



Chemistry and Biochemistry

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Chemistry 410 Physical Chemistry Syllabus

last update: Spring 2018

Class meetings:

- **lecture:** MWF 12-12:50pm in GMCS-314
- **optional examples session:** M 5-5:50pm (room to be determined)

Instructor:

- [Andrew Cooksy](#); CSL-310; 619-594-5571; office: hours Mon/Wed 9:30-10:30am

Materials:

- **Book:**
 - **CHEM 410A Textbook:** *Physical Chemistry: Quantum Mechanics and Molecular Interactions* by Cooksy, with access to the *Mastering Chemistry* online homework system. The course code that you will use to find my problem sets in Mastering is **COOKSY410ASPRING2018**.
 - **CHEM 410B Textbook:** *Physical Chemistry: Thermodynamics, Kinetics, and Statistical Mechanics* by Cooksy, with access to the *Mastering Chemistry* online homework system. **(You probably already have access to Mastering if you took Chem 410A with me the previous semester. Check before you pay a second time.)**
 - **CHEM 410A Lab manual:** *Chem 410A Laboratory Projects Manual*

These materials will be available through Aztec Bookstore. Any form of the textbook (hardcover, loose-leaf, e-book) is fine. If you plan to buy a used copy, **make sure you also get access to the online homework.** Buying the homework access separately can cost almost as much as buying the new book bundle. However, the homework access should be good for a year, so will cover both Chem 410A and Chem 410B if you take 410B in Fall 2018. You may want to check out the bookstore's [price matching offer](#).

- **Solutions to the end-of-chapter problems:** are available online from [Pearson](#).
- **Reserve materials:** A few of the more recent Physical Chemistry texts are on reserve at Love Library, for those of you wishing to see an alternative presentation of the same material. Note that most of these texts cover both semesters of p-chem in one volume, with

quantum in the middle and thermodynamics at the beginning of the book. Also, we will give more attention to statistical mechanics (at the beginning of Chem 410B) than is typical.

- **Blackboard** will be used to post announcements, assignment scores, and final grades. Please be aware that I keep a separate gradebook, where I make adjustments such as dropping low scores, and therefore *the point total evaluated by Blackboard is not the number I use to assign a grade.*

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Catalog Description

CHEM 410A. Physical Chemistry (4)

Three lectures and three hours of laboratory. Prerequisites: Chemistry 232, 232L, 251; Mathematics 252 (Mathematics 150, 151; 252 or Physics 195, 195L, 196, 196L for chemistry teaching major); Physics 195, 195L and 196, 196L. Recommended: Physics 197 and 197L. Theoretical principles of chemistry with emphasis on mathematical relations. Theory and practice in acquisition and statistical analysis of physical measurements on chemical systems.

CHEM 410B. Physical Chemistry (3)

Three lectures. Prerequisites: Chemistry 232, 232L, 251, 410A. Theoretical principles of chemistry with emphasis on mathematical relations. Theory and practice in acquisition and statistical analysis of physical measurements on chemical systems

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Student Learning Objectives:

In this course, encompassing Chem 410A and Chem 410B, we will examine in detail the theoretical framework that justifies *all* chemical laws. The student successfully completing the course will be able to accomplish the following outcomes.

Outcome	Activity	Assessment
Analyze diverse chemical systems and reduce them to their principal chemical and physical components and interactions for the purposes of mathematical description.	Students will be presented with derivations of fundamental principles through lecture and reading, with example applications discussed with the class as time permits.	New applications of these principles will be presented as word problems for the students to solve on examinations.
Predict the outcome of molecular processes (including diffusion, interaction with radiation, and chemical reaction) from a set of initial conditions.	Lecture will demonstrate how principles of chemistry and physics aid in predicting the dynamics of molecular systems. Students will practice applying these concepts in online homework problems with unlimited attempts.	New systems and initial conditions will be presented as problems for the students to solve on examinations.
Calculate or estimate structural properties of individual molecules and small groups of molecules using principles of quantum mechanics. (Chem 410A)	Lecture will demonstrate how quantum mechanics describes systems at the molecular scale. Students will practice applying these concepts in online homework problems with unlimited attempts.	New applications of these principles will be presented as word problems for the students to solve on examinations.
Use Excel and Maple to carry out several basic operations for the analysis and visualization of scientific data (Chem 410A lab).	Students will work through several guided problems of growing complexity in data analysis, data presentation, and numerical simulations.	Most activities will include a final component where data is given to the student to analyze as part of their score for the day's project. In addition, quizzes on selected topics will be presented throughout the semester following the guided portion of the relevant lab.

