CHEM 3070

Physical Chemistry: Statistical Thermodynamics and Chemical Kinetics
Fall 2023, 4.0 Credit Units

This course meets the **Quantitative Intensive (QI)** requirement.
This course addresses the following **Essential Learning Outcomes**: Quantitative Literacy, Problem Solving, Oral Communication, and Foundations and Skills for Lifelong Learning

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Time and Place Monday, Wednesday, & Friday 8:35AM-9:25AM JFB B-1
Section 2: Tuesday & Thursday 7:30AM – 8:20AM CSC 25
Section 3: Tuesday & Thursday 8:35AM - 9:25AM MCD 130

Prerequisites ("C-" or better in (CHEM (1220 OR 1221) OR AP CHEM score of at least 5) AND (PHYS 2220 OR PHYS 3220)) AND ("C" or better in (MATH 1260 OR MATH 1321 OR MATH 2210)).

Class Overview

Course Outcomes

Physical Chemistry is concerned with explaining and predicting the behavior of atoms and molecules from basic laws of physics. While CHEM 3060 explores the quantum-mechanical nature of molecular energy levels, structure, and interactions, the overarching goal of CHEM 3070 is to provide you with the tools to *understand the collective behavior of many molecules*. At the end of the course, the student will be able to...

- Understand the dominant role of microscopic fluctuations.
- Calculate the entropy of a macroscopic system from the statistics of microscopic fluctuations.
- Understand the role of the energy scale set by k_BT and use it to predict chemical phenomena.
- Count microstates in discrete and continuous model systems.
- Determine if a system should be treated with quantum mechanics or can be understood with classical statistical mechanics.
- Write down the partition function of a simple system and derive important properties from it.
- Explain the Second Law of Thermodynamics in terms of the likelihood of microscopic fluctuations.
- Understand concepts of work and heat.
- Understand the connection between entropy and thermodynamic potentials like enthalpy and Gibbs free energy.
- Understand how microscopic fluctuations dictate properties of materials like a rubber band.
- Interpret phase diagrams.

- Explain why systems can coexist in different phases and why the distinction between phases vanishes at the critical point.
- Predict the distribution of material from knowledge of the chemical potential. • Predict interactions between charged solutes.
- Understand the implications of the long-ranged nature of Coulomb interactions.
- Use the microscopic energy landscape of a chemical reaction to calculate its macroscopic rate.
- Estimate molecular speeds of particles in the gas phase and in solution.
- Connect macroscopic rate laws to microscopic collision and reaction mechanisms.

Required Materials

No textbook is required! The lectures and discussion sections will teach you all you need to know. However, books are always great as a reference, to get a different perspective, or to read up on something ahead of time. Here are my suggestions for a few good books that cover most of the course material:

- Physical Chemistry: A Molecular Approach (McQuarrie & Simon). Good classic PChem book that also includes Quantum Mechanics. Profs. Steele/Morse/Anderson use this book in Chem 3060. Some of the material discussed in class is not or only sparsely included.
- Thermodynamics and Statistical Mechanics (Shell). This book takes a viewpoint that is close to the lectures on some topics.
- Molecular Driving Forces (Dill & Bromberg). Good book written from a molecular viewpoint. It also has useful math chapters.
- Physical Chemistry (Atkins). Good and well-known book. Does not go very deep on some topics.
- Introduction to Modern Statistical Mechanics (Chandler). Condensed, advanced, and challenging text, but full of insights. Comes with lots of challenging problems.

Required Effort

Experience suggests that you might find this class more challenging than most other courses you have taken so far. The class requires you to develop accurate mental models of molecular fluctuations, to describe these models using challenging mathematical concepts, and to creatively apply a relatively small number of fundamental principles in a range of different situations. **To be successful in this class, you should plan to work at least 10 hours per week out of class (i.e., in addition to the lectures and discussions) on the material.**

Extensions and Accommodations

To be fair to all students in the course, I will rarely grant homework extensions or make-up exams. Yet, I realize that often things come up that are out of your control. **Therefore, your lowest problem set grade and lowest midterm grade will be dropped from your final grade.** To ensure fairness, no accommodations can be made, or extensions given after an assignment is due or an exam has begun. Please also get in touch with me via email if you have any concerns about your progress in class, your grade, or your ability to succeed in the class. The sooner we start a conversation, the easier it will be for us to find solutions that help you achieve your goals and succeed in class.

COVID Accommodations

Although the COVID pandemic seems to be easing up, there are still many cases in Utah and the rest of the United States. Please do not come to class or the discussion sections if you have COVID symptoms or test positive for COVID. Please email the instructor if you feel sick or test positive so we can figure out a plan. Missing class, discussion sections, or exams due to COVID will not negatively impact your grade. We will make appropriate accommodations on a case-by-case basis.

Student Mental Health Resources

Rates of burnout, anxiety, depression, isolation, and loneliness have noticeably increased during the pandemic. If you need help, campus mental health resources are available, including counseling, trainings, and other support (https://studentaffairs.utah.edu/mental-health-resources/index.php). Consider participating in a Mental Health First Aid or other wellness-themed training provided by Student Affairs' Center for Student Wellness to help contribute to creating a healthier and safer campus community. These are designed to equip you to better recognize and respond to signs and symptoms of mental health and substance abuse challenges.

