Instructor: Steve Scheiner, Chemistry Building 273
797-7419, steve.scheiner@usu.edu
T, Th 1:30 - 2:45 Widtsoe 330

Office Hours: T Th 2:45 - 3:45, and other times by drop-in or appointment

other relevant sources are on Reserve at the USU Library

Content: The course is designed to provide the student with both background and practical knowledge about computational chemistry. Each student will design (with the guidance of the instructor) and carry out an original computational chemistry research project.

Material to be presented in class will be organized as follows:
- Foundations of molecular orbital theory
- Ab initio implementation of Hartree-Fock theory
- Methods of electron correlation
- Extracting chemical properties from calculations
- Density functional theory (DFT)
- Means of including solvation effects
- Molecular mechanics
- Hybrid quantum and classical methods (QM/MM)
- Semiempirical procedures
- Dynamics and statistical methods

Grading: Students will be evaluated on the basis of:
1) a research paper to be submitted at the conclusion of the course
2) an in-class presentation of a paper from the literature

Learning Objectives
- Formulate a set of calculations that can address a relevant research question
- Use one or several computer programs and extract useful information
- Write a research paper that describes methods, results, and interpretation
- Assess the meaning and validity of calculations that appear in the chemical literature

Assessment
- Student learning will be measured via the quality of the research paper turned in at the conclusion of the semester, and the acuity with which they analyze a paper in the literature.

In accordance with the Americans with Disabilities Act, reasonable accommodation will be provided for all persons with disabilities in order to ensure equal participation in Chemistry 5100. A student who requires an accommodation must contact the Instructor. The disability must be documented by the Disability Resource Center. In cooperation with the Disability Resource Center, reasonable accommodation will be provided for students with Disabilities. Course material may be requested in alternate formats through the Disability Resource Center. The administration of Chemistry 5100 will adhere strictly to the academic regulations stipulated in the most recent USU General Catalog. The complete code of Policies and Procedures for Students can be viewed at:
http://www.usu.edu/studentservices/studentcode