Fundamentals of Computational Statistical Mechanics (300)

Instructor: Balasubramanian Sundaram

1. Ideal Monoatomic Gas (3)
    a. Translational Partition Function
    b. Born-Oppenheimer Approximation
    c. Thermodynamic Functions
2. Classical Statistical Mechanics (4)
    a. Classical Partition Function
    b. Phase Space and Liouville Equation
    c. Equipartition of Energy
3. Ideal Polyatomic Gas (4)
    a. Vibrational Partition Function
    b. Rotational Partition Function
    c. Thermodynamic Functions
4. Chemical Equilibrium (3)
    a. Equilibrium Constant and Partition Function
5. Imperfect Gases (4)
    a. Virial Equation of State
    b. Virial Coefficients
    c. Hard Sphere Potential
    d. Quantum Corrections to B2(T)
    e. Law of Corresponding States
6. Classical Monoatomic Liquids (5)
    a. Distribution Functions
    b. Thermodynamic Functions and g(r)
    c. Radial Distribution Functions and Potential of Mean Force
7. Time Correlation Function Formalism (15)
    a. Absorption of Radiation
    b. Light Scattering - Classical Theory
    c. Raman Scattering
    d. Response Functions and TCFs
    e. Dielectric Relaxation
    f. Molecular Spectroscopy
    g. Neutron Scattering

Books:

1. Statistical Mechanics by D.A. Mcquarrie, Viva Books
2. Physical Chemistry by I.N. Levine
3. Introduction to Modern Statistical Mechanics by David Chandler