## SCHEME OF TEACHING M.TECH (NANOSCIENCE AND NANOTECHNOLOGY) AND EXAMINATION SCHEME-2015-2016

### FIRST SEMESTER

<table>
<thead>
<tr>
<th>Course No</th>
<th>SUBJECT</th>
<th>SCHEDULE FOR TEACHING</th>
<th>THEORY</th>
<th>PRACTICAL</th>
<th>Subject Credits</th>
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<tr>
<td>MNT6101</td>
<td>Foundation of Nanoscience Quantum and Statistical Mechanics</td>
<td>3</td>
<td>–</td>
<td>3</td>
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<tr>
<td>MNT6102</td>
<td>Basics of Biology and Biotechnology in Nanoscience &amp; Nanotechnology</td>
<td>3</td>
<td>–</td>
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<td>50</td>
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<tr>
<td>MNT6103</td>
<td>Foundation of Nanoscience Physical chemistry aspects</td>
<td>3</td>
<td>–</td>
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<tr>
<td>MNT6104</td>
<td>Synthesis and Characterization of Nanomaterials</td>
<td>4</td>
<td>–</td>
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<tr>
<td>MNT6105</td>
<td>Scientific Computation and Simulation in Nanoscience &amp; Nanotechnology</td>
<td>2</td>
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<td>MNT6106</td>
<td>Laboratory - I</td>
<td>_</td>
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Total marks = 425; Total credits = 17
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<th>Course. No.</th>
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<tr>
<td>MNT6201</td>
<td>Chemistry of Nanomaterials and Fabrication</td>
<td>4 _ 4</td>
<td>50 50 100</td>
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<tr>
<td>MNT6202</td>
<td>Nanobio-technology</td>
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<tr>
<td>MNT6203</td>
<td>Physics of Nanomaterials</td>
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<tr>
<td>MNT6204</td>
<td>Semiconductor Devices in Nanoscience &amp; Nanotechnology MEMS and NEMS</td>
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<td>50 50 100</td>
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<td>MNT6205</td>
<td>Carbon Nanotube, its Functionalization and Nanofluidics</td>
<td>4 _ 4</td>
<td>50 50 100</td>
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<td>MNT6206</td>
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<td>MNT6207</td>
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Total marks = 575; Total credits = 23
### THIRD SEMESTER

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<tr>
<td>MNT7101</td>
<td>Supramolecular and Surface Chemistry of Molecular Devices</td>
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<tr>
<td>MNT7102</td>
<td>Nanocomposites: Structure Properties &amp; Performance</td>
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<td>MNT7104</td>
<td>Laboratory - III</td>
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Total marks = 400; Total credits = 15

### FOURTH SEMESTER

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<tr>
<td>MNT7202</td>
<td>Seminar</td>
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Total marks = 100; Total credits = 20

* No numerical marks are to be assigned to thesis work. It is either “accepted” or “rejected”. Quality of work reported in the thesis can be graded in terms of “Very Good”, “Good” or “Average”.

Total Marks (all semesters) = 1500

Total Credits (all semesters) = 75

- In case of project, ‘lecture’ means theoretical work connected with it; e.g., literature survey, preparation of presentation material, etc.
 COURSE CONTENTS

MNT 6101  FOUNDATION OF NANOSCIENCE: QUANTUM & STATISTICAL APPROACH

The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question.

The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed.

**Section A**

**Introduction to quantum mechanics**: Failure of classical mechanics, brief discussion of general ideas such as wave particle duality, uncertainty principle, superposition principle, solutions of Schrödinger equation for 1-D and 3-D square wells and potential barriers, H-atom problem, operators, eigen values and eigen vectors, exchange operator and identical particles. Introduction to angular momentum operators, eigen values and eigen vectors of $L^2$, $L_Z$, $J^2$, $J_z$.

**Approximation methods**: Non degenerate and degenerate perturbation theory and applications and harmonic oscillator; variational method and its application to harmonic oscillator and hydrogen atom.

