Ph.D. Course Work Syllabus

Department of Chemistry

KISHKINDA UNIVERSITY, BALLARI

Ph.D. Course Work Syllabus

Effective From

2024-25

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Dept. of Chemistry
Faculty of Engineering & Technology
Kishkinda University, BITM-Campus,
Near Allipur, Hosapete Road, Ballari-583104

Paper-I: Nanomaterial and Synthesis

Course Title:	**Nanomaterial and Synthesis**	Credits:	**04**
Course Code:	**24CHE01**	SEE Marks:	**100**
Course Type:	**Self-Study**	Exam Duration:	**03**

Objectives:

This course work introduces PhD Scholars to nanomaterials, emphasizing their unique nanoscale properties compared to bulk materials and the principles guiding their synthesis. It covers both chemical and physical approaches to nanomaterial fabrication, detailing mechanisms, advantages, and challenges of various techniques. Students will learn how to tailor nanomaterial properties through surface functionalization, doping, and composite formation, highlighting the significance of surface chemistry for enhancing performance in diverse applications. The module also explores the wide-ranging applications of nanomaterials in fields such as energy, electronics, medicine, and environmental science, along with advanced characterization techniques for assessing their properties in complex environments.

Module 1: Introduction to Nanomaterials and their Properties

Nanomaterials Classification: 0D (Quantum Dots), 1D (Nanowires, Nanotubes), 2D (Graphene, Nanoplates), 3D (Nanoparticles, Nanospheres), Carbon-based nanomaterials (Graphene, CNTs, Fullerenes), Metal and metal oxide nanoparticles, Hybrid and composite nanomaterials

Properties of Nanomaterials: Surface area-to-volume ratio, Quantum effects, Optical, electrical, mechanical, and thermal properties at the nanoscale, Size and shape-dependent properties (e.g., surface plasmon resonance, catalytic activity)

Module 2: Chemical Synthesis: Bottom-up Approaches

Chemical Vapor Deposition (CVD): Process, types (e.g., thermal CVD, plasma-enhanced CVD), Applications: Graphene, CNTs, thin films

Solvothermal and Hydrothermal Synthesis: Precursor selection, solvent choice, reaction conditions, Synthesis of nanoparticles (e.g., TiO_2, ZnO, metal oxides)

Sol-Gel Process: Chemistry behind sol-gel process, Fabrication of nanostructured materials (e.g., silica, ceramics, composites)

Template-Assisted Methods: Hard vs. soft templates, Nanowires, nanotubes, nanorods

Controlled Precipitation and Co-Precipitation: Nucleation and growth control, Examples: Metal and metal oxide nanoparticles

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Module 3: Physical Methods of Synthesis: Top-down Approaches

Laser Ablation: Mechanism of laser ablation in liquids and gases, Applications: Gold nanoparticles, quantum dots

Ball Milling and Mechanical Alloying: Process, advantages, and limitations, Production of nanoparticles via high-energy milling

Electrospinning: Process principles, nanofiber production, Applications in tissue engineering, filtration, and energy storage

Plasma Synthesis: Plasma-assisted chemical vapor deposition (PACVD), Synthesis of carbon nanomaterials, thin films

Magnetron Sputtering: Thin-film deposition, nanostructuring, Applications in semiconductors and photovoltaic devices

Atomic Layer Deposition (ALD): Deposition of uniform thin films at the atomic level, Applications in semiconductor and nanostructure growth

Top-down vs. Bottom-up Approaches: Definition and comparison of these strategies, Applications of each approach in nanomaterial fabrication

Module 4: Nanomaterial Functionalization and Modification

Surface Functionalization: Covalent vs. non-covalent functionalization, Attachment of functional groups, polymers, or biomolecules, Examples: Carbon nanotubes, graphene oxide

Doping and Alloying: Doping metal oxides and semiconductors to improve electronic, catalytic, and optical properties, Alloying techniques and their effects on nanomaterial properties

Nanocomposites: Hybrid nanomaterials: Organic-inorganic, metal-oxide, polymer composites, Examples: Carbon nanotube-based composites, graphene-polymer hybrids

Self-Assembly Techniques: Directed and spontaneous assembly of nanoparticles and nanostructures, Applications: Sensors, photonic devices, and catalysis

Module 5: Applications of Nanomaterials and Catalysis

Thermo-/Phot-/Electro-catalysis: Thermocatalysis Fundamentals, Catalytic mechanisms: adsorption, reaction, and desorption, Kinetics and thermodynamics of thermocatalytic reactions, Photocatalysis Fundamentals, Photonic energy and its interaction with materials, Band gap theory and semiconductor photocatalysts, Excitation and charge separation processes, Water splitting and hydrogen production, Electrochemical principles and cell design, Electrode materials and their properties Reaction mechanisms and kinetics.

