20CY105 PHYSICAL CHEMISTRY - 1

Hours Per Week :

L	T	P	C
3	1	-	4

Course Description and Objectives:

This course introduces students to the core area of physical chemistry, based around the themes of systems, states and processes. Topics covered are chemical thermodynamics, statistical thermodynamics, chemical kinetics, electrochemistry, and solid state chemistry. Throughout the course, the relationship between physical phenomena and the molecular structure and reactions underpinning advanced materials will be highlighted. The laboratory component provides training in a range of physical chemistry techniques which are relevant to both industrial and research settings.

Course Outcomes:

Upon completion of the course, the student will be able to achieve the following outcomes

COs	Course Outcomes
1	Understand the laws of thermodynamics and understand interrelationships between different thermodynamic properties.
2	Analyze physical interpretation of partition functions and calculate thermodynamic properties of model systems.
3	Apply the concepts of chemical kinetics to understand integrated rate equations of different orders, activation energy and purpose of catalyst.
4	Apply the knowledge of electrochemistry to study the concepts of free energy, cell potential, and conductance.
5	Apply the knowledge of various crystal systems and understand the basic crystallographic concepts and defects in solid state structures.

Unit- I :

Chemical Thermodynamics :

The laws of thermodynamics; enthalpy, entropy, internal energy, free energy, heat capacities, Carnot cycle; Carnot engine; Kelvin – Planck and Clausius Clapeyron equation and equivalence of the two statements with entropic formulation, Maxwell's relations; Gibbs- Helmholtz equation chemical potential, fugacity, chemical reaction equilibrium, phase equilibria; mixtures, solutions, Thermodynamic derivation of Raoult's law.

Unit - II :

Statistical Thermodynamics :

Partition functions, relation between partition functions and thermodynamic functions, the internal energy, statistical entropy, Maxwell-Boltzmann statistics, Bose-Einstein statistics, ensembles and Fermi-Dirac statistics, classical statistical thermodynamics, entropy and probability.

Unit - III :

Chemical Kinetics :

Basic definitions, differential equation view of rate, rate constant, rate law, reaction order, half-life, empirical determination of reaction order and reaction kinetics: initial rates, kinetic analysis, and experimental methods, Arrhenius equation, concept of activation energy, Lindeman theory, enzyme-substrate catalysis, Michaelis-Menten constant, steady-state approximation, collision theory, transition state theory.

Unit – IV :

Electrochemistry :

Components of electrochemical cell, concept of galvanic and electrolytic cells, standard electrode potential, redox reaction, redox potential, electrode-electrolytic interface, electromotive force, electrochemical series, Nernst equation, polarizable and non-polarizable electrodes, types of reference electrodes, IUPAC convention of electrode potentials, thermodynamics of electrochemical cells and applications.

Ion conductance, specific and molar conductance, Kohlrausch's law, Debye-Huckel theory, conductometric titrations.

Unit – V :

Solid State Chemistry :

Crystal structure: crystalline and amorphous solids, one and two dimensional lattices, crystal systems, Bravais lattices, point groups: FCC, BCC and HCP metals and packing efficiency, ionic radii ratios, structure types of ionic solids: CsCl, NaCl, ZnS, Na_2O, CaF_2, $CdCl_2$, TiO_2, perovskite ABO_3, spinel and olivine. Powder X-ray diffraction, Bragg's law, indexing the powder XRD pattern.

Defects and Non-Stoichiometery - Point, Line and Plane defects; Intrinsic and Extrinsic defects - Vacancies, Schottky and Frenkel defects - Charge Compensation; Non-stoichiometry and defects.

Text Books:

1. Atkins, P. W. & Paula, J. de Atkins' Physical Chemistry, 10th Edition, Oxford University Press
2. R, West, Solid State Chemistry and its Applications, john Wiley & Sons, 1984 (Reprint Edition)
3. Puri, Sharma, and Pathania, Principles of Physical Chemistry

Reference Books:

1. Gileady, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH – 2011
2. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley 2001
3. Kapoor K.L, A Text Book of Physical Chemistry, McGraw Hill India.
4. Levine, I. N. Physical Chemistry, 6th Edition, McGraw-Hill India.
5. Castellan, G. W. Physical Chemistry, Narosa
6. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press.