Chemistry 684: Chemical and Statistical Thermodynamics

Syllabus: Fall 2019

Instructor:	Prof. John D. Weeks	Office: 1108 IPST (Bldg 085)
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Office hours:	Thurs 2:30-4:00pm or by appt	Lecture: Tu Thurs 11:00 am-12:15 pm Chem 0124

Required textbook: (1) Thermodynamics – H. Callen ISBN: 978-0471862567

Highly recommend: (2) Introduction to Modern Statistical Mechanics - D. Chandler ISBN: 978-0195042771

Other good texts (3) Principles of Chemical Equilibrium – K. Denbigh ISBN: 978-0521281508

(4) Thermodynamics and Statistical Mechanics: An Integrated Approach – M. Scott Shell ISBN: 978-1107656789

Class Format

Lecture attendance is important and expected. The lectures will supplement the texts with much new material and will try to emphasize the important conceptual issues and clarify tricky points.

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

Homework*:* Problem sets will be handed out about every week to ten days, and you will have at least five 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 will usually grade only one problem in the set in detail but will look at the other problems 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 thermodynamics in particular is subtle, and students often feel they understand what is going on until they have to do a problem. I will use the homework in particular to help decide those close calls between a B+ and an A- or a C+ and a B-.

Exams: There will one midterm exam in addition to the final exam, which is set by the University to take place on Wed. Dec 11 from 8:00am-10:00 am. The final exam will cover mainly the material discussed since the midterm exam, but earlier material may also be included, since thermodynamics 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. The final exam will count 45% of the final grade, the midterm exam 35%, with my assessment of the homework and class participation making up the remainder. Grades will be scaled, and since this is a graduate course I hope I will not have to give any C's!

Academic Honor Principle*:* Students are expected to observe the University's Code of Student Conduct. See http://osc.umd.edu/OSC/AcademicDishonesty.aspx. 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. These discussions will often help you understand some of the subtle concepts you will encounter in this course.

COURSE OUTLINE (Tentative)

I. General introduction to the course

A. How to think about macroscopic systems
B. Macroscopic mechanical and thermodynamic variables
C. Equilibrium state; analogy to mathematical functions of many variables

II. Energy and first law of thermodynamics

A. Work and heat; adiabatic processes
B. Energy as state function
C. Empirical temperature

III. Entropy and second law of thermodynamics

A. Adiabatic paths between arbitrary states
B. Callen form of second law; internal constraints
C. Relation to other descriptions; Carnot Cycles
D. Mathematical consequences: convex and concave functions
E. Stability

IV. Free energies

A. Usefulness of change of variables in describing experiments
B. General thermodynamic potentials and Legendre transforms
C. Geometric and other interpretations of Legendre transforms

V. Selected applications of thermodynamics

A. Phase transitions
B. Mixtures
C. Other

VI. Entropy and ensembles in statistical mechanics

A. Phase space and ergodic hypothesis
B. Microcanonical ensemble and Boltzmann entropy formula
C. Changing variables in statistical mechanics: other ensembles