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
3) quality of in-class participation

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,
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