Chemistry 175/273: Winter 2025

Statistical Mechanics
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office hours: Tuesday 4:30pm

Course overview and objectives

Statistical mechanics connects microscopic chemical properties to macroscopic, thermodynamic properties. Your goal in this course is to develop tools to analyze, calculate, and predict such properties (e.g., phase equilibria, equilibrium constants, rates, and free energies) from microscopic molecular information. The first part of this course will focus on constructing statistical ensembles and highlighting the implications of those ensembles for thermodynamic properties. We will first cover phenomenology, describing the laws of thermodynamics and stability, and then we will build from the ground up, starting with quantum mechanics. In the second half of the quarter, we will focus on kinetics in the gas phase and liquid phase. You will seek to master strategies for dealing with the complexity of molecular interactions, from approximations like mean-field theory to numerical techniques like molecular dynamics. We will study both diffusion limited and activated processes, with the objective of highlighting the role of statistical fluctuations in reactivity. By the end of the course, the goal is that you will have a sense of the extraordinary information contained in partition functions and you will be able to use analytical and numerical techniques to make predictions about the thermodynamics and kinetics of equilibrium chemical systems.

Logistics

Communication

Announcements for this course will be made either in lecture or on the course website https://rotskoff.github.io/chem175-263/. All major dates for assignments and exams are available in the course calendar on Canvas. I will hold office hours weekly on Tuesday 4:30pm to 5:30pm.

Resources and textbooks

Lectures notes for the quarter are available on the course webpage. While no textbooks are required, you may find the following textbooks useful as a supplement: *Introduction to Modern Statistical Mechanics* by David Chandler or *Statistical Mechanics: A Concise Introduction for Chemists* by Benjamin Widom.

Synchronicity

You are expected to attend lecture three times per week from 12:30pm - 1:20pm PST. It is expected that you will attend all in person lectures.

Assessments

There will be weekly problem sets due each Wednesday before the synchronous class session (12:30 PM PST, sharp). Problem sets must be turned in before the class; there is a link on the

course webpage with instructions for submission. We will have two take-home midterm exams. There will be a final exam. For the quizzes, you will have the opportunity to revise and resubmit your solutions to the quiz after receiving feedback. While I encourage you to work collaboratively on problem sets, you are expected to abide by the Stanford honor code on all assignments and must write your own solutions. You are encouraged to complete the quizzes without consulting your notes as they are intended to help you evaluate your own understanding.

Students with Documented Disabilities

Students who may need an academic accommodation based on the impact of a disability must initiate the request with the Office of Accessible Education (OAE). Professional staff will evaluate the request, review appropriate medical documentation, recommend reasonable accommodations, and prepare an Accommodation Letter for faculty. The letter will indicate how long it is to be in effect. Students should contact the OAE as soon as possible since timely notice is needed to coordinate accommodations. Students should also send your accommodation letter to instructors as soon as possible. The OAE is located at 563 Salvatierra Walk (phone: 723-1066, and online http://oae.stanford.edu).

Outline of the course

Statistical Mechanics, Fluctuations, and Ensembles

1. Thermodynamics
2. Quantum mechanical energy levels and the microcanonical ensemble
3. Deriving the canonical ensemble from the microcanonical axiom
4. Computing partition functions for idealized particles
5. Using partition functions: fluctuation-response relations

Noninteracting systems

1. Computing partition functions for gases: monoatomic, diatomic, polyatomic
2. Computing the equilibrium constant
3. Deriving the ideal gas law

Interacting systems and molecular dynamics

1. Models of interactions
2. Phase transitions
3. Molecular dynamics simulation and Monte Carlo methods
4. Structure and theory of simple liquids

Kinetics

Diffusion limited processes

1. Collision theory
2. The Boltzmann equation

Activated processes

1. Transition state theory
2. Free energy differences and importance sampling