SIKKIM UNIVERSITY

(A Central University Established by an Act of Parliament of India, 2007)

LEARNING OUTCOME - BASED CURRICULUM

PH.D. (CHEMISTRY) COURSEWORK

(With effect from Academic Session 2023-24)

DEPARTMENT OF CHEMISTRY
SIKKIM UNIVERISTY
6TH MILE, TADONG - 737102
GANGTOK, SIKKIM, INDIA

Table of Contents

Sr. no	Content	Page number
1	Preamble	1
2	Programme Outcomes (POs)	1-2
3	Program Learning Outcomes (PLOs)	2
4	Structure of Ph.D. Coursework program	2
5	Course Details	3-31

1. Preamble

Through the PhD program, students embark on a transformative journey of discovery, critical thinking, and intellectual exploration. The program is characterized by its emphasis on independent and original research, supported by a strong foundation in theoretical frameworks, research methodologies, and advanced disciplinary knowledge. Students are encouraged to pursue novel research questions, explore uncharted territories, and challenge existing paradigms within their field of study.

2. Programme Outcomes (POs)

PO1: Acquisition of In-depth Knowledge: Doctoral candidate will acquire advanced and specialized knowledge in their specific field of study, as well as in allied subject areas relevant to their research.

PO2: Advanced Problem Analysis: Doctoral candidate will develop advanced skills in identifying, formulating, critically reviewing research literature, and analyzing complex problems within their field of study, demonstrating a high level of scientific rigor.

PO3: Research Investigation and Innovation: Doctoral candidate will conduct original and innovative research using advanced research methodologies, techniques, and approaches to explore and provide novel solutions to complex research problems.

PO4: Environmental and Societal Impact: Doctoral candidate will critically assess the environmental and societal implications of their research, demonstrating an understanding of sustainable development principles and promoting responsible and ethical practices in their scientific pursuits.

PO5: Ethical Conduct: Doctoral candidate will adhere to the highest standards of scientific integrity, ethics, and professional conduct, upholding the principles of responsible research and maintaining confidentiality when necessary.

PO6: Individual and Collaborative Research Skills: Doctoral candidate will demonstrate advanced skills in conducting independent research, as well as the ability to collaborate effectively with multidisciplinary teams, fostering a culture of knowledge sharing and collaboration.

PO7: Effective Scientific Communication: Doctoral candidate will effectively communicate their research findings to the scientific community and broader society through high-quality scientific presentations, publications, and reports, demonstrating strong oral and written communication skills.

PO8: Continuous Learning and Professional Development: Doctoral candidate will demonstrate a commitment to lifelong learning and professional development, actively seeking opportunities to enhance their knowledge, skills, and expertise in their field of study.

PO9: Societal Impact and Engagement: Doctoral candidate will recognize and fulfill their societal responsibility by utilizing their research outcomes and expertise to address social challenges, contribute to the well-being of communities, and actively engage with stakeholders to promote the application of scientific knowledge for the betterment of society.

3. **Program Learning Outcomes**

PLO1: Students will be able to demonstrate clear understanding of fundamental concepts, and in-depth knowledge in their specific field.

PLO2: Students will be able to demonstrate their mastery over experimental and theoretical techniques of their research filed of interest.

PLO3: Students will be able to formulate new research problems and develop strategy for its solution adding new values to their respective field.

PLO4: Students will be able to communicate and defend their research work in both written and oral form to different category of audience.

4. **Structure of PhD program**

Code	**Course Name**	**Credits**	**In-Sem Marks**	**End-Sem Marks**	**Total Marks**
CHE-C-701	Research Methodology	4	50	50	100
CHE-C-702	Research & Publication Ethics	2	25	25	50
CHE-C-703	Review of Literature & Research Proposal	2	25	25	50
CHE-E-7XY	**Elective Papers (Choose any one course from E-704 – E 712)**	4	50	50	100
CHE-E704 CHE-E705 CHE-E706 CHE-E707 CHE-E708 CHE-E709 CHE-E710 CHE-E711 CHE-E712	Advanced Physical Chemistry Advanced Topics in Organic Chemistry Bio-Inorganic Chemistry Computational Chemistry Nanomaterials and Nanotechnology Strategies in Organic Synthesis Supramolecular Chemistry Material Chemistry Concepts in Catalysis				

5. Course Details

Course Name Research Methodology **Code:** CHE-C-701

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 **=** 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): On completion of the course, students will be be able to:

1. Understand the fundamental concepts and principles of research methodology in chemistry.
2. Identify and formulate research questions and hypotheses.
3. Design appropriate experiments and methodologies for chemical research.
4. Collect, analyze, and interpret experimental data using statistical methods and software tools.
5. Evaluate and critique scientific literature.
6. Communicate research findings effectively through written articles and oral presentations.
7. Apply ethical guidelines and practices in scientific research.

