

Welcome to Chemistry 444 - Elementary Statistical Mechanics!

Instructor: Prof. Todd Gingrich, Ryan 4018, todd.gingrich@northwestern.edu

TA: Camelia Roy, cameliaroy2030@u.northwestern.edu

Office Hours: We will settle times for Camelia's office hours and mine at the first lecture, once we can see who can come when.

Lecture: Tuesday/Thursday, 9:30 - 10:50 am, Tech LG66

First Lecture: Tuesday, September 29 (I am away at a conference the first week)

Course Websites: I will maintain two separate websites for the course:

1. The canvas site is the official course website and will be the portal for submitting assignments.
2. That canvas site has extra bells and whistles, so I will also post the essentials (notes and assignments) to this minimalist site: <http://gingrich.chem.northwestern.edu/teaching/444/2026>.

Textbook: Students take this course with a variety of motivations. Some seek a high-level overview and others want a deep dive that will strongly inform their research interests. To split this difference, the course will be centered around a set of lecture notes and problem sets that only scratch the surface of statistical mechanics and thermodynamics. Those students whose research interests warrant additional study would be well-served to supplement the course by reading (and solving problems from) David Chandler's Introduction to Modern Statistical Mechanics.

Notes: Lectures will be at the chalkboard. Last year I found that students engaged much more when I left the iPad behind, so I am doing it again. That means the notes I post will be last year's notes, put up on the course website ahead of each lecture so you can read along or ahead. The content will match closely, but I will not hit every seam in the same place, so next to each set of notes on the website I will mark the dates we covered it.

I. Rationale: This graduate-level course develops a quantitative framework for characterizing equilibrium states of chemical, physical, and biological systems. The emphasis throughout will be on connecting behavior at macroscopic length scales, where most observations take place, and microscopic length scales, where material properties originate. Specifically, the course will cover analytical and computational methods from probability theory to derive macroscopic properties from relatively simple microscopic models. In doing so, we will clarify conceptual connections between entropy, free energy, work, heat, and phase transitions while developing the framework for computational methods that are employed in a research setting.

II. Course Aims and Objectives

Aims: To use statistical mechanics to predict the typical value of macroscopic order parameters at thermal equilibrium, the magnitude of fluctuations away from this typical value, and the expected response to perturbations.

Specific Learning Objectives: By the end of this course, students should have acquired the ability to:

1. Explain the importance and ubiquity of the Boltzmann distribution.
2. Demonstrate how the thermodynamics of ideal systems relates to decorrelated fluctuations.
3. Compute partition functions for non-interacting systems and thereby derive thermodynamic properties.

4. Rationalize the existence of phase transitions using mean field theory.
5. Describe one or more strategies for extracting free energies from computer simulations.

III. Format and Procedures: The course will consist of two in-person lectures per week, each one about eighty minutes long. The notes are posted online ahead of each lecture, as described above. Students are encouraged to not only attend but to be active participants in the lectures.

Problem solving is a critical component of the course. These skills will be developed through weekly problem sets, which will mix analytical calculations with some numerical computations. Students are strongly advised to seek assistance during office hours, which should be considered a co-equal part of the course.

My Assumptions:

My assumption is that students in this course have had exposure to elementary ideas of statistical thermodynamics including study of entropy, the Boltzmann distribution, free energy, work, heat, and phase transitions. I assume, however, that most students have not had the opportunity to explore derivations of these topics nor applications to complex systems. Because we will not shy away from mathematics, I expect that some students will want to refresh their understanding of multivariable calculus and probability. In some cases our study will be aided by computations and simulations that will require modest amounts of programming and plotting. I assume the students have a wide diversity of comfort levels with computational skills. Google Colab is the environment Camelia and I will actively support, but you are welcome to use whatever you like, including chatbots that write code for you, so long as you understand what you submit. Problem Set 0 says more about this.