Energy Applications: Nanomaterials in energy storage (e.g., batteries, supercapacitors), Nanocatalysis in fuel cells, hydrogen production, and CO_2 capture

Electronics and Photonics: Nanomaterials in semiconductors, sensors, and transistors, Plasmonics and light-matter interactions in nanostructures

Nanocosmetics: Anti-Aging Effects of Nanocosmetics, mechanisms of nanomaterials to enhance the efficacy of anti-aging ingredients and their effects on skin rejuvenation, safety and toxicology of nanomaterials in cosmetics, synthesis and characterization of nanoparticles for cosmetic applications ex: silver, zinc oxide, and titanium dioxide, analyze their properties and efficacy in cosmetic formulations.

References:

1. Roco, M. C., & Bainbridge, W. S. (Eds.). (2013). *Nanotechnology: Societal Implications and Applications* (Vol. 3). Springer.
2. Iijima, S. (1991). *Helical Microtubules of Graphitic Carbon*. Nature.
3. Chen, Z., et al. (2014). *Nanomaterials: Synthesis, Properties and Applications*. Wiley-VCH.
4. Wang, Y., & Liu, Y. (2017). *Nanotechnology in Medicine: An Introduction to the Medical Applications of Nanomaterials*. Springer.
5. Introduction to Nanomaterials and Nanotechnology by Challa S. S. R. Kumar
6. Nanomaterials: Synthesis, Properties, and Applications – *Nature Nanotechnology*
7. Nanomaterials Synthesis: Top-down and Bottom-up Approaches by L. S. S. Kumar et al.
8. Chemical Synthesis and Applications of Nanomaterials – *Journal of Materials Chemistry A*
9. Physical Methods for Nanomaterial Synthesis by J. H. Chen
10. The Role of Physical Vapor Deposition and Electrospinning in Nanomaterials Synthesis – *Materials Science & Engineering R*
11. Functional Nanomaterials: Synthesis, Characterization, and Applications by K. R. R. Anjaneyulu
12. Functionalization of Nanomaterials for Biomedical Applications – *Advanced Materials*
13. Nanomaterials: Applications in Energy, Environmental, and Medical Engineering by M. M. Pillai et al.
14. Applications of Nanomaterials in Energy, Medicine, and the Environment – *Nature Materials*

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Paper-II: Advanced Topics in Materials Science and Engineering

Course Title:	**Advanced Topics in Materials Science and Engineering**	Credits:	**04**
Course Code:	**24CHE02**	SEE Marks:	**100**
Course Type:	**Self-Study**	Exam Duration:	**03**

Objectives:

This cpurse work introduces research scholars to advanced techniques for analyzing and characterizing materials at various length scales, emphasizing both theoretical foundations and practical applications to contemporary materials challenges. It covers thermodynamic principles and kinetic processes linking macroscopic properties to atomic behavior, equips students with simulation tools for modeling material behavior at different scales, and explores materials science's role in energy and sustainability, particularly in developing next-generation materials for energy storage and environmental applications. Additionally, it delves into the design and fabrication of nanomaterials and their diverse applications across fields like electronics and medicine.

Module 1: Advanced Material Characterization Techniques

Microscopy Techniques: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), and Scanning Tunneling Microscopy (STM).

X-ray Diffraction (XRD): Techniques for phase identification, strain analysis, and crystal structure determination.

Neutron and Synchrotron Techniques: Neutron diffraction, Small-Angle X-ray Scattering (SAXS), and X-ray tomography for 3D imaging.

Solid-state NMR for Techniques nanomaterials: Basics of NMR: Principles and concepts, Differences between solution and solid-state NMR, Magnetic interactions: Chemical shift, dipolar coupling, and J-coupling, Spin systems and relaxation mechanisms, NMR Techniques for Solids: Magic Angle Spinning (MAS), Cross-polarization (CP), 2D NMR techniques

Module 2: Molecular absorption spectroscopic tools

Raman Analysis: Basic principles: scattering of light, Stokes vs Anti-Stokes scattering, Key differences between Raman and Infrared spectroscopy, Raman spectra and their interpretation, Advanced Raman Techniques.