Course Description: The Research Methodology in Chemistry course is designed to provide students with a comprehensive understanding of the principles, techniques, and tools required to conduct effective research in the field of chemistry. This course aims to equip students with the knowledge and skills necessary to design, plan, execute, and analyze scientific research projects. Through a combination of theoretical lectures, practical exercises, and case studies, students will gain a solid foundation in research methodology and develop critical thinking, problem-solving, and data analysis skills.

Course Outline:

Unit 1: Introduction to Research Methodology. Literature review. Understanding research questions and objectives. Recent trends in Chemistry publication. Research Formulating Hypotheses and testing. Defining variables and controls. Experimental Design. Independent, dependent, and controlled variables. Techniques for data collection in chemistry experiments. Calibration and quality control procedures. Use of SI units. Concept of moles. Preparation of solutions. Data organization and management. Writing and maintaining laboratory record book.

Unit 2: Descriptive statistics and graphical representation of data. Statistical Analysis in Chemistry Research. Interpreting experimental results. Graphical representation of data using software tools. Drawing conclusions and making inferences. Presenting data in tables. Using graphs to visualize data. Basic software for drawing chemical structure, drawing graphs, writing articles and presentation.

Unit 3: Laboratory Safety and Ethics. Importance of safety protocols in chemical research. Ethical considerations and responsible conduct of research. Institutional and government regulatory boards and compliance. Safety gears, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass ware, centrifuge safety, treated biomedical wastes. Emergency response, Chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency, accident reporting.

Unit 4: Reporting and Presenting Research Findings. Writing scientific research reports and publishing. Authorship and Publication Ethics. Creating effective oral presentations. Poster design and presentation skills.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., and Jones, A. 2002 Practical Skills in Chemistry, Pearson Education Ltd. [Prentice Hall]
2. OSU safety Manual 1.01.
3. Kothari, C. R. Research Methodology. Methods and Techniques
4. Singh, A. K. Tests, Measurements and Research Methods in Behavioural Sciences:

Course Name Research and Publication Ethics **Code:** CHE-C-702

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 1+1+0 = 2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): On completion of the course, students will be able to:

1. Understand the fundamental ethical principles and guidelines governing research and publication.
2. Identify and address ethical challenges and dilemmas that may arise during the research process.
3. Demonstrate knowledge of responsible conduct of research and research integrity.
4. Understand the importance of data management, privacy, and confidentiality in research.
5. Comprehend the ethical considerations related to human subjects, animal research, and biosafety.
6. Apply ethical guidelines to the process of authorship, acknowledgments, and peer review.
7. Recognize and manage conflicts of interest in research and publication.
8. Develop strategies for promoting ethical behavior and fostering a culture of research integrity.

Course Description: The Research and Publication Ethics course aims to provide participants with a comprehensive understanding of the ethical principles and practices involved in conducting research and publishing scholarly work. The course will cover various topics related to research integrity, responsible conduct of research, ethical considerations in data collection and analysis, authorship and publication ethics, and addressing conflicts of interest. Through interactive discussions, case studies, and practical exercises, participants will develop the knowledge and skills necessary to navigate ethical challenges in the research and publication process.

Course Outline:

Unit 1: Introduction to Research and Publication Ethics. Ethical principles and guidelines in research and publication. Historical cases of research misconduct. The importance of ethics in maintaining scientific integrity. Responsible Conduct of Research. Understanding research misconduct and questionable research practices. Data fabrication, falsification, and plagiarism. Ethical considerations in experimental design and data analysis

Unit 2: Ethical Considerations in Animal Research. Ethical guidelines for animal research. Animal welfare and minimizing harm. Alternatives to animal research. Chemical and Biosafety and Ethical consideration. Laboratory safety and risk assessment. Handling and disposal of hazardous materials

Unit 3: Authorship and Publication Ethics. Criteria for authorship and acknowledgments. Plagiarism and self-plagiarism. Duplicate publication and salami slicing. Peer Review and Editorial Processes. The role of peer review in ensuring research quality. Ethical responsibilities of peer reviewers and editors. Conflicts of interest in peer review.

Unit 4: Conflicts of Interest and Research Funding. Identifying and managing conflicts of interest. Disclosure requirements in research funding. Balancing objectivity and financial considerations. Ethics in Data Management and Sharing. Data ownership and intellectual property rights. Patents.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Research and Publication Ethics (2021) by Wakil Kumar Yadav
2. Research and Publication Ethics in Social Science 2nd Edition-2022. Sumanta Dutta.
3. Manual for Research Ethics Committees: Centre of Medical Law and Ethics, King's College London (2011) by Sue Eckstein (Editor)

Course Name Review of Literature & Research Proposal **Code:** CHE-C-703

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 1+1+0 = 2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Research

Course Learning Outcomes (CLOs): On completion of the course, students should be able to:

1. Critically evaluate and present recently published scientific research studies.
2. Identify research gaps and formulate research questions.
3. Conduct a comprehensive review of literature on a specific topic of interest.
4. Develop a detailed research proposal incorporating the literature review.
5. Present their research proposal effectively in a seminar setting.
6. Enhance their oral communication and presentation skills.
7. Strengthen their understanding of research methodology and scientific writing.

