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

Office Hours: due to Covid issues, by 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
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.

There are University policies regarding responses to the Covid crisis as well as other issues that are spelled out
at this site:
http://www.usu.edu/provost/faculty-life/syllabus.cfm
and you will find information about the Department's safety provisions:
https://chem.usu.edu/safety/SafetyNew-working