**Section B**

**Theory of ensembles**: The microcanonical ensemble theory and its application to ideal gas; the canonical ensemble and its thermodynamics, Partition function; energy fluctuations; equipartition; harmonic oscillator as canonical ensemble; grand canonical ensemble and significance of statistical quantities.

**Quantum statistics**: Briefly discuss quantum ensemble; statistics of occupation, thermodynamical behavior of ideal Bose gas; Bose-Einstein condensation; discussion of a gas of phonons; thermodynamics of a Fermi gas; free electron gas and Pauli paramagnetism.

**Books and Suggested Readings:**

2. *Quantum Mechanics* – Leonard I. Schiff, TataMcgraw Hill
3. *Quantum Mechanics: Theory and Applications*– S. Lokanathan and A. Ghatak, Macmillan India Limited
5. *Statistical Physics* by K. Huang, Wiley
The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section, and the compulsory question.

The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed.

**Section A**

**Cell structure and physiology:**

**Cell structure:** Prokaryotic and eukaryotic cells, plant and animal cells. Cell multiplication- binary fission, mitosis and meiosis, biomolecules- carbohydrates, proteins, lipids, nucleic acids, cellular metabolism, bioenergetics- metabolism of glucose, pyruvate, alcoholic and lactic acid fermentation. Cellular transport- diffusion, osmosis, facilitated diffusion, passive and active transport.

**Enzymology:** Classification, kinetics- Michalis-Menten equation, mechanism of action- acid base catalysis, metal ion catalysis, purification techniques- PAGE, gel-filtration, electrophoresis, ion-exchange chromatography, ligand based chromatography, Industrial applications of enzymes.

**Microbes:** Kindommonera, protista, protozoa and fungi- characteristic features of the groups and their importance. Growth curve of microbes in culture, isolation, preservation, DNA replication, genetic recombination.

**Section B**


**DNA engineering:** Gene cloning technology restriction enzymes, vectors for cloning DNA – plasmid, bacteriophage and cosmids, PCR, DNA probes, molecular beacon, DNA sequencing, oligonucleotide synthesis, DNA microarray systems- technique and application. Monoclonal antibodies and their importance.

**Books and Suggested Readings:**
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The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed.

Section A

Atomic and molecular Basics:
Particles and bonds: Electronegativity, different scales and methods of determination. Recent advances in electronegativity theory, variation of electronegativity, Group electronegativity. Polarities of bonds and molecules, dipole moments. Percentage of ionic character form dipole moment and electronegativity difference.


Chemical bonds in nanotechnology: Van der Waals interactions, dipole–dipole interactions, ionic interactions, metal bonds, covalent bonds, coordinative bonds, hydrogen bridge bonds and polyvalent bonds.

Colloids: Classification of colloids, preparation of colloidal solutions, purification of colloidal solution (dialysis, electrodialysis, ultrafiltration), properties of colloidal solution (physical properties, optical properties, electrokinetic properties), electrical double layer, zeta potential, precipitation of sols by electrolytes, other methods of precipitation, concept of gold number. Emulsion, gels, uses of colloids, micelle formation.

Crystalline structure: Crystalline and amorphous solids, isotropy and anisotropy, crystal systems, elements of symmetry, space lattice and unit cell, Bravais lattice, Miller indices. Defects in crystals: intrinsic and extrinsic defects, point defects, line and plane defects, vacancies-Schottky and Frankel defects, color centres and other defects in non-stoichiometric crystals. Metals insulators and semiconductors, band theory, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, high temperature super conductors.

Section B


homogenous and heterogeneous nucleation, critical radius in homogeneous and heterogeneous nucleation, growth modes, introduction to various scattering techniques in surface science.

