Statistical Mechanics, CHEM 6481, Fall 2012

Professor Christine Payne
christine.payne@chemistry.gatech.edu
MWF 10:05-10:55am, MoSE 1224
Office Hours: TBA, MoSE G026
Course website: T-Square

Prerequisites:
Advanced quantum mechanics (can be taken concurrently), advanced thermodynamics, multivariate calculus. McQuarrie's "Quantum Chemistry" and McQuarrie and Simon's "Molecular Thermodynamics" are considered background material.

Required Text:
"Introduction to Modern Statistical Mechanics," David Chandler (Oxford, New York, 1982)

Recommended Text:
"Statistical Mechanics," Donald McQuarrie (HarperCollins, New York, 1976).
"Thermodynamics and an Introduction to Thermostatistics, 2nd ed." Herbert Callen (Wiley, New York, 1985).

Course Outline:
1. Introduction, mathematics, thermodynamics
2. Equilibrium and stability
3. Statistical mechanics
4. Ideal systems
5. Phase transitions and Ising model
6. Mean field theory and applications
7. Renormalization group theory
8. Monte Carlo method
9. Classical fluids
10. Non-equilibrium systems
11. Chemical kinetics and transition state theory
12. Langevin equation

Grading:
20% Problems sets and seminar critiques
20% Midterm-Fri., October 12
20% Final- Mon., December 10, 11:30-2:20pm
20% Research paper
20% Ising model simulation

Problem Sets and Exams. Problem sets will be assigned roughly every 10 days and will be due one week after they are assigned. Homework will be graded on a 1 (problems are attempted, but not correct), 2, 3 (majority of problems are correct) scale. Please feel free to work on problem sets with your classmates, but make sure you hand in your own copy for grading. Completing and understanding the problem sets will be essential for doing well on exams. Exams will be closed book. You may bring a single sheet of notes.

Current Research in Statistical Mechanics. A. Seminars. You will be required to attend your choice of two seminars describing research in Statistical Mechanics and write a brief (500 words) summary of the science presented. These summaries will be graded as problem sets. **B. Research paper.** You will choose a statistical mechanics paper from the Journal of Chemical Physics or the Journal of Physical Chemistry. The paper must have been published in 200-2012 and it cannot be a paper you have used in a previous course or published by your current or former research group. You will discuss the scientific context of this paper, review and critique the important findings, and propose future research. A 3-page paper will be due **November 21.** Use the style and reference guidelines provided in JPC. The final paper should look like it is ready for publication in JPC. Before **September 24**, please email me three proposed papers (links or pdfs). I will approve one or ask for more papers. An abstract of your paper will be due **October 22**.

Using Statistical Mechanics. Each student will write a computer simulation of an Ising model. The choice of computer language is up to you.

Attendance and absence. Attendance at lecture is strongly recommended as lectures will include material that is not in the textbook and will be on exams. If you have a valid excuse for missing an exam, an oral exam at a later time will be scheduled. Late problem sets will not be accepted.