ANNA UNIVERSITY, CHENNAI

AFFILIATED INSTITUTIONS

R - 2009

CURRICULUM I SEMESTER

M.TECH. NANOSCIENCE AND TECHNOLOGY

SEMESTER I

SL. NO	COURSE CODE	COURSE TITLE	L	T	P	C
THEORY						
1.	MA9320	Mathematical Modeling and Simulation	3	0	0	3
2.	NT9311	Quantum Mechanics	3	0	0	3
3.	NT9312	Physical Chemistry	3	0	0	3
4.	NT9313	Physics and Chemistry of Materials	3	0	0	3
5.	NT9314	Synthesis and Applications of Nanomaterials	3	0	0	3
6.	NT9315	Biological Systems	3	0	0	3
PRACTICAL						
7.	NT9317	Computation and Simulation Laboratory	0	0	4	2
8.	NT9318	Material Synthesis and Experiments	0	0	4	2
		TOTAL	**18**	**0**	**8**	**22**

MA9320 MATHEMATICAL MODELING AND SIMULATION L T P C
3 0 0 3

UNIT I FUNDAMENTAL PRINCIPLES OF NUMERICAL METHODS 9

Scientific Modeling - Numerical data and Numerical operations -Numerical Algorithms - Numerical Programs -Numerical Software - Approximations in Mathematical Model building- Numerical integration -Differentiation -Variational finite element methods- Rayleigh's method-Ritz method.

UNIT II MATHEMATICAL MODELING 9

Mathematical modeling - physical simulation - advantages and limitations - process control - Transport phenomena- concept of physical domain and computational domain - assumptions and limitations in numerical solutions – Finite element method and Finite difference method.

UNIT III DIFFERENTIAL EQUATIONS & APPLICATIONS 9

Euler method, Runge-Kutta method, Multi step-differential equations-boundary values-Elliptic equations-one dimensional parabolic equation-hyperbolic equation- partial differential equations -separation of variables-wave equation-Laplace equation-nonlinear partial differential equations - approximation methods of nonlinear differential equations.

UNIT IV SIMULATION 9

Basic concepts of simulation- data manipulation, data exchange of the structure, properties and processing of materials**-**Three dimensional model for capillary nanobridges and capillary forces. Molecular dynamics simulation.

UNIT V MONTE CARLO METHODS 9

Basics of the Monte Carlo method-Algorithms for Monte Carlo simulation-Applications to systems of classical particles-modified Monte Carlo techniques-percolation system-variation Monte Carlo method-diffusion Monte Carlo method - Quantum Monte Carlo method.

TOTAL : 45 PERIODS

REFERENCES

1. S.C. Chapra and R.P.Canale, "Numerical methods for Engineers", Tata McGraw Hill, New Delhi, 2002.
2. Erwin Kreyzig, "Advanced Engineering Mathematics", John Wiley & Sons, 2004.
3. R.J. Schilling and S.L. Harris, "Applied Numerical Methods for Engineers using MATLAB and C", Thomson publishers, New Delhi, 2004.
4. D. Frenkel and B. Smith, "Understanding molecular simulation from algorithm to applications", Kluwar Academic Press, 1999.
5. K. Ohno, K. Esfarjani and Y. Kawazoe, "Introduction to Computational Materials Science from ab initio to Monte Carlo Methods", Springer-Verlag, 1999.

NT9311 QUANTUM MECHANICS L T P C
3 0 0 3

UNIT I INTRODUCTION 9

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

UNIT II BASICS OF QUANTUM MECHANICS 9

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.

UNIT III SOLUTION OF TIME INDEPENDENT SCHRÖDINGER EQUATION 9

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

UNIT IV APPROXIMATE METHODS 9

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

UNIT V QUANTUM COMPUTATION 9

Concept of quantum computation, Quntum Qbits etc.

TOTAL : 45 PERIODS

TEXT BOOKS AND REFERENCES

1. Modern Physics - Beiser
2. Quantum Mechanics - Bransden and Joachen
3. Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles, 2nd Edition by Eisberg, Robert; Resnick, Robert
4. Quantum Physics – A. Ghatak
5. Principles of Quantum Mechanics 2nd ed. - R. Shankar
6. Quantum Mechanics - Vol 1&2 - Cohen-Tannoudji

NT9312 PHYSICAL CHEMISTRY L T P C
3 0 0 3

UNIT I INTRODUCTION TO THERMODYNAMICS 9

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 eqations.

UNIT II ELEMENTARY STATISTICAL MECHANICS 10

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.

UNIT III THEORY OF SOLUTION AND RELATED TOPICS 8

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

UNIT IV DIFFUSION 9

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.

UNIT V PHASETRANSFORMATIONS 9

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.