Books and Suggested Readings:
1. **Physical Chemistry** by P. W. Atkins, Oxford Press
2. **Introduction to Modern Colloid Science** by Robert J. Hunter, Oxford University Press.
3. **Thermodynamics and Statistical Mechanics** by A N Tikhonov, Peter Theodore Landsberg
4. **Thermodynamics and Statistical Mechanics** by John M. Seddon, J. D. Gale

**MNT 6104 SYNTHESIS AND CHARACTERIZATION OF NANOMATERIALS**
The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section, and the compulsory question.
The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed

**Section A**

**Classification of nanostructures:** Fundamental basis of classification (metallic and nonmetallic), 0-D (nanoclusters), 1-D (nanowires), 2-D (thin films & multilayers), and 3-D materials. Introduction to size and shape dependent phenomena in nanostructures. Magnetic, electrical and electronic and optical properties of Nanomaterials, introduction to nanoplasmonics.

**General methods of synthesis:** Metal nanoparticles, metals and inter-metallics, ceramics, Nanocomposites, magnetic particles, synthesis of semiconductor nanoparticles, bio-synthesis, and synthesis using porous materials (zeolite hosts) and membranes (anodized alumina membrane). Size distribution – methods for uniform size distribution, superlattice formation.

**Fabrication techniques:** Working principles of chemical vapor deposition, physical vapor deposition, RF sputtering, arc-discharge, laser ablation, thermal evaporation, e-beam techniques (focused ion beam), MBE, MOCVD, self-assembly formation, nano-patterning (screen printing, e-beam lithography), nano-indentation, membrane techniques using anodized alumina. Wet chemical, electrochemical, and chemical bath technique.

**Processing techniques:** Mechanical attrition, high energy ball milling, mechano-chemical pulverization, mechanism of grain size reduction, solution blending, melt mixing, extrusion & molding.

**Section B**

**Characterization techniques:**
**Structural and morphological:** Various surface forces and introduction to scanning probe microscopes (AFM, MFM, STM & STS, and CFM), SEM, HRTEM, powder x-ray diffraction (XRD).
Surface probes: Electron energy loss spectroscopy (EELS), low energy electron diffraction (LEED), Reflection High energy electron diffraction (RHEED) X-ray photoelectron and auger electron spectroscopy (XPS, AES).

Optical and electrical: UV visible, Infrared/Raman, surface enhanced Raman scattering, Photoluminescence, Hall Effect, IV and CV.

Size exclusion and purification: Membrane filtration, selective solvent precipitation, size exclusion chromatography, HPLC.

Patterning techniques for nanoscale devices: Introduction to optical/UV electron beam and X-ray lithography systems and processes, wet etching, dry (plasma/reactive ion) etching, etch resists-dip pen lithography.

Preparation environments: Clean rooms - specifications and design, air and water purity, requirements for particular processes, vibration free environments: working practices, sample cleaning, chemical and biological contamination and purification.

Books and Suggested Readings
1. Springer Handbook of Nanotechnology by Bharat Bhushan
4. Handbook of Semiconductor Nanostructures and Nanodevices Vol 1-5- A. A. Balandin, K. L. Wang

MNT 6105 SCIENTIFIC COMPUTATION AND SIMULATION IN NANOSCIENCE & NANOTECHNOLOGY - 1
The question paper for end-semester examination will consist of seven questions of equal marks, viz.05. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question.
The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed

Section A
Tools: Practical approach to learning operating systems (DOS, UNIX, Windows) and Graphical packages (Origin, Gnuplot)
Programming: Fortran and C++: Character set, variables, constants, Data types and their declarations, relational operators, logical operators, arithmetical operations, built in functions, input output statements, functions, subroutine, Array handling.

Section B
Random numbers: Monte-carlo integral methods, importance sampling, fast fourier transform.
Physical simulations: N body methods and particle simulations, Verlet algorithm, molecular dynamics and monte-carlo methods. Simulation of small system and Ab initio methods.
Laboratory: Five open ended experiments based on FORTRAN, C++ and on numerical methods.

