Chemistry 6485: Computational Chemistry

Instructor

Meetings:	MWF 9:05-9:55, MoSE G021
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Description

This introductory course in computational chemistry will discuss molecular mechanics, semiempirical, and particularly *ab initio* approaches for molecular modeling. The course will be project-based, and students will be encouraged to pursue projects related to their own research if possible. The course will highlight the computational algorithms used to implement the theoretical methods. This is a graduate-level course but should be accessible to advanced undergraduates. Graduate-level quantum mechanics is not required, but students will need to become familiar with some basic concepts from quantum chemistry such as eigenvectors and eigenvalues, the Schrödinger equation, orbitals, and variational and perturbational methods. This material will be reviewed briefly at appropriate times during the course. Students will learn the basic theory and algorithms behind computational chemistry methods, and they will also learn the advantages and disadvantages of these methods and how to use them to solve problems of interest in chemistry and molecular science and engineering. The course project may be in one of two areas: (1) the application of computational chemistry, or (2) a programming project to implement computational chemistry algorithms.

Requirements and Grading Scheme

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

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 must attend a minimum of 1/2 of the lectures. 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

- Introduction (1 lecture): Scope of computational chemistry; course topics; review of key concepts from linear algebra
- Molecular Mechanics / Force Field Methods (3 lectures): Introduction to molecular mechanics; comparison of popular force fields; performance of molecular mechanics (slides)
- Molecular dynamics (2 lectures)
- Review of postulates of quantum mechanics (1 lecture)
- The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states, and Hessian indices (1 lecture) (slides)
- Review of the variational method (1 lecture)
- Slater Determiants, Slater's Rules, one- and two-electron integrals, and permutational symmetry of integrals (1 lecture)
- Hartree-Fock molecular orbital theory (4 lectures): Deriving the Hartree-Fock equations, Hartree-Fock energy expressions for arbitrary spin-orbital configurations, spin integration, restricted and unrestricted references, self-consistent-field (SCF) procedure
- Basis sets (2 lectures): Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange (slides)
- Molecular integrals (1 lecture): Gaussian product theorem, evaluating integrals computationally
- The Hartree-Fock algorithm (1 lecture)
- Electronic spin (1 lecture): $\hat{S}^2$ operator, degeneracy, evaluating the spin of Slater determinants

- Electron configurations, term symbols, Aufbau principle, diatomic MO diagrams, Walsh's rules (2 lectures)
- Geometry optimization (1 lecture) (slides)
- Molecular properties (1 lecture): dipole moment, polarizability, hyperpolarizability, magnetic moment, NMR shifts, methods for computing properties
- Semiempirical methods (1 lecture)
- Density-functional theory (2 lectures)
- Vibrational frequency analysis (2 lectures): symmetry analysis, harmonic vs. fundamental frequencies, zero-point vibrational energies (ZPVE's), Hessian index, distinguishing minima from transition states (slides)
- Practical advice about electronic structure computations (1 lecture) (slides)
- Comparing the performance of electronic structure theories (1 lecture) (slides)
- Transition state theory, statistical mechanics, and thermodynamic properties (2 lectures) (slides)
- Introduction to electron correlation; configuration interaction (2 lectures) (slides)
- Many-body perturbation theory (1 lecture)
- Coupled-cluster theory (2 lectures)
- Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory (1 lecture) (slides)
- Excited state methods (1 lecture)
- Example applications (1 lecture)

Textbooks

1. F. Jensen, *Introduction to Computational Chemistry*, 2nd Edition, (Wiley, New York, 2007). 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.

Supplementary Books that may be of interest

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. 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.