

# MODEL COURSE OUTLINE (THEORY)

FOR

## M.TECH. PROGRAMME IN NANOSCIENCE & NANOTECHNOLOGY

### 1<sup>st</sup> SEMESTER

#### QUANTUM MECHANICS

##### Course Contents:

##### Introduction

Wave-particle duality, Schrödinger equation and expectation values, Uncertainty principle

##### Basics of Quantum mechanics

Solutions of the one-dimensional Schrödinger equation for free particle, particle in a box, particle in a finite well, linear harmonic oscillator. Reflection and transmission by a potential step and by a rectangular barrier.

##### Solution of Time independent Schrödinger equation at higher dimensions and more complicated systems

Particle in a three dimensional box, linear harmonic oscillator and its solution, density of states, free electron theory of metals. The angular momentum problem. The spin half problem and properties of Pauli spin matrices.

##### Approximate methods

Time independent and time dependent perturbation theory for non-degenerate and degenerate energy levels, the variational method, WKB approximation, adiabatic approximation, sudden approximation

##### Quantum computation

Concept of quantum computation, Quantum Qbits etc.

#### PHYSICS AND CHEMISTRY OF SOLIDS

##### Course Contents:

##### Structure of Matter

Amorphous, crystalline, crystals, polycrystals, symmetry, Unit Cells, Crystal Structures (Bravais Lattices), Crystallographic Directions, Crystallographic Planes, Miller Indices, Bragg's Law, Single Crystal and Powder X-ray Diffraction

##### Chemical Bonding

Atomic Bonding in solids, Types of bond: Metallic, Ionic, Covalent and Van der Waals bond; Hybridisation; H-bonding Molecular orbital theory for simple molecules such as diatomic molecule etc.

### **Types of Material**

Different types of materials: Metals, Semiconductors, Composite materials, Ceramics, Alloys, Polymers.

### **Imperfections in solids**

Imperfections of crystal structure: point defects, Grain boundaries, phase boundaries, Dislocations Screw, Edge and Mixed Dislocations generation of defects by quenching, by plastic deformation and by radiation, interaction between point defects and dislocations.

## **ELEMENTS OF PHYSICAL CHEMISTRY**

### **Course Contents:**

#### **Introduction to Thermodynamics**

The first and second laws of thermodynamics. Thermodynamic functions, heat capacity, enthalpy, entropy. Equilibrium in one phase system, real gasses, the reactions between gases, reactions of solid-state phases, Phase rule, Phase diagram, reaction kinetics, rate equations.

#### **Elementary Statistical Mechanics**

Microstates and entropy and its statistical definition, Entropy of mixing, Gibb's free energy, Gibb's paradox, phase space density, ergodic hypothesis, Liouville's theorem, The microcanonical-, canonical- and grand canonical- ensemble and their connections, Fluctuations. Classical Statistical systems, Boltzman statistics and quantum statistical systems, Fermi-Dirac and Bose-Einstein Statistics and their applications.

#### **Theory of Solution and related topics**

The theory of solutions, Free energy as a function of composition. Methods for calculation of thermodynamic equilibrium. Electrochemical processes.

#### **Diffusion**

Fick's Law, mechanisms of diffusion; generation of point defects; self-diffusion; the influence of the pressure and pressure gradient; Kirkendall effect; fast diffusion; influence of isotropic state; experimental methods of investigation of diffusion.

#### **Phase Transformations**

Mechanisms of phase transformation; homogeneous and heterogeneous nucleation; spinodal decomposition; grain growth; precipitation in solid solution; transformation with constant composition; order-disorder transformations; Martensitic transformation.

## **2<sup>nd</sup> SEMESTER**

### **SYNTHESIS AND CHARACTERIZATION OF NANOMATERIALS**

#### **Course Contents:**

##### **Physical Methods:**

Inert gas condensation, Arc discharge, RF-plasma, Plasma arc technique, Ion sputtering, Laser ablation, Laser pyrolysis, Ball Milling, Molecular beam epitaxy, Chemical vapour deposition method and other variants, Electrodeposition.

