COMPUTATIONAL CHEMISTRY. CHM6586

Instructor : Dr. Adrian E. Roitberg

CLB 313C

Tuesdays is on 7th period, 1:55 PM to 2:45 PM
Thursdays 4 and 5th periods (10:40am-->12:35 pm)

Course objectives
This course, for graduate students and advanced undergraduate students, is intended to cover modern methods of computational chemistry and its applications to chemical bonding and spectra, based on quantum mechanics, and an introduction to molecular dynamics.

Course description
The main components of this course are: (a) an introduction to software packages for computational chemistry; (b) model building and molecular mechanics; (c) molecular orbitals and electronic structure; (d) Optical, infrared and magnetic resonance spectra; (e) solvation effects and molecular dynamics; and (f) building large systems (polymers and solid surfaces).

NOTE: The following contents are meant as a guideline, to be refined as the course is taught.

COMPUTATIONAL CHEMISTRY

CONTENTS

1. Introduction to software packages: HyperChem, Spartan, Gaussian, ACES, etc.
2. Model building and molecular mechanics
3. Geometry optimization and potential energy surfaces
4. Semi-empirical molecular orbitals: Huckel, differential overlap approximations; bonding and properties.
5. Atomic orbital basis sets and electron integrals
6. Hartee-Fock and density functional calculations of bonding and properties
7. Optical, infrared and magnetic resonance spectra
8. Survey of electron correlation methods and sample results; potential energy surfaces and reaction paths.
9. Solvation effects. Reaction field approximation.
10. Molecular dynamics and Monte Carlo methods for large systems.
11. Building large systems: polymers, polysaccharides, polunucleotides; solid surfaces.