

DISCIPLINE-SPECIFIC ELECTIVE COURSE - 25 (DSE-25)

Fundamentals of Solid-State and Materials Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Fundamentals of Solid-State and Materials Chemistry (DSE-25)	4	2	--	2	--	--

Learning Objectives:

- To introduce solid-state and wet chemical synthesis methods, and basics of nanomaterials.
- To explain electronic properties of solids using band theory.
- To understand crystal structures, symmetry, and structure determination via diffraction techniques.
- To use thermal and spectroscopic techniques to characterize materials.
- To explore magnetic properties and structure via electron and atomic force microscopy.

Learning outcomes:

By the end of the course, students will be able to:

- Apply solid-state and chemical synthesis methods to create nanomaterials.
- Interpret band structures and explain properties of metals, insulators, and semiconductors.
- Analyze crystallographic data using symmetry concepts and X-ray/electron diffraction.
- Characterize materials using TGA, DSC, UV-Vis, FTIR, PL, and NMR.
- Evaluate magnetic ordering and interpret SEM, TEM, and AFM data.

SYLLABUS OF DSE 25

Unit 1: Materials Synthesis and Nanochemistry

(Hours: 6)

Solid state reaction and wet chemical synthetic routes, Top down and bottom-up approach to prepare different kinds of nanomaterials, Fundamental concept of nanoscience including quantum confinement effect, Examples: ZnO, TiO₂, Ag nanoparticles.

Unit 2: Structure and Bonding in Solids

(Hours: 12)

Fundamentals of lattice including Bravais Lattices, crystal's direction and planes, symmetry operations and symmetry elements, point group, space group and crystal structures, Miller indices, Types of closed packed structures, Factors which influence crystal structures, Introduction to band theory. Metals, insulators and semiconductors, Electronic structure, k-space and Brillouin zones (qualitative).

Bragg condition and Bragg method, Laue method, PXRD: principles and instrumentation, Crystallite size (Scherrer) and Williamson-Hall method to determine lattice strains from diffraction patterns, Basics of Single Crystal X-ray diffractometer (SCXRD), electron and neutron diffraction.

Unit 3- Spectroscopy and Thermal Analysis

(Hours: 6)

UV-Visible, FTIR, Photoluminescence (PL) and NMR techniques to understand materials properties, Thermogravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), principles and interpretation, Examples: thermal decomposition, phase changes.

Unit 4: Advanced Characterization and Magnetic Properties

(Hours: 6)

Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Atomic Force Microscope (AFM): working principles and applications, Magnetic behaviour: Curie and Curie-Weiss laws, magnetic ordering, exchange interactions, Hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism.

Practical Component

Hands-on experiment

1. Synthesis of oxide nanomaterials (e.g., ZnO, TiO₂) using solid-state or sol-gel methods.
2. Preparation of semiconducting CdSe, ZnSe, In₂S₃ (any of one) nanomaterials by any soft chemical approach (emulsion based, co-precipitation etc.).
3. Preparation of metal nanoparticles (e.g., Ag, Cu, or Ni) using standard reduction and capping agents.
4. Studying photocatalytic degradation of environmentally pollutant dye (Crystal Violet, Rhodamine B, methyl orange etc.) by any semiconducting (In₂S₃, CdSe, ZnO- any one) or metallic nanoparticles under visible light irradiation and using UV-Visible spectrophotometer.

5. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
6. Determination of glass transition temperature of a given salt (e.g. CaCl_2) conductometrically.
7. Understanding the differences of functional groups by FTIR analysis of different organic compounds (For example, acids, carbonyls, esters, phenolic OH groups etc.).
8. Determination of band gap of a semiconducting nanoparticle (in solution) using UV-visible spectrophotometer.
9. Determination of band gap of a semiconducting nanoparticle (in solid) using UV-visible spectrophotometer (DRS mode).

Analysis of Compounds/Sample with pre-recorded spectra/diffraction patterns and images subject to availability of instruments

1. Measurement and interpretation of different spectra from UV-Vis, IR and NMR using organic, inorganic compounds and molecules. [At least 6 spectra (two from each category) to be provided to students for analysis].
2. Analysis of diffraction pattern obtained from Powder X-ray diffractometer etc (calculation of crystallite size using Scherer equation and lattice strain calculation using Williamson-Hall equation etc). [At least two diffraction patterns of known sample can be provided to students for analysis]
3. Thermogravimetric analysis of compound, molecules etc.
4. Structural analysis using SEM images, EDX analysis of known samples. Students can be provided SEM images and others for analysis.
5. Calculation of particle sizes, aspect ratio from low magnification TEM images of known samples and lattice plane/d spacing calculations from HRTEM images.
6. Facility (PXRD, SCXRD, TEM, SEM and NMR) visits of the students.

Recommended References and Textbooks: (For theory)

1. H. V. Keer, Principles of the Solid State, Wiley Eastern.
2. W. D. Callister, Materials Science and Engineering, Wiley.
3. C. N. R. Rao, Nanomaterials Chemistry: Recent Developments and New Directions, Wiley-VCH.
4. R. S. Drago, Physical Methods in Chemistry, Saunders College.
5. Ray Egerton, Physical Principles of Electron Microscopy, Springer.
6. Principles of Fluorescence Spectroscopy by Joseph R Lakowicz
7. Fundamentals of Molecular Spectroscopy by C. N. Banwell
8. Introduction to Molecular Spectroscopy, G. M. Borrow, McGraw Hill.

Supplementary reading

1. Ashcroft & Mermin, Solid State Physics, Saunders College

Recommended References and Textbooks: (For practical)

1. B.D. Khosla, V.C. Garg and Adarsh Gulati, Senior Practical Physical Chemistry, R. Chand & Co.
2. J.N. Gurtu, Advanced Physical Chemistry Experiments, Pragati Prakashan.
3. G.N. Mukherjee, University Handbook of Undergraduate Chemistry Experiments, Univ. of Calcutta.
4. Ian M. Watt, The Principles and Practice of Electron Microscopy.
5. Ray F. Egerton, Physical Principles of Electron Microscopy – An Introduction to SEM, TEM and AFM.
6. Yoshio Waseda et al., X-ray Diffraction Crystallography: Introduction, Examples and Solved Problems.
7. Journal articles and datasets from ACS, RSC, Elsevier, as applicable (Ind. Eng. Chem. Res. 2014, 53, 3131–3139; ChemSusChem 2011, 4, 1796–1804; ACS Appl. Mater. Interfaces 2017, 9, 11651–11661; Journal of Luminescence 2007, 124, 327–332)