Chem 126/226: Computational Chemistry

When: **Fall 2013; MWF 11:00 – 11:50**

Where: **Arts 1535**

Instructor: **Prof. Bernie Kirtman**

Office hrs: **TW 1:30-2:30 pm**

Computational chemistry is a broad subject that includes not only actual numerical calculations but also the theory and molecular modeling on which they are based. With the rapid advance in high speed number-crunching capabilities and the accessibility of numerous multi-faceted software packages it is now routine for experimental projects to have an important computational aspect. Thus, it has become increasingly imperative for all advanced students of chemistry to have at least a cursory knowledge of the computational tools that are available. This course will survey the field and, at the same time, provide the basic theoretical underpinnings as well as the strengths and weaknesses of the methods employed. It will be assumed that the student has a background in quantum and statistical mechanics at the level of an introductory course in physical chemistry. Grades will be based entirely on homework exercises. These exercises will involve, in part, the use of standard computational chemistry computer codes.

Since there is much more material than can be included in a one-quarter class it is necessary to make a selection of what will be covered. Roughly the first 2/3 will be devoted to molecular structure and microscopic properties, the last 1/3 to dynamics and macroscopic properties A brief course outline follows (some of the topics may not be covered for lack of time):

I. Potential Energy Surfaces (PES)/Molecular Mechanics (MM)
Born-Oppenheimer approximation; classical models for PES; geometry optimization

II. Molecular Orbital (MO) Model for Electronic Structure
electron spin; electron exchange; Hartree-Fock model; canonical molecular orbitals

III. Hybrid MO/MM and Related Models
boundaries through space; boundaries through bonds

IV. Electrical, Magnetic and Other Electronic Structure Properties
dipole moments and polarizabilities; chemical shifts, spin-spin coupling, hyperfine coupling, magnetic susceptibility; atomic charges; ionization potentials and electron affinities

V. Beyond the MO Model for Electronic Structure
configuration interaction (CI); multi-reference CI; many-body perturbation theory/coupled clusters

VI. Excited Electronic States
single excitation states; time-dependent Hartree-Fock; double excitations

VII. Density Functional Theory
Hohenberg-Kohn theorems; local density approximation; Kohn-Sham model; gradient approximations; hybrid approximations and Jacob's ladder; general performance overview

VIII. Molecular Dynamics (MD) and Monte Carlo (MC) Simulations of Molecular Ensembles
phase space and trajectories; Verlet and leapfrog MD; Metropolis sampling for MC; simulating annealing and basin filling

IX. Thermodynamic Properties
microscopic-macroscopic connection; ensemble properties

X. Implicit and Explicit models for Condensed Phases
continuum models; explicit solvent; relative merits