APRCET 2023-24

46-MATERIAL SCIENCE AND NANOTECHNOLOGY

Unit 1: Quantum Mechanics: Operator algebra, Eigen values and Eigen functions, Operators for momentum and energy, The Schrodinger wave equation and the postulates of Quantum Mechanics, Discussion of solutions of the Schrodinger equation to some model systems, viz., particle in a box, harmonic oscillator, rigid rotor, hydrogen atom. Ordinary Angular momentum, Generalised Angular momentum, Eigen functions and Eigen values of angular momentum, Ladder operator, addition of angular momenta, Spin, antisymmetry and Pauli Exclusion Principle.

Unit 2:Thermodynamics: Basic concepts of laws of thermodynamics, free energy, chemical potential and entropy, partial molar properties: their significance and determination of partial molar volume, fugacity and its determination. Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, Postulates of ensemble averaging, canonical, grand canonical and micro-canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, and calculation of thermodynamic properties in terms of partition functions, Heat capacity, chemical equilibria and equilibrium constant in terms of partition functions, Entropy of monatomic gases. Maxwell-Boltzman, Bose-Einestein and Fermi- Dirac statistics.

Unit 3:Condensed Matter Physics: Chemical bonding and Shapes of Molecules: Ionic or electrovalent, covalent and vander walls bonds; Inert pair effect; Lattice energy of ionic crystals; Ion deformation or polarization of ions; Fajan’s rules; Hydrogen bond, Odd electron bonds; Bonding in metals-Metallic bond. olecular orbital theory (MOT): Molecular orbital configuration of some homonuclear diatomic species; Bond order or bond multiplicity; Molecular orbital configuration of some hetro-nuclear diatomic species; Hybridization of atomic orbital’s - Types of hybridization and shapes of some common molecules with σ-or σ+ _ bonds.

Unit 4:Crystal Systems: Translational vectors; Lattice and Basis; Unit cell; Bravais lattices; Lattice constants, Crystal planes; Miller indices; Symmetric operations; Point groups; Packing fraction; Simple cubic structures; Body centered cubic structure, Face centered cubic structure; Hexagonal close packed tructure. Imperfections in Crystals:Point defects: Impurities; Vacancies - Frenkel and Schottky intrinsic vacancies; Equilibrium concentration of defects; Ionic conductivity in alkali halides; Color centers: Classification-F,F', V centers-Production of color centers. Line defects: Edge and Screw dislocations; Burger vector; Stress field around dislocations; Dislocation energy - Estimation of dislocation densities, Expression for strain energy of dislocation; Role of dislocations in crystal growth. Plane defects: Stacking faults; Grain boundaries – Low angle grain boundaries

Unit 5:Magnetic Properties of Materials: Classification; Weiss filed theory; Temperature dependence of spontaneous magnetization; Heisenberg model; Exchange; Exchange interaction; Exchange integral; Concept of ferromagnetic domains. Antiferromagnetism: Molecular field theory of Antiferromagnetism; Ferrimagnetism – Introduction; Structure of ferrites; Curie temperature and susceptibility of ferromagnets; Garnets; Occurrence of super paramagnetism; Effect of nano size particles on domain structures and other magnetic Properties

Unit 6:Nanomaterials: Nanomaterials definitions - Classification of Nanomaterials - dimensions, confinement - Surface to volume ratio - Energy at bulk and nano scale - Nature Nanophenomena – Size dependent variation in Physical and Chemical properties. Synthesis of Nanomaterials: Chemical Methods: Colloidal precipitation - Sol-Gel process - Reduction method- Hydrothermal - olvothermal - Templated - Combustion route and photochemical method. Physical and Mechanical Methods: Arc discharge – Lithography – Chemical Vapor Deposition - High Energy Ball milling – Mechano-chemical reactions – Special Nanostructures - Quantum dots.

Unit 7:X-ray diffraction: Bragg conditions, Miller Indices, Laue method, Bragg method, Description of procedure for Debye Scherrer method of X-ray structural analysis of crystals, Index reflections, identification of unit cells from systematic absences in diffraction pattern-structure of simple lattices and X ray intensities-structure factor and its relation to intensity and electron density.

Unit 8: UV-Visible spectroscopy: Introduction, Types of electronic transisitons, Effect of conjugation, Concept of chromophore and Auxochrome, Bathochromic, Hyperchromic and

Hypsochromic shifts, Theory, Instrumentation, Double beam spectroscopy; Sources of radiation, Detectors, Monochromators, Applications to organic compounds and Chemical kinetics and disadvantages.

Unit 9:Infrared Spectroscopy: Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero-point energy, force constant, bond strengths, anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, PQR branches, Selection rules, exclusion principle.

Unit 10:Raman Spectroscopy: Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational – rotational Raman spectra, selection rules.

Nuclear Magnetic Resonance spectroscopy: Introduction to NMR nuclear spin and magnetic moment, quantum description of NMR, theory of NMR, chemical shift, spin lattice (T1), spin spin (T2) couplings, the Bloch equations, the theory of relaxations, relaxation mechanisms for spin1/2 nuclei, proton NMR applications.

Microscopic Techniques: Surface topography, Principle, Instrumentation and applications of Electron microscopy, Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Atomic force microscopy (AFM).