Chemical & Biomolecular Engineering 532

Statistical Thermodynamics

Fall 2011

Tuesday & Thursday 12:40 – 2:10 p.m.

DO 314

Instructor: Dr. Stephen J. Paddison

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Office Hours: Wednesday 2:00 - 4:00 p.m., DO 321, or by appointment.

Textbook: Statistical Mechanics, Donald A. McQuarrie

Other Reference Books: Statistical Mechanics, R. A. Pathria & P. D. Beale; An Introduction to Statistical Thermodynamics, Terrell L. Hill

Attendance: Attendance is optional but **highly recommended**.

Lectures: Tuesday and Thursday: 12:40 – 2:10 PM; Dougherty 314. **Please no cell phones or pagers** during lectures. If you come late, please respect your fellow students and minimize disturbance.

Examinations: There will be a midterm exam and a final exam. The former will be a 2 hr exam scheduled during the regular lectures and the latter a comprehensive exam scheduled by the registrar's office but likely to be administered on a mutually agreed upon date and time. The examinations will be based upon class lectures (including handouts), textbook reading, and homework problems. **Failure to take the final exam will lead to a non-passing grade!** There will be NO make-up, early, or late exams!

Homework Problems: They will be assigned throughout the course with the typical frequency of one set every other week.

Grading:

Midterm Exam	25 %
Homework Problems	30 %
Participation	10 %
Final Exam	35 %

Final letter grades will be assigned according to the following scale: 85-100% = A, 70-84% = B, 55-69% = C, 40-54% = D, below 40% = F.

Misconduct: Cheating on examinations will not be tolerated. Anyone found cheating (copying another exam, asking others for answers, or using textbook or notes during exams) will be asked to leave and will receive a failing grade (i.e. F) for the course.

Extra Credit: There will be NO individual extra credit work assigned.

Course Objectives: Statistical mechanics is the study of macroscopic systems from a micro or molecular point of view and statistical thermodynamics is that branch of statistical mechanics that deals with systems at equilibrium. Statistical mechanics is the theory with which one may analyze the behavior of natural or spontaneous fluctuations. This theory allows one to understand the magnitudes and time scales of these fluctuations and the concomitant stability or instability of structures that spontaneous fluctuations inevitably destroy. The goals of statistical mechanics are the understanding and prediction of macroscopic phenomena and properties from individual molecules, atoms, or particles that make up a system.

Topics:

(1) Review: classical mechanics (Lagrangian and Hamiltonian formulations), quantum mechanics, thermodynamics, mathematics (probability distribution, Stirling's approximation, bi- and multi-nomial distributions, Lagrange multipliers, maximum term method)
(2) Canonical Ensemble: averages of ensembles, method of most probable distribution, thermodynamic connections
(3) Other Ensembles: Grand canonical, microcanonical, isothermal/isobaric ensemble
(4) Fluctuations
(5) Statistics: Boltzmann, Fermi-Dirac, and Bose-Einstein statistics
(6) Ideal monoatomic gas
(7) Ideal diatomic gas
(8) Classical statistical mechanics – phase space and the Liouville equation
(9) Ideal polyatomic gases
(10) Chemical equilibria
(11) Quantum statistics
(12) Transition State Theory