Chemistry 5220: Advanced Physical Chemistry II
Statistical Mechanics

Why do hot things cool? Why don't the oceans evaporate into the atmosphere? Can entropy ever give rise to order?

In this course we will answer these questions and more while we seek to understand how the collective physical behaviors that we know as "thermodynamics" emerge from simple physical laws and statistical rules. As our understanding grows, you will use the tools we discuss to pose well-defined questions related to your research interests and develop approaches to answer them. In the end, my goal is that you will come to appreciate the power, utility, and beauty of this statistically-based understanding of the physical world.

LEARNING OBJECTIVES

After successfully completing this course, students will be able to:

(1) Explain the concept of entropy and how it governs processes in the world to your grandparents. Be able to calculate entropy in various situations and use those calculations to generate and/or disprove hypotheses about the expected behavior of large collections of particles.
(2) Identify when a system is at equilibrium and explain what that means in terms of the kinds of measurements and calculations that are possible.
(3) Choose and make use of appropriate ensembles, free energies, and partition functions to explore and predict the behavior of a given system under specific conditions.
(4) Explain the role of temperature in thermodynamics and predict temperature-dependent effects.
(5) Demonstrate how phase changes emerge from simple physical rules governing the interactions between particles in a system.
(6) Recognize and articulate the role of statistical mechanics in both your research and in your every-day life.
(7) Critically evaluate the use of and developments in modern statistical mechanics through the careful reading of current research articles.

INSTRUCTOR INFORMATION

Prof. Kateri H. DuBay
Chemistry Bldg, Suite 388, Left-Hand Office
243-2159
Office Hours (to be confirmed): 12:00pm – 2:00pm on Tuesdays

CLASS MEETING TIMES

Class will be held Tuesday and Thursday from 9:30-10:45 am in 411 Chemistry.

TEXTS

D Chandler, ***Introduction to Modern Statistical Mechanics***. Oxford University Press, Oxford, UK 1987.
This text is an essential and required resource for the course.

COURSE TIMELINE

This course has been divided into three Units. At the start of each Unit, a detailed list of the readings and other assignments within the unit will be distributed. We will also spend the first week setting up a conceptual framework and reviewing important mathematical tools that will be essential to our efforts this semester.

Week 1 -- Prelude: Setting the Stage
Where are we going and what tools do we need to get there?

Weeks 2-6 -- Unit 1: Thermodynamics and Statistical Mechanics
What does the free energy tell us about a system? How can we use partition functions to calculate various quantities? What IS entropy? And why does the Boltzmann constant show up just about everywhere?
(IMSM Chapters 1, 2 & 3)

Midterm Exam 1 – in and after class on Thursday, Oct. 1 (tentative)

Weeks 7-11 -- Unit 2: Non-Interacting and Interacting Systems
What do these approaches tell us about non-interacting systems? And what happens when they start to interact? Why do we have phase changes? And what can we do when a problem is too difficult to solve analytically?
(IMSM Chapters 4, 5, & 6)

Ising Model Project

Midterm Exam 2 – in and after class on Thursday, Nov. 5 (tentative)

Weeks 12-16 -- Unit 3: Classical Fluids and Non-Equilibrium Stat Mech
What is a liquid and how does it differ from a gas or a solid? What happens to a system that is not at equilibrium? Is there anything we can know or say about it?
(IMSM Chapters 7 & 8)

Research Article Presentation

Final Exam – Friday, December 18th, 2pm – 5pm, 411 Chemistry

PREREQUISITES

A year-long course in upper-level physical chemistry or the equivalent in chemical engineering or physics.

RESOURCES

This syllabus, practice problems and solutions, exam solutions, project descriptions and grading rubrics, and other helpful materials will be posted on the UVa Collab site for this course. This is also where the online forums will be located ("Reading Questions," "Logistical Questions," "Substantive Questions," and "Excused Absences" – see details below).

COURSE COMPONENTS

***Textbook Readings and Question Posting*:** Readings will be assigned before most of our class times. When a reading is assigned, you are responsible for completing:

(1) a careful and thoughtful reading of the assigned sections;
(2) a serious attempt to work through all derivations and any suggested Exercises included in the assigned sections;
(3) the posting of your sincere questions about the material covered in the reading to the Reading Question forum on Collab **by 5pm the night before lecture**. You may include any question you have, from "what is an ensemble?" to "how do I get from line 10 to line 11 in the derivation on p. 27?" Posting at least one question per reading is required for full participation credit on this assignment, but feel free to post more.