##### **Chemical Methods:**

Metal nanocrystals by reduction, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, , Liquid-liquid interface, Hybrid methods, Solvated metal atom dispersion, Post-synthetic size-selective processing. Sol-gel, Micelles and microemulsions, Cluster compounds.

##### **Biological Methods of Synthesis:**

Use of bacteria, fungi, Actinomycetes for nanoparticle synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Mechanism of formation; Viruses as components for the formation of nanostructured materials; Synthesis process and application, Role of plants in nanoparticle synthesis

##### **Characterization Techniques**

X-ray diffraction, Scanning Probe Microscopy, SEM, TEM, Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-VIS-IR Spectrophotometers, Principle of operation and application for band gap measurements, Magnetic and electrical measurements.

##### **Lithographic Techniques**

AFM based nanolithography and nanomanipulation, E beam lithography and SEM based nanolithography and nanomanipulation, Ion beam lithography, oxidation and metallization. Mask and its application. Deep UV lithography, X-ray based lithography.

### **PROPERTIES OF NANOMATERIALS**

#### **Course Contents:**

##### **Introduction**

Properties of materials & nanomaterials, role of size in nanomaterials.

##### **Electronic Properties**

Classification of materials: Metal, Semiconductor, Insulator, Band structures, Brillouin zones, Mobility, Resistivity, Relaxation time, Recombination centers, Hall effects.

##### **Confinement and transport in nanostructure**

Current, reservoirs, and electron channels, conductance formula for nanostructures, quantized conductance. Local density of states. Ballistic transport, Coulomb blockade, Diffusive transport, Fock space.

#### **Dielectric Properties**

Polarization, ferroelectric behaviour.

#### **Magnetic Properties**

Fundamentals of magnetism, Different kind of magnetism in nature: Dia, Para, Ferro, Antiferro, Ferri, Superpara. Important properties in relation to nanomagnetism.

#### **Optical Properties**

Photoconductivity, Optical absorption & transmission, Photoluminescence, Fluorescence, Phosphorescence, Electroluminescence.

#### **Thermal Properties**

Concept of phonon, Thermal conductivity, Specific heat, Exothermic & endothermic processes.

#### **Mechanical Properties**

Young's modulus, Bulk Modulus, Modulus of rigidity. Tensile Testing and Tensile Strength, Yield Strength, Breaking Strength, Plastic Deformation, Statistical Analysis of Failure Data, True Stress and Strain Bend Testing – Flexural Strength and Modulus, Brinnell Testing – Hardness, Impact Testing – Toughness, Resilience, Scratch Test.

### **3<sup>rd</sup> SEMESTER**

#### **ELECTIVES**

##### **CARBON NANOTUBE AND ITS FUNCTIONALIZATION**

#### **Course Contents:**

##### **Preparation of Carbon Nano-Tubes**

CVD and other methods of preparation of CNT

##### **Properties of Carbon Nanotubes**

Electrical, Optical, Mechanical, Vibrational properties etc.

##### **Applications of Carbon Nanotubes**

Field emission, Fuel Cells, Display devices

##### **Functionalization of Carbon Nanotubes**

Carbon Nanotubes, Functionalization of Carbon Nanotubes, Reactivity of Carbon Nanotubes,

Covalent Functionalization -Oxidative Purification

Defect Functionalization –Transformation and Modification of Carboxylic Functionalization like Amidation, Thiolation, Halogenations, Hydrogenation, Addition of Radicals, Addition of Nucleophilic Carbenes, Sidewall Functionalization through Electrophilic Addition, Cycloadditions, Carbenes Addition, Addition of Nitrenes, Noncovalent Exohedral Functionalization, Endohedral Functionalization

**Other Important Carbon based materials:**

Preparation and Characterization Fullerene and other associated carbon clusters/molecules, Graphene-preparation, characterization and properties, DLC and nanodiamonds.

**NANOPARTICLES AND MICROORGANISMS, BIONANOCOMPOSITES****Course Contents:****Microorganisms for synthesis of nanomaterials and for toxicity detection**

Natural and artificial synthesis of nanoparticles in microorganisms; Use of microorganisms for nanostructure formation, Testing of environmental toxic effect of nanoparticles using microorganisms;

**Nanocomposite biomaterials, teeth and bone substitution**

Natural nanocomposite systems as spider silk, bones, shells; organic-inorganic nanocomposite formation through self-assembly. Biomimetic synthesis of nanocomposite material; Use of synthetic nanocomposites for bone, teeth replacement.