Books and Suggested Readings:
3. Introductory Computational Physics Andi Klein and Alexander Godunov (Cambridge)

MNT 6106: LABORATORY I
Each student is required to perform the following open-ended experiments.
1. Hall effect
2. Four probe conductivity
3. ESR measurements
4. XRD setup
5. Preparation of nano-oxides by sol-gel method and their characterization
7. Study of Langmuir and Freudlich adsorption isotherms for adsorption of oxalic acid on activated charcoal.
8. Visualisation and study of protein structures.
9. Enzyme Kinetics

MNT 6201 CHEMISTRY OF NANOMATERIALS
The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question.
The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed.
**Section A**

**Basic building blocks:** Covalent architecture, coordinated architecture and weakly bound aggregates, interactions and topology.

**Chemical properties:** Origin of chemical reactivity, catalytic activity at nanoscale and specific examples of anomalous catalytic reaction, supported nanoscale catalysts, mass transport.


**Section B**

**Chemistry of applied nanomaterials**

Application of organic nanoparticles- lipids, proteins, peptides, dendrimers, cyclodextrin, and polysaccharide based organic nanoparticles in nanomedicine and drug delivery through nanoscopic structure and nanoformulation.

Applications of zero-dimensional nanoparticles: Quantum dots for molecular electronics, nanoparticles as catalysts.

Applications of one dimensional nanotubes and nanowires: nanotube/nanowire-based field effect transistors for biosensing, gas sensing, piezoelectric nanowires as nanogenerator, thermoelectric nanowires, quantum dots for bio-sensing.

Application of nonporous materials: a Single nanopore for DNA sequencing, nonporous anodized aluminum oxide, nonporous metal-organic framework for gas absorption, photographic materials, magnetic particles for recording media, pigments, nanostructured materials as new chemical reagents, fluids, inks and dyes, block copolymers and dendrimers. Analytical and environmental chemistry of nanoparticles: chemical and biological nanosensors, controlled pore size materials like zeolites (MCM-41, ZSM) and other controlled pore silicates, pillared clays, green chemistry, environmental impact of fine particles.

**Books and Suggested Readings**


5. **Novel Nanocrystalline Alloys and Magnetic Nanomaterials** by Brian Cantor

MNT 6202  NANOBIO TECHNOLOGY
The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question. The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed.

Section A
Biophysics and bioengineering: Bioelectromagnetism-concept and importance, biomechanics-types including sports biomechanics, biotribology and applications, biomaterials-biomineralization, applications and importance of compatibility, biological/circadian rhythms and its phase markers, neurotransport: nerve impulse conduction and conduction across synapse, EEG, ECG and its association with the working of the heart.

Tissue engineering: Concept of tissue engineering- cell types, scaffolds and bioreactors, nanopump, molecular motors- types and examples, nanoscale biostructures, self-healing structures.

Applications: Lab-on-a-chip, organic molecular based computing - amorphous computing, DNA fingerprinting, bio-imaging, bioassays, nanovectors & drug delivery, nano-diagnostics & therapeutics, DNA molecular therapy, photodynamic therapy, smart materials, biosensors, nanorobotics.

Section B
Introduction: Overview of nanoparticles in biomedical applications, limitations and challenges in using nanoparticles in biomedical fields, biocompatibility/toxicity of nanomaterials

Bioconjugation: Introduction to bioconjugation, interaction of biomolecules with nanoparticles, surface functionalization/modification of nanoparticles by ligand exchange or ligand modification; reactions of bioconjugation, types of cross linkers- homofunctional,
heterofunctional, zero length; bioconjugation using covalent, non-covalent, biological approaches; examples of bioconjugation with metallic, semiconducting, magnetic nanoparticles and liposomes, modification and conjugation of antibody, enzyme, nucleic acid and oligonucleotide coupling reactions, fluorescent probes and their use in nanotechnology, ligand immobilization on chromatography supports, PEGylation and synthetic polymer modification, characterization of nanobioconjugates using electrophoresis, chromatography and various spectroscopic techniques.

Bioinspired nanomaterials: Superhydrophobic materials such as lotus leaf structure, bioinspired superglues (adhesive nanostructures), ultra hard materials, organic and inorganic natural nanomaterials, natural fibers (spider silk, sponge fibers), nanomaterials derived from cell walls.

