Chemistry 4021/8021 **Computational Chemistry** 3/4 Credits
Spring Semester 2009

Time and Location: MWF 0905-0955, 331 Smith Hall.
(Computer Laboratory is in 101D Smith, and the internet is everywhere)

Instructor: Chris Cramer (215 Smith Hall, 624-0859, cramer@umn.edu).

TA: Zahid Ertem (147 Smith Hall, 624-1535, mzertem@gmail.com).

Office Hours: By arrangement -- you are welcome to look up me or Zahid at any time.

Textbook: Cramer, *Essentials of Computational Chemistry*, 2nd Ed., Wiley, 2004.

Class Website: http://pollux.chem.umn.edu/8021 -- site includes hand-outs, problem sets, exams, and answers from this and many previous years.

Coursework: There will be three software-based problem sets assigned during the semester. These practical exercises will be accomplished on either microcomputers or the hardware of the Minnesota Supercomputing Institute (students will be provided with MSI accounts). For 8021 students *only*, there will be a requirement for an analysis of a computational paper within the student's area of interest due on the date of the final (approx. 4-8 pages). There will be one midterm and one final exam; the former will be in class and the latter will be of the take-home variety and make use of data developed by the class over the course of the last two problem sets. Finally, there will be one to three quizzes given randomly. Possible dates for quizzes are indicated in the course outline.

My intent is *not* to foster memorization of specific details within the field, but to provide the student with the background and resources necessary both to *apply* and to *assess critically* computational methodologies from a *chemistry* standpoint. There will be almost no emphasis on algorithms other than that required for basic understanding of models and methods. Several classes will focus on discussion of recent applications and will **require** the prior reading of journal articles handed out in class. The quizzes will allow you to demonstrate having engaged the assigned reading prior to class.

Grading: For 8021, the three labs will each contribute 10% to your overall grade. The critical analysis will contribute an additional 15%, as will each of the two exams and also the sum of your quiz scores. The final 10% will be assigned by me based on classroom participation in lecture and discussions. Chem 4021 grading will use the same weightings of one exercise relative to another, but there is no analysis paper. You are welcome to discuss your performance with me at any point and I will provide feedback as graded exercises begin to accumulate.

Academic Misconduct: I rigorously adhere to the IT policy on scholastic conduct. This is a challenging course affording significant opportunity for individual initiative. Insofar as many of the graded requirements are to be completed outside of class, you will have the opportunity to discuss them with your peers. This does not become inappropriate *unless* it is designed to arrive at the required results without actually performing the antecedent work. I trust you to act within what should be common-sense limits.