TIP: Statistical Mechanics is a conceptually difficult field, and you will find this text challenging. To succeed in this course, you MUST spend significant time wrestling with the readings and the calculations, derivations, and problems contained therein.

***In-Class Activities*:** During most classes, I will present the material you have just read in a short and interactive lecture format, paying special attention to the areas you have questions on (as communicated to me on the Reading Question Forum). We will then consider the exercises and derivations in the text in more detail. Before class ends, we will conclude with a summary of the major points covered in class that day and then briefly set the stage for your next reading assignment.

I will ask you to participate in various ways during class time and expect you to come prepared to talk about what you have understood about the readings and where you are stuck, etc... I utilize cold-calling, a technique in which I will pose questions to the class and then randomly (according to a randomly-ordered roster) ask one of you to answer it. There will also be a handful of short exercises designed for me to assess your understanding before we get to a high-stakes exam. Your engagement in these in-class activities will count towards your participation grade. Full credit is awarded for full participation NOT for correct

answers. In fact, I view incorrect answers as more informative than correct answers, since it gives me feedback on things we still need to spend time on.

If you are absent from class for good reason, please let me know by posting on the **Excused Absence Forum** (see **Email/Communication Policy** below) so I can adjust your grade appropriately. [Note: Good reasons include illnesses, a family emergency, sporting event for a UVA team, etc... Bad reasons include sleeping in, on vacation, etc…]

***Practice Problems*:** A few additional problems will be assigned at the end of most Thursday classes, with the idea that, after the lecture time that week, you should have acquired the foundational knowledge needed to approach these additional problems (and I must emphasize "approach," not necessarily "solve"). Your answers will be due by the following Tuesday's class. You will receive credit for these problems as part of your participation grade if you turn in an assignment that makes a credible attempt to answer each of the questions.

Solutions to these problems will be posted online a week after they are assigned. You are encouraged to work on them with your peers, but please remember that the reason you are doing them is to improve your understanding and to give you practice in solving problems in preparation for the exams and projects. This goal would be best served if you first (1) spend time wrestling with the problems alone, then (2) meet with some of your peers once a week to work through them and get past any difficulties you have, and only THEN (3) look at the answer key and work by yourself and with your peers, if need be, to understand the solutions. You will need to understand how to approach and complete these problems in order to succeed on the exams. At the end of each Unit, we will spend one class reviewing and talking through these problems to address any remaining questions.

***Reflective Journaling*:** You will be keeping a reflective journal with a brief entry required once a week, due by noon on Monday. You will post an entry to the collab forum entitled "Student Journals." This will be a private forum visible only to each student and myself. In each entry you will respond briefly to the following questions:

(1) Where have you encountered principles of Statistical Mechanics during your week (outside of class), either in your every-day, non-academic, life or in the course of your daily academic life (in research talks, articles that you read, your research, etc...)?

(2) How has your learning of course material progressed over the previous week? Are there any roadblocks that are holding you back? If so, how do you plan to address them in the coming week?

The purpose of part (1) is for you to start seeing the implications of Statistical Mechanics around you and its utility for your future endeavors in science. You

will also use your responses here to guide you as you decide on the topic of your research article presentation. The purpose of part (2) is for you to reflect regularly on your learning and consider how to improve it. Your entire entry should take no more than 30 minutes to write and should be no more than a page of text. This journal is your opportunity to reflect on your evolving understanding of Stat Mech, and there are no right or wrong answers here. If you take the exercise seriously, you will receive full credit. This exercise might be most helpful if you take brief notes for yourself throughout the week as you encounter Stat Mech in the World or as you do your readings and practice problems.

***Exams*:** Exams are designed to assess your mastery of the material, both conceptually and in terms of your ability to solve problems. Your understanding and skill should build throughout this course, and therefore each exam will be cumulative. Anything covered in the assigned readings, lectures, or practice problems are fair game for examination -- including the content of student presentations.

Each exam will contain an in-class portion, followed immediately by an out-of-class take-home portion. You should expect the take-home portion to push the boundaries of your understanding.

As soon as each midterm exam is graded, it will be returned and the exam key will be posted on the same day. There will then be an opportunity for you to attend my office hours and earn back some of your points. You can receive up to a fourth of your missed points back for each question if you can explain to me how you went wrong and why, and you can receive another fourth of your missed points back for each question if you can articulate for me the correct way to answer the question and why it is correct. So, in total, you can earn back up to half of the points you missed on the exam. You will only be able to do this during the next two office hours after the exams are returned (if you cannot make one of those two office hours, let me know and we can schedule another appointment during that time-window).