TOTAL : 45 PERIODS

REFERENCES

1. Thermodynamics and Statistical Mechanics - A N Tikhonov, Peter T Landberg, Peter Theodore Landsberg
2. Thermodynamics and Statistical Mechanics by John M. Seddon, J. D. Gale
3. Thermodynamics by Zymansky
4. Statistical Physics by K. Huang
5. Statistical Mechanics-Landau &Lifshitz
6. Physical Chemistry – Atkins Peter, Paula Julio
7. Physical Chemistry, 1st Edition –Ball

NT9313 PHYSICS AND CHEMISTRY OF MATERIALS L T P C
3 0 0 3

UNIT I PHYSICAL PROPERTIES 9

Melting point and phase transition processes- quantum-size-effect (QSE). Size-induced metal-insulator-transition (SIMIT)- nano-scale magnets, transparent magnetic materials, and ultrahigh-density magnetic recording materials-chemical physics of atomic and molecular clusters.

UNIT II PHYSICAL CHEMISTRY OF SOLID SURFACES 9

Surface energy – chemical potential as a function of surface curvature-Electrostatic stabilization- surface charge density-electric potential at the proximity of solid surface-Van der Waals attraction potential.

UNIT III CHEMISTRY ASPECTS 9

Photochemistry; Photoconductivity; Electrochemistry of Nanomaterials-Diffusion in Nanomaterials; Nanoscale Heat Transfer; Catalysis by gGold Nanoparticles; Transport in Semiconductor Nanostructures; Transition Metal Atoms on Nanocarbon Surfaces; Nanodeposition of Soft Materials; Nanocatalysis.

UNIT IV NANOSTRUCTURES 9

Electronic Structure of Nanoparticles- Kinetics in Nanostructured Materials- Zero dimensional, one-dimensional and two dimensional nanostructures- clusters of metals and semiconductors, nanowires, nanostructured beams, and nanocomposites-artificial atomic clusters-Size dependent properties-size dependent absorption spectra-phonons in nanostructures.

UNIT V NANOSYSTEMS 9

Nanoparticles through homogeneous nucleation-Growth controlled by diffusion-growth controlled by surface process-influences of reduction reagents-solid state phase segregation-kinetically confined synthesis of nanoparticles-template based synthesis.

TOTAL : 45 PERIODS

REFERENCES

1. K.W. Kolasinski, "Surface Science: Foundations of Catalysis and Nanoscience", Wiley, 2002.
2. Joel I. Gersten, "The Physics and Chemistry of Materials", Wiley, 2001.
3. A. S. Edelstein and R. C. Cammarata, "Nanomaterials: Synthesis, Properties and Applications", Institute of Physics Pub., 1998.
4. S.Yang and P.Shen: "Physics and Chemistry of Nanostructured Materials", Taylor & Francis, 2000.
5. G.A. Ozin and A.C. Arsenault, "Nanochemistry : A chemical approach to nanomaterials", Royal Society of Chemistry, 2005.

NT9314 SYNTHESIS AND APPLICATIONS OF NANOMATERIALS L T P C
3 0 0 3

UNIT I BULK SYNTHESIS 9

Synthesis of bulk nano-structured materials –sol gel processing –Mechanical alloying and mechanical milling- Inert gas condensation technique – Nanopolymers – Bulk and nano composite materials.

UNIT II CHEMICAL APPROACHES 9

Self-assembly, self-assembled monolayers (SAMs). Langmuir-Blodgett (LB) films, clusters, colloids, zeolites, organic block copolymers, emulsion polymerization, templated synthesis, and confined nucleation and/or growth. Biomimetic Approaches: polymer matrix isolation, and surface-templated nucleation and/or crystallization. Electrochemical Approaches: anodic oxidation of alumina films, porous silicon, and pulsed electrochemical deposition.

UNIT III PHYSICAL APPROACHES 9

Vapor deposition and different types of epitaxial growth techniques- pulsed laser deposition, Magnetron sputtering - Micro lithography (photolithography, soft lithography, micromachining, e-beam writing, and scanning probe patterning).

UNIT IV NANOPOROUS MATERIALS 9

Nanoporous Materials – Silicon - Zeolites, mesoporous materials - nanomembranes and carbon nanotubes - AgX photography, smart sunglasses, and transparent conducting oxides –molecular sieves – nanosponges.

UNIT V APPLICATION OF NANOMATERIALS 9

Molecular Electronics and Nanoelectronics – Nanobots- Biological Applications – Quantum Devices – Nanomechanics - Carbon Nanotube – Photonics- Nano structures as single electron transistor –principle and design.

TOTAL : 45 PERIODS

REFERENCES
1. S.P. Gaponenko, Optical Properties of semiconductor nanocrystals, Cambridge University Press, 1980.
2. W.Gaddand, D.Brenner, S.Lysherski and G.J.Infrate(Eds.), Handbook of NanoScience, Engg. and Technology, CRC Press, 2002.
3. K. Barriham, D.D. Vvedensky, Low dimensional semiconductor structures: fundamental and device applications, Cambridge University Press, 2001.
4. G. Cao, Nanostructures & Nanomaterials: Synthesis, Properties &Applications , Imperial College Press, 2004.
5. J.George, Preparation of Thin Films, Marcel Dekker, Inc., New York. 2005.