Calculate or estimate dynamic properties of large sets of molecules using principles of statistical mechanics, chemical thermodynamics, and reaction kinetics. (Chem 410B)

Lecture will demonstrate how classical physical chemistry describes systems at the laboratory scale. Students will practice applying these concepts in online homework problems with unlimited attempts.

New applications of these principles will be presented as word problems for the students to solve on examinations.

Meeting these objectives should allow the student to eventually build a meaningful intuition regarding chemical behavior based on a unified foundation of chemical theory.

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Prerequisites

Physical chemistry is a fairly demanding course, and we spend little time reviewing material from the foundation courses that come earlier. Enforcing the prerequisites allows us to better match the course to those students who have at least partly established that foundation through their prior coursework. We do not enforce all the prerequisites at registration because this would make it impossible for many qualified transfer students to register. However, students who do not fulfill the course requirements listed as detailed below may be **dropped from the course** by the instructor:

- **MATH 151, PHYS 196, and CHEM 231** and their prerequisites (MATH 150, PHYS 195, CHEM 200 and 201). To take CHEM 410A, a student must have **already passed** all of these courses. Concurrent enrollment is not sufficient. If you are missing only the **PHYS 196L** lab, you may enroll in CHEM 410A, but to register for CHEM 410B in the spring, you *must* either have completed or be enrolled in PHYS 196L by then.
- **MATH 252, CHEM 251**. We are currently enforcing these prerequisites. If seats are still available by the first day of classes, we *may* relax this requirement. If this is the only course blocking you from registering for CHEM 410A and you would like to enroll in 410A, [email me](#).
- **CHEM 410A** is a prerequisite for CHEM 410B.

If you satisfy any of these requirements by coursework at a different institution, it may be necessary to show the transcripts for that work to the instructor.

This is not a math class, and so I try to avoid unnecessarily lengthy mathematics in the problems. Usually. However, mathematics is our principal tool, and you need to be very comfortable with elementary algebra, geometry, and calculus (up to derivatives, simple integrals, and power series). The math is all manageable one step at a time, but there will sometimes be many steps.

This is pretty much a physics class, however. In Chem 410A in particular we will call on results from mechanics and electromagnetism to justify some of our conclusions about atomic and molecular structure. You are probably familiar with the concepts if you've taken first-year physics, and we will introduce (but rarely prove) any equations from physics that we'll need before we use them.

There is an introductory chapter ("Chapter A") to the text that summarizes the prerequisites we

will rely on most often. Your texts for previous math and physics courses should help you if you're rusty in those areas.

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Course Material

In one sentence, the course covers principles of atomic and molecular structure, molecular interactions, statistical mechanics, chemical thermodynamics, and chemical kinetics.

TOPICS

The Chem 410A/B sequence covers the fundamental physics of chemical systems, including structure, energetics, and interactions of molecules. The material can be applied to inorganic, organic, and biochemical molecules and reactions. In fact, most of the important results in physical chemistry will already be familiar to you from general chemistry. If you find the details of our work in this class obscure the results, you may want to go back and look at the relevant section of a general chemistry text.

The primary reference for the course is still the lectures themselves. No material is covered on the tests that has not been discussed in class, and occasional lecture topics may appear on the tests even if they are not included in the reading. But if you read ahead, you may find the lectures more useful, and your note-taking may be reduced to adding comments to the text rather than recording the entire lecture.

ORGANIZATION

Physical chemistry examines chemical phenomena both on the scale of individual atoms and molecules (the microscopic limit) and on the scale of thousand-gallon chemical reactors (the bulk or macroscopic limit) and bigger, as well as everywhere in between. In this class, we build from the microscopic limit to the macroscopic:

1. quantum mechanics of atoms
2. quantum mechanics of molecules
3. molecular interactions at microscopic scale
4. statistical mechanics and extrapolation to the macroscopic limit
5. thermodynamics and bulk properties of non-reactive systems
6. bulk reaction thermodynamics and kinetics.

