Chemistry 522: Statistical Mechanics

Syllabus: Spring 2022

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Office hours:	Mon 10:00am-12:00pm or by appt	Lecture: Mon/Wed 8:40-10:00am, CCB 1203

Course Textbook: (1) *Introduction to Modern Statistical Mechanics* – D. Chandler

Other texts: (2) Statistical Mechanics – D. McQuarrie
(3) Statistical Physics of Particles – M. Kardar
(4) Statistical Mechanics: Theory and Molecular Simulation – M. E. Tuckerman

Materials Covered in Lecture and Assigned reading: Students are responsible for all materials covered in the lecture and the assigned reading materials, including any handouts.

Homework*:* Problem sets will be handed out roughly every week or two, and you will have at least 5 days to complete them. You are expected to hand in the worked problems at the start of the lecture on the day the problem set is due. **Your solution sheets must be stapled together.** I may not grade all assignments in detail (I will record who does and does not turn it in!), but I will at least look it over to get a general impression of how you are doing and what points need to be discussed more in class. It's important to do the homework since statistical mechanics and thermodynamics in particular are subtle. Students often feel they understand what is going on until they have to do a problem.

Exams: There will be one midterm exam and possibly one final exam (TBD), in addition to a final project. Any and all exams may include any material covered in class to that point, since statistical mechanics is a subject that builds on what is already known. The best way to prepare for all the exams is to attend the lectures, do the problem sets, and ask questions in class and in office hours about what is confusing you.

Final Project: The final project will require you to find the use of a classic model, concept, etc. within a modern context. For example, the use of a "classic" statistical mechanical relation in a molecular simulation paper or a "classic" model used to interpret experimental results. Thoroughly understand the origins of the classic result, the context of its original derivation/discovery including any approximations, and how/why it is used in the modern context. Do you envision further generalizations of this result or model? Write a detailed report on this subject. Give an oral presentation to the class on your selected works in the format of a symposium talk. The project format will be discussed in more detail in class.

Grades: The midterm exam will count as 30% of the final grade, the final exam and/or project 40%, with my assessment of the homework and class participation making up the remaining 30%. Grades will be scaled, and since this is a graduate course I hope I will not have to give a C!

Academic Honor Principle*:* Students are expected to observe the University Code of Student Conduct. Cheating on the exams or problem sets is not acceptable and will be met with zero tolerance. *However, discussing and working together on homework is encouraged provided you put the results of those discussions in your own words and turn in your own work.* Many times, these discussions will help you understand the subtle concepts encountered in this course.

COURSE OUTLINE (Subject to Change)

I. Brief Review of Mathematics and Thermodynamics (Lecture 1)

II. Foundations of statistical mechanics (Lectures 2-5)

A. Macroscopic and microscopic variables and review of thermodynamics
B. Phase space and ergodic hypothesis
C. Ensemble approach

III. Non-interacting (ideal) systems (Planned for lectures 6-9, Midterm lecture 10?)

A. Introduction; occupation numbers; Fermi and Bose statistics
B. Quantum Ideal gases
C. Bose-Einstein condensation
D. Phonons in harmonic solid; Einstein and Debye models
E. Free electron model for metals
F. Classical limit
G. Classical ideal gases of atoms and molecules

IV. Phase transitions and critical phenomena (Part 1) (Planned for Lectures 11-14)

A. Ising model and lattice gas
B. Computer simulations of Ising Models
C. Range of correlations
D. Critical phenomena and exponents
E. Mean field theory + intro to scaling and the renormalization group
F. Isomorphisms

V. Interacting systems: classical fluids (Planned for Lectures 15-19)

A. Computer Simulations: Molecular dynamics and Monte Carlo simulations
B. Distribution functions + Properties of pair distribution functions
C. Density fluctuations and compressibility
D. Low density limit; virial coefficients
E. Hard sphere model and van der Waals picture
F. Perturbation methods, free energy calculations, and solvation
G. Molecular fluids and water

VI. Nonequilibrium Systems (Planned for Lectures 20-23)

A. Linear response theory + fluctuation dissipation
B. Time correlation functions, spectroscopy, kinetics, transition state theory
C. Fluctuations theorems + nonequilibrium work relations

VII. Phase transitions and critical phenomena (Part 2) (Planned for Lecture 24-25)

A. Scaling
B. The Renormalization Group