Books and Suggested Readings


MNT 6203 PHYSICS OF MATERIALS AND NANOMATERIALS

The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section, and the compulsory question.

The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed

Section A

Resume of structure, binding, lattice dynamics and thermal properties: Lattice structures, bindings in solids, elastic constants, lattice vibrations, normal modes, density of states, conductivity and band gap, metal to insulator transition, mechanical properties, magnetic and electronic transport properties, thermal expansion.


Transport theory: Electronic transport from classical kinetic theory, calculation of relaxation time in metals and insulators, Hall effect and magnetoresistance.

Basic ideas of dielectric and magnetic properties of metals: Polarization mechanisms, Dielectric function from oscillator strength, clausiusmosotti relation, piezo, pyro and ferroelectricity, basics of ferromagnetism in materials.
Section B

Nanomaterials foundations:
Introduction: Definition, historical perspective, effects of nanoscience and nanotechnology on various fields; top down and bottom up approaches in nanosciences.


Renewable energy engineering: Introduction to photovoltaics, working principles, theory and device characteristics, calculation of various parameters and terminology used in photovoltaics, efficiency determination, types of solar cells- 1st, 2nd and 3rd generation solar cells, inorganic and organic solar cells, dye-sensitized solar cells, role of various parameters on efficiency, application of Nanomaterials (quantum dots, semiconductor oxides, plasmonic nanoparticles) in solar cells, MIM devices and current trend.

Books and Suggested Readings
1. Introduction to Solid State Physics VIIIth Ed. by C. Kittel
2. Introduction to Nanotechnology by Owen and Poole, Wiley
4. Quantum Wells, Wires & Dots: Theoretical & Computational Physics of Semiconductors Nanostuructures by Paul Harrison, Wiley International
5. Nanostructures and Nanomaterials - Synthesis, Properties and Applications by Cao, Guozhong

MNT 6204 SEMICONDUCTOR DEVICES IN NANOTECHNOLOGY: MEMS AND NEMS

The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question.

The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed

Section A

Review: review of physics and properties of semiconductor, formation of energy band diagram, intrinsic carrier concentration, donors and acceptors, nondegenerate and degenerate semiconductors, mobility, carrier diffusion, current density, recombination processes, continuity equation.
Junctions: p-n junction diode, thermal equilibrium condition, depletion region, depletion capacitance current voltage characteristics and temperature effect, charge storage and transit behavior, junction breakdown.
**Heterostructures:** Metal semiconductor contacts, basic characteristics, Schottky barrier, ohmic contact, MOS structure, MIS diode, operation and its characteristics, MOSFET scaling and modeling, scaling effects, charge coupled device (CCD). Hetero-junction and hetero structure devices, quantum and nanoelectronics.

**Section B**

**Transistors:** Bipolar transistor, fabrication techniques of bipolar transistor, transistor action, static characteristics of bipolar transistor, frequency response and switching of bipolar transistor, heterojunction bipolar transistor.

**MEMS and NEMS:** Overview, working principle of sensors and microactuation, scaling laws, materials for MEMS, active substrate materials, polymers as MEMS and NEMS materials, Consideration for microfabrication materials, LIGA process, microsystem packaging, die, device and system level packaging, interfaces in microsystem packaging for different application, signal mapping and transduction, micro system design consideration, process design, mechanical design, mechanical design using Fem, design considerations for optical, fluidic, RF and bio MEMS, overview of CAD tools for MEMS and NEMS design and simulation.

**Books and Suggested Readings:**

2. *Introduction to Semiconductor Materials and Devices* by S.M. Tyagi
7. *MEMS & MOEMS Technology and Applications* - P. RaiChoudhury
8. *Processing Technologies* - Gandhi

**MNT 6205 CARBON NANOTUBE, ITS FUNCTIONALIZATION AND NANOFUIDICS**

The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question. The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed.
Section A

Introduction to carbon nanotubes

**Structure of carbon nanotubes:** bonding in CNTs, vector notation, unit cell, defects in carbon nanotubes, density of states.

