   -0.164960   -0.806060          rs, h11s, h22s, h33s
0.846641    0.864420   -0.540969    0.000000          rp, h11p, h22p, h33p
              0.207711    0.012948    0.000000          k11p, k22p, k33p
0.971939    0.374967    0.000000    0.000000          rd, h11d, h22d, h33d
              0.029256    0.000000    0.000000          k11d, k22d, k33d
0.000000    0.000000    0.000000    0.000000          rf, h11f, h22f, h33f
              0.000000    0.000000    0.000000          k11f, k22f, k33f
```

Sample PBS Job script

```
#PBS -l nodes=1:ppn=2
#PBS -l walltime=4:00:00
#PBS -j oe
#PBS -N test_abinitp
#
cd $PBS_O_WORKDIR
#

mpirun /usr/global/abinit/5.4/bin/abinip < tparal_1.files > tparal_1.log

exit
```


Molecular Mechanics Packages

- AMBER
- CHARMM
- DL_POLY
- GROMACS
- LAMMPS
- NAMD
- XPLOR
- Towhee (MC)

AMBER (Assisted Model Building with Energy Refinement)

- Classical molecular dynamics simulations (NVT, NPT, etc)
- Force field for biomolecular simulations (proteins, nucleic acids, carbohydrates and organic molecules)
- Combined Quantum Mechanics/Molecular Mechanics (QM/MM) implementation
- Parallelized dynamics codes
- Explicit Solvent Models with particle-mesh Ewald sum (PME), Implicit Solvent models with Poisson-Boltzmann and Generalized Born approach
- Enhanced sampling (replica exchange MD, Locally Enhanced Sampling)
- Free energy calculation (MM/PBSA, etc.)
- Structural and trajectory analysis
-

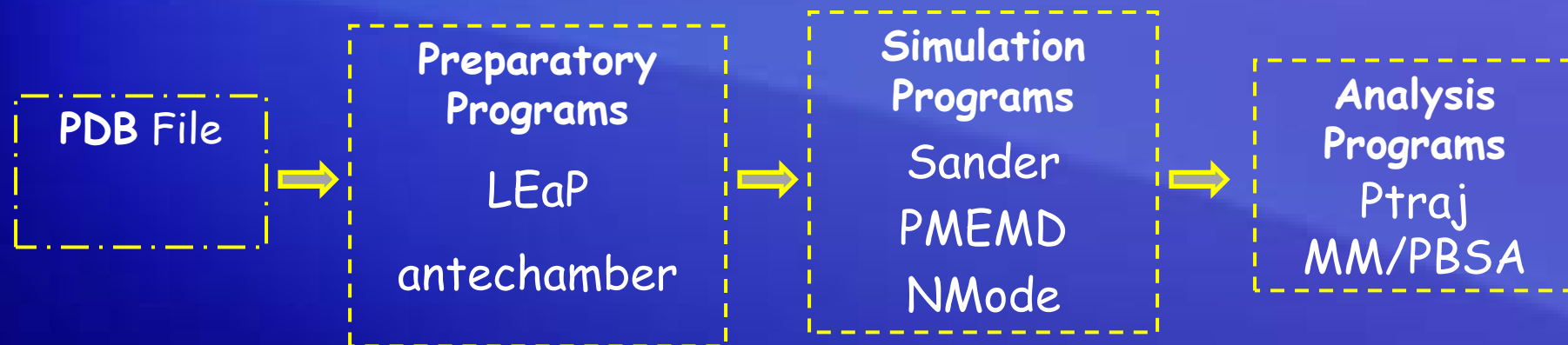
Normal procedure to set up a simulation

Step 1, obtain and edit initial structure

Step 2, prepare input parameter and topology file

Step 3, run simulations and save production trajectory

Step 4, analyze output and trajectory files



Preparation using Leap

Leap command script

```
source leaprc.ff03
oxy = loadPdb oxyt.pdb
bond oxy.1.SG oxy.6.SG
charge oxy
check oxy
saveAmberParm oxy oxy_vac.top oxy_vac.crd
solvateOct oxy TIP3PBOX 9.0
saveAmberParm oxy oxy.top oxy.crd
quit
```

Sander Input

