

Introduction to Computational Chemistry

Computational chemistry covers both *cheminformatics* and more traditional *chemical calculations*.

Cheminformatics

Cheminformatics uses informatics tools such as data mining to assist with chemistry research. Although this is a growing area of chemistry it is beyond the scope of this guide.

Chemical Calculations

We can use chemical calculations to determine three types major chemical information:

- Structure
- Properties
- Reactivity

Methods

Computational chemistry methods can be broken down into four broad types:

- **Ab Initio Quantum Methods** – A mathematical solution to the Schrödinger equation is generated. This gives access to all the structure, properties and reactivity of the system. The result is entirely based on theoretical approaches.
- **Semi-empirical Quantum Methods** – Experimental data is used to supplement theoretical methods and significantly reduce the computational cost.
- **Density Functional Theory (DFT)** – Here, a *functional* (function of a function) is used to relate the electron density to the quantum mechanical description of the system. This functional allows us to determine all the structure, properties and reactivity of the system from the electron density (which can be cheaper to calculate than the wavefunction.)
- **Molecular Mechanics** – Uses classical (Newtonian) mechanics to study the chemical system. Basically amounts to spheres attached by different types of springs.

Tools on the EaStCHEM RCF

These include: the calculation software packages; software that allows the visualization of results and provide an interface to the calculation codes; and the computing hardware that the calculations run on.

- **Software** – Gaussian, MOLPRO, CASTEP, CRYSTAL, CPMD, VASP, Amber, DL_POLY
- **Interface/Visualization** – ArgusLab, ChemSketch, VMD, Chem3D

- **Hardware** – RCF Facilities: dual-core AMD Opteron, 2GB per processor, lots of disk, fast interconnects, Globus Toolkit