Chemistry 4597, Statistical Thermodynamics

Randall Hall, LSU

September 13, 2011

Chemistry 4597, Fall Semester, 2011 Introduction to Statistical Thermodynamics

8-10 AM TTh

Lead instructor: Randall Hall LSU 427 Choppin Hall, 578-3472 office hours: any time

General Information: Statistical mechanics provides tools to understand and predict macroscopic properties and phenomena from the behavior of individual atoms and molecules. This course will cover the elementary principles of statistical mechanics, its application to ideal systems and liquids, and molecular simulations of strongly interacting systems.

Textbook: There will be no required textbook.

Supplementary textbooks: Statistical Thermodynamics by Donald A. McQuarrie (University Science Books, 1973) Statistical Mechanics by Donald A. McQuarrie (HarperCollins, 1976). This is the standard reference text for statistical mechanics and you should consider purchasing a copy of this book.

Introduction to Modern Statistical Mechanics by D. Chandler (Oxford Univ. Press, 1987) An introduction to statistical thermodynamics by Terrel L. Hill (Dover, 1960) Computer simulations of liquids by M.P. Allen & D.J. Tildesley (Oxford Univ. Press, 1987)

Examinations: One 50-minute mid-term exam will be given and a final exam. Calculators are required.

Homework: Homework assignments will be distributed on Thursday throughout the semester. Assignments will be collected on the date to be specified.

Project: A simulation project will be given in the middle of the semester. You will be asked to give a short presentation of the project before the week of the final exam.

Grading: Final Grades will be calculated from a weighted average of the performances on the homework assignments (15%), the simulation project (25%), the midterm exam (30%), and the final exam (30%).

Exams are open notes.

Schedule:

1. Derivation and Understanding of Partition Functions
Review of thermodynamics, quantum mechanics, and mathematics (120 min)
Derivation of Boltzmann statistics and the canonical ensemble (100 min)
Grand canonical and isobaric-isothermal ensembles (50 min)
Fluctuations (50 min)
Fermi and Bose statistics (50 min)
2. Theoretical Applications of Statistical Mechanics 2.a) Main topics to be covered
Ideal monatomic and diatomic gas (only polyatomic if time allows) (200 min)
Classical statistical mechanics (100 min)
Equilibrium (100 min)
Reaction rates (50 min)
Crystals (100 min)
2.b) Extra topics if time permits
Quantum statistics (chap 10) (100 min)
Cell theory of liquids? (50 min)
Liquid state perturbation theories ? (50 min)
Ising model (50 min)
Mean field theory (50 min)
Polymers ? (50 min)
Renormalization theory (50 min)
3. Molecular Simulation
Intro to molecular simulation (50 min)
Hit-and-miss/importance sampling (50 min)
Non-Boltzmann sampling (50 min)
Calculation of thermodynamic properties (50 min)
Distribution functions like g(r), classical liquid state theory (50 min)
Advanced simulation methods (100 min)
Project Presentations (100 min)