```
sander [-help] [-O] [-A] -i mdin -o mdout -p prmtop -c inpcrd -r restrt  
-ref refc -x mdcrd -y inptraj -v mdvel -e mden -inf mdinfo -radii radii  
-cpin cpin -cpout cpout -cprestrt cprestrt -evbin evbin
```

```
molecular dynamics run  
&cntrl  
  imin=0,  irest=1,  ntx=5,                (restart MD)  
  ntt=3,  temp0=300.0,  gamma_ln=5.0,      (temperature control)  
  ntp=1,  taup=2.0,                (pressure control)  
  ntb=2,  ntc=2,  ntf=2,            (SHAKE, periodic bc.)  
  nstlim=500000,                (run for 0.5 nsec)  
  ntwe=100,  ntwx=100,  ntpr=200,        (output frequency)  
/  

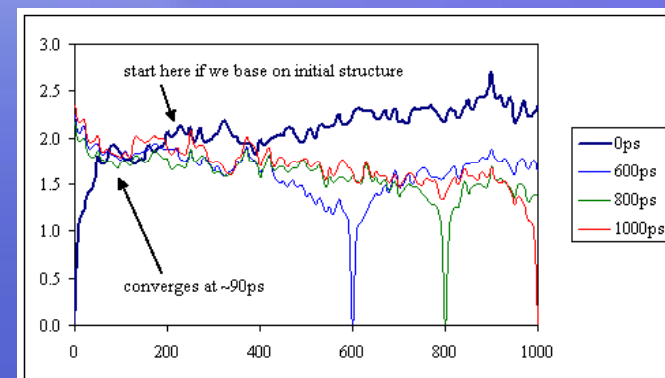
```

- General minimization and dynamics parameters.
 - General flags describing the calculation.
 - Nature and format of the input.
 - Nature and format of the output.
 - Frozen or restrained atoms.
 - Energy minimization.
 - Molecular dynamics.
 - Self-Guided Langevin dynamics.
 - Temperature regulation.
 - Pressure regulation.
 - SHAKE bond length constraints.
 - Water cap.
 - NMR refinement options.
- Potential function parameters
 - Generic parameters
 - Particle Mesh Ewald.
 - Using IPS for the calculation of nonbonded interactions
 - Extra point options
 - Polarizable potentials.
 - Dipole Printing
- Weight change information.
- File redirection commands.
- Getting debugging information

Analysis using ptraj

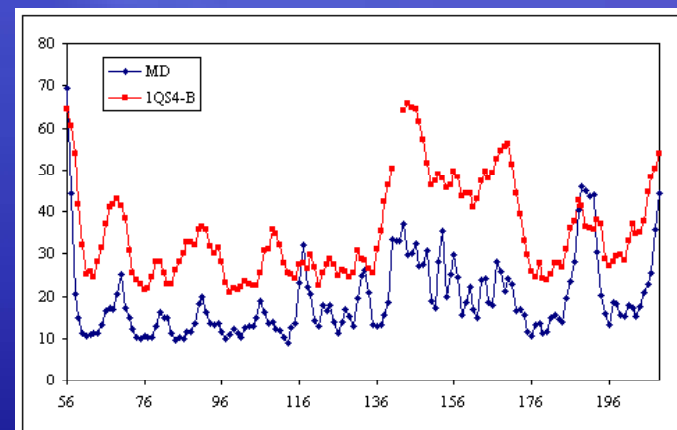
RMSD analysis (ptraj 1qs4A.top ptraj.input2)

```
trajin 1qs4A_md01_nowat.mdcrd  
reference 1qs4A.crd  
rms reference out 1qs4A_md01_RMSD.dat  
:1-154  
go
```



B-factor calculation

