

Chemistry 883 Fall 2008

Computational Quantum Chemistry

In this course we will discuss modern theories of the electronic structure of atoms and molecules and their implementation in representative computer programs such as MOLPRO, GAUSSIAN, and GAMESS. There will be two lectures a week (Tuesday and Thursday, 3:00-3:50) and one scheduled computational Laboratory (Wednesday, 3:00-5:50). Lecture topics include:

Hartree-Fock Theory
Moller-Plesset Perturbation Theory
Configuration Interaction
Multi-Configuration Self Consistent Field Theory
Coupled Cluster Theory
Density Functional Theory

The laboratory period will provide an opportunity to learn how to use the various codes and to illustrate and reinforce the lecture topics. The goal of the course is to develop an understanding of the accuracy, range of applicability and information content of the various theories. Familiarity with the basics ideas of Quantum Mechanics will be assumed.

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Recommended Text: *Introduction to Computational Chemistry*
Frank Jensen
John Wiley

The first class will meet Tuesday, August 29 at 3:00 PM in room 136, Chemistry. If you are interested in the course, please attend.