Spectroscopic Techniques: Raman Spectroscopy, X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES), and Fourier-transform infrared spectroscopy (FTIR).

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BET Method of Material Analysis: Surface Area Determination, Pore Size Distribution, Porosity Studies and their application to nanomaterial characterization.

Module 3: Thermodynamics and Kinetics of Materials

Thermodynamics of Phase Transitions: Free energy concepts, phase diagrams (binary and ternary systems), and Gibbs' phase rule.

Solidification and Crystallization: Nucleation, growth mechanisms, and kinetics of phase transformations.

Diffusion in Solids: Fick's laws, Kirkendall effect, and diffusion in alloys and polymers.

Defects and Non-Equilibrium Thermodynamics: Point defects, dislocations, grain boundaries, and non-equilibrium processes.

Kinetics of Reactions: Rate laws, reaction mechanisms, and control of microstructure through processing.

Module 4: Computational Materials Science

Molecular Dynamics (MD) Simulation: Principles, force fields, and applications in predicting material behavior at the atomic scale.

Density Functional Theory (DFT): Quantum mechanical modeling of materials' electronic structure and properties.

Monte Carlo Methods: Statistical simulations for studying phase transitions, surface processes, and other phenomena.

Finite Element Method (FEM): Simulation of macroscopic mechanical behavior, including stress-strain analysis and failure modeling.

Materials Informatics: Using machine learning and big data to predict materials properties and design new materials.

Module 5: Advanced Materials for Energy and Sustainability

Energy Storage Materials: Lithium-ion batteries, solid-state batteries, supercapacitors, and next-generation energy storage devices.

Photovoltaics and Solar Cells: Organic, perovskite, and thin-film solar cells, materials for light harvesting and conversion.

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Fuel Cells and Hydrogen Storage: Electrochemical energy conversion, materials for proton exchange membranes (PEM), and hydrogen storage solutions.

Materials for Carbon Capture and Environmental Remediation: Carbon nanomaterials, catalysis for CO_2 reduction, and materials for waste remediation.

Circular Economy in Materials: Recycling and reuse of materials, sustainability metrics, and life-cycle analysis.

References:

1. Callister, W. D., & Rethwisch, D. G. (2020). Materials Science and Engineering: An Introduction (10th ed.). Wiley.
2. Meyer, E. M., & Ward, R. M. (2014). Introduction to Materials Science for Engineers (8th ed.). Pearson.
3. Raghavan, V. (2015). Materials Science and Engineering: A First Course (5th ed.). Prentice-Hall.
4. Shackelford, J. F. (2015). Introduction to Materials Science for Engineers (8th ed.). Pearson.
5. Buchanan, R. A., & Schmid, F. (2011). Fundamentals of Materials Science and Engineering. Wiley-IEEE Press.
6. Zhao, Y., & Zhang, L. (2023). "Advanced Techniques in Nano-Structured Materials for Energy Storage Applications." Journal of Materials Science, 58(2), 402-420.
7. Gao, X., et al. (2021). "The Role of Additive Manufacturing in Metal Matrix Composites: Current Trends and Future Prospects." Materials Science and Engineering: A, 812, 141293.
8. Smith, R. M., & Lee, Y. H. (2020). "The Impact of High-Entropy Alloys on Structural Materials: A Review of Recent Developments." Materials Today, 45(5), 232-244.
9. Brunauer, S., Emmett, P. H., & Teller, E. (1938). *Adsorption of gases in multimolecular layers*. Journal of the American Chemical Society, 60(2), 309–319.

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Paper-III: Polymers and Composites and Their Modern Applications

Course Title:	**Polymers and Composites and Their Modern Applications**	Credits:	**04**
Course Code:	**24CHE03**	SEE Marks:	**100**
Course Type:	**Self-Study**	Exam Duration:	**03**

Objectives:
This course work provides foundational knowledge in polymer science, covering polymerization techniques, molecular structure, and properties. It explores polymer blends, alloys, and nanocomposites, emphasizing their impact on material performance. Scholars will learn about processing technologies for polymer-based materials and composites, including advanced techniques, and examine the relationship between material structure and mechanical performance. Additionally, the module highlights cutting-edge applications of polymers and composites across various industries, focusing on technological innovations and sustainability.

