Welcome to Chemistry 444 - Elementary Statistical Mechanics! 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. Students should come away with a visceral understanding of: entropy, free energies, the relationships between statistical mechanics and thermodynamics, and phase transitions. The topics are intrinsically technical and rely on some mathematical tools that may be unfamiliar, but effort will be made to keep things as simple as possible (and no simpler). To aid with the intuitive understanding, we will make use of computational techniques for simulating and visualizing these concepts, which will require that students have (or develop) some familiarity with basic computer programming.

Instructor: Prof. Todd Gingrich, Ryan 4018, todd.gingrich@northwestern.edu
Office Hours: Mondays 11 am, Tuesdays 3:30 pm (or by appointment)
Lecture: Tuesday/Thursday, 9:30 - 11:00 am, Tech L158
Course Website: http://gingrich.chem.northwestern.edu/teaching/444/444.html.

Textbook(s): The lectures will not directly follow a single book. The first week will loosely follow Chapter 1 of Frederick Reif's Fundamentals of Statistical and Thermal Physics. Motivated students may also appreciate Hugo Touchette's review paper "The large deviation approach to statistical mechanics". Most of the rest of the course will follow David Chandler's Introduction to Modern Statistical Mechanics (IMSM), primarily Chapters 3-6. We will intersperse some review/crash courses in thermodynamics, which will roughly follow Chapters 1-2 of IMSM. Many students find IMSM to be too terse, so you may also find it useful to consult McQuarrie's Statistical Mechanics, Widom's Statistical Mechanics: A Concise Introduction for Chemists, Dill and Bromberg's Molecular Driving Forces, and Frenkel and Smith's Understanding Molecular Simulation. A very good thermodynamics book is Herbert Callen's Thermodynamics and an Introduction to Thermostatics.

Notes Particularly because we will not be following any one textbook, I will endeavor to post notes on the course website that more or less go along with each lecture. Because this is my first time teaching this course, the notes may not be typeset. Please forgive me.

Evaluation: There will be weekly problem sets. I reserve the right to grade these for completeness or for accuracy, and it may vary week by week. Solutions will be posted, so you should always be able to evaluate the accuracy of your own work. There will also be a midterm exam and a final assessment. The form of the final (exam, final project/paper, or a combination) will be determined later. Final grades will be determined by weighting the homeworks and exams:

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

Collaboration: 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.

Programming Assignments: Relatively simple computer simulations can help illuminate several phenmomena we will discuss, so some assignments will include a computational component. **I do not expect you to be an expert programmer.** I am not picky about what programming language you use to complete these assignments. To make things as easy as possible for beginners, I will support a single programming environment—Mathematica—and will provide a basic framework to build off of. If you do not already have Mathematica, you can install it on a personal computer for free through Northwestern's site license.

Course Outline (subject to change):

1. Stochastic dynamics
   (a) Random walks and basic probability
   (b) Large deviations
   (c) Diffusion and mean squared displacement
2. Basic principles of statistical mechanics
   (a) Density fluctuations, decorrelation, and lattice gasses
   (b) Entropy and the second law
   (c) The Boltzmann distribution
   (d) Statistical independence and the ideal gas law
3. Pulling on polymers
   (a) Hamiltonian dynamics
   (b) Langevin dynamics
   (c) Work, heat, reversible work, and free energy
   (d) Nonequilibrium work relations
4. Thermodynamics
   (a) Fundamental laws
   (b) Conditions for equilibrium
   (c) Heat capacity
5. Phase transitions
   (a) Ising model
   (b) Markov chain Monte Carlo
   (c) Importance sampling
   (d) Phase equilibria