

Time and Location: Generally (but always check!) WF 0905–0955, STSS 530B.
M (optional) 0905–0955, 101D Smith (Computer Lab)

Instructor: Chris Cramer (215 Smith Hall or 105B Walter Library, phone: 624-0859 or 624-9371, email: cramer@umn.edu, Twitter: @ChemProfCramer)

IMPACTor/TA: Allison Dzubak (101 Smith Hall, phone: 624-5923, email: dzub0005@umn.edu)

Office Hours: By arrangement — you are welcome to schedule mutually convenient time with either myself or Allison.

Textbook: Cramer, *Essentials of Computational Chemistry*, 2nd Ed., Wiley, 2004. Note that I have assigned a textbook for which I am the author and thereby earn royalties on sales of new copies (about \$4–6 per book). In accordance with University conflict of interest policy, I take this opportunity to inform you, in writing, of that situation.

Video Presentations: Lectures are recorded as video and delivered online, *not* in the classroom. The non-scheduled class times *may* be used by students to watch class videos, or to work on problem sets.

As this course will have a decidedly “flipped” flavor, students are responsible for reading/viewing relevant material *before* discussion in class. See the course outline for assigned reading/viewing.

Class Website: <http://pollux.chem.umn.edu/8021> — the site includes lecture notes, hand-outs, problem sets, exams, and answer keys from this and many previous years (.../4021 works, too). You will need to use the website a *lot*. Video links are there, associated slide presentations are there, the course outline is there, discussion assignments are there, the course seating chart is there, etc.

Coursework: There will be three software-based problem sets assigned during the semester. These practical exercises will be accomplished on either microcomputers or using the hardware of the Minnesota Supercomputing Institute (students will be provided with MSI accounts). **Start these well ahead of their due dates as they require a substantial time investment to complete.**

There will be two midterms and one final exam. **The date/time of the final exam is May 15, 2013, 1:30–3:30 PM.**

In-class discussions of literature papers will include short, written assignments to be completed prior to class and turned in after the discussion (details are provided separately).

In addition, a portion of the grade (see below) will be awarded based on attendance and classroom participation in discussions.

For 8021 students *only*, there will be a requirement for a written analysis of a computational paper within the student's area of interest due at the time of the final exam (approx. 4-8 pages; details will be provided separately).

Note that in developing and administering graded content, 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 computational algorithms other than that required for the most basic understanding of models and methods. Several classes will focus on discussion of recent applications and will **require** the **prior** reading and analysis of journal articles specified in the course outline.

Grading: For 8021, the three labs will be worth 100 points each. All three exams will be worth 100 points each, as will the critical analysis paper for 8021 students. Each written summary of a literature paper discussion task will be worth 50 points. Finally, 100 points will be assigned by me based on attendance and classroom participation and engagement in lectures and discussions. (1000 pts total for 4021, 1100 for 8021)

I grade each class, 4021 and 8021, based on the distribution of student performance (you can call that a "curve", if you like, but the numbers in each class are sufficiently small that a normal distribution is not really expected). Historically, 4021 has had grades distributed roughly 20/40/30/10 A/B/C/other, and 8021 has had grades distributed roughly 45/50/5 A/B/C (noting that C is a failing grade for a graduate student).

You are welcome to discuss your performance with me at any point and I will provide feedback as graded exercises begin to accumulate. If an absence that is excused under University policy causes you to miss a graded exercise, please come see me to arrange a plan for dealing with that circumstance.

Academic Misconduct: I rigorously adhere to the CSE 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 (because I want to live in that kind of world; don't you?)

Anything unclear? If so, just ask me.

Appendix. There are a number of items intended for inclusion on every University of Minnesota syllabus. You can find them at:

http://www.policy.umn.edu/Policies/Education/Education/SYLLABUSREQUIREMENTS_APPA.html

and you should read them there.