CHEM-GA 2600: Statistical Mechanics

Glen Hocky

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E-mail: `hockyg@nyu.edu`
Office Hours: Thurs 1pm-3pm   Class Hours: T/Th 9:30 AM-10:45 AM
Office: Waverly 1066B   Class Room: GCASL 365

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 is no class scheduled for Thanksgiving (November 22) but there is class scheduled on November 20. I will be traveling on Tuesday, December 11, so there will not be a regularly scheduled class that day.

The final will happen during the week of December 10 (probably December 13).

Grading

There will be weekly problem sets. These will be graded for completeness but not accuracy. They are for your own benefit, but I would like to collect them every week to see how the class is doing.

Some computational exercises may be found at https://github.com/hockyg/chem-ga-2600.

Grading will be based on the midterm and the final (the form of the final, whether it is an exam, final project/paper, or a combination of these, will be determined later).

- Homeworks, 20%
- Midterm, 35%
- Final, 45%

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.