



PES UNIVERSITY

**Ph.D. / MTech by Research course work
Chemistry**

List of courses

#	Course Code	Course Title
1	UE23CY841A	Nanoscience & Nano Materials
2	UE23CY842A	Analytical Techniques
3	UE23CY843A	materials Degradation and Protection

UE23CY841A: Nanoscience and Nanomaterials

This course covers the most recent advances in the synthesis, fabrication, characterization, properties and applications of nanomaterials with an emphasis on recent technological breakthroughs in the field.

Course Objectives :

- To have an updated knowledge of the state-of-the-art in nanomaterials and their synthesis and applications
- To understand the deviation in properties of nanostructured materials from their bulk counterparts

Course Outcomes:

After the successful completion of this course, the student will be able to:

- Appreciate the history, background and nature of Nanoscience and technology.
- Understand various properties of nanostructures.
- Explain the various physical and chemical methods used for the synthesis of nanomaterials.
- Know various metal, metal oxide and carbon nanostructures and their applications in catalysis, sensor, energy storage.

Course Outline

Unit I : Introduction and properties of nanomaterials: Origin of Nanotechnology, Introduction to Nano-science; History and Scope, Interdisciplinary nature, Nanosized effects on surface to volume ratio, atomic structure, molecules and phases, energy at the nanoscale molecular and atomic size, quantum effect. Classification of nanostructures - Zero dimensional, one-dimensional and two dimensional nanostructure materials – semiconductors, ceramics and nanocomposites, size dependent phenomena, quantum dots, nanowires, nanotubes, nanosheets, nano and mesopores. Mechanical properties, Thermo physical properties, Electric properties, Electrochemical properties, Magnetic properties, Optical properties and Catalytic properties of nanomaterials.

Unit 2 : Synthesis of Nanomaterials: Synthesis of nanomaterials: Bottom-up approach and Top-down approach with examples. Physical methods: Inert gas condensation, Arc Discharge, RF-plasma, plasma arc technique, electric explosion of wires, lasers ablation, laser pyrolysis, ball milling, molecular beam epitaxial, electro deposition, chemical vapour deposition. Sol-gel technique, Combustion synthesis, ultrasonic precipitation process. Microwave synthesis, sonochemical synthesis, photochemical synthesis, synthesis in supercritical fluids. Fabrication of Nanofibers by Electrospinning method.

Unit 3 : Characterization of Nanomaterials: Structural characterization techniques: X-Ray photoelectron Spectroscopy(XPS), X-Ray topography, Energy Dispersive X-Ray Analysis(EDAX), Principles and applications of X- Ray Diffraction: Small angle X-Ray Diffraction and Wide angle X-Ray Diffraction; Electron Diffraction, Electro probe microanalysis (EPMA), Ion beam techniques: RBS. Surface characterization Techniques: Scanning electron microscopy (SEM), Transmission electron microscopy, Basic principles and applications of scanning probe techniques (SPM), Atomic force microscopy, and scanning tunneling microscopy. Spectroscopic techniques: UV-Visible spectroscopy, Infrared (IR) & Fourier Transform infrared (FTIR) Spectroscopy, Raman Spectroscopy techniques: Photo luminescence Spectroscopy, Diffuse reflectance spectroscopy.

Unit 4 : Carbon nanostructures, Nanooptics and Nanocatalysis: Carbon nanostructures : Allotropes of Carbon, synthesis, and applications of Graphene and fullerenes. Carbon nanotubes: types, structure synthesis and purification of carbon nanotubes and applications. Nanooptics: Absorption: direct and indirect bandgap transitions - Emission: photoluminescence and Raman Scattering, Emission: Chemiluminescence and Electroluminescence, Shape dependent optical properties, Optical absorption, Optical emission, Surface plasmon resonance (SPR) - Surface enhanced Raman scattering (SERS). Nanocatalysis: Introduction, nanomaterials in catalysis, metals, recent progress, nanostructured adsorbant, metals, controlled pore size materials, pelletized nanocrystal, nanoparticles as new chemical reagents, metals, metal oxide reactions, nanocomposite polymers, fluids, inks and dyes, block co polymers and dendrimers, nano crystal super lattices.

Unit 5 : Applications of Nanomaterials: Nanoelectro mechanical systems (NEMS)- Data storage devices – diskettes and tapes. Applications of CNT/metal oxide nanocomposites, Graphene/metal oxide nanocomposite, CNT/polymer composites, Graphene/polymer composites in catalyst support, gas storage, biosensors. Biological applications of nanomaterials, Drug delivery, nanodevices in medicine. Gold nanoparticles in medicine. Catalysis using nanomaterials – metal/metal oxide nanoparticles for heterogeneous catalysis. Nanofibers for biomedical applications as an implant material. Nanomaterials for environmental applications. Carbon nanofibers and its applications.

Reference books:

1. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Guozhong Cao , Imperial College Press (2004)
2. Nanomaterials- Synthesis, Properties and Applications, Edited by A.S. Edelstein and R.C. Cammarata, Institute of Physics Publishing, London, 1998 (paper back edition)
3. Chemistry of nanomaterials : Synthesis, properties and applications C. N. R. Rao, Achim Muller, A. K Cheetham, Wiley-VCH, 2004

4. Carbon nanotubes: Basic concepts and Physical properties, Reich, S., Thomsen, C. Maultzsch, J., Weinheim: Wiley-VCH, 2004
5. Nanostructured Materials and Nanotechnology: Concise Edition, Nalwa, Hari Singh Diego: Academic Press, 2002
6. Springer Hand Book of Nanotechnology, Bharat Bhushan ,4th edition,2017

UE23CY842A: Analytical Techniques

Analytical chemistry is one of the important divisions of chemistry that aids researchers in experimental (classical and applied) chemistry to characterize chemical compounds. It deals with qualitative as well as quantitative measurements.

