BASIC STATISTICAL MECHANICS

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TYPE OF COURSE : New | Both | UG/PG
COURSE DURATION : 12 weeks (20 Jul' 20 - 9 Oct' 20)
EXAM DATE : 18 Oct 2020

PRE-REQUISITES : Thermodynamics, Basic Algebra and Calculus

INTENDED AUDIENCE : Chemistry, Physics, Material Science, Chemical Engineering

INDUSTRIES APPLICABLE TO : Pharmaceutical and fuel cell companies will recognize this course vey useful.

COURSE OUTLINE :

In order to understand natural phenomena like phase transitions or nucleation or many biological reactions like protein folding, enzyme kinetics, we need to understand how many particles interact and behave together in certain specified manner. For example, ice melts at 00 C and water boils at 1000 C, at low temperature the rain drops form in the upper atmosphere. Enzyme beta-galactosidase allows the breaking of the C-O bond that leads to the digestion of lactose .These are complex processes which involve many particles to behave in a collective fashion. This could happen because of the interaction among particles. However, these cannot be solved by Newton's equations, because we cannot solve Newton's equations even for three particles interacting system. So the forefathers of this field, Maxwell, Boltzmann and Gibbs introduced probabilistic approach and combined it with mechanics to form the 'Statistical Mechanics.' This a branch of theoretical science that parallels Quantum Mechanics and these two together form the main tools at our disposal to understand why things happen and how they happen. The present course will address the basic postulates of Statistical Mechanics and then will show how starting from the basic postulates one builds a formidable framework which can be used to explain phenomena mentioned above.

ABOUT INSTRUCTOR :

Prof. Biman Bagchi is internationally known in the area of physical and biophysical chemist, particularly in the study of phase transition and nucleation, solvation dynamics, mode-coupling theory of electrolyte transport, dynamics of biological macromolecules, protein folding, enzyme kinetics, supercooled liquids and protein hydration layer. He has been working on these areas for more than 35 years, and received a large number of awards. He has published around 470 papers in reputed journals with h-index 73 and has authored 22 major review articles. Besides several scientific articles, he has authored three books: (i) Molecular Relaxation in Liquids, (ii) Water in Biological and Chemical Processes: From Structure and Dynamics to Function and (iii) Statistical Mechanics for Chemistry and Materials Science.

COURSE PLAN :

Week 1: Preliminaries: Objectives of Statistical Mechanics (SM), probability and statistics

Week 2: Probability and Statistics, Fundamental concepts of SM

Week 3: Phase Space and Trajectories, postulates

Week 4: Postulates of Statistical Mechanics, Microcanonical ensemble

Week 5: Microcanonical Ensemble, Canonical Ensembles

Week 6: Canonical Ensemble, Grand Canonical Ensemble, isothermal-isobaric ensemble

Week 7: Fluctuation and Response Functions, ideal monatomic gas

Week 8: Ideal Monatomic Gas: Microscopic Expression of Translational Entropy, ideal gas of diatomic molecules

Week 9: Ideal Gas of Diatomic molecules: Microscopic Expression of Rotational and Vibrational Entropy and Specific Heat

Week 10: Non-ideal gas, Cluster Expansion and Mayer's Theory

Week 11: Mayer's Theory for Interacting Systems: Phase Transition

Week 12: Landau Theory of Phase Transitions: Order Parameter Expansion and Free Energy Diagrams, Nucleation