Chemistry 687: Statistical Mechanics and Chemistry

Syllabus: Spring 2010

Instructor:	Prof. John D. Weeks	Office: 1109 IPST (Bldg 085)
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Office hours:	Thurs 3:30-4:30pm or by appt	Lecture Tu Thurs 2:00 -3:15 pm

Required textbooks: (1) Introduction to Modern Statistical Mechanics - D. Chandler
ISBN: 0195042778
(2) Introduction to Statistical Thermodynamics- T. Hill
ISBN: 0486652424

Other suggested texts: (3) Statistical Mechanics - D. McQuarrie
(4) Molecular Driving Forces – K. Dill

Class Format

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

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

<u>Homework</u>*:* Problem sets will be handed out about every two weeks, and you will have at least a week 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 not grade the homework in detail (but will record who does and does not turn it in!) and will 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, and students often feel they understand what is going on until they have to do a problem. I will also use the homework to help decide the close calls between a B+ and an A- or a C+ or a B-.

<u>Exams:</u> There will be two midterm exams during the semester in addition to the final exam. These exams will cover mainly the material discussed since the last exam, but earlier material may also be included, since statistical mechanics is a subject that builds on what is already known. The best way to prepare for 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. One or both exams may be a take-home exam. The tentative dates for the exams are Mar. 2 and Apr. 6. These two exams will count 60% of the final grade, the final exam 35% and 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!

<u>Academic Honor Principle</u>*:* Students are expected to observe the University's Code of Student Conduce. 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 some of the subtle concepts you will encounter in this course.

COURSE OUTLINE (Tentative)

I. Foundations of statistical mechanics

A. Macroscopic and microscopic variables and review of thermodynamics
B. Phase space and ergodic hypothesis
C. Ensemble approach
 a. microcanonical ensemble and Boltzmann entropy formula
 b. canonical and grand canonical ensembles
 c. relation to thermodynamics
 D. Fluctuations

II. Non-interacting (ideal) systems

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

III. Interacting systems: classical fluids

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

IV. Phase transitions and critical phenomena

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
F. Scaling picture and introduction to renormalization group
 a. Kadanoff scaling picture
 b. RG solution of d=1 Ising model
 c. approximate RG treatment of d=2 Ising model