CHEM-GA 2600: Statistical Mechanics

Glen Hocky

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Office Hours: TBD
Class Hours: T/Th 9:30 AM-10:45 AM
Office: Waverly 1166B
Class Room: 12 Waverly, L111

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 25), but there is class scheduled on November 23. There will also **not** be class on Sept 7 or 16 due to Jewish holidays. I will probably assign some extra readings those weeks. There will also **not** be class on October 12, because the *University is on a Monday Schedule*. We will plan to have almost every class in person for now, but will have to be flexible about switching to remote lectures as circumstances dictate.

All lectures and assignments will be posted on my group website at the URL above. There will be an NYU Brightspace page which may be used for submitting assignments and certain other remote contingencies.

A written problem set will be assigned most weeks, and should be turned in before class on the due date. These can be turned in in-person, but it may be possible/needed to turn them in through the Brightspace site in certain circumstances. As in past years, *the final exam will likely be a longer programming assignment* which shows that you can apply concepts you've learned in a real setting. This will be a one-week at-home assignment that will be assigned around the week of December 13 (last week of classes).

Remote contingencies

If you are sick, of course do not come to in-person class. All class notes will be available online and we can have extra office hours to make sure you catch up on any lectures missed.

If I am unable to teach in person or NYU transitions to remote lectures, the class will be given over Zoom. The meeting will be scheduled through Brightspace, and so should appear in your NYU zoom account if you are logged in, and the link will also be available through the course site; the lecture will be recorded, and posted to Brightspace automatically.

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 can be done on an NYU run course site that will be sent out later. Copies of the exercises will also be available from:
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.