Special Topics in Computational Chemistry and Biophysics
CHEM 6670 (Fall 2007)

Times: M/W/F 12:30 to 1:20 pm
Location: PHSC 119

Course Instructor: Dr. Jana Khandogin
Chemistry building room 309
Office hour: M/W/F 3-4 pm
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Description

This course covers the fundamentals of statistical mechanics and quantum mechanics theories as well as their applications in molecular simulations and quantum calculations. The second half of the course offers practical training in quantum calculations for small molecules and molecular dynamics simulations for macromolecules (proteins) using leading software packages. Depending on the interests and background of audience, small programming exercises in molecular simulations may also be offered.

Pre-requisites

At least one undergraduate-level physical chemistry course is required.

Grading Scheme

Problem sets: 25%
Midterm: 25%
Final (presentation): 25%
Projects: 25%

Topics

1. Introduction to statistical mechanics: postulates, ensembles, partitions, connection to macroscopic properties, Boltzmann statistics
2. Introduction to quantum chemistry: Configuration-Interaction, Hartree-Fock, Many-body perturbation theory, Density Functional theory, semi-empirical methods
3. Force fields, molecular dynamics, Monte Carlo methods, Brownian dynamics
4. Free energy simulations, conformational sampling techniques
5. Implicit solvent models, Normal mode analysis
6. Applications of electronic structure calculations and molecular simulations

Reference Textbooks

The following text books are recommended for reference. Handouts will be given throughout the course.

1. A. R. Leach, “Molecular Modeling”, Prentice Hall, Second Edition, 2001.
2. M .P. Allen and D. J. Tildesley, “Computer Simulation of Liquids”. Oxford University Press, 1987.
3. D. Frenkel and B. Smit, “Understanding Molecular Simulation: From Algorithms to Applications”, Academic Press, Second Edition, 2002.
4. C. Cramer, “Essentials of Computational Chemistry”, Wiley, second Edition, 2004.
5. A. Szabo and N. Ostlund, “Modern Quantum Chemistry”, Dover Publications, 1996.

Course Schedule

Date	Week	Topics
August	1	Quantum mechanics: postulates, Born-Oppenhermeier approximation, Schrodinger equation, eigenfunctions, eigenvalues, variational principle
	2	Computational quantum methods: orbitals, basis sets, Hartree-Fock, Configuration-Interaction theories
Sept	3	Computational quantum methods: Density functional, perturbation, semi-empirical theories
	4	Electronic structure calculations: case study
	5	Statistical mechanics: postulates, ensembles, partition functions, entropy, temperature
	6	Statistical mechanics: connection to macroscopic quantities, Boltzmann statistics, statistical quantities
Oct	7	Computer simulation methods: Monte-Carlo, molecular dynamics, Brownian dynamics
	8	Force fields, potential energy functions, basic algorithms, free energy simulation methods
	9	Advanced simulation techniques: implicit solvent models, replica-exchange conformational sampling, normal mode analysis
	10	Molecular dynamics simulations: case study
Nov	11	Mid-term exam; introduction to computational chemistry software
	12	Projects in quantum calculations and molecular simulations
	13	Projects in quantum calculations and molecular simulations
	14	Projects in quantum calculations and molecular simulations
Dec	15	Projects due
	16	Final presentation