This differs from the organization of most textbooks in the field, which start with classical thermodynamics and kinetics, and then introduce quantum mechanics and statistical mechanics in the second half. I hate that, so instead we're using my own textbook as your reference. But no single teaching style or book works for everyone, so some other textbooks will be on 3-day reserve at Love Library (see below).

A more detailed breakdown of the course topics follows the chapters of the 2-volume textbook in sequence:

Chemistry 410A: Microscopic Systems

Physical Chemistry: Quantum Mechanics and Molecular Interactions

chap	topic
Part I: Atomic Structure	
1-2	Introduction to quantum mechanics
3	One-electron atoms
4	Many-electron atoms
Part II: Molecular Structure	
5	Chemical bonds
6	Molecular symmetry
7	Electronic states
8	Vibrational states
9	Rotational states
Part III: Intermolecular Interactions	
10	Intermolecular forces in gases
11	Clusters and macromolecules
12	Structure of liquids
13	Structure of solids
Chemistry 410B: Macroscopic Systems	
<i>Physical Chemistry: Thermodynamics, Stat Mech, and Kinetics</i>	
Part I: Extrapolation to Macroscopic Systems	

- 2 Introduction to statistical mechanics
- 3 Partitioning the energy
- 4 Stat mech and molecular interactions
- 5 Mass transport
- 6 Energy transport

Part II: Non-reactive Macroscopic Systems

- 7 Introduction to thermodynamics
- 8 Energy and enthalpy
- 9 Entropy
- 10 Phase transitions
- 11 Solutions

Part III: Reactive Macroscopic Systems

- 12 Chemical thermodynamics
- 13 Chemical kinetics: elementary reactions
- 14 Chemical kinetics: multistep reactions

For a tentative lecture schedule, please see the course calendar for [CHEM 410A](#) or [CHEM 410B](#).

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Grading Scheme**OVERALL GRADING SCHEME**

Final grades will be assigned on the following scale:

A 85-100%

B 70-84%

C 50-69%

For CHEM 410A, the totals from the lecture and the lab parts of the course are combined in a 75:25 ratio before determining the final grade.

LECTURE GRADING SCHEME

Note that for CHEM 410A the following table applies only to the lecture part of the course:

#	assignment	points each	points total	% lecture grade
6	homework sets	20 pts (drop lowest score)	100	10%
4	drills	25 pts	100	10%
6	20-minute exams	100 pts (drop lowest score)	500	50%
1	cumulative final	300 pts	300	30%

LAB GRADING SCHEME (410A ONLY)

The lab grade is based on several 10-point labs, and a few 10-point quizzes. The lab and lecture instructors (not always the same person) will determine the grading scale for the labs, and at the end of the semester the total lab scores will be normalized to the lecture grading scale below (so that for example a high B in lab is converted to a high B on the lecture grading scale). The final score will then be computed as $0.25(\text{normalized lab score}) + 0.75(\text{lecture score})$.

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Assessments

DRILLS

These are 10-minute quizzes on the most basic material, mostly review material from prerequisite classes such as General Chemistry. These are sometimes directly relevant to the lecture material, and the dates on which they are given may be changed during the semester to accommodate the variable lecture schedule. Because it should not be necessary to spend a lot of time preparing for these, I will allow myself to give a drill on only three day's notice. Drill material will usually *not* be reviewed in lecture.

- 410A drill topics may include:
 - unit analysis and conversions,
 - stoichiometry,
 - reasonable values for physical quantities,
 - basic integrals and derivatives,
 - electron configurations for atoms,

- Lewis structures and VSEPR theory for molecules.
- 410B drill topics may include:
 - more unit conversions and reasonable values,
 - more basic calculus, including power series approximations,
 - balancing chemical reactions,
 - calculating enthalpies, energies, and entropies of reaction,
 - elementary kinetics with rate laws.

PROBLEM SETS (ONLINE HOMEWORK)

One problem set of online *Mastering Chemistry* homework problems will be given before each exam. I will make available a number of problems, worth 1 or 2 points each, with a maximum score of 20 points per problem set. You are encouraged to try as many problems as you can manage, but you only need to complete *20 points' worth* of problems to get full credit. These will normally be due the **Monday** before each exam, and the initial problems will be posted about two weeks before that. I may continue to add problems to the set up until it is due, but you will have at least one full week to work to complete your 20 points. No credit will be given for late problem sets, so please get your 20 points done before the due date.

