

**Instructor:** Steve Scheiner, Chemistry Building 273  
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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/studentservices/studentcode>