**Nanobio Systems**

Nanoparticle-biomaterial hybrid systems for bioelectronic devices, Bioelectronic systems based on nanoparticle-enzyme hybrids; nanoparticle based bioelectronic biorecognition events. Biomaterial based metallic nanowires, networks and circuitry. DNA as functional template for nanocircuitry; Protein based nanocircuitry; Neurons for network formation. DNA nanostructures for mechanics and computing and DNA based computation; DNA based nanomechanical devices. Biosensor and Biochips.

**Drug Delivery, Therapeutic action of nanoparticles and nanodevices**

Targeted, non-targeted delivery; controlled drug release; exploiting novel delivery routes using nanoparticles; gene therapy using nanoparticles; Nanostructures for use as antibiotics; Diseased tissue destruction using nanoparticles;

**Diagnostics using nanomaterial, Nanoparticles for bioanalytical applications**

Nanodevices for sensing and therapy. Use of nanoparticles for MRI, X Ray, Ultrasonography, Gamma ray imaging. Nanoparticles as molecular labels; biological labeling using quantum dots as molecular labels;

**Tissue Engineering:**

Major physiologic systems of current interest to biomedical engineers: cardiovascular, endocrine, nervous, visual, auditory, gastrointestinal, and respiratory. Useful definitions, The status of tissue engineering of specific organs, including bone marrow, skeletal muscle, and cartilage. Cell biological fundamentals of tissue engineering

## **NANOSENSORS AND NANODEVICES**

### **Course contents:**

#### **Micro and nano-sensors**

Fundamentals of sensors, biosensor, micro fluids, MEMS and NEMS

#### **Packaging and characterization of sensors**

Method of packaging at zero level, dye level and first level.

#### **Sensors**

Sensors for aerospace and defense: Accelerometer, Pressure Sensor, Night Vision System, Nano tweezers, nano-cutting tools, Integration of sensor with actuators and electronic circuitry, Sensor for bio-medical applications: Cardiology, Neurology and as diagnostic tool, For other civil applications: metrology, bridges etc.

#### **Biosensors**

Clinical Diagnostics, generation of biosensors, immobilization, characteristics, applications, conducting Polymer based sensor, DNA Biosensors, optical sensors

#### **Biochips**

Metal Insulator Semiconductor devices, molecular electronics, information storage, molecular switching, Schottky devices

#### **Quantum Structures and Devices**

Quantum layers, wells, dots and wires, Mesoscopic Devices, Nanoscale Transistors, Single Electron Transistors, MOSFET and NanoFET, Resonant Tunneling Devices, Carbon Nanotube based logic gates, optical devices. . Connection with quantum dots, quantum wires, and quantum wells

## **MOLECULAR NANO ELECTRONICS**

### **Course Contents:**

#### **Introduction**

Recent past, the present and its challenges, Future, Overview of basic Nanoelectronics.

#### **Molecular Electronics Components**

Characterization of switches and complex molecular devices, polyphenylene based Molecular rectifying diode switches.  
Technologies, Single Electron Devices, Quantum Mechanical Tunnel Devices, Quantum Dots & Quantum wires

#### **Nanoelectronic & Nanocomputer architectures and nanotechnology**

Introduction to nanoelectronic and nanocomputers, Quantum DOT cellular Automata (QCA), Single electron circuits, molecular circuits Nanocomputer Architecture.

#### **Spintronics**

Introduction, Overview, History & Background, Generation of Spin Polarization Theories of spin Injection, spin relaxation and spin dephasing, Spintronic devices and applications, spin filters, spin diodes, spin transistors.

## **SEMICONDUCTOR NANOSTRUCTURES & NANO-PARTICLES**

### **Course Contents:**

#### **Semiconductor nanoparticles Synthesis**

Cluster compounds, quantum-dots from MBE and CVD, wet chemical methods, reverse micelles, electro-deposition, pyrolytic synthesis, self-assembly strategies.