**Preparation of carbon nano-tubes (CNT):** Chemical vapor deposition, arc discharge and other methods of preparation, growth mechanisms: solid phase model, liquid phase model, crystallization model, VLS model, tip growth and root growth methods, purification methods.

**Properties:** Electrical, optical, mechanical and vibrational properties.

**Functionalization of CNTs:** 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, cyclo additions, carbenes addition, addition of nitrenes, non covalent exohedral functionalization, endohedral functionalization.

**Applications:** Fuel cells, display devices, super-capacitors, hydrogen storage.

Section B

Transport phenomena in nanofluidics: Confined fluids at nanoscale and capillary flows, intermolecular forces, surface tension and Marangoni flow, Ficks law, hydrodynamic equations and governing equations in nanofluidics, scaling laws.

**Nanofluidics engineering and applications:** Various fabrication methods; carbon nanotube and nanofluidics, fabrication of silica nanofluidics tubings. Applications: chemical reactions in confined fluids, single molecule detection, transport of ions, DNA, and microtubules, biomolecular motors, biomolecule separation and detection, optofluidic devices for single molecule sensing, nanopillars and nanoballs for DNA analysis.

Books and Suggested Readings

1. **Synthesis, functionalization and surface treatment of nanoparticles** - Marie Isabelle Baraton
2. **Physical properties of Carbon Nanotube** - R Satio
4. **Carbon Nanotubes: Properties and Applications** - Michael J. O’Connell
5. **Nanotubes and Nanowires** - CNR Rao and A Govindaraj, RCS Publishing
7. **Physical chemistry of surfaces** by Arthur W, Adamson and Alice P. Gast (John Wiley and Sons, 1997)
8. **Nanofluids: Nanoscience and Nanotechnology** by Joshua B Edel and Andrew J deMello (RSC Publishing 2009)

MNT 6206: LABORATORY II
Each student is required to perform the following open-ended experiments.
1. Thin film setups
2. Characterization based on FTIR
3. Production of nanoparticles by chemical route
4. Size determination of microbes/ nanoparticles
5. Sequence analysis of proteins
6. Prediction of protein secondary and tertiary structures
7. Molecular docking.

MNT 6207 SCIENTIFIC COMPUTATION AND SIMULATION IN NANOSCIENCE & TECHNOLOGY- II
Twelve open ended experiments based on FORTRAN, Mathematica or C++ and on numerical methods.
Books and Suggested Readings:
3. Introductory Computational Physics Andi Klein and Alexander Godunov (Cambridge)
4. Handbook of Mathematica
5. Modelling Molecular Structures by Allan Hinchliffe (Wiley)
6.

MNT 7101 SUPRAMOLECULAR AND SURFACE CHEMISTRY OF MOLECULAR DEVICES
The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question.
The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed

Section A
Basics of supramolecular chemistry: Receptors, coordination and the Lock and Key Analogy, binding constants and measurement of binding constants, cooperativity and the chelate effect.
preorganisation and complementarity, non-covalent interactions (ion–ion interactions, ion–dipole interactions, dipole–dipole interactions, hydrogen bonding, cation–π interactions, anion–π interactions, π–π Interactions, Van der Waals forces and crystal close packing, closed shell interactions).

Host – Guest chemistry: guests in solution, macrocyclic versus acyclic hosts, complexation of cations, anions & neutral molecules (crown ethers template effect). Metal-containing receptors, simultaneous cation and anion receptors, supramolecular catalysis and enzyme mimics.

Supramolecular chemistry: structures & design
Catenanes, rotaxanes, molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic, molecular analogues of mechanical machines.

Nanochemistry: Nanoscale photonics, assembly and manipulation on the nanoscale, chemistry with a microscope tip, self-assembly on surfaces, single molecules, atomic-level assembly of materials, graphene, fullerenes, supramolecular design strategy & nanotechnology, supramolecular polymers, gels and fibers.