Course objectives:

- To introduce students to the methods and concepts of analytical chemistry
- To understand various techniques of analysis
- To get an overview of the instruments involved for characterization and analysis of experimental data

Course Outcomes:

After the successful completion of this course, the student will be able to:

- Understand various molecular spectroscopic studies
- Explain the usage of electro-analytical methods in analysis
- Know to employ surface analysis, thermal analysis to structures
- Comprehend various chromatographic techniques

Course outline:

Unit 1: Spectroscopy: Infra-red spectroscopy- Theory; Instrumentation; Sample Handling; Interpretation of Spectra; Characteristic group absorptions of molecules. Mass spectroscopy- Instrumentation; Mass spectrum; Determination of molecular formula; Recognition of molecular ion peak; Ionization techniques; Fragmentation and rearrangements; Quantitative applications of mass spectrometry. Nuclear Magnetic Resonance spectroscopy- NMR spectrometry; Relaxation; Pulsed Fourier Transform Spectrometry; Rotating Frame of Reference; Instrumentation and sample handling; Chemical shift; Spin coupling; Chemical shift equivalence; Magnetic equivalence; Geminal and vicinal coupling; ^{13}C NMR spectroscopy U-V Visible spectroscopy- Fundamental laws of Photometry; quantitative methodology; radiation sources, detectors, U-V Visible spectrophotometers Atomic Absorption spectroscopy- Atomic Absorption spectrophotometer, analysis

Unit 2 : Electroanalytical Chemistry: Potentiometry; Coulometry ; Polarography; Linear Potential Sweep Voltametry; Cyclic Voltametry; Impedance measurements; AC Voltametry.

Unit 3: Chromatographic techniques Chromatographic separations; Gas chromatography; Gas chromatographic columns and stationary phases; Principles and applications of gas-liquid chromatography; High- Performance Liquid Chromatography (HPLC); Thin Layer and column Chromatography; Ion-Exchange Chromatography; Size-Exclusion chromatography.

Unit 4: Surface Characterization by Spectroscopy and Microscopy: X-ray diffraction- Lattice; Lattice symmetry; Characterization of powder and thin films; Line shape analysis, surface area measurement(SBET), XPS, AFM, STM, SEM, TEM

Unit 5: Thermal Methods : Thermogravimetric methods; Differential thermal analysis; Differential Scanning Calorimetry

Reference books:

1. Principles of Instrumental Analysis by Douglas A. Skoog, F. James Holler, Timothy A. Nieman; Saunders Golden Sunburst Series.
2. Modern Analytical Chemistry by David T Harvey; McGraw-Hill Science.
3. Spectrometric Identification of Organic Compounds by R. M. Silverstein, F. X. Webster; John Wiley and sons
4. Analytical Chemistry by Gary D. Christian; John Wiley and sons
5. Instrumental methods of analysis by Willard, Merit and Dean, 7th edition, 1998

UE23CY843A - Materials Degradation and Protection

Course objectives:

- To understand the corrosion process, thermodynamics and electrochemical aspects of corrosion, environmental effects and corrosion control.
- To become familiar with corrosion rate expressions, corrosion rate measurements and corrosion mechanism in sea water.

Course Outcomes:

Students obtain a basic understanding of the corrosion mechanism, corrosion rate expressions and measurements.

Unit 1: Introduction and mechanism of corrosion: Definition of corrosion, corrosion damage, corrosion rate expressions, classification of corrosion, electrochemical aspects, electrochemical reactions, Pourbaix diagrams, mixed potential theory, polarization, Evan's diagrams, passivity.

Unit 2: Factors affecting corrosion: Environmental effects - oxygen and oxidizers, temperature, corrosive concentration, cathode/anode area ratio, galvanic coupling using mixed potential theory.

Unit 3: Forms of corrosion: Uniform, galvanic, crevice, intergranular, pitting, selective leaching, erosion, stress corrosion, corrosion fatigue, fretting, hydrogen damage, microbial corrosion.

Unit 4: Corrosion testing: Materials and specimens. Surface preparation, measuring, weighing, exposure techniques. Corrosion rate measurements - Tafel and linear polarization, AC impedance, small amplitude cyclic voltammetry, interpretation of results.

Unit 5: Corrosion protection: Materials selection, alternative environment – organic and inorganic inhibitors, green inhibitors, design, cathodic and anodic protection, coatings. Corrosion in sea water and high-temperature corrosion -mechanisms and kinetics, materials for protection against sea water and high – temperature corrosion.

Reference books:

1. Mars G. Fontana, Corrosion, McGraw - Hill Book Company 1986.
2. Denny A. Jones, Principles and Prevention of Corrosion, Maxwell Macmillan 1992.
3. Metals Handbook, Vol.13, Corrosion, ASM Metals Book, Ohio, 1987.
4. John O'M Bockris and Amulya K. N. Reddy, Modern electrochemistry, second edition, volume 2B, Kluwer Academic/Plenum Publishers, New York, 1998.