#### **Semiconductor nanoparticles- size–dependant physical properties**

Melting point, solid-state phase transformations, excitons, band-gap variations-quantum confinement, effect of strain on band-gap in epitaxial quantum dots, single particle conductance.

#### **Semiconductor nanoparticles – applications**

Optical luminescence and fluorescence from direct band gap semiconductor nanoparticles, surface-trap passivation in core-shell nanoparticles, carrier injection, polymer-nanoparticle, LED and solar cells, electroluminescence, barriers to nanoparticle lasers, doping nanoparticles, Mn-Zn-Se phosphors, light emission from indirect semiconductors, light emission from Si nanodots.

#### **Semiconductor nanowires**

Fabrication strategies, quantum conductance effects in semiconductor nanowires, porous Silicon, nanobelts, nanoribbons, nanosprings.

## **OPTICAL PROPERTIES OF NANOMATERIALS, NANOPHOTONICS AND PLASMONICS**

### **Course Contents:**

#### **Metal Nanoparticles**

Metal Nanoparticles, Alloy Nanoparticles, Stabilization in Sol, Glass, and other media, Change of bandgap, Blueshift, Colour change in sol, glass, and composites, Plasmon Resonance.

#### **Semiconductor nanoparticles – applications**

Optical luminescence and fluorescence from direct, bandgap semiconductor nanoparticles, surface-trap passivation in core-shell nanoparticles, carrier injection, polymer-nanoparticle LED's and solar cells, electroluminescence; barriers to nanoparticle lasers; doping nanoparticles, Mn-ZnSe phosphors; light emission from indirect semiconductors, light emission from Si nanodots.

#### **Physics of Linear Photonic Crystals**

Maxwell's Equations, Bloch's Theorem, Photonic Band Gap and Localized Defect States, Transmission Spectra, Nonlinear Optics in Linear Photonic Crystals, Guided Modes in Photonic Crystals Slab

#### **Technology, Materials, and Fabrication of Photonic Crystals**

Choices of Materials: Semiconductors, Amorphous, and Polymers, Fabrications of Photonic Crystals Structures (1-D, 2-D, 3-D)

### **Applications of Photonic Crystals Devices**

1-D Photonic Crystals, Couplers, Waveguides, High-Q Cavities, etc, 2-D Photonic Crystals, Photonic Crystal Fibers, 4 Tunable Photonic Crystal Filters

### **Physics of Nonlinear Photonic Crystals**

1-D Quasi Phase Matching, Nonlinear Photonic Crystal Analysis, Applications of Nonlinear Photonic Crystals Devices, Materials: LiNbO<sub>3</sub>, Chalcogenide Glasses, etc, Wavelength Converters, etc

### **Elements of Plasmonics**

Introduction: Plasmonics, merging photonics and electronics at nanoscale dimensions, single photon transistor using surface plasmon, nanowire surface plasmons-interaction with matter, single emitter as saturable mirror, photon correlation, and integrated systems. All optical modulation by plasmonic excitation of quantum dots, Channel plasmon-polariton guiding by subwavelength metal grooves, Near-field photonics: surface plasmon polaritons and localized surface plasmons, Slow guided surface plasmons at telecom frequencies.

## **NANOCOMPOSITES**

### **Course Contents:**

#### **Metal based nanocomposites**

Metal-Oxide or Metal-Ceramic composites, Different aspects of their preparation techniques and their final properties and functionality.

Metal-metal nanocomposites, some simple preparation techniques and their new electrical and magnetic properties.

#### **Design of Super hard materials**

Super hard nanocomposites, its designing and improvements of mechanical properties.

#### **New kind of nanocomposites**

Fractal based glass-metal nanocomposites, its designing and fractal dimension analysis. Electrical property of fractal based nanocomposites. Core-Shell structured nanocomposites.

#### **Polymer based nanocomposites**

Preparation and characterization of diblock Copolymer based nanocomposites; Polymer-carbon nanotubes based composites, their mechanical properties, and industrial possibilities.

## **4<sup>th</sup> SEMESTER**

### **Project**