Semester	JAN 2022
Open to semester	8,12,14,22
Course code	**CH4224/CH6284**
Course title	**Advanced Material Science**
Credits	4 /4
Course Coordinator & participating faculty (if any)	Ramanathan Vaidhyanathan* R. Boomi Shankar
Nature of Course	Lectures and Tutorials
Pre-requisites	None
Objectives (goals, type of students for whom useful, outcome etc)	The course aims to teach the concepts and practices behind the study of crystalline, porous materials, and other functional solid-state materials. The student would be taught the concepts of x-ray crystallography in-depth and breadth. Most powerful material characterization technique. They will be taught the principles and methods of thermal analysis, characterization and property investigation of porous and polarizable solids. Chemistry of ferroelectric solids, cage compounds would be taught. The relevance of these materials in a variety of energy research and applications would be covered. Different chemical and material characterization methods such as Mass Spectrometry, X-ray Photoelectron Spectroscopy, Inductively Coupled Plasma- would be discussed in depth. These are all relevant to any student pursuing research in physical, chemical or biological materials science. At the end, the student will have substantial knowledge on crystallography, material characterizations and working principles of such methods, these all pertain to the state-of-the-art techniques that are being employed in various areas of material science.
Course contents (details of topics /sections with no. of lectures for each)	Introduction: Molecules to Materials Part 1: Cage compounds and coordination driven self-assemblies. Families of cationic, anionic and neutral cage compounds. Analysis of metallosupramolecular assemblies by using advanced mass spectrometric and NMR techniques. Examples for cage-compounds utilized in host-guest chemistry and materials applications. (5 hrs). Part 2:

	(a) Special solid-state materials. Polyhedral solids: vertex-, edge- and face-sharing octahedra and tetrahedra. Comparison of packing of spheres in metals, alloys and compounds. Hume-Rothery and Laves phases. Spheres with occupied interstices: spinels, perovskites and other interstitial compounds. (b) Polar functional solids. Fundamental principles of non-linear dielectric properties. Perovskites and other oxides as dielectric, piezoelectric and ferroelectric materials.(6 hrs) Molecular ferroelectrics. Single- and multi-component ferroelectric materials, ferroelectric polymers, organic-inorganic hybrid ferroelectrics. Ferroelectric and ferroelastic substances and their characterization. Utilization of ferroelectrics in memory devices, sensors and energy-harvesting applications. (6 hrs) Crystalline solids: Zeolites, Metal Organic frameworks, Covalent Organic Frameworks. Understanding their structure and properties - Amorphous, poly crystalline & single crystalline materials. (1 hr) Crystallography as a tool to understand crystalline materials: Point groups to unit cell symmetry to space groups. Structure solution from X-ray diffraction- (PXRD indexing, Understanding and interpreting Space group representation, Reciprocal Space, Structure Factor, Phase Problem, Thermal modeling). TWIN refinement and disorder modeling. Quizzes and practical tutorials on crystallography and problem solutions. (12 hrs) Adsorption concepts and application: Surface area, surface tension, contact angles. Fundamentals of adsorption; theory; isotherms, fundamental adsorption models, types of isotherms. Adsorbents: Micro, Meso and Macroporous Materials. (6 hrs) Introduction to advanced characterization techniques: Plasma and photoelectron spectroscopy and Mass Spectrometry. Includes Spectroscopy of Solid State compounds with special emphasis on X-ray Photoelectron, a vital surface characterization technique for many materials research areas. Thermal Analysis (TGA, DSC, DTA similarities and differences). (6 hrs)

Evaluation /assessment	End-Sem Examination-35% Mid-Sem Examination-30% Others-Mid-sem Quiz: 15% End-sem Quiz: 15% Paper presentation: 5%%
Suggested readings (with full list of authors, publisher, year, edn etc.)	1. "X-ray Structure Determination: A practical guide", Second Ed. Wiley Interscience, Authors: G. H. Stout and L. H. Jensen. 2. “Characterization of Porous Solids and Powders: Surface Area, Pore Size and Density” (S. Lowell et al.). Kluwer Academic Publishers, Springer. 3. "Atomic Absorption and Plasma Spectroscopy", Wiley India Ed., Second Ed., John R. Dean 4. Supramolecular Engineering: Discrete Molecular Assemblies, Comprehensive Supramolecular Chemistry II, Volume 6, 2017, Edited by Scott J. Dalgarno, Elsevier Press. 5. Inorganic Structural Chemistry, Second Edition by Ulrich Muller, 2006, John Wiley & Sons, England. 6. The Physics and Chemistry of Materials by Joel I. Gersten and Fredrick W. Smith, 2001, John-Wiley & Sons, New York. 7. Principles and Applications of Ferroelectrics and Related Materials by M. E. Lines and A. M. Glass, 1977 (reprinted in 2009), Oxford university Press, U.K. Note: Additionally, the slides will be made available online (internal) and several relevant teaching materials would be shared as pdf via online platform.