CHEM 5920 Computational Chemistry

Course Description:

This course is designed to train students to do practical quantum chemistry calculations. An overview will be provided about the basic principles, with emphasis on the basic concepts, rather than the mathematical details. Practical problems are covered, so that a student learns how to solve chemical problems by computation.

Main Course Outline:

1. Theoretical Overview: Many electron problems, the Slater determinants, the calculation of one-centre and two-centre integrals, Hartree-Fock method, Linear combination of atomic orbitals, the variation principle. Post-Hartree-Fock treatment and Density Functional Theory.

2. Practical consideration: choice of basis sets; typical xc-functional for DFT. Practical problems: geometry optimization, potential energy surface, optimization of transition states, calculation of harmonic frequencies, energetics.