```
trajin 1qs4A_md01_nowat.mdcrd  
rms first out 1qs4A_md01_CA.dat :1-  
154@CA  
atomicfluct out 1qs4A_md01.bfactor @CA  
byatom bfactor  
go
```



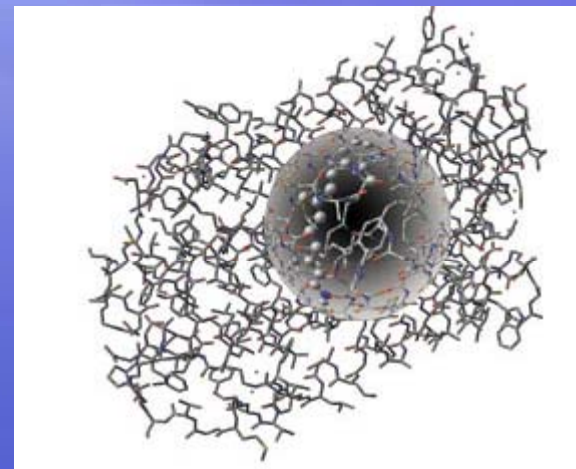
Other Packages

- 3D-DOCK
- AUTODOCK
- Gaussview
- HADDOCK
- Molden
- Pymol
- Rosetta
- VMD

Quantum mechanics/molecular mechanics method

- **Enhanced ONIOM Method (Gaussian)**

- able to model large molecules by defining two or three layers within the structure that are treated at different levels of accuracy;
- applicable in many other areas, including enzyme reactions, cluster models of surfaces and surface reactions, photochemical processes, substituent effects and reactivity of organic and organometallic compounds, and homogeneous catalysis.



- **Q-Chem/CHARMM, Gaussian/Tinker, ChemShell, NWChem, etc.**

- Interface Quantum mechanics with molecular mechanics directly with special treatment at the boundary

Gaussian – ONIOM Input

Two-Layer ONIOM
specification

