# Computational chemistry

It is a branch of *theoretical chemistry* whose major goals are to create efficient mathematical approximations and computer programs that calculate the properties of *molecules* (such as total energy, atomization energies, dipole and quadrupole moment, vibrational frequencies, reactivity and spectroscopic quantitities etc …) and to compare to experimental results.

The *Computational chemistry* term is generally used when a mathematical method is sufficiently well developed that it can be automated for implementation on a computer. The computational cost of its use grows *factorially* (even faster than *exponentially*) with the number of electrons. Therefore, a great number of approximate methods are used to achieve the best trade-off between accuracy and computational cost.

Several major areas may be distinguished within computational chemistry:

- The computational representation of atoms and molecules *(our goal in this lab course)*
- Storing and searching for data on chemical entities
- Identifying correlations between chemical structures and properties
- Theoretical elucidation of structures based on the simulation of forces
- Computational approaches to help in the efficient synthesis of compounds
- Computational approaches to design molecules that interact in specific ways with other molecules

The most popular classes of *ab initio electronic structure* methods are:

- Hartree-Fock (HF)
- Møller-Plesset perturbation theory (MP)
- Multi-configurational self-consistent field (MCSCF)
- Configuration interaction
- Multi-Reference Configuration Interaction
- Coupled cluster
- Quadratic configuration interaction
- Quantum Monte Carlo
- Density functional theory
- Generalized Valence Bond (GVB)
- Modern valence bond theory

**In this lab course we will focus only on two methods; HF and MP2 to perform calculations. Calculated quantities will be compared to literature or you own experimental values.**