WISCONSIN
UNIVERSITY OF WISCONSIN-MADISON

Syllabus

CHEM 775 (Electronic Structure of Molecules)

Spring Semester, 2019

Credits: 3 credits (including course hours and a final project).

Course Designation and Attributes: None

Meeting Time and Location: MWF 9:55-10:45 AM, Chemistry 8335

Instructional Mode: The course will be taught in-person, with additional course materials provide on line.

The objective of this course is to prepare you to use state-of-the-art electronic structure methods in your research. You leave the course with an appreciation of the capabilities (and limits) of current electronic structure techniques, basic guidelines for choosing an appropriate computational method, and the practical skills necessarily to put this knowledge into practice. The level of the course is aimed at continuing graduate students with an understanding of quantum mechanics at the level of CHEM 675 (or equivalent).

Course Learning Outcomes:

- Appreciate the underlying quantum-mechanical and mathematical basis for modern electronic structure methods
- Understand the capabilities and limitations of common wavefunction and density functional theory (DFT) methods
- Apply wavefunction and DFT methods to molecular systems to predict chemical properties and reactivity

Instructor: J.R. Schmidt, 8305d Chemistry, 262-2996, *schmidt@chem.wisc.edu*.

Instructor Office Hour: By appointment.

Suggested References:

1. Modern Quantum Chemistry, Szabo and Ostlund (required, low-cost Dover book)
2. Introduction to Computational Chemistry, Frank Jensen
3. Essentials of Computational Chemistry, Chris Cramer
4. Density-Functional Theory of Atoms and Molecules, Parr and Yang

Lectures: The lectures in this class will be somewhat formal (in the mathematical sense), developing the theoretical underpinnings of various computational techniques. Certainly, we will also devote substantial class time to *qualitative* discussions regarding the capabilities and limits of various approaches, and practical issues such as basis sets, etc. The homework sets will provide the best opportunity for you to gain expertise with computational best practices – through direct experience. In class questions and discussion are strongly encouraged and will benefit the class as a whole. *Please feel free to speak up at any time!*

Problem Sets: Homework assignments will be given (approximately) weekly and are the most important component of the class from a pedagogical point of view. Assignments will be due in class one week after distribution. You may discuss homework with other students in the class, but you must write up your answers independently (unless otherwise specified). Solutions will be posted to Learn@UW.

The homework will combine occasional conceptual pencil-and-paper exercises with frequent computations. We will focus on the Gaussian 09/16 computational package, but the ideas and approaches we learn are equally applicable to all packages (aside from the detailed formatting of the input file).

You are encouraged to use the Sunbird computer cluster for your computations. The cluster has all relevant software already installed and configured for easy use. See https://hpc.chem.wisc.edu/using-the-clusters/ for details on how to login and submit jobs.

Exams and Grading: There will be one midterm and a final project. Your final course grade will be based approximately on the following criteria: midterms (25%), problem sets (50%), and final project (25%). The required final project constitutes the 3rd credit for the course.

Topics: Below is a list of topics that will be covered. This list may be altered according to time constraints, etc. but is intended to provide a general outline for the course.

1. Review of relevant QM
2. Introduction to electronic structure theory
3. The Hartree-Fock (HF) approximation
4. Basis sets in quantum chemistry
5. Configuration interaction (CI)
6. Pair and coupled-pair theories
7. Density functional theory (DFT)
8. Calculation of properties
9. Excited states
10. Intermolecular interactions
11. Solvation and QM/MM
12. Materials and solids