```
# oniom(blyp/3-21g:amber)
geom=connectivity
```

```
# oniom(blyp/3-21g/dgal:amber) geom=connectivity opt=loose
```

```
blyp/3-21g:amber with density fitting from Luecke
```

```
3 1 1 1
```

```
N-N3-0.181200 22.076181 24.563316 -13.077047 L
```

```
C-CT-0.003400 20.736756 24.514869 -13.699982 L
```

```
C-C-0.616300 20.734957 25.313129 -14.988472 L
```

```
O-O--0.572200 20.731825 24.680955 -16.030293 L
```

```
.....
```

```
C-CT--0.043900 19.775830 32.473200 7.920456 L
```

```
C-CT--0.015800 18.776883 33.512258 7.403331 L H-HC 0 0. 0.
```

```
C-CT--0.082400 17.966350 32.942557 6.232525 H
```

```
C-CT-0.377886 16.928731 33.900731 5.689445 H
```

```
N-N2--0.693824 17.521649 35.160530 5.191031 H
```

```
N-N--0.415700 22.301376 31.316157 8.955475 L
```

```
.....
```

```
H-HW-0.417000 10.154733 46.125705 25.662719 L
```

```
H-HW-0.417000 11.339041 47.039598 25.433539 L
```

```
H-H-0.274700 21.866560 34.137178 7.953109 L
```

