Chem 601: Theory of Chemical Bonding
Course Outline - Fall 2007

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Recommended Book: Molecular Modelling: Principles and Applications, Second Edition, Andrew Leach, Prentice Hall, 2001.

Additional reading material:
Quantum Chemistry, I. N. Levine, Prentice Hall, 2000.

Topics to be covered include:

(1) Molecular Orbital Calculations
- Hartree-Fock equations
- Basis sets

(2) Advanced *ab initio* methods
- Electron correlation
- Density Functional Theory

(3) Exploring potential energy surfaces
- Locating and characterizing local minima
- Frequency calculations
- Transition structures and reaction pathways

(4) Empirical and semi-empirical computational methods
(5) Examples of molecular modelling using computational chemistry software

The course grade will be based on:

(1) Graduate level problem sets involving setting up and running computational chemistry software (30%)
(2) Computational project seminar (20%)
(3) Computational project final report (20%)
(4) Final (30%)