Welcome to Chemistry 444 - Elementary Statistical Mechanics!

Instructor: Prof. Todd Gingrich, Ryan 4018, todd.gingrich@northwestern.edu
Office Hours: Mondays 11 am, Fridays 10 am (or by appointment)
Lecture: Tuesday/Thursday, 9:30 - 11:00 am, Tech LG62
Course Website: http://gingrich.chem.northwestern.edu/teaching/444/2019/.

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 lectures per week, each one hour and twenty minutes long. All of the lecture notes will be posted online immediately following lecture. 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 need 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, so I will provide assistance in the Python language using Google Colab.

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 assign weekly problem sets every Tuesday, due the following Tuesday at the beginning of class (unless otherwise stated). These problems are an integral part of the course.
3. Final Project: In lieu of a final exam, each student will complete a final project. Under consultation with Todd, each student will select a topic of interest and develop a series of problem set questions 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 **Tuesday, November 19**. More details about the project will be shared later in the course.

V. Grading Procedures: Grades will be based on:

- Homeworks: 30%
- Midterm: 35%
- Final: 35%

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!). 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.

VII. Accommodations for student 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 Accessible NU to verify their eligibility for appropriate accommodations.

VIII. Course Outline (subject to change):

1. Basic principles of statistical mechanics

   (a) Dynamics in chemistry
   (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