CHEM-GA 2600: Statistical Mechanics

Glen Hocky

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Class Hours: T/Th 9:30 AM-10:45 AM
Class Room: Virtual

Course Description

This course will be a modern introduction to the topic of *statistical mechanics*, that is, the way in which the interactions between sufficiently large sets of molecules give rise to experimentally observable properties of a system.

I will strive to make this course as directly useful for understanding research going on in the department, be it in theoretical, physical, materials, or biological chemistry. Hence special emphasis will be given to how theory and computation connects to experiments, e.g. in the areas of phase transitions, spectroscopy, self-assembly, polymers, etc.

Books

The main text for the course is **Statistical Mechanics: Theory and Molecular Simulation by Mark E. Tuckerman**.

There are many other great books worth looking at. These can provide alternative explanations, derivations, and many practice problems.

- B.J. Berne and R. Pecora, Dynamic Light Scattering
- D. Chandler, Introduction to Modern Statistical Mechanics
- R.P. Feynman, Statistical Mechanics, A set of lectures
- J.-P. Hansen, and I.R. McDonald, Theory of Simple Liquids
- T.L. Hill, Statistical Mechanics
- D.A. McQuarrie, Statistical Mechanics
- R. Zwanzig, Nonequilibrium statistical mechanics

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Course Structure

Logistics

Class will generally be every Tuesday and Thursday. There will not be class on Thanksgiving (November 26), but there is class scheduled on November 24.

Because of remote learning this year, there may or may not be midterm or final exams. It is more likely that there will be extra projects or assignments instead. If there were a midterm, it would around Oct 13-20, depending on where we are in the course. The final would happen or be assigned around the week of December 7th (final week of regular classes).

Grading

Any written problem sets will be graded for completeness but not accuracy. They are for your own benefit, but I will to collect them every week to see how the class is doing.
There will also be computational exercises, which may be found at https://github.com/hockyg/chem-ga-2600.

Grading will be based on the midterm and the final projects, as well as the problem sets.

- Homeworks and participation, 40%
- Midterm, 25%
- Final, 35%

Topics Outline

Topics that will be covered:

Connection between classical mechanics and thermodynamics, statistical definition of thermodynamic quantities, the concept of thermodynamic ensembles, molecular dynamics simulations, Monte Carlo sampling, enhanced sampling for thermodynamic quantities, phase transitions, linear-response theory, and fluctuation dissipation theorems.

Topics that may be covered:

Theory of simple liquids, non-ideal liquids, time correlation functions, generalized Langevin equation, random walks and diffusion, polymer theory.