

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
- Text:** “Essentials of Computational Chemistry”, by C. Cramer, 2nd Ed, Wiley
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
3) quality of in-class participation
- Learning Objectives** Students will learn to do the following:
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, as well as their comments and questions in class.

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/studentervices/studentcode>