Chemistry 8561: Thermodynamics, Statistical Mechanics, and Kinetics I

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Class Hours: 13:00-14:15 on Monday & Wednesday and Friday 13:25 - 14:15 on Friday
Class Room: 111 Smith Hall

Course Description

Chemistry 8561 is an introduction to statistical mechanics course. The goal of this course is to learn how to (1) calculate thermodynamic properties of chemical systems, (2) calculate reaction rates, and (3) programing in Python. To accomplish this goal, the course will cover basic statistics, ensembles and fluctuations, ideal and real gases, liquids and crystals, and molecular simulations. Broadly, the course will involve an active learning format on Monday and Wednesday. Friday will focus on computational projects; starting at basic programming and progressing to molecular simulations.

Textbooks

- "Statistical Mechanics" by Donald A. McQuarrie (University Science Books, 2000 (1976)) is the recommended textbook.

- "An Introduction to Statistical Thermodynamics" by Terrell L. Hill (Dover, 1986) is a great book and less than $15. Additionally, an eBook can be found from the library by going to https://reserves.lib.umn.edu/
Examinations (15% + 25%)

- Midterm 15%: Tentatively scheduled for October 25th. This will be a 75 minute exam given in class during the normal lecture period.
- Final 25%: Tentatively scheduled to be distributed December 14th. This will be a 24-hour take home exam. You are allowed to use your notes, textbooks, any source, or computer program. You are not allowed to work with anyone, all work must be independent. The exam will be distributed on December 14th and has to be submitted 24 hours later.

Homework (10%)

7-10 Homework assignments will be distributed each Monday throughout the semester. Homework assignments can be carried out in small groups (consisting of no more than 3 students). Assignments (one per group) will be collected on the following Monday (unless otherwise noted on the schedule).

Presentation of Special Topics (10%)

Several classes will focus on the discussion of papers from the literature. Several topics will be available ranging from seminal papers to more recent advances. These papers will be presented in groups of 2 or 3 students and last approximately 30 minutes long with 10 minutes of questions. The students may present a chalk talk, use slides, other teaching aids, or any combination.

Computation Projects (15% + 25%)

In the classroom we will walk through writing a program which will do a molecular simulation of a Lennard-Jones liquid in Python. As we build upon this code, short ‘side-projects’ will be assigned which will extract information from these simulations. Students can use the CSE workstations or their own computers.

- Project 1: 15% Lennard-Jones Analysis Projects (radial distribution function, a model of water). These projects will be carried out individually.
- Project 2: 25% Groups (of 2 or 3 students) will choose a project which involves development of code, analysis of results, and then presentation of results to the class. The students are encouraged to develop their own project; however, several project options will also be provided.

Grading

Final grades will be calculated from the weighted average of the performances in the exams (40%), homework (10%), the presentation of special topics (10%), and computational projects
(40%). Any registered student who does not complete the course will receive an F, unless if they officially withdraw from the course.

Schedule

**Week 01, 09/04 - 09/08:** Introduction and Postulates of Statistical Mechanics / Python

**Week 02, 09/11 - 09/15:** Canonical Ensemble / Lennard-Jones Energy and Potential

**Week 03, 09/18 - 09/22:** Grand Canonical Ensemble and Fluctuations / Monte Carlo

**Week 04, 09/25 - 09/29:** Boltzmann, Fermi-Dirac, Bose-Einstein statistics / Radial Distribution Functions

**Week 05, 10/02 - 10/06:** Ideal Gases / Molecular Dynamics

**Week 06, 10/09 - 10/13:** Real Gases / Diffusion

**Week 07, 10/16 - 10/20:** Chemical equilibrium / Modified Lennard Jones

**Week 08, 10/23 - 10/27:** Review and Midterm / No Class October 27th

**Week 09, 10/30 - 11/03:** No Class

**Week 10, 11/06 - 11/10:** Crystals: Einstein and Debye models / Thermostats

**Week 11, 11/13 - 11/17:** Computation Projects

**Week 12, 11/20 - 11/24:** Special Topic Presentations

**Week 13, 11/27 - 12/01:** Advance Simulation Methods

**Week 14, 12/04 - 12/08:** Computational Project Presentation

**Week 15, 12/11 - 12/15:** Final Exams