BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI K. K. BIRLA GOA CAMPUS

FIRST SEMESTER 2020-2021

COURSE HANDOUT

Date: 01/08/2020 **Course No.: CHEF415**

Course Title: Molecular and Statistical Thermodynamics **L P U: 3 0 3**

Instructor-in-Charge: Paramita Haldar

1. **Course Description:** Introduction of Statistical Thermodynamics, Boltzmann Factor and Partition Functions, Concept of Ensembles, Canonical Partition Function and Ensemble, Partition functions and Ideal gases, Applications of Statistical Thermodynamics: i) Thermo-physical property calculations in ensembles, ii) Chemical Reactions in Ideal gases, Grand Canonical Partition Function and Ensemble, Micro Canonical Partition Function and Ensemble, Other ensembles, Ising model, Phase Equilibria, Gibbs Ensemble (VLE), Thermodynamic Integration, Gibbs-Duhem Integration, Free Energy calculation; Virial EOS: second virial coefficient; Intermolecular Potential Energy functions; Distribution functions: Radial Distribution Function, (RDF); Classical Wave Equation, Schrodinger Equation, Intermolecular Potential, Molecular Simulation Techniques: Molecular Dynamics and Monte Carlo Simulation, Monte Carlo Simulation in various ensembles, Special Applications: From Surface Adsorption: Adsorption Isotherm, Diffusion of Porous Media.

2. **Scope and Objective:** The course will introduce the students to the principles, methods and applications of statistical thermodynamics. After introducing the fundamental of Statistical Thermodynamics and concept of ensemble averages, the connection between thermodynamic quantities and different partition function will be established, following which other ensembles and fluctuations will be discussed. The application of Boltzmann statistics to ideal gases and chemical equilibrium will be described. Interatomic Potentials between atoms will be introduced then. Molecular dynamics and Monte Carlo Simulation will be described at various ensemble situations. The application of Statistical Thermodynamics will be described.]

3. **Text Book:** **1.** "Statistical Mechanics", Donald A McQuarrie, Viva Books Pvt. Ltd.
   2. "Introduction to Statistical Thermodynamics", Terrell L Hill, Addison Wesley.

4. **Reference Books:**
   1. "Introduction to modern statistical Mechanics", D. Chandler, Oxford University Press, NY.
   2. "Understanding Molecular Simulation: From Algorithms to Applications", Berend Smit and Daan Frenkel, Academic Press.
   3. "Computer Simulation of Liquids", D. J. Tildesley and M.P. Allen, Oxford Science Publications.
   4. "An Introduction to Applied Statistical Thermodynamics", Stanley I. Sandler, John Wiley & Sons, Inc.

5. **Course Plan:**

Lecture no.	Topics to be covered	Learning Objectives	Chapter in Text Book and Reference Book
1	Introduction to Statistical Thermodynamics	Brief Description about Thermodynamics	McQuarrie Chapter 1 and Class Notes
2	The Boltzmann Factor and Partition Functions	Understanding of Partition Function and postulates	McQuarrie Chapter 1 and Class Notes
3	Partition Functions and Ideal Gases	Understanding of Partition Functions for ideal gases	McQuarrie Chapter 1 and Class Notes
4 - 7	Ensemble and Thermodynamics	Understanding different types of ensembles and way of calculating	McQuarrie Chapter 2 and Class Notes

