KEMS4180: Chemical dynamics and molecular interactions (3 ECTS)

Course plan

- 10 lectures
- 10 homework exercise sets (discussed in lecture)
- Final exam (4 hours, open book, internet access)

Topics

- Statistical Mechanics (Mandl Book)
  - Laws of Thermodynamics
  - Ensembles
  - Partition Function
  - Chemical Reactions
- Transition State Theory (Hill Book)
  - Arrhenius equation
  - Eyring equation
  - Kramer's theory (lecture notes)
- Methods of approximation (Lecture notes)
  - Molecular Interactions
  - Monte Carlo
  - Molecular Dynamics
  - Free Energy Calculations

- Electron transfer (Lecture notes)
  - Marcus Theory
- Photochemistry (Lecture notes)

Literature

- Mandl Statistical Physics, 2nd
  - Chapter 1: The First Law of Thermodynamics
    - 1.1 Macroscopic Physics
    - 1.2 Some Thermal Concepts
    - 1.3 The First Law
  - Chapter 2: The Second Law of Thermodynamics I
    - 2.1 The Direction of Natural Processes
    - 2.2 The Statistical Weight of a Macrostate
    - 2.3 Equilibrium of an Isolated System
    - 2.5 Equilibrium of a System in a Heat Bath
  - Chapter 4: The Second Law of Thermodynamics II
    - 4.1 The Second Law for Infinitesimal Changes
    - 4.2 The Clausius Inequality
    - 4.3 Simple Applications
    - 4.4 The Helmholtz Free Energy
    - 4.5 Other Thermodynamic Potentials
    - 4.6 Maximum Work
    - 4.7 The Third Law of Thermodynamics
    - 4.8 The Third Law of Thermodynamics (continued)

- Chapter 5: Simple Thermodynamic Systems
    - 5.1 Other Forms of the Second Law
    - 5.2 Heat Engines and Refrigerators
    - 5.4 Some Properties of Perfect Gases
- Chapter 7: The Perfect Classical Gas
    - 7.1 The Definition of The Perfect Classical Gas
    - 7.2 The Partition Function
    - 7.3 Validity Criterion for the Classical Regime
    - 7.4 The Equation of State
    - 7.5 The Heat Capacity
    - 7.6 The Entropy
    - 7.7 The Maxwell-Boltzmann Velocity Distribution
    - 7.8 Real Gases
    - 7.9 Classical Statistical Mechanics
- Chapter 9: The Perfect Quantal Gas
    - 9.1 Introductory Remarks
    - 9.2 Quantum Statistics
    - 9.3 The Partition Function
- Chapter 11: System with Variable Particle Numbers
    - 11.1 The Gibbs Distribution
    - 11.7 Thermodynamics of the Gibbs Distribution
    - 11.9 Chemical Reactions

- T. Hill Statistical Introduction to Statistcal Thermodynamics.
    - Chapter 11: The Rate of Chemical Reaction in Ideal Gas Mixtures

- Handouts.