Chemistry 394-01. Computational Chemistry

INSTRUCTOR: Prof. Keith T. Kuwata, Olin-Rice 318, 696-6768, kuwata@macalester.edu
Web page: www.macalester.edu/~kuwata (for class handouts and overheads)

REQUIRED TEXTS: (1) James B. Foresman and Aeleen Frisch, *Exploring Chemistry with Electronic Structure Methods*, 2nd ed., Gaussian, Inc., Wallingford, CT, 1996 (purchase at the Lampert Building Bookstore). (2) William F. Polik and Jordan R. Schmidt, *WebMO Users Guide*, Version 3.3, WebMO LLC, Holland, MI, 2003 (provided free of charge).

DESCRIPTION: Computation plays a key role in chemistry research today, with many articles in the chemical literature using computer modeling to make predictions of chemical behavior and to interpret experimental results. Arguably the most powerful subfield of computational chemistry is what as known as quantum chemistry—the application of quantum mechanics to atoms and molecules. This course has the following goals: (1) introducing students to the basic concepts of quantum chemistry; (2) illustrating the power and limitations of different quantum chemical methods; (3) giving students experience in applying quantum chemistry to a variety of systems. The emphasis throughout the course will be on the use of computers to make predictions, instead of the mathematics and physics underlying quantum mechanics.

The software we will be using for the quantum chemical calculations is *Gaussian 03*, the most popular, and perhaps the most versatile, computational chemistry program in the world. The late Professor John A. Pople, who helped create the original version of *Gaussian* in 1970, shared the 1998 Nobel Prize in Chemistry in part for this contribution. The graphical user interface we will use is WebMO, written principally by Professor William F. Polik of Hope College.

CLASSES: Mondays from 7:00 to 10:00 p.m. in Olin-Rice 301 and 341. Class times will typically consist of a lecture on the basic concepts to be considered that week, a demonstration of how to perform specific calculations using WebMO, and time to start on that week's assignment. **Attendance every week is mandatory**, unless you have a valid excuse (such as sickness or bereavement).

You should do the assigned reading (out of the Foresman and Frisch book) before coming to class, but the goal of the reading is to gain some familiarity with the material and figure out what questions you have, rather than mastering the material.

PROBLEM SETS: Assignments (usually consisting of exercises that I have adapted from the *WebMO Users Guide*) will be handed out on a given Monday, and be due in class the following Monday. Unless otherwise noted, each of the problems sets will be weighted equally in determining this percentage of your cumulative score. **There will be a 20% per day penalty for late homework.**

As in all Macalester chemistry classes, you are encouraged to work with your classmates on homework. However, you must turn in your own work.

FINAL PROJECT: During the second half of the semester, you will begin work on an independent project in which you choose a topic from the chemical literature, pose specific questions about that topic, perform calculations to answer your question, and present your results in both an oral presentation and a paper. More details to come!

GETTING HELP: I will be available in my office Monday 1:10-2:10 p.m., Tuesday 9:00-10:00 a.m., Wednesday 2:20-3:20 p.m., Thursday 1:10-2:10 p.m., and Friday 3:30-4:30 p.m. If you can't make one of

these office hours, please make an appointment with me, or just come by—I'll usually be somewhere in Olin-Rice during business hours.

GRADING: **Class Participation: 10%** **Problem Sets: 55%** **Final Project: 35%**
Note that there are no quizzes or tests. Since this is an advanced elective course, I anticipate all final grades will be B or higher—but this is not guaranteed!

ACADEMIC INTEGRITY: Copying another student's homework, fabricating computational data, or plagiarizing materials for either your oral presentation or final paper all constitute cheating and are expressly forbidden. Following college policy, I will report any clear violation of academic integrity standards to Ann Minnick, the Director of Academic Programs.

COURSE SCHEDULE (timing of topics may vary)

Date	What's Due?	Reading	Topics/Event
1/26		pp. 3-22 (skim)	Introduction; single-point energies and charge distributions
2/2	**PS 1**	39-45	Geometry optimizations and conformational analysis
2/9	**PS 2**	46-49; 70-73	Introduction to transition structures and vibrational frequencies
2/16	**PS 3**	169-180	Locating transition structures and making rate predictions
2/23	**PS 4**	61-69; 166-168	Chemical significance of vibrational frequencies
3/2	**PS 5**	97-102; 261-262	Basis sets; start literature search for final projects
3/9		93-96; skim 111-121	Levels of theory and highly accurate methods
3/16		**NO CLASS (Spring Break)**	
3/23	**PS 6**	**NO CLASS (I'll be at the American Chemical Society National Meeting)**	
3/27	**Proposal**		(Note Friday due date)
3/30			Begin final project calculations
4/6	**Intro**		Present a brief introduction to your project; continue calculations
4/13			Continue final project calculations
4/20	**Draft**		Continue final project calculations
4/27	**Talk**		In-class oral presentations
5/4	**Talk**		In-class oral presentations
5/8	**Paper**		(Note Friday due date)