Introduction to Computational Chemistry

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Third Trimester, Spring 2008
Thursdays, 6:30 – 9:30 PM

Course description (courtesy of Professor Hai Lin, Chemistry, University of Denver, Comp Chem 5510).
This course provides the essential theoretical background of computational chemistry and the practical skills to perform computations to solve chemical problems. The intended audiences are both students who need a background for studying more advanced computational techniques and students who are doing experiments but also have interests in computations. Students need not memorize specific theoretical details and algorithms, however, by the end of the course, the students should be able to critically assess the applicability of computational methods to specific questions from a chemistry point of view, and successfully apply appropriate computational techniques in their academic and scientific careers.

The content includes discussions of molecular mechanics, Hartree-Fock theory, semi-empirical methods, density functional theory (DFT), basis sets, geometry optimization and transition state searches, and molecular property calculations. In addition, students will learn how to read the professional literature in computational chemistry, with a focus on the Journal of Computational Chemistry. Students will be expected to plan and complete a small research project, with a journal-type article as the deliverable.

The structure of the course is a combination of lecture and lab (in the same classroom). Hands-on training will be given in the application of computations using available software packages on the North Carolina High School Computational Chemistry Server (http://chemistry.ncssm.edu). Packages include GAMESS (General Atomic and Molecular Electronic Structure System), Gaussian 03, MOPAC (Molecular Orbital PACkage), and Tinker. All four are heavily used in the academic and research communities. You may also buy a computational chemistry software package (Spartan) for $20.00. For some labs you will be required to use the Comp Chem server.

Topics Schedule (see Moodle for more detailed assignment list):

Class	Date	Topic
1	March 2 (Tues)	Introductions; guiding questions; computational chemistry procedure
2	March 13	Applications of computational chemistry
3	April 10	Fundamental mathematics and methods; approximations
4	April 17	Basis Sets
5	May 1	Basis Sets (cont.); methods (cont.); PROJECT TOPIC DUE
6	May 8	Codes and Software
7	May 15	Transition States
8	May 22	Thermochemistry
9	TBD	Applications in medicine, environmental science, biology
10	May 29	Review and project work

Grade Distribution

- Weekly quizzes 20%
- Homework/Journal articles 15%
- Labs 25%
- Final exam 15%
- Final project with paper 25%

Grading Scale:

A+ = 97 A = 93 A- = 89 B+ = 85 B = 81 B- = 77C+ = 73 C = 69 D= 65

General class schedule (subject to change as needed):

Time	Activity	Minutes
6:30 - 6:50	Quiz	20
6:50 - 7:30	Lecture	40
7:30 - 8:10	Lab	40
8:10 - 8:25	BREAK	15
8:25 - 8:55	Journal Article	30
8:55 - 9:30	Project	35

More to know:

- Office Hours: I teach A, B, and F blocks, and am out of the building on Friday afternoons. Appointments can be made by arrangement. I am also available by email regularly (although I typically stop reading email after 9:30 pm, because I'm old.). My schedule is posted on my office door
- Textbook: Gotwals, R., and Sendlinger, S. "A Chemistry Educator's Guide to Molecular Modeling", in press, 2007. This book is available electronically via the Moodle.
- Lab: The structure of the course is a combination of lecture and lab (in the same classroom). There will typically be a small structured lab in the first part of the course, then a larger lab during the second part (see schedule above). For the second lab, students will be required to prepare a 250-300 word written abstract of the lab activity.
- Homework: Homework typically includes reading assigned textbook chapters and a weekly journal article (usually with a short comprehension quiz and discussion), and answering related questions on the Moodle.
- Quizzes: there is a weekly 20-minute quiz, based on the previous week's lecture, lab activities, textbook reading, and journal article reading.
- Journal articles: We will discuss theory and applications of computational techniques to solve chemical problems. This requires the prior reading of journal articles handed out in class. We will frequently have a short open-article quiz on the week's article.
- Notebook: you are required to purchase a bound notebook (composition book, for example). In this notebook, you should keep class notes, comments and observations from journal articles, and ALL of your labs (following the lab sample found on the Moodle). Your notebooks will be graded twice each trimester, with each grade counting as one quiz grade. Collection dates are posted on the Moodle.
- Final Project: Every student is required to work on a small project within the student's area of interest due on the date of the final and submit a short journal-style report (6 to 10 pages), due on the final exam day. Students can work in collaborative groups of NO MORE THAN THREE (3).
- Comments on Grading: this course requires active participation, and your grade will reflect that. *Recognizing that senioritis is an insidious disease, understand that it is **fatal** in a course like this*. This is, after all, a course in quantum chemistry! You should anticipate at least **six** hours a week (one hour a day) of work outside of class. Some weeks may be more, some may be less.
- Classroom materials: you will absolutely need to have a charged laptop every class. I will bring extra power strips to class if you need to plug in, but will not have enough for the entire class. **Mozilla Firefox** should be loaded on your machine. Other software will be installed as needed during the class.
- Classroom computer usage: computers may be used ONLY during computational activities. Computers may not be open during lectures or other activities unless so directed. Notes need to be taken in the bound notebook.
- Miscellaneous: we start on time. Also, do not bring dinner to class. Drinks and "discrete" snacks are OK. Surfing the net, IMing, and otherwise doing things online not related to chemistry are violations of honor code and otherwise strongly discouraged (see note above regarding computer usage).
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ACADEMIC HONESTY: Individual ownership of your work is important. You will learn more effectively by taking your own notes and struggling with the problems and assignments yourself. Faculty and student tutorials are available to help you but it will be to your advantage to make a serious attempt at the assignment before seeking help. If you are having trouble making progress, seek help as soon as possible. It is important to get notes for any class missed and to make up any work missed as soon as possible.

The following will be considered a breach of academic honesty:

1. Giving or receiving help during a test or quiz.
2. Discussing the contents of a test or quiz with members of the class or with other sections of the course who have not taken it.
3. Programming information into your calculator to be used during a test or quiz.
4. Completing assignments to be graded for other students is a violation for both the giver and the recipient of the work.

You will be given a detailed honesty policy and will be asked to sign an honesty form. You will also be asked to sign an honesty pledge on tests, quizzes, and exams.