Module 1: Introduction to Polymers and Polymer Chemistry

Polymer Chemistry: Types of polymerizations (addition vs. condensation), free radical, ionic, and coordination polymerizations.

Polymer Structures and Morphology: Amorphous and crystalline structures, chain configurations (linear, branched, crosslinked), and the influence of molecular weight on properties.

Polymer Properties: Mechanical (tensile, elongation, modulus), thermal (glass transition temperature, melting point), and chemical stability.

Module 2: Polymer Blends and Nanocomposites

Polymer Blends and Alloys: Types of blends (miscible vs. immiscible), phase behavior, compatibilizers, and industrial applications.

Nanocomposites: Introduction to nanofillers (nanoclays, carbon nanotubes, graphene, nanoparticles), their dispersion in polymer matrices, and their impact on properties (mechanical, thermal, electrical).

Applications of Polymer Nanocomposites: Electronics, automotive, aerospace, and packaging industries.

Module 3: Advanced Polymer Processing Techniques

Polymer Processing Fundamentals: Injection molding, extrusion, blow molding, compression molding, and thermoforming.

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Advanced Processing Techniques: Additive manufacturing (3D printing of polymers and composites), electrospinning, melt-electrospinning, and nanoimprinting.

In-Situ Polymerization: Fabrication of polymer composites via in-situ polymerization of monomers in the presence of reinforcing phases.

Processing-Property Relationships: The effect of processing on the mechanical, thermal, and chemical properties of polymers and composites. structure-property relationships in polymers.

Module 4: Mechanical Properties and Performance of Polymers and Composites

Stress-Strain Behavior of Polymers: Tensile testing, viscoelasticity, time-temperature superposition, and rheological properties.

Fracture and Failure Mechanisms: Crack propagation in polymers, fatigue, environmental stress cracking, and impact resistance.

Reinforced Composites: Fiber-reinforced composites (carbon, glass, aramid fibers), failure mechanisms in composites, and hybrid composites.

Design and Optimization: Tailoring mechanical properties for specific applications (e.g., lightweight structures, high-strength materials).

Module 5: Modern Applications of Polymers and Composites

Polymers in Electronics: Conductive polymers, flexible electronics, organic light-emitting diodes (OLEDs), and wearable devices.

Polymers in Medicine: Biodegradable polymers, drug delivery systems, tissue engineering, and medical implants.

Polymers in Aerospace and Automotive: High-performance composites, lightweight materials, and fuel efficiency.

Sustainable Polymers and Green Composites: Recycling of polymeric materials, and the development of sustainable composites.

References:

1. Polymer Composites: From Design to Processing by M. P. Mathew, L. S. T. Stanciu, and S. M. R. Shamsuddin

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2. Introduction to Polymers by Robert J. Young and Peter A. Lovell
3. Polymer Nanocomposites: Synthesis, Characterization, and Applications by Visakh M. P., Rashmi S.
4. Baker, D., & Rankin, W. J. (2019). Recent Advances in Polymers and Polymer Composites for Structural Applications. Composites Science and Technology, 181, 107675.
5. Shen, X., & Hu, G. (2020). Advanced Polymer Composites for Electronics and Photonics Applications." Journal of Materials Science, 55(3), 1052-1075.
6. Sung, K. & Cho, W. (2022). Polymers and Composites for Environmental Sustainability: Challenges and Future Directions. Composites Part B: Engineering, 232, 109586.
7. Advanced Polymers in Medicine by Muaz A. Razzak
8. Polymer Composites in the Automotive Industry by R. L. Shanks
9. Mechanical Properties of Polymers and Composites by Laurence W. McKeen
10. Principles of Polymer Engineering by N. G. McCrum, C. P. Buckley, and C. B. Bucknall
11. Mechanical Properties of Polymers and Composites by Laurence W. McKeen
12. Principles of Polymer Engineering by N. G. McCrum, C. P. Buckley, and C. B. Bucknall
13. Polymer Blends and Alloys by S. K. Varma
14. Polymer Nanocomposites edited by L. T. Drzal, M. P. A. G. Carreau
15. Introduction to Polymers by Robert J. Young and Peter A. Lovell
16. Polymer Chemistry: An Introduction by Paul C. Hiemenz and Timothy P. Lodge

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