Statistical Thermodynamics (Ch/ChE 164) Winter 2008

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The principal textbooks are T. L. Hill, Introduction to Statistical Mechanics (Addison-Wesley, 1960) (A Dover edition is also available) and D. Chandler, Introduction to Statistical Mechanics (Oxford Univ. Press, 1987). A few good references are: D. A. McQuarrie, Statistical Mechanics (Harper & Row, 1976), L. E. Reichl, A Modern Course in Statistical Physics (Univ. of Texas Press, 1980); M. Plischke and B. Bergersen, Equilibrium Statistical Mechanics (Prentice-Hall, 1989); L. D. Landau and E. M. Lifshitz, Statistical Physics (Part I) (Pergamon Press, 1980). K. A. Dill and S. Bromberg, Molecular Driving Forces – Statistical Thermodynamics in Chemistry and Biology (Garland Science, 2003). All these reference books are on reserve at the new Sherman Fairchild Library.

Credit of the course will consist of four components: homework, a midterm exam, a final exam, and a project. A minimum of 10% of the credit will be deducted if the homework is not handed in on the due date.

You are not to refer to homework and exams of this course from previous years. You may collaborate on the homework; however, the solutions you write must reflect your own understanding. For your own benefit, it is recommended that you think through the homework problems independently before collaborating.

1. Preliminaries: fundamentals of classical and quantum mechanics, fundamentals of thermodynamics, elementary probability theory;
2. Formulation of statistical mechanics: postulates of statistical mechanics; derivation of various ensembles; connection to thermodynamics; statistical fluctuations; equivalence of ensembles;
3. Simple applications: Bose-Einstein gas, Fermi-Dirac gas, Maxwell-Boltzmann gas, heat capacity of solids;
4. Classical statistical mechanics: phase space, Maxwell velocity distribution, equipartition theorem;
5. Non-interacting systems: diatomic gases, chemical reaction equilibrium, Langmuir adsorption isotherm;
6. Interacting systems: lattice models, mean-field (self-consistent) theory, statistical thermodynamic variational principle, exact solution for 1-dimentional models;
7. Correlation and response functions: linear response theory;
8. Classical fluids: distribution functions, structure factor S(k) (or pair correlation function g(r)), measuring S(k), approximate schemes for calculating g(r);
9. Computer simulation: molecular dynamics, Monte Carlo method and importance sampling.