Course Description:

The Review of Literature & Research Proposal course is designed to provide students with an opportunity to enhance their research skills by critically analyzing and presenting recently published scientific research studies. Students will learn how to conduct a thorough literature review, identify research gaps, and formulate research questions. This course emphasizes active student participation and encourages students to explore diverse areas of scientific research.

Course Outline:

Unit 1: Course Introduction and Overview. Discussion on selecting research areas and topics for presentations. Students will present well-cited scientific research studies from journals with high impact factors. Topics of the presentations to be decided by students in consultation with teachers. Feedback and discussions on the presented research studies.

Unit 2: Research Proposal Development and Seminar Presentation. Introduction to research proposal development. Importance of literature review in research proposals. Guidelines for writing a comprehensive literature review. Students develop their research proposals incorporating the literature review. Preparation of research proposal and Research Proposal Seminar. Peer feedback, discussion and suggestions for improvement

Suggested-teaching learning strategy

1. Self-Study of research and review articles
2. Presentations and Seminars
3. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Research proposal writing	Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	Seminar		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings: Cited scientific research studies and reviews from journals with high impact factors.

Course Name Advanced Physical Chemistry **Code:** CHE-E-704

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs): Upon completion of this course, students will be able to:

1. Explain the concepts of internal heat, entropy production, and their relationship with fluxes and forces in chemical systems.
2. Apply phenomenological equations and understand the Onsager reciprocal relation in the context of irreversible thermodynamics.
3. Analyze non-equilibrium stationary states using Prigogine's principle of minimum entropy production.
4. Utilize scattering techniques and potential energy surfaces to investigate molecular collision dynamics.
5. Understand experimental techniques such as molecular beam and chemiluminescence techniques for studying reaction dynamics.

6. Apply trajectory calculations and state-to-state kinetics in the analysis of molecular collisions.
7. Comprehend the properties of lasers and their applications in reaction kinetics, including the study of fast and ultrafast reactions.
8. Demonstrate knowledge of techniques such as flow and stopped-flow techniques, relaxation techniques, and pump-probe techniques in the study of reaction kinetics.
9. Explain the properties and functions of biopolymers, biomembranes, and their role in biochemical processes.
10. Understand active and passive transport processes and multiple equilibria in biochemistry.
11. Analyze self-organizing systems and their interactions, including micelles, lipids, cyclodextrins, liquid crystals, reverse micelles, coacervates, and proteins.
12. Apply various surface and biophysical

Course Description: This course provides a comprehensive understanding of various concepts and principles in irreversible thermodynamics, molecular collisions, lasers in reaction kinetics, and thermodynamics in biochemistry.

Course Outline:

Unit 1: Irreversible Thermodynamics: Internal heat and entropy production; Relation of entropy production with Fluxes & Forces; Phenomenological equation; Onsager reciprocal relation; Prigogine's principle of minimum entropy production at non equilibrium stationary state.

Unit 2: Molecular collisions: Scattering as a probe of collision dynamics, Potential energy surface, Experimental techniques in reaction dynamics: molecular beam and chemiluminescence techniques, trajectory calculations, state to state kinetics, some case studies.

Unit 3: Lasers: its properties and applications in reaction kinetics, Techniques for the study of fast and ultrafast reactions: Flow and stooped flow technique, relaxation technique, pump-probe technique , single photon counting and fluorescence up- conversion techniques, femtochemistry.

Unit 4: Thermodynamics in Biochemistry (Fundamentals and Applications): Biopolymers (Proteins, Enzymes, DNA, Carbohydrates); Biomembranes (Structure and Function); Active transport and passive transport, Multiple equilibria, Specific examples of multiple equilibria, Transport processes; General features of transport processes; Optical systems for the study of transport processes. Self organizing systems (Micelles, Lipids. Cyclodextrins, Liquid crystals, Reverse micelles, coacervates, Proteins etc) their interactions and solutions properties. Preparation, Characterization and Application of nanoparticles Surface and Biophysical Techniques: CD, SEM, TEM, EDAX, DLS, Gel Electrophoresis, Radioactivity, XPS.