```
H-H-0.377886 17.847763 35.188083 4.238902 H
```

```
H-H-0.341200 18.066775 49.503351 -1.731201 L
```

```
H-HO-0.474700 15.931300 31.668829 17.328019 L
```

```
1 2 1.0 1770 1.0 1771 1.0 1772 1.0
```

```
2 3 1.0 5 1.0 1769 1.0
```

```
3 4 2.0 8 2.0
```

```
4
```

```
5 6 1.0 7 1.0 1764 1.0
```

```
6 1768 1.0
```

Three-Layer ONIOM specification

```
# ONIOM(mp2/6-311g**:b3lyp/6-31g*:
```

Introduction to Con

Visualization tools

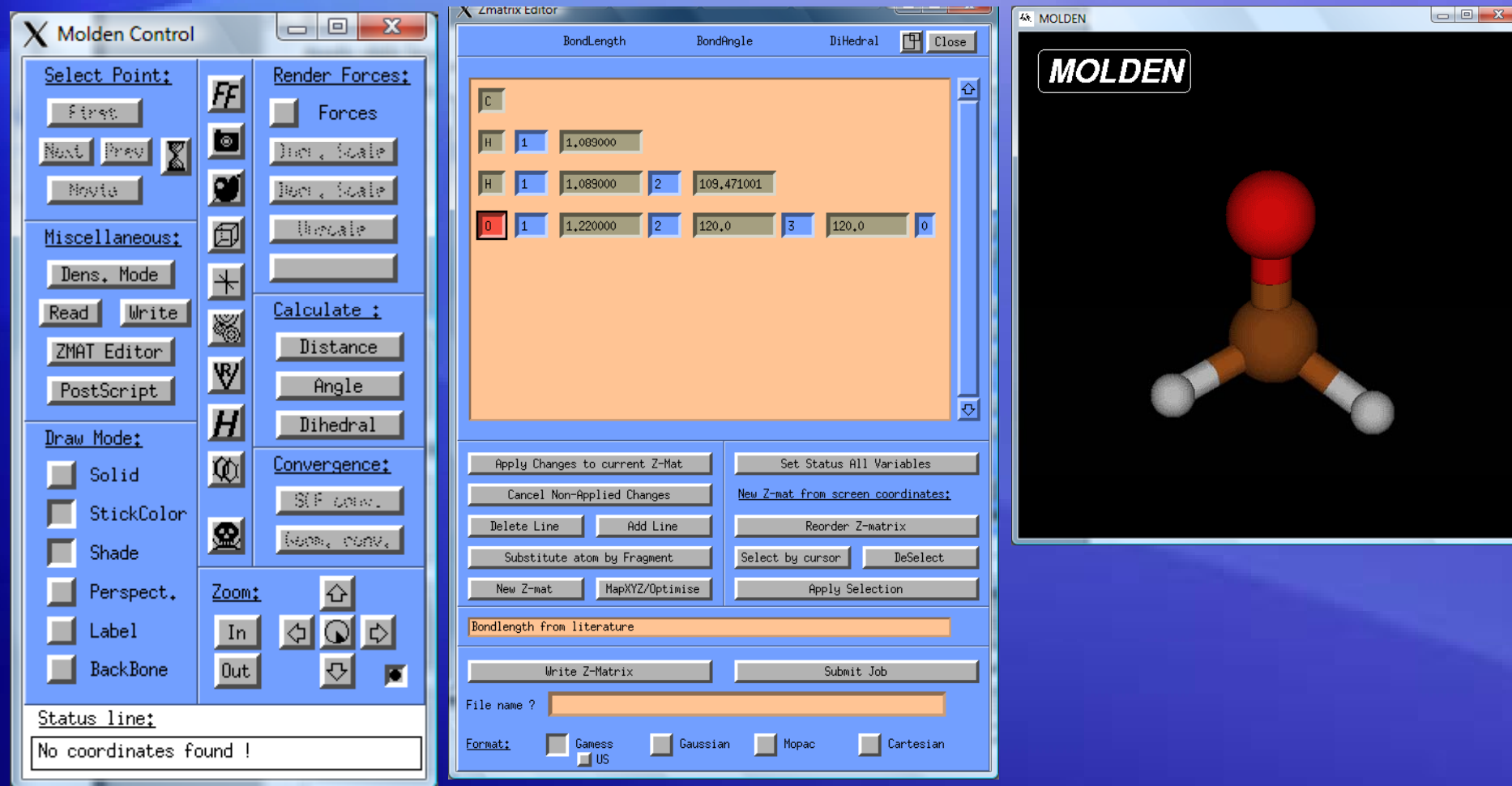