Most of these will be based on the more straightforward lecture material. The primary goal of the homework is to encourage the class to prepare for the exam more than two days in advance. The homework problems are **not** intended to exactly represent problems that will appear on the exams. Studying solutions to these assignments *alone* will be of only partial benefit in preparing for the exams.

The homework also provides an opportunity to illustrate some applications drawn from material covered in lecture, and these may contain tougher mathematics than will be necessary on the exams. If you're spending more than 15 minutes on one problem and not making progress, please come to the office hours or email me or use the Blackboard discussion forum.

EXAMS AND FINAL

There will be six 20-minute exams and one 2-hour final. CHEM 410B has an additional, *optional* [ACS final exam](#). For all exams and the final:

- Attempt all the questions.
- You are permitted to consult your own notes and our textbook during the exams, but additional textbooks are not allowed (only because students would then not have equal access to the same information).
- The exams will begin with several short-answer problems, dealing with the most fundamental concepts in as straightforward a manner as I can manage. This section will count for 40% of the exam. Although there may be exceptions, in general partial credit is not available on these problems.
- There will then be 2 or 3 longer problems, counting towards the remaining 60% of the available points. These problems draw from more specific topics and require varying amounts of math. Partial credit is always available on these problems. These are not all intended to be of equal difficulty, but the prepared student will recognize the questions they know how to answer.
- For full credit, please put down your pen or pencil as soon as I say the exam is over.

Although the exams are all open-book, you **must** come to them prepared. You will have time only for very brief consultation of your notes. Attached to each 20-minute exam are what I deem all necessary tables, constants, and complicated equations. The final exam will offer you

almost twice as much time per question, so will feel less rushed. But I find that the added time does not tend to greatly raise students' scores.

The 20-minute exam on which you get your lowest score will be dropped from calculation of the final grade. If you are unable to take an exam for any reason, that exam will become your dropped score. There are no make-up exams. Please beware of purposely dropping any exam to make room in your schedule for something else. Throughout the two-semester sequence, what we cover on one exam is always based on material that the previous exams covered, so it doesn't pay to purposely neglect any section of the course.

The final exam will review all of the course material for the semester, and provides an opportunity to improve recorded scores on *some* problems from the short exams. Your exam scores are recorded question-by-question. After writing the final, I will match some of those questions to questions on the 20-minute exams which covered the same topic. If you score higher on one such question on the final than you did on the corresponding question on the 20-minute test, I will raise your grade on the 20-minute test. But don't count on a lot of help from this: because there are not nearly as many questions on the final as on the set of 20-minute tests, the final will not be able to correct substantially for routinely poor performance on the 20-minute tests. Also, the final is not capable of changing grades as much as one might think. The wide grade ranges of the grading scheme (with a 20% range for a B, for example) make it hard for any one assignment to shift the final total by a whole letter grade.

ACS FINAL EXAM IN CHEM 410B

Two final exams will be offered in CHEM 410B only:

- My own final exam, in the same format as the 20-minute exams, covering only the material from CHEM 410B and given on *the last two days of class*. This is the official final exam for the course, and attendance at this exam is mandatory.
- The ACS standardized, multiple choice examination in physical chemistry, covering material from *CHEM 410A and CHEM 410B*. This exam will be offered during the 2-hour slot scheduled for our final exam, to adhere to the testing procedures stipulated by the ACS. Attendance at this exam is optional (because it covers material from 410A as well as 410B) but encouraged.

Your best score of the two finals will be your score on the final for CHEM 410B. Therefore, it cannot hurt your grade to take the ACS exam. A review of CHEM 410A material will be offered between the two exams. Scores from the earlier, official final exam will be made available only after the ACS exam.