Class Structure and Grading

No-screens policy

To create a focused learning environment, I ask that you please do not interact with your phones during lecture and discussion meetings. Please use only those devices in class that contribute to learning (e.g., any type of note-taking device). I will not enforce this policy in any way but I highly recommend you follow it as research clearly demonstrates the learning benefits of this approach.

In-person lectures and lecture slides

I will deliver all class content in the form of in-person lectures. For the best educational experience, I highly recommend you attend lectures regularly. Lecture slides (pdf) will be made available on Canvas.

Weekly Canvas quizzes

At the end of every week of classes, I will post a short quiz (5-10 questions) on Canvas. While the homework will mostly concentrate on practical applications of what you learned in class, weekly Canvas quizzes will focus on concepts. You should be able to answer some of the questions straightforwardly from what is covered during lectures; other questions will require you to think a little deeper.

Homework and discussion meetings

Problem sets will be posted weekly. Some of the problems are quite challenging and designed to not only illustrate points made during lectures, but also to further develop certain ideas and to introduce new facets of a topic. Please take these problems seriously! To succeed in exams you will need to solve problems of similar caliber. To guide you through the problems and address any questions and difficulties, we will work on homework problems in groups during our discussion meetings (Tuesdays and Thursdays). Roughly half of the problems will be marked with labels "Day 1" or "Day 2". These labels indicate that we will discuss these problems in either the Tuesday ("Day 1") or Thursday ("Day 2") discussion sections. I urge you to come prepared to the discussion meetings and ready to interact with others. The material covered in this course is not a collection of separated pieces of information that need to be memorized. Rather, physical chemistry consists of a few fundamental principles that, once mastered, will enable you to independently think about and explain phenomena that are new to you. The best way to become familiar with these principles is not by watching a video or studying a book, but rather through discussions with people who work on the same scientific problems. To get the most out of group work during discussion meetings, I urge you to start working on the problems before you come to discussion, so you can ask meaningful questions and are able to assist others.

Written solutions to all problems are due at the end of Friday and will be submitted as a single PDF file on Canvas. If you prefer, you may hand in a hardcopy of your solutions Friday before or after class. Keys will be posted on the course website and graded homework will be returned electronically within a week's time. Two notes on homework format:

- Please, print legibly! It is at the sole discretion of your TA to decide that they cannot grade a particular problem because of bad handwriting.
- Please order your pages according to problem number.

Exams

Exams will be based on material covered during in-person lectures. There will be two mid-term exams in addition to the final exam. Exams will be administered in the classroom. Midterms will be administered during regular class hours. The date and time of the final exam is set by the University. During exams, you cannot use any electronic devices, including calculators, phones, laptops, tablets, etc. **The lowest midterm score will be dropped from your final grade. The final exam cannot be dropped.**

Academic Honesty

Any form of cheating on exams and homework (including, but not limited to, copying from old homework keys) will not be tolerated. Please refer to the University regulations for more information. (www.regulations.utah.edu/academics/6-400.html)

Participation

It is a requirement of this class to attend the live lectures and the discussion section. We will not be taking attendance, but we may have in-class or discussion section worksheets that we will collect as part of your participation grade. We will also use Poll Everywhere (https://www.polleverywhere.com/) in this course to poll the class. Poll Everywhere questions will be graded purely on participation. The last component to the participation grade is an open-ended question on the Canvas Quiz reflecting on the week.

Grades

The final grade will be calculated from the following approximate contributions:

- Participation 10%
- Weekly Canvas quizzes 15%
- Written Homework 25%*
- Midterm exam 1 or 2 25%**
- Final exam 25%

*The written homework with the lowest score will not be considered as part of your grade.

The midterm with the lower score will not be considered as part of your final grade. The final exam **cannot be dropped.

The following key will be applied to determine final grades: This key can be modified to consider class performance.

Points (%)	93-100	90-92	87-89	83-86	80-82	77-79	73-76	70-72	60-69	< 60
Grade	A	A-	B+	B	B-	C+	C	C-	D	E

Class Schedule

Important Dates

Last day to drop class or elect CR/NC	Fri, 9/1
Mid-term exam 1	Fri, 9/27

Last day to withdraw	Fri, 10/20
Mid-term exam 2	Fri, 11/20
Last day to reverse CR/NC	Fri, 12/1
Last day of class	Thurs, 12/7
Final exam	Tues, 12/12 8:00 AM to 10:00 AM