Molecules

- Gaussview
- Molden
- Molekel
- Pymol
- ECCE
- ArgusLab
- VMD
- VegaZZ
- DeepView
- Discovery Studio
- Jmol

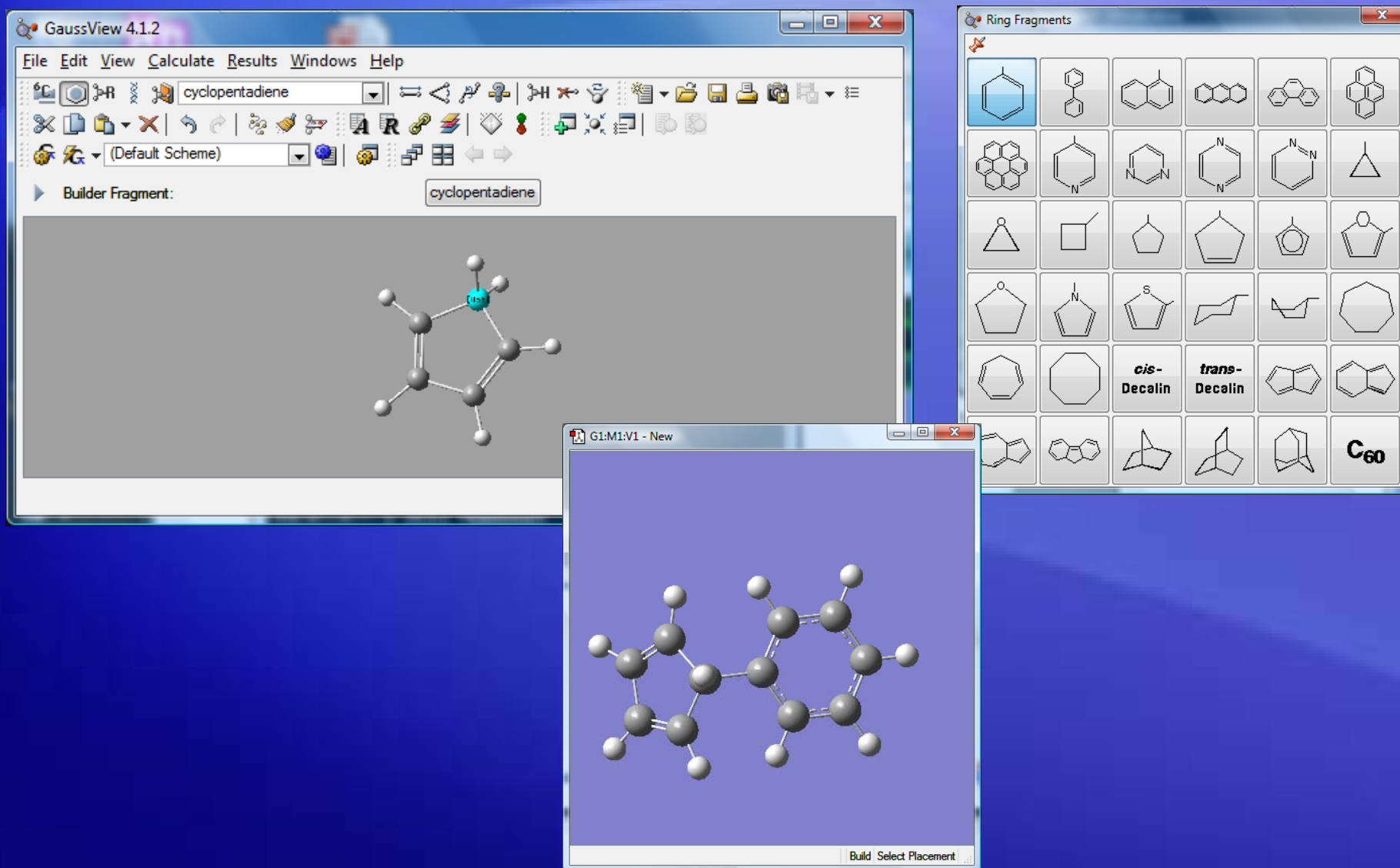
Periodic Systems

- Materials Studio
- Crystal Maker
- VMD

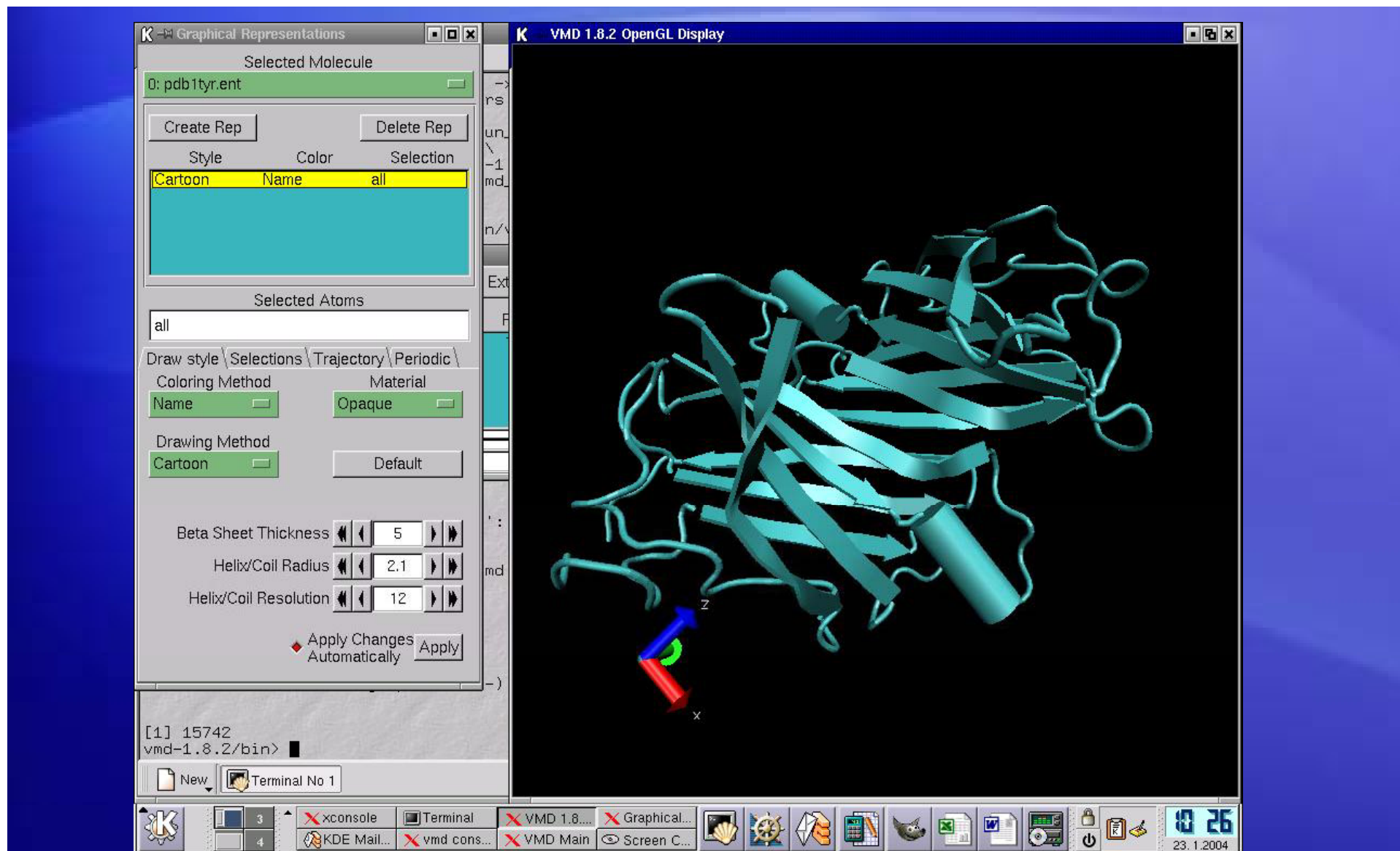
MOLDEN



Gaussview

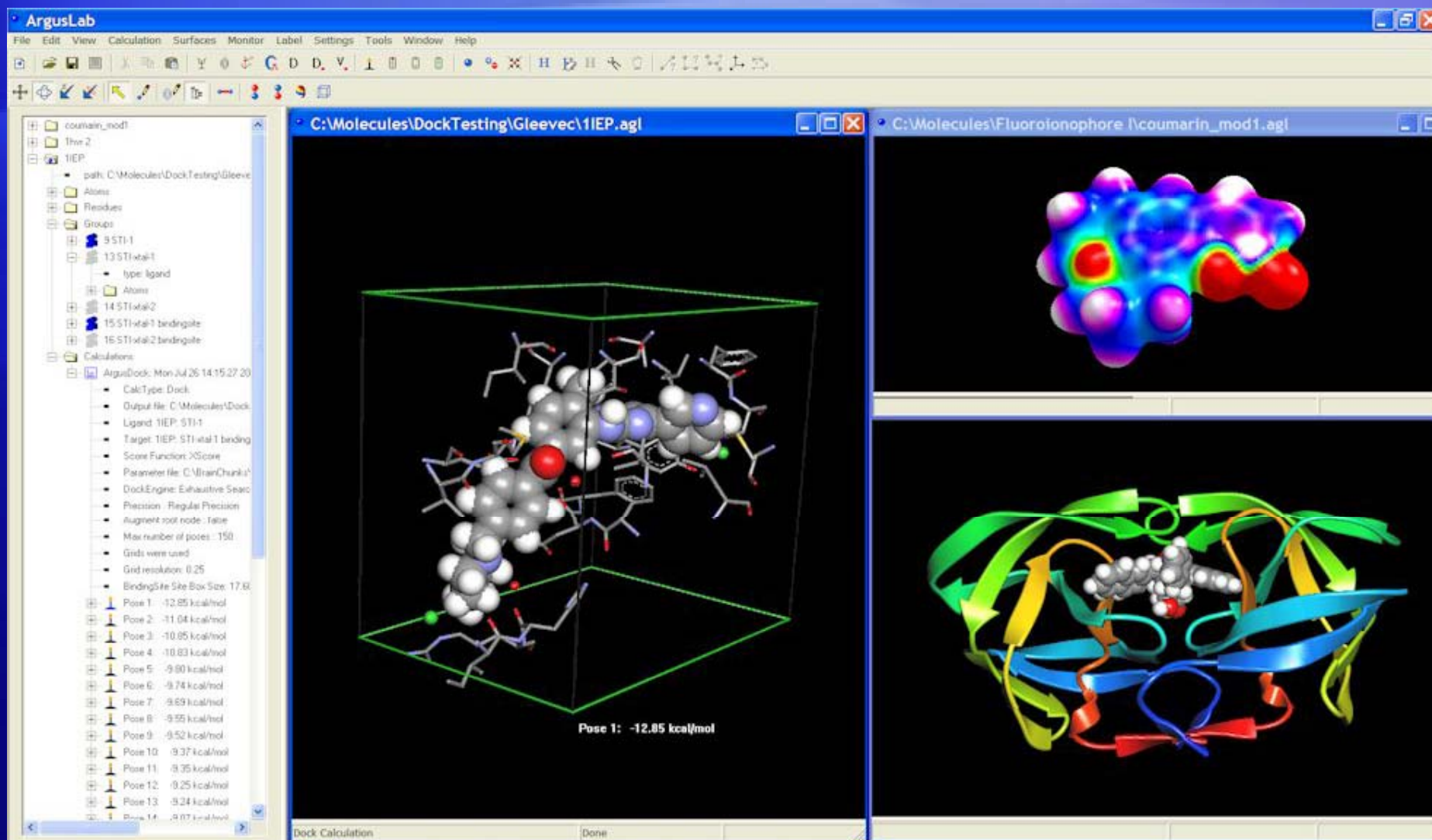


VMD



Introduction to Computational Chemistry

ArgusLab



Acknowledgement

Some slides have used pictures and graphics from other authors.