LABS (410A ONLY)

The lab manual will allow you to prepare for each lab. While you may consult with each other before the lab, full credit will not be given for lab assignments that appear to be largely copies of the same file. Any part of the assignment may be modified upon your arrival in lab in order to encourage everyone to be ready to do their own work. The labs must be completed during the class period, in the assigned classroom; *exceptions require prior consent of the instructor*. If more than one lab section is being offered, then changing sections for a particular lab to accommodate a personal schedule conflict is allowable, provided that consent is obtained from the instructor(s) for both sections and that there are enough computers available.

Lab outline

1. **Introduction to Excel.** Entering and evaluating formulas; naming cells.

2. **Numerical integration.** Using the Newtonian integration scheme to evaluate integrals along one coordinate.
3. **Experimental measurements.** These are quick measurements to acquire data for later analysis by Excel.
4. **Introduction to error analysis.** Gaussian error distributions; calculating averages and standard deviations by formula and using the internal Excel functions.
5. **Introduction to linear least squares fitting (LINEST).** Finding best-fit slope and intercept for a linear data set, and plotting trend lines.
6. **More linear least squares fitting.** Linearizing non-linear equations, and resulting propagation of errors.
7. **Introduction to non-linear least squares fitting (Solver).** Evaluation and minimization of chi squared.
8. **More non-linear least squares fitting.**
9. **Introduction to symbolic math program Maple.** Plotting wavefunctions, calculating basic physical properties from the wavefunction.
10. **More Maple.** 3D plots, animated plots.
11. **Introduction to quantum chemistry computations (Gaussian 09).**
12. **More quantum chemistry computations (Gaussian 09 and Solver).**

MISSED ASSIGNMENTS

This course cannot always be your top priority, and in consideration of this, the lowest score from each of (a) the problem sets, (b) the 20-minute exams, and (c) the regular CHEM 410A labs (not lab practical or lab quizzes) are all dropped. If you do not turn in one of these assignments for any reason, that becomes the dropped assignment. This is intended to accommodate emergencies such as illness, as well as professional obligations such as out-of-town conferences. In the event that other obligations or emergencies compel you to miss multiple assignments and you are concerned about your grade, then you may meet with me during office hours to discuss the possibility of taking an incomplete.

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SDS ACCOMMODATION

Students who may qualify for special accommodations for these assignments should first seek authorization by contacting Student Disability Services at 619-594-6473 (Calpulli Center, Suite 3101). Students with that authorization should then contact me as early as possible so that we can agree on a suitable protocol for drills, quizzes, labs, and exams. We cannot retroactively apply special consideration for assignment scores. You are welcome to email me if you would like to set up an appointment outside regular office hours for that discussion.

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Additional Hours: Examples Session and 410A Calculus Boot Camp

We have a lot of material to cover, and we will cover almost all of it. Lectures are therefore rather fast-paced, and it is often not possible to work through example problems during class time. To make up for this, please take advantage of my office hours to go over lecture material, sample problems, and to review quizzes and exams.

Examples Session. In addition to the regular office hours, a totally optional examples session is held each Monday evening (starting the second or third week of class) from 5-6pm. This allows us to go over additional problems, and at a more leisurely pace. New material for tests is never introduced at these sessions, and attendance is not expected or required. If you choose to come, you may arrive and leave anytime during the session, but please bring questions about

the material or suggestions for problems to work through.

Calculus Boot Camp (Chem 410A only). A 4-day, 7am-8am review of basic calculus, focusing on the rote methods rather than the mathematical theory. This is completely optional. Nothing is graded, and no sign-up or regular attendance is required. The idea is to provide a chance for students who are concerned about their calculus skills to exercise them before it really matters. I do not try to make this interesting; it's just math drills, available for those who feel they might need it and are willing to make some extra effort.

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Studying Physical Chemistry

You've reached a level of coursework where there's no reliable formula for success. I will be trying to grade each student based on their understanding of fundamental concepts that underlie all of chemistry, and their ability to apply those concepts to different situations. This is a lot to ask. I appreciate that your time is limited, and you want your study time to be wisely used, but it will be up to you to find what works best. It is possible to study many hours and still be disappointed by performance on the exam, so you need be honest with yourself about how to make your studying most effective. For example, reading the homework problems and then reading the solutions can feel very rewarding, but often does not prepare a student for the demands of putting together the solution on their own. Detailed solutions to many problems in the book are provided in the solutions manual, but I always try to write new problems and new *kinds* of problems for the exams.

