

Time and Location: MWF 0905–0955, Kolthoff Hall 140

Instructor: Laura Gagliardi (229 Smith Hall email: gagliard@umn.edu)

IMPACTs or/TAs: Hung Pham (101 Smith Hall email: phamx494@umn.edu) and Debmalya Ray (101 Smith Hall email: rayxx332@umn.edu)

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

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

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.

The videos are recorded by Professor Christopher J. Cramer and can be found at:
https://www.youtube.com/playlist?list=PLkNVwyLvX_TFBLHCvApmvafqqQUHb6JwF

Students are responsible for reading/viewing relevant material *before* discussion in class. See the course outline for assigned reading/viewing.

Class Website: On Canvas — the site includes lecture notes, hand-outs, problem sets, exams, and answer keys 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 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 final exam will take place on 5/15 (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.

The following material has been adapted from:

<https://policy.umn.edu/education/syllabusrequirements>

Student Conduct Code: The University seeks an environment that promotes academic achievement and integrity, that is protective of free inquiry, and that serves the educational mission of the University. Similarly, the University seeks a community that is free from violence, threats, and intimidation; that is respectful of the rights, opportunities, and welfare of students, faculty, staff, and guests of the University; and that does not threaten the physical or mental health or safety of members of the University community.

As a student at the University you are expected adhere to Board of Regents Policy: *Student Conduct Code*. To review the Student Conduct Code, please see: http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf.

Note that the conduct code specifically addresses disruptive classroom conduct, which means "engaging in behavior that substantially or repeatedly interrupts either the instructor's ability to teach or student learning. The classroom extends to any setting where a student is engaged in work toward academic credit or satisfaction of program-based requirements or related activities."

Use of Personal Electronic Devices in the Classroom

Using personal electronic devices in the classroom setting can hinder instruction and learning, not only for the student using the device but also for other students in the class. To this end, the University establishes the right of each faculty member to determine if and how personal electronic devices are allowed to be used in the classroom. For complete information, please reference: <http://policy.umn.edu/education/studentresp>.

Scholastic Dishonesty

You are expected to do your own academic work and cite sources as necessary. Failing to do so is scholastic dishonesty. Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or

using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis. (Student Conduct

Code: http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf)

If it is determined that a student has cheated, the student may be given an "F" or an "N" for the course, and may face additional sanctions from the University. For additional information, please see: <http://policy.umn.edu/education/instructorresp>.

The Office for Community Standards has compiled a useful list of Frequently Asked Questions pertaining to scholastic dishonesty: <https://communitystandards.umn.edu/avoid-violations/avoiding-scholastic-...>. If you have additional questions, please clarify with your instructor for the course.

Makeup Work for Legitimate Absences

Students will not be penalized for absence during the semester due to unavoidable or legitimate circumstances. Such circumstances include verified illness, participation in intercollegiate athletic events, subpoenas, jury duty, military service, bereavement, and religious observances. Such circumstances do not include voting in local, state, or national elections.

For complete information, please see: <http://policy.umn.edu/education/makeupwork>.

Appropriate Student Use of Class Notes and Course Materials

Taking notes is a means of recording information but more importantly of personally absorbing and integrating the educational experience. However, broadly disseminating class notes beyond the classroom community or accepting compensation for taking and distributing classroom notes undermines instructor interests in their intellectual work product while not substantially furthering instructor and student interests in effective learning. Such actions violate shared norms and standards of the academic community. For additional information, please see: <http://policy.umn.edu/education/studentresp>.

Grading and Transcripts

The University utilizes plus and minus grading on a 4.000 cumulative grade point scale in accordance with the following:

A	4.000
A-	3.667
B+	3.333
B	3.000
B-	2.667
C+	2.333
C	2.000
C-	1.667
D+	1.333
D	1.000
S	.

For additional information, please refer to:

<http://policy.umn.edu/education/gradingtranscripts>.

Sexual Harassment

"Sexual harassment" means unwelcome sexual advances, requests for sexual favors, and/or other verbal or physical conduct of a sexual nature. Such conduct has the purpose or effect of unreasonably interfering with an individual's work or academic performance or creating an intimidating, hostile, or offensive working or academic environment in any University activity or program. Such behavior is not acceptable in the University setting. For additional information, please consult Board of Regents Policy:

https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf

Equity, Diversity, Equal Opportunity, and Affirmative Action

The University provides equal access to and opportunity in its programs and facilities, without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression. For more information, please consult Board of Regents Policy: https://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity_Diversity_EO_AA.pdf.

Disability Accommodations

The University of Minnesota views disability as an important aspect of diversity, and is committed to providing equitable access to learning opportunities for all students. The Disability Resource Center (DRC) is the campus office that collaborates with students who have disabilities to provide and/or arrange reasonable accommodations.

- If you have, or think you have, a disability in any area such as, mental health, attention, learning, chronic health, sensory, or physical, please contact the DRC office on your campus (UM Twin Cities - [612.626.1333](tel:612.626.1333)) to arrange a confidential discussion regarding equitable access and reasonable accommodations.
- Students with short-term disabilities, such as a broken arm, **can** often work with instructors to **minimize** classroom barriers. In situations where additional assistance is needed, students should contact the DRC as noted above.
- If you are registered with the DRC and have a disability accommodation letter dated for this semester or this year, please contact your instructor early in the semester to review how the accommodations will be applied in the course.
- If you are registered with the DRC and have questions or concerns about your accommodations please contact your (access consultant/disability specialist).

Additional information is available on the DRC website: sdzavada@r.umn.edu, UM Twin Cities - drc@umn.edu) with questions.

Mental Health and Stress Management

As a student you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance and may reduce your ability to participate in daily activities. University of Minnesota services are available to assist you. You can learn more about the broad range of confidential mental health services available on campus via the Student Mental Health Website: <http://www.mentalhealth.umn.edu>.

Academic Freedom and Responsibility: *for courses that do not involve students in research*

Academic freedom is a cornerstone of the University. Within the scope and content of the course as defined by the instructor, it includes the freedom to discuss relevant matters in the classroom.

Along with this freedom comes responsibility. Students are encouraged to develop the capacity for critical judgment and to engage in a sustained and independent search for truth. Students are free to take reasoned exception to the views offered in any course of study and to reserve judgment about matters of opinion, but they are responsible for learning the content of any course of study for which they are enrolled.*

Reports of concerns about academic freedom are taken seriously, and there are individuals and offices available for help. Contact the instructor, the Department Chair, your adviser, the associate dean of the college, or the Vice Provost for Faculty and Academic Affairs in the Office of the Provost.

Laura Gagliardi