

Chemistry 8843: Computational Chemistry

Instructor

Meetings: MWF 10:05-10:55, Boggs 3-46
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Description

This introductory course in computational chemistry will discuss molecular mechanics, semiempirical, and particularly *ab initio* approaches. The course will be project-based, and students will be encouraged to pursue projects related to their own research if possible. This is a graduate-level course but should be accessible to advanced undergraduates. Graduate-level quantum mechanics is not required, but a good undergraduate-level quantum chemistry background is expected.

Requirements and Grading Scheme

Problem sets and labs	20%
Midterm	25%
Final	25%
Project	30%

A substantial part of the grade will be determined by a class project in computational chemistry which is to be carried out during the course of the semester. A different project will be selected by each student in the first few weeks of the semester, with the approval of the instructor. Students are encouraged to select a class project relevant to their own research, if feasible. Auditors are required to take the midterm and final and demonstrate a minimal understanding of the subject, *or* they may turn in a satisfactory class project. Pass/fail students are required to turn in a class project and take both the midterm and the final and receive an overall passing grade.

Topics

Because this is a special topics course, there is some room to adjust the topics to be covered. At the first meeting, a discussion will be held about whether any additional topics are of interest to the class.

I. Introduction and Review of Quantum Chemistry

- (A) Introduction to computational chemistry
- (B) Operators, commutators, Dirac notation, linear vector spaces
- (C) Postulates
- (D) Analytically soluble problems (particle in a box, etc.)
- (E) Variation and perturbation methods

II. Molecular Quantum Mechanics

- (A) Born-Oppenheimer Approximation
- (B) Force Field methods (Molecular Mechanics)
- (C) Molecular dynamics
- (D) Electronic structure of atoms
- (E) Electronic structure of diatomics
- (F) Group theory and molecular point groups
- (G) Electronic structure of polyatomics
- (H) Hartree-Fock theory, part I

III. Analysis and Properties

- (A) Geometry optimization

- (B) Vibrational frequencies: symmetry analysis, harmonic vs. fundamental frequencies, zero-point vibrational energies (ZPVE's), Hessian index, distinguishing minima from transition states
- (C) Intrinsic reaction coordinate (IRC) analysis
- (D) Electrostatics: dipole moment, polarizability, hyperpolarizability
- (E) Transition state theory, statistical mechanics, and thermodynamic properties

IV. Computation of Electronic Structure

- (A) Hartree-Fock method and various notations for one- and two-electron integrals
- (B) Basis sets
- (C) Semi-empirical methods
- (D) Intro to electron correlation methods
 - (1) Dynamical correlation and configuration interaction (CI)
 - (2) Many-body perturbation theory (MBPT)
 - (3) Coupled-cluster methods (CC)
 - (4) Density functional theory (DFT)
 - (5) Valence-bond theory (VB)
 - (6) Extrapolation methods (G2, G3, CBS, focal-point analysis).
- (E) Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF)
- (F) Comparing the performance of electronic structure theories

V. Selected Special Topics

Textbooks

1. F. Jensen, *Introduction to Computational Chemistry*, (Wiley, New York, 1999). Good introductory textbook covering a variety of topics.
2. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st ed., revised (Dover, 1989). More mathematical detail for many of the *ab initio* electronic structure methods.

Recommended Supplementary Books

1. D. A. McQuarrie, *Quantum Chemistry* (University Science Books, Mill Valley, CA, 1983). Very readable introductory text for undergraduate-level quantum chemistry.
2. I. N. Levine, *Quantum Chemistry*, 4th ed. (Prentice Hall, Englewood Cliffs, NJ, 1991). Covers some of the topics in this course.
3. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd ed. (Wiley, New York, 1990). Classic reference on the subject.
4. E. B. Wilson, J. C. Decius, and P. C. Cross, *Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra* (Dover, New York, 1980). Classic reference on the subject, in affordable Dover paperback form.