Course Requirements:

1. **Class attendance and participation:** There is no required attendance policy for lectures or for office hours. You are, however, strongly encouraged to attend and participate actively.
2. **Problem Sets:** I will post problem sets on Thursdays, due at 5 pm on Wednesday of the following week (unless otherwise stated). The first one is posted Tuesday, September 29 and due Wednesday, October 7. Camelia will grade them and return comments. These problems are an integral part of the course.
3. **Final Project** Each student will complete a final project. In consultation with Todd, each student will select a topic of interest and develop a multi-part problem set around that topic. The expectation is that students will first need to learn the topic then identify illustrative example problems, computations, or simulations around which they will base their problem set (and accompanying solutions!). The topic for the final project must be approved by **Wednesday, November 4**, and the project is due **Friday, December 4 at 5 pm**. More details about the project will be shared later in the course.
4. **Final Oral Exam:** During exam week (**Monday, December 7 through Wednesday, December 9**) I will sit down with each of you for about twenty minutes. We will talk about the arc of the lectures, about your problem sets, and about your project. I will not ask everyone the same things. If I have watched you fight through the problem sets in office hours, seen your questions in lecture or by email, or heard about your work from Camelia, I already know a good deal about how you think, and we can spend most of the time on your project. If I have seen less of you, or if I suspect a chatbot did more of your problem sets than you did, I may hand you a piece of one

and ask you to work through it with me.

IV. Grading Procedures: Grades will be based on:

- Problem Sets: 30%
- Final Project: 30%
- Final Oral Exam: 40%

Academic Integrity

Each student in this course is expected to abide by the [Northwestern University Code of Academic Integrity](#). Any work submitted by a student in this course for academic credit will be the student's own work.

This is a graduate course. The primary purpose is to empower you, not to judge you with grades. I am attempting to create assignments that will improve your understanding. This is best achieved by collaborating early and often, with your classmates and with me. COME TO OFFICE HOURS! Camelia and I are there to help you.

Figure out how to solve the problems with others. Write the solutions/code for yourself to confirm that you actually get it. Should copying occur, both the student who copied work from another student and the student who gave material to be copied will both automatically receive a zero for the assignment. Penalty for violation of this Code can also be extended to include failure of the course and University disciplinary action.

Generative AI: The goal for this course is for you to build capabilities by the end that you didn't have at the beginning, not just for you to produce correct answers. Generative AI can be a tremendous resource, but I caution you that it can also prevent you from experiencing the struggle that gives you the best opportunity to learn. Before you ask anyone or anything for help on a problem, I urge you to exert a serious individual effort to solve it independently. If you get stuck, chatbots can be a piece of getting you unstuck, alongside office hours and your classmates. After getting unstuck, your final answer should again be developed and written independently by you. You're smart enough to realize that it is virtually impossible to police your behavior (and entirely uninteresting, I might add). But you're also smart enough to realize that the oral exam is going to be a very challenging wake-up call if you've grown accustomed to adopting a chatbot's hallucinations as your own. Resist the urge to outsource your thinking to Silicon Valley's latest neural network, and you'll walk out of this course with a new and improved one of your own.

V. Accommodations for students with disabilities In compliance with the Northwestern University policy and equal access laws, I am available to discuss appropriate academic accommodations that may be required for students with disabilities. Requests for academic accommodations are to be made during the first three weeks of the quarter, except for unusual circumstances. Students are encouraged to work with [AccessibleNU](#) to verify their eligibility for accommodations. This applies to the oral exam as well as to written work.

VI. Course Outline (subject to change):

1. Basic principles of statistical mechanics
 - (a) Dynamics in chemistry

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- (b) Counting microstates in the thermodynamic limit
 - (c) The Boltzmann distribution
 - (d) Spontaneity, constraints, and the ideal gas law
2. Connecting statistical mechanics to thermodynamics
 - (a) Entropy and the second law
 - (b) Conditions for macroscopic equilibrium: temperature, pressure, chemical potential
 - (c) Reversible and irreversible work
 - (d) Helmholtz free energy and the connection to partition functions
 - (e) Nonequilibrium work relations
 - (f) Ensembles, generating functions, and Legendre transforms
 3. The importance of interactions
 - (a) Cross-overs and phase transitions
 - (b) The Ising model and universality
 - (c) Mean field theory
 - (d) Phase equilibria, phase diagrams, and Maxwell constructions
 4. Making use of computers
 - (a) Markov Chain Monte Carlo
 - (b) Molecular dynamics