Preliminary schedule of lectures and exams

Date	Topic
8/21	Introduction and Microscopic Fluctuations (***asynchronous***, ***virtual***)
8/23	The Boltzmann Distribution
8/25	Introduction to Entropy
8/28	Entropy
8/30	Molecular Speed
9/1	Boltzmann Distribution Derived
9/4	**No Class – Labor Day**
9/6	Partition Functions
9/8	Classical vs. QM Partition Functions
9/11	Indistinguishability, rotations, and equipartition theorem (***asynchronous***, ***virtual***)
9/13	Vibrations, Gibbs entropy, and transition to Thermodynamics (***asynchronous***, ***virtual***)
9/15	First Law of Thermodynamics (***asynchronous***, ***virtual***)
9/18	Thermodynamics Demos
9/20	Pulling a Polymer
9/22	Auxiliary Functions
9/25	Midterm 1 Review and Q&A
9/27	**Midterm 1 (Content of 8/21-9/14)**
9/29	Spontaneous Processes and the Second Law
10/2	Extensivity and Gibbs-Duhem Equation
10/4	Maxwell Relations and Rubber Bands
10/6	Phase Transitions and Phase Diagrams
10/9	**No Class – Fall Break**
10/11	**No Class – Fall Break**
10/13	**No Class – Fall Break**
10/16	Coexistence Curves and Critical Points
10/18	Phase Transitions in Mixtures
10/20	Nucleation and Growth
10/23	Visualizing Phase Transitions
10/25	Solutions and the Ideal Chemical Potential
10/27	Chemical Equilibrium (***asynchronous***, ***virtual***)
10/30	Ideal Solutions/Mixtures
11/1	Colligative Properties
11/3	Dynamics/Kinetics
11/6	Diffusion
11/8	Bimolecular Reactions and Rate Laws
11/10	Effusion
11/13	Transition State Theory
11/15	Rate Laws and Reaction Mechanisms

11/17	Midterm 2 Review
11/20 11/22 11/24	**Midterm 2 (9/29-11/10 Content)** Detailed Balance and Complex Rate Laws **No Class – Thanksgiving Break**
11/27 11/29 12/1	Spectroscopy for Chemical Reactions Crystal Structures and X-Ray Diffraction Reactions at Surfaces
12/4 12/6 12/8	Review Statistical Mechanics and Thermodynamics Review Thermodynamics and Kinetics **Reading Day!**
12/12	**Final Exam (8:00-10:00 AM)**

Please note that the course schedule is preliminary. I may modify it with reasonable notice to you. Any changes will be announced in class and posted on Canvas under Announcements.

Additional Information and University Regulations

The Americans with Disabilities Act
The University of Utah seeks to provide equal access to its programs, services, and activities for people with disabilities. If you will need accommodations in this class, reasonable prior notice needs to be given to the Center for Disability Services, 162 Olpin Union Building, (801) 581-5020. CDS will work with you and the instructor to make arrangements for accommodations. All written information in this course can be made available in an alternative format with prior notification to the Center for Disability Services. Please notify me of any requested accommodations within the first week of class.

Sexual Misconduct, Discrimination, and Related Retaliation
The University of Utah is committed to fostering a positive and welcoming learning, working, and living environment. Sexual Misconduct, Discrimination and Retaliation are prohibited by University Policy. Faculty and staff have a responsibility to inform the Office of Equal Opportunity and Affirmative Action (OEO/AA) when made aware of incidents of sexual misconduct, discrimination, and related retaliation, to ensure that individuals impacted receive information about options for reporting and supportive resources. Incidents may come to the attention of faculty and staff in any way, including through face-to-face conversations, admissions or scholarship applications or essays, a written class assignment or paper, class discussion, email, text, or social media post. This obligation applies regardless of where or when an incident occurred, including if it occurred off campus and/or before they were a member of the campus community. Additional information can be found on the OEO website, or you may contact oeo@utah.edu or 801-581-8365. If you wish to seek support confidentially, please contact the Victim-Survivor Advocates 801.581.7776 or advocate@sa.utah.edu

Campus Safety
The University of Utah values the safety of all campus community members. To report suspicious activity, call campus police at 801-585-COPS (801-585-2677). You will receive important emergency alerts and safety messages regarding campus safety via text message. For more information regarding safety and to view available training resources, including helpful videos, visit safeu.utah.edu.

Inclusivity
It is my intent that students from all diverse backgrounds and perspectives be well served by this course, that students' learning needs be addressed both in and out of class, and that the diversity that students

bring to this class be viewed as a resource, strength, and benefit. It is my intent to present materials and activities that are respectful of diversity: gender, sexuality, disability, age, socioeconomic status, ethnicity, race, and culture. Your suggestions are encouraged and appreciated. Please let me know ways to improve the effectiveness of the course for you personally or for other students or student groups. In addition, if any of our class meetings conflict with your religious events, please let me know so that we can make arrangements for you. **Student Names & Personal Pronouns** Class rosters are provided to the instructor with the student's legal name as well as "Preferred first name" (if previously entered by you in the Student Profile section of your CIS account, which can be managed at any time). While CIS refers to this as merely a preference, I will honor you by referring to you with the name and pronoun that feels best for you in class or on assignments. Please advise me of any name or pronoun changes so I can help create a learning environment in which you, your name, and your pronoun are respected. If you need any assistance or support, please reach out to the LGBT Resource Center at https://lgbt.utah.edu/campus/faculty_resources.php

Changes to the Syllabus This syllabus is meant to serve as an outline and guide for our course. Please note that I may modify it with reasonable notice to you. I may also modify the course schedule to accommodate the needs of our class. Any changes will be announced in class and posted on Canvas under Announcements.