

Statistical Thermodynamics and Kinetics

Course Outline and Reading Assignments

I. Thermodynamic Equilibrium (Chandler Chap. 1)

- A. Microscopic and Thermodynamic Variables
- B. Types of Equilibrium Systems
- C. Five Laws of Thermodynamics
- D. Heat and Work as Path Functions
- E. Types of Paths: Reversible, Adiabatic, ...
- F. Applications of the Second Law to Equilibrium
- G. Mathematics of Extensive and Intensive Functions

II. Thermodynamic Stability (Chandler Chap. 2, 2.4*)

- A. Stability Criteria and Conjugate Variables
- B. Auxiliary Functions: Enthalpy and Free Energies
- C. Heat Capacity, Bulk Modulus and Henry Coefficient
- D. Maxwell's Relations
- E. Chemical Equilibrium
- F. Phase Equilibrium and the Phase Rule

III. Statistical Mechanics (Chandler Chap. 3, 3.7*)

- A. Ergodic Hypothesis, Spatial and Ensemble Averages
- B. Microcanonical Ensemble
- C. Canonical Ensemble
- D. Quantum and Classical Averages
- E. Generalized Ensembles as Legendre Transforms

IV. Ideal Systems: Gases and Solids (Chandler Chap. 4)

- A. Statistics of Ideal Systems
- B. Bosons and Fermions
- C. Electromagnetic Radiation as a Photon Gas**

- D. Vibrations in Solids as a Phonon Gas
- E. Ideal Gas of Atoms and Molecules
- F. Chemical Equilibrium in Gases

V. Non-Ideal Systems: Liquids (Chandler Ch. 7.1-7.2, 5.1-5.2, 5.4, 6.1-6.2)

- A. Intermolecular Interactions
- B. Equations of State
- C. Virial Theorem
- D. Radial Distribution Functions
- E. Molecular Simulations: Molecular Dynamics and Monte Carlo**

VI. Dynamics and Relaxation (Chandler Chap. 8, 8.7*)

- A. Correlation Functions
- B. Regression Hypothesis
- C. Fluctuation-Dissipation Theorem**
- D. Chemical Kinetics, Dynamics and Transition State Theory
- E. Fick's Law and Diffusion
- F. Langevin Equation and Friction**

*Optional reading

**Time permitting