

TCIS, Hyderabad

Course: Statistical Mechanics I

Start Date: 9th August 2017

Coordinates (Preferred): Monday, Wednesday, 11.30-1.00 pm, FReTB

Instructor: Jagannath Mondal

Syllabus:

Total number of lectures: 24 ; Duration of each lecture: 1hr 30 minutes

Short description: An introductory course of statistical mechanics with some applications in chemical and macromolecular systems. This course is generally offered as 'statistical mechanics I' in Physics. Here the course outline is slightly revised so that it can act as a bridge course between physics and chemistry.

1. Brief overview of equilibrium thermodynamics: Extensive and intensive properties, Laws of thermodynamics, entropy and free energy, phase-equilibrium, chemical potential (2 lectures)
2. Ensembles in statistical mechanics: Introduction to micro canonical, canonical and grand canonical ensembles, partition function and establishing their connections to thermodynamic variables, fluctuations (5 lectures)
3. Application of statistical mechanics to ideal gas, rotational and vibrational spectroscopy, heat capacity of crystals and chemical reaction equilibrium. (3 lectures)
4. Statistical mechanics of quantum system : Introduction to Fermion and Boson, Ideal Fermi gas and Ideal Bose-einstein gas and discussion of classical limit, Introduction to Bose-Einstein condensation (4 lectures)
5. Statistical mechanics of interacting systems 1: non-ideal gas: Introduction to classical partition function and configuration integral, statistical mechanics of second and third virial coefficients and laws of corresponding states. (3 lectures)
6. Statistical mechanics of interacting systems 2: simple liquids: radial distribution function ($g(r)$). Relation of thermodynamic functions to $g(r)$, Brief introduction of integral equation theories and perturbation theories in classical liquids, relation between free energies and $g(r)$ (4 lectures)
7. Application of statistical mechanics in computer simulation: Introduction to molecular dynamics simulation, connection with statistical mechanics, application of simulations to free energy calculations. Case study in chemical and biological systems (3 lectures)

Primary Text / Reference Books:

Main Text:

- 1) Statistical Mechanics: Donald Mcquarrie
- 2) Statistical Mechanics: R. K. Pathria
- 3) Introduction to Modern Statistical Mechanics: David Chandler

Books for Special topics:

1. Understanding Molecular simulation: From Algorithms to Applications: Daan Frenkel and Berendt Smit

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

- 4 assignments (2 before mid term and 2 after mid term), 30 %
- 2 closed-book exams (1 mid term (30%) and 1 final exam (40%))