NT9315 BIOLOGICAL SYSTEMS L T P C
3 0 0 3

UNIT I INTRODUCTION TO DNA STRUCTURE 15

DNA double helix, genome structure and organization in prokaryotes and eukaryotes, Central dogma DNA is a genetic material-Experiments, DNA replication-Mechanism of replication, different types in prokaryotes and eukaryotes, Enzymes involved and its details, Mechanism of transcription in prokaryotes and eukaryotes, splicing and transcriptional factors, transcriptional inhibitors, mechanism of translation, translational factors, Prokaryotic and eukaryotic translation machinery, Co and post translational modifications.

UNIT II INTRODUCTION TO AMINO ACIDS AND PROTEINS 8

Physical and chemical properties of amino acids, different types of protein, Proteins of pharmaceutical importance, role of covalent and non covalent interactions important to protein structure and functions.

UNIT III PROTEIN STRUCTURE 8

Primary, secondary, super secondary, tertiary, quaternary structures and the methods to determine, including prediction methods and utilization of genomic databases.

UNIT IV LIPIDS AND CARBOHYDRATES 6

Structure – function – biosynthesis – Metabolism.

UNIT V CELL STRUCTURE AND FUNCTION OF ORGANELLES 8

Eukaryotic and Prokaryotic cells, Principle of membrane organization, cytoskeletal proteins, types of cell division, mitosis and meiosis, cell cycle and molecules that control cell cycle, structural organization and multiplication of bacteria, viruses, algae and fungi.

TOTAL : 45 PERIODS

REFERENCES
1. R. Cantor, P.R.Samuel, “Biophysical Chemistry”, W.H., Freeman & Co., 1985.
2. Watson, James, T.Baker, S.Bell, A.Gann, M.Levine, and R.Losick. “Molecular Biology of the Gene”, 5th ed., San Francisco: Addison-Wesley, 2000.
3. Alberts, Bruce, Alexander Johnson, Julian Lewis, Martin Raff, Keith Roberts, and Peter Walter. Molecular Biology of the Cell. 4th ed. New York: Garland Science, 2002.
4. Branden, Carl-Ivar, and John Tooze. Introduction to Protein Structure. 2nd ed. New York: Garland Pub., 1991.
5. Creighton, E, Thomas, “Proteins: Structures and Molecular Properties”, 2nd Ed. New York: W.H. Freeman, 1992.
6. B.Lewin, “Genes IX”, International Edition. Sudbury: Jones & Bartlett, 2007.

NT9317 **EXPERIMENTS FOR PRACTICAL – I**
COMPUTATION AND SIMULATION LABORATORY **L T P C**
0 0 4 2

1. MATLAB programme to plot the first four eigenfunctions of a one - dimensional rectangular potential well with infinite potential barrier.
2. Numerical solution of the Schrodinger wave equation for a rectangular potential well with infinite potential barrier using MATLAB programme.
3. Toy model in molecular electronics: IV characteristics of a single level molecule
4. To determine the lattice constant and lattice angles for atomically resolved STM image of HOPG (Highly Oriented Pyrolytic Graphite using offline Scanning Probe Imaging Processor (SPIP) Software.
5. To determine the surface roughness of raw and processed AFM images of glass, silicon and films made by different methods using offline SPIP software.
6. Simulation of I-V Characteristics for a single Junction circuit with a single quantum Dot using MOSES 1.2 Simulator.
7. Study of Single Electron Transistor using MOSES1.2 Simulator.

TOTAL : 60 PERIODS

NT9318 **EXPERIMENTS FOR PRACTICAL - II MATERIAL SYNTHESIS AND EXPERIMENTS**

L T P C
0 0 4 2

1. Chemical synthesis of Ag nanoparticles; UV-Visible absorption of the colloidal sol; Mie formalism; Estimation of size by curve fitting
2. Chemical synthesis of CdS nanoparticles; Optical absorption spectra; Band gap estimation from the band edge
3. Aqueous to organic phase transfer of Ag and CdS nanoparticles; Confirmation by UV- Visible absorption
4. Synthesis of Au and Ag nanoparticles at aqueous-organic liquid interface; UV-visible spectroscopy of the colloidal film; comparison with the corresponding colloidal sol.
5. Sol gel synthesis of ZnO nanoparticles
6. Micellar route to Pt nanoparticles
7. A bioroute to Au nanoparticles
8. Room temperature B-H loops for □-Fe_2O_3 nanoparticals of different sizes (5-50nm).

TOTAL : 60 PERIODS