ANDHRA PRADESH RECRUITMENT OF ASSISTANT PROFESSORS IN THE UNIVERSITY SYLLABUS FOR THE SCREENING TEST

MATERIAL SCIENCE AND NANOTECHNOLOGY SUBJECT CODE – 36

<u>UNIT - 1</u>

Physics and Chemistry of Materials

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, anti symmetry and Pauli Exclusion Principle.

<u>UNIT - 2</u>

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. Molecular 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 + π bonds.

<u>UNIT - 3</u>

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 structure. 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.

<u>UNIT – 4</u>

Synthesis of Nanomaterials and their Significance in Nanoscience: Chemical Methods: Colloidal precipitation - Sol-Gel process - Reduction method- Hydrothermal - Solvothermal -Templated - Combustion route and photochemical method. Gaseous and Physical Methods: Arc discharge – Chemical Vapor Deposition - Lithography – High Energy Ball milling – Mechanochemical reactions. Biological methods: plant extract and microorganisms for synthesis of metal and metal oxide nanoparticles. Significance of Nanoscience: Classification of Nanomaterials dimensions, confinement - Surface to volume ratio - Energy at bulk and nanoscale - Nature Nanophenomena – Size-dependent variation in Physical and Chemical properties.

Types and properties of bulk and Nanomaterials: Types - Metals, alloys, semiconductors, ceramics, composites, polymeric materials, carbon nanostructures and thin films.

Dielectric properties: Dielectric polarization; Dielectric constant and displacement vector; Atomic or molecular polarizability; Clausius Mossotti relation; Types of polarizability - Dipolar polarizability, Frequency dependence of dipolar polarizability; Ionic polarizability; Electronic polarizability.

Ferroelectric properties: Classification and properties of ferroelectrics; Ferroelectric domains; Dipole theory of ferroelectricity; Theory of BaTiO3; Dielectric behavior of BaTiO₃ and determination of transition constants; Titanium and oxygen ion displacement theories; Anti-ferroelectricity and piezoelectricity; Effect of particle size on ferroelectrics.

Magnetic Properties: 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.

Mechanical Properties: Concept of stress and strain; Hook's law; Stress strain behaviour; Anelasticity; Elastic properties of materials -Young's modulus, bulk modulus, shear modulus and

Poissson's ratio; Plastic deformation - Yielding and yield strength, tensile strength, ductility, resilience, toughness, true stress and strain and hardness; Creep of soft materials; Effect of nanodimensions on mechanical properties- Elastic properties, hardness and strength, tensile ductility and strain hardness, creep and super-plastic behaviour, fracture and toughness.

Thermal Properties: Specific heat of solids – The classical model, the Einstein model, the Density of states; The Debye's model; Thermal conductivity of solids; Conductivity due to electrons and phonons; Thermal expansion of solids; Thermal properties of nonmaterial.

Optical Properties: Optical absorption, band gap, luminescence

<u>UNIT – 5</u>

Characterization techniques for bulk and nanomaterials

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.

Diffuse Reflectance UV-Visible spectroscopy: Principle, instrumentation, band gap calculation of semiconductors, Measurement of surface plasmon resonance of metal nanoparticles.

Raman Spectroscopy: Classical and quantum theories of Raman effect, selection rules, Structural strain and disorder in nanomaterials.

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

X-ray photoelectron spectroscopy: Principle, Instrumentation, core level shifts, electron spectroscopy of chemical analysis; applications of XPES to qualitative analysis; chemical shift; application to surface studies and structural analysis.

BET surface area analysis: Theory, types of isotherms, BET equation, classification of pores, determination of single and multi-point surface area, pore-size distribution.

Particle size analyzer and Zeta potential: Principle, particle size distribution measurement, pH_{ZPC} (Zero point Charge).

<u>UNIT – 6</u>

Applications of Materials and Nanomaterials

Solar Cells: Importance of solar cells; Principle of operation; Current-voltage characteristics,; Comparison of inorganic and organic solar cells, silicone solar cells - manufacture of polycrystalline and nanocrystalline silicon; Conjugated polymer solar cells - Concept of heterojunction (dispersed and molecular heterojunctions); Function of dye sensitized solar cells (DSSC); Perovskite solar cells.

Catalytic Water Splitting: Electrocatalytic, photocatalytic and photoelectrochemical methods, band gap engineering, types of Heterojunctions, Size and shape effects, Efficiency calculations-quantum yield, relative quantum efficiency, Turnover frequency.

Fuel Cells: Fuel Cell principles; Types of fuel cells - Alkaline Electrolyte, Phosphoric acid, Molten Carbonate, solid oxide and direct methanol fuel cells; Principle and operation of Proton Exchange Membrane (PEM) fuel cell -Construction of PEM fuel cell stack, efficiency characteristics of PEM fuel cells; Direct methanol fuel cells.

Batteries: Principles of battery operation; Battery components; Types of batteries – Primary and secondary batteries; Lead acid, Nickel-cadmium and Lithium ion batteries.

Supercapacitors: electrical double layer model, Principles and materials design, Nanostructured Carbon-based materials, Nano-Oxides, Novel hybrid electrode materials.

Nanosensors: Micro and nano-sensors, Mechanical sensors - pressure sensors, gas and liquid flow sensors, position sensors - Chemical sensors - Optical and radiation sensors- Gas Sensor-Bio Sensors- DNA based biosensors-Packaging and method of packaging.

Environmental and health care applications: Heterogeneous catalytic degradation of pollutants in aqueous and gas phase, Water purification, Self-cleaning, anti-microbial, health diagnosis and drug delivery, precision agriculture farming, societal implications.