		thermodynamics properties using these ensemble.	
8	Fluctuations and Thermodynamic Equivalence of Ensembles	Understanding Fluctuations in the energy of an assembly	McQuarrie Chapter 2 and Class Notes
9 - 10	2_{nd} and 3_{rd} Law of Thermodynamics	Explanation of entropy and partition function	(Ref.) Hill Chapter 2 and Class Notes
11	Energy Distribution among Molecules	Discussion on energy distribution in molecules in relation to chemical reactions	(Ref.) Hill Chapter 3 and Class Notes
12 - 14	Thermodynamics Functions for Ideal Gas	Establish of thermodynamics properties for ideal monoatomic, diatomic and polyatomic gas	McQuarrie Chapter 5, 6, 8 and Class Notes
15	Chemical Equilibrium in Ideal Gas Mixture	How to calculate chemical equilibrium constant for ideal gas mixture	McQuarrie Chapter 9 and Class Notes
16	Rate of Chemical Reactions in Ideal Gas Mixtures	How to calculate rate of chemical reactions for ideal gas mixtures	(Ref.) Hill Chapter 11 and Class Notes
17	Virial Expansion	Understanding of compressibility factor, first and second virial coefficient for ideal gas	McQuarrie Chapter 12 and Class Notes
18	Vander Waals Equation of State	Understanding of Vander Waals equation of state for ideal gas	(Ref.) Hill Chapter 16 and Class Notes
19	Radial Distribution Function (RDF)	How density varies as a function of distance, Calculation of radial distribution function, (or pair correlation function), structure factor, Higher-order distribution functions	(Ref.) Hill Chapter 17 and Class Notes
20	Ising Model	Use of thermodynamics properties on Ising Model	(Ref.) Sandler Chapter 10 and Class Notes
21	Lattice Theory of Solutions	How to establish Lattice theory for solutions/ Liquids	(Ref.) Hill Chapter 14 and Class Notes
22	Intermolecular Potential (a) Lennard-Jones, (b) Hard Spheres, (c) Harmonic, (d) Coulombic	Understanding of different types of inter-atomic potential between atoms	(Ref.) Frenkel & (Ref.) Allen and Class Notes
23- 25	Molecular Dynamics Simulation	Basic of Molecular Dynamics simulation, MD simulations at various ensembles and how to perform the simulation	(Ref.) Frenkel and Class Notes
26 – 28	Monte Carlo Simulation	Basic of Monte Carlo simulation, MC simulations at various ensembles and how to perform the simulation	(Ref.) Allen and Class Notes
29 – 30	Application of Statistical Thermodynamics -Adsorption	Understanding of Adsorption in terms of molecular thermodynamics	(Ref.) Frenkel and Class Notes
31 - 32	Application of Statistical Thermodynamics -Diffusion	Understanding of Diffusion in terms of molecular thermodynamics	(Ref.) Frenkel and Class Notes

6. **Evaluation Scheme:**

EC. No.	**Evaluation Component**	**Duration**	**Weightage**	**Remarks**
1.	Test 1 (September 14, 16)	30 Minutes	10	Open Note
2.	Test 2 (October 12, 14)	30 Minutes	10	Open Note
3.	Test 3 (November 11, 13)	30 Minutes	15	Open Note
3.	Project (November 18)		30	
4.	Attendance		5	
5.	Comprehensive Examination	3 Hours	30	Closed Book

***Instruction for Project:**
Project will be assigned by the IC after discussion with individual groups. If anyone misses his/her presentation-date assigned by the IC, then he/she will be recorded as absent. Inconvenience (if any) should be informed the IC beforehand.
Projects will be majorly computer programming based. FORTRAN / C/ Python or Matlab programming can be used to solve the assignments. Discussion during the class and with IC is high recommended. **Sample Code will be discussed in the class and provided on the course website (Moodle or Google Classroom).**

7. Consultation Hour: Tuesday & Thursday 5.30 pm. – 7.00 pm. Appointments can be changed as per requirement if only a prior request mail is sent to the IC.

8. Notices: Notices, if any, concerning the course will be displayed on the course website (Moodle and Google Classroom.

9. Makeup Policy: Make-Up's are not given as a routine. It is solely dependent upon the GENEUINENESS of the circumstances under which a student fails to appear in a scheduled test.

10. Lectures: The class meets on Monday, Wednesday and Friday from 3.00 pm. To 4 pm. Attendance is strongly recommended as discussions and group activities will be part of the classroom activity.

Paramita Haldar
Instructor-in-charge