There will be two Midterm Exams and one Final:
Midterm Exam 1 (tentative): Thursday, Oct. 1st (after completion of Unit 1)
Midterm Exam 2 (tentative): Thursday, Nov. 5th (after Unit 2 & Ising Modeling)
Final Exam: Friday, December 18th, 2pm – 5pm, 411 Chemistry.

***Ising Magnet Project*:** This project will expose you to numerical simulations in one of the simplest and most elegant models used in Statistical Mechanics, namely, the Ising Model. In pairs, you will work to explore the Ising Model using a few different techniques, answer various questions, and report your findings back to the entire class. You will be working on this project in stages over the course of about two weeks.

***Research Article Presentations and Discussions*:** At the end of the course, each student will present a current research article to the class that is enabled by the principles of stat mech. Each presenter will highlight how the tools of statistical mechanics made the work

possible, and will also propose concrete improvements and stat-mech-enabled extensions to the work. My hope is that each presenter will choose an article within their own research subfield in order to explore specifically how stat mech is used in that field. The class as a whole will also be required to participate during the presentation by asking seminar-style questions and participating in the discussion. Each student's grade will reflect the quality of both their presentation and their contributions to the discussions after others present.

GRADING

20% Participation (in-class work; journal; question-posting, practice problems)
15% Midterm Exam 1
15% Midterm Exam 2
5% Ising Model Project
15% Research Article Presentations and Discussions
30% Final Exam

HONOR CODE

The University of Virginia has a robust Honor Code system regulated by the students, and I expect all students to adhere to this code. Specifically, in this course:

(1) you may not work with others on the **exams**, for both the in-class and take-home portions. You will be asked to sign a pledge attesting to that.
(2) you may discuss the following work with your classmates, but it is expected that the final online posting or what you turn in or your classroom presentation will be in your own words and will truly reflect your own thoughts and questions: **(a) journal entries**, **(b) reading question forum**, **(c) practice problems**, and **(d) research article presentation**.
(3) you may do **all other work** in consultation with your fellow students.

EXAM REGRADE POLICIES

Regrade Policy: Exam solution sets will be posted when the graded exams are returned to you. These will include details on how points were awarded for each question, including the partial credit given for common not-quite-right answers. If, **after** reviewing your exam in light of this solution set, you feel you did not receive the correct grade, please bring this to my attention. Requests for re-grades should be made **in person** (with exam in hand) immediately following class or during office hours and must be made **within one week** after the exams are returned. Note: All exams are subject to photocopying before they are returned.

Alternative Exam Times: Alternative exam times will only be available to students who are unable to make the exam due to illness or some other extreme circumstance. Should something come up, please email me as soon as possible, **before the exam**, and we will work out alternative arrangements.

EMAIL/COMMUNICATION POLICY

Emails to professors often include questions regarding course material or questions on course policies and assignments. The answers to both kinds of questions are of interest to the entire class and are therefore not best addressed over email. Please bring these questions to class or post them online. In addition to the Reading Question forum and the Journal Forum, there will also be three other forums on the Collab site that are designed to function better than email would:

(1) "Logistical Questions" is the place for you to post your administrative or logistical questions regarding the course and any assignments. This forum will be visible to your classmates.

(2) "Substantive Questions" is the place for any substantive questions that arise after we cover a particular set of material. This forum will also be visible to your classmates.

(3) "Excused Absences" is simply a place for me to keep a record of any excused absences you have (otherwise they are in danger of getting lost in my overly-full inbox). If you need to miss class for a good reason (illness, family emergency, any kind of crisis, etc...), please post the date and reason on that forum and I will take that into account when calculating your participation grade for that day. This forum is private (i.e. I can see what you post and respond to it, but your classmates cannot see it), however, if you would prefer not to write your reason down (there may be cases when, despite the privacy settings, that is not a comfortable option for you), please still post your absence and just note, "reason to be communicated [in person]/[over email]/etc..."

NOTE: This is **not** the best way to notify me about your need to reschedule an exam or a presentation -- for those absences, please email me as soon as you become aware of such a need so we can make alternative plans ASAP.

I will be regularly checking these forums and responding to any questions posted there in a timely manner, ***except for the 24 hours before any exam.*** However, if you feel your questions are not fully or clearly answered there, please bring them to my office hours.

If you need to get in touch **for some other reason** – e.g. perhaps you would like to request a time to meet outside of regular office hours (because the set times conflict with other classes) or have concerns of a personal nature that cannot be addressed in class or office hours – then you may email me: dubay@virginia.edu.