Section B

Surface chemistry
Colloidal State: Determination of size of colloidal particles, types of surfactants: anionic, cationic, gemini, zwitterionic & non-ionic (non-ionic), theory of surfactants, phase behavior of concentrated surfactant systems, micelle formation- micelle type, micellar growth, micellar solution saturation, structure of liquid crystalline phases, surfactant geometry & packing.
The critical micellization concentration (CMC), factors affecting cmc, effect of chemical structure, temperature, Kraft temperature, emulsions & gels, microemulsions.

Books and Suggested Readings

MNT7102 NANOCOMPOSITES : STRUCTURE, PROPERTIES & PERFORMANCE

The question paper for end-semester examination will consist of seven questions of equal marks, viz. 10. The first question will be compulsory and will consist of several short questions/problems covering the entire syllabus. The rest of the questions shall be distributed evenly over the whole syllabus, such that there are at least three questions from each unit. The candidates will attempt five questions in all, selecting at least 02 questions from each section and the compulsory question.
The books indicated as text-book(s) are suggestive of the level of coverage. However, any other book may be followed

Section A

Introduction to nanocomposites
Various types of Nanocomposites, nanocomposites based on various fillers and polymers, reinforcement, carbon nanotubes, fullerenes, and grapheme based nanocomposites, Nanocomposites based on metal and metal oxide nanoparticles, magnetic nanoparticles, organic-inorganic nanoparticles, silicates, calcium carbonate, clays, bio-nanocomposites, Nanocomposites thin films and coatings. Rheology and rheology control in nanocomposites.

Processing of nanocomposites
Various techniques and methods of processing of nanocomposites (solution blending-thermoplastic and thermosetting polymers, melt mixing, extrusion, injection molding, compression molding, in situ polymerization, electro-polymerization, inverse micro-emulsion, mechanochemical pulverization), methods of deposition for thin films, processing of bio-nanocomposites, environmental life-cycle assessment. Alignment of CNTs in nanocomposites (melt drawing, magnetic & electric field induced alignment, doctor blade technique, layer-by-layer assembly, polar solvent exposure, solution spinning, transverse alignment).

Section B
Properties of nanocomposites
Mechanical – elastic modulus, tensile strength, stiffness, impact resistance; swelling behavior, barrier properties and permeability, thermal, electrical and electronic, wear and scratch resistance, flame retardant, photo-degradation resistance, corrosion resistance, biodegradability, optical, and rheological, wetting behavior.

Nanocomposites in fuel cells: Working principle of fuel cells, cell reactions, cell characteristics and design, calculation of various parameters and terminology used, cell output or efficiency determination, types of fuel cells. Various nanocomposites used in fuel cells. Other applications of nanocomposites: as flame-retardant materials - role of nanoparticles, and mechanism of fire-retardant, in packaging industry, nanocomposites for coating & biomedical applications, aerospace applications, optical applications.

Books and suggested readings
5. Polymer Nanocomposites: Synthesis, Characterization, and Modeling (Acs Symposium Series) (Hardcover) by Ramanan Krishnamoorti (Editor) and Richard A. Vaia (Editor), An American Chemical Society Publication (2001)
10. Reference Research Articles/papers from Journals

### Additional Recommended texts & References


### MNT 7104 LABORATORY III

**Introduction to Universal Safety Standards:** Hazard classification-flammable, combustible, explosive, bio-hazard, carcinogens, ion and laser radiation, etc. Standard laboratory practices – chemicals classification for storage, safe bulk solvent storage, ventilation requirement, first aid practices.

1. XRD
2. SEM
3. STM
4. TEM
5. Carbon based nano material production
6. Mass spectrometry
7. Fluorescence microscope

### MNT 7103 and MNT 7201 PROJECT and DISSERTATION

Each student will be required to work on major project approved by department faculty that will span third and fourth semesters during which periodic progress reports will be monitored. At the end of third semester, project progress will be evaluated by department faculty. At the end of IV semester, the student will submit the thesis based upon his/her project work

### MNT 7202 SEMINAR

Each student will be required to present his/ her project work/ dissertation in the form of a seminar