To pass the course it is usually enough to make sure that you can do the basic calculations. But to get an A, you will need to demonstrate that you can apply the principles we cover to new situations of my choosing. That requires testing yourself not just on how to use particular equations, but on why those equations work for particular situations, and what would happen if the situations were different. My hope is that an A will reflect a deep grasp of the most fundamental ideas in chemistry. I hope you'll agree that this is a goal worth considerable effort.

My recommendations:

1. **Work lots of problems, but don't spend a lot of time on any particular one.** The most difficult part of a good exam problem is right at the beginning: seeing what concepts we've covered that relate to the question. For that purpose, I think it's more valuable to see lots of different examples than to go into depth on a few.
2. **Don't assume that understanding a solution is the same as being able to solve a problem.** It is much easier to make sense out of a solution that is presented to you than to come up with another similar solution on your own. Concentrate on how *how you would start solving the problem* that particular way. What in the problem makes it clear which equations are useful?
3. **Don't memorize a particular approach.** Learning recipes for solving particular kinds of problems (a strategy that works well in General Chemistry) is only a small part of succeeding in Physical Chemistry. Some of these problems can be solved by rote, but not the really interesting ones, and I try to make the exam questions interesting.
4. **Try to ask yourself qualitative questions about the material.** This is difficult, but once you get to the point that you can solve the purely numerical problems, you should be able to ask yourself what that answer means. Would the final value be larger or smaller if you changed the system somehow (more massive particle, bigger container, ...)? What if we asked the same question, but about a different system? These are the kinds of questions I ask myself when coming up with the problems.
5. **Make the lectures worthwhile by reading ahead** if you can, and asking questions in

lecture when you need to.

6. **Study with others and ask each other questions** about the material. Test each other. The end-of-chapter problems begin with a set of "discussion questions." These would be terrible exam questions because they look mostly for qualitative, essay-like solutions (difficult to grade), but they are suggestions for the sort of questions you should be asking each other.
7. **Come to office hours and/or the Monday afternoon examples session**, at least once, early in the semester. At least find out if it's worth it before you look for alternatives.
8. **Keep thinking about the material.** The material should make sense, if you can give yourself the time to think it through. That's the most rewarding thing about the class -- it shows how chemistry all fits together into one cohesive picture.

Ultimately, the only way to guarantee success in the course should be to understand the material really, really well. Try to honestly assess your own understanding of the material, for example by seeing how reliably you can productively start to solve problems at the end of each chapter, and use that as your guide to what study techniques work best for you.

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Conduct of Class

Please ask questions. If we really are in too much of a hurry, or if I just can't come up with a better explanation than I've already given, we may need to postpone the discussion until office hours. However, if the class is exceptionally quiet, it only encourages me to keep on talking and talking and talking.

Please always disable any noisy electronic devices you have, such as cell phones and watch alarms, before you come into class so that they will not disturb us during lecture or lab. If you must use your phone during lab, please leave the room first. If you must use your phone during lecture, please stay away.

The goal of the labs is for you to understand how to use the software to accomplish a specific task, and the assignment is there to keep your efforts focused. Please get assistance if you need it. In addition to asking the instructor questions, you are welcome to confer with each other during the regular labs, but only you and your instructor are permitted to edit your assignment. For example, other students should not type an expression into your Excel spreadsheet, or use your mouse to demonstrate how to change the appearance of your chart. Please also remember that the lab quizzes test the skills introduced by the regular labs, and for the quizzes no assistance from classmates is permitted, so you will want to know how to do your own work for these assignments.

I prefer not to invest class time in discussing the course administration. Of course you may ask me to justify any aspect of the syllabus, but please reserve those questions for office hours or email, outside of our limited lecture time. Lab tends to quiet down towards the end of the lab period, and so I am also often available then for questions then about the lecture material or administrative issues.

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Add/Drop Procedures

If you are unable to enroll in the course because you are blocked, or the sections are full, or the schedule number is hidden, [email me](#). To drop the course, use your [WebPortal](#) account.

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Academic Honesty

Students are expected never to represent someone else's work as their own nor to assist others in doing so. Violations of this rule will be documented and may result in grade reduction (including failure) and disciplinary review by the University. Please see the [SDSU academic honesty page](#) for further information.

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