Suggested teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Prigogine, I. Introduction to Thermodynamics of Irreversible Processes.
2. Levine, R.D. and Bernstein, chemical kinetics and dynamics Molecular Reaction Dynamics and Chemical Reactivity, Oxford
3. Cantor, C. R. Schimmel, P. R. Biophysical Chemistry: Part I: The Conformation of Biological Macromolecules.
4. Cantor, C. R. Schimmel, P. R. Biophysical Chemistry: Part II: Techniques for the Study of Biological Structure and Function
5. Cantor, C. R. Schimmel, P. R. Biophysical Chemistry: Part III: The Behavior of Biological Macrolmolecules Somorjai, G.A. Li, Y. Introduction to Surface Chemistry and Catalysis

Course Name: Advanced Topics in Organic Chemistry **Code:** CHE-E-705

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs): Upon completion of this course, students will be able to:

1. Demonstrate an understanding of various synthetic approaches to drug discovery, such as total synthesis, combinatorial synthesis, and diversity-oriented synthesis.
2. Evaluate the importance and applications of current topics in organic synthesis, including photoredox catalysis, C-H activation, photo-electrochemistry, organocatalysis, and continuous flow chemistry.
3. Critically analyze the concepts of molecular asymmetry and dissymmetry and determine absolute configurations of chiral molecules.
4. Evaluate different methods for introducing chirality and generating new chiral centers in molecules, including asymmetric synthesis using chiral substrates, chiral auxiliaries, chiral reagents, and chiral catalysts.
5. Describe the principles of green chemistry and its application in organic synthesis, including the use of green synthetic methods, catalysis, organics reactions in aqueous media, ionic liquids, supercritical fluids, microwave radiation and solid phase synthesis.
6. Apply the principles of green chemistry in organic synthesis, including the use of catalysis, organic reactions in aqueous media, ionic liquids, supercritical fluids, and microwave radiation. Apply solid-phase organic reactions and catalysis in synthetic chemistry.
7. Apply spectroscopic techniques (UV, IR, PMR, CMR, 2D NMR, and Mass spectrometry) for structure elucidation and analysis in multi-step synthesis and reaction monitoring.
8. Integrate multiple spectroscopic techniques for comprehensive analysis and structure elucidation of organic compounds.

Course Description:

The students will learn diverse synthetic techniques and advantage and disadvantage of the processes. Different aspects of stereoselective synthesis and pros and cons of different strategies will be dealt in detail. Different aspects of green chemistry with special emphasis on solid state synthesis will be taught. Various types of spectroscopic techniques used in monitoring of reaction and elucidation of structure will dealt in detail.

Course Outline:

Unit: 1

Unit I: Various synthetic approaches to drug discovery:

Total synthesis, Combinatorial synthesis, Diversity oriented synthesis and their importance, utilities, advantages and disadvantages.

Introduction and potential uses of current topics in organic synthesis like Photoredox catalysis. C-H activation, Photo-electro chemistry, Organocatalysis, Continuous flow chemistry

Unit II: Special topics on stereoselective synthesis:

General consideration of molecular asymmetry and dissymmetry, Determination of Special chiralities- axial, planner and helical chiralities, determination of their absolute configurations and uses in stereoselective synthesis

Different methods to introduce chirality or generate new chiral centres in a molecule. Asymmetric synthesis using chiral substrate, chiral auxiliaries, chiral reagents and chiral catalysts with various examples. Advantages and disadvantages of each of these techniques., Application of each of these techniques in synthesis of various natural products.

Unit III: Green Chemistry and solid phase reactions

Green Chemistry: Overview. Set of principles of green chemistry, green synthetic methods, catalysis, organics reactions in aqueous media, ionic liquids, supercritical fluids and under microwave radiations. Solvent free organics reactions, solid phase organics reaction and catalysis.

Unit IV: Advances in the Application of Spectroscopic Techniques in organic synthesis

Application of different spectroscopic methods like UV, IR, PMR, CMR, 2D NMR and Mass spectrometry.in multi-step synthesis and reaction monitoring. Structure elucidation through the combined use of spectroscopic techniques for comprehensive analysis

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Combinatorial Chemistry: From Theory to Application, Volume 26, Second Revised Edition; Willi Bannwarth, Berthold Hinzen; Wiley-VCH Verlag GmbH & Co. KGaA, 2006
2. Diversity-Oriented Synthesis: Basics and Applications in Organic Synthesis, Drug Discovery, and Chemical Biology Andrea Trabocchi, Wiley, 2013
3. Organic chemistry; Clayden, J., Greeves, N. , Warren, S. and Wothers, P.; Oxford University Press, 2000
4. Multicomponent Reactions in Organic Synthesis; Jieping Zhu, Qian Wang, Mei-Xiang Wang; WileyVCH Verlag GmbH & Co. KGaA, 2015
5. Advanced Organic Chemistry; 5th Ed. Carey F. A. and Sundburg R. J.; Springer, 2007 9.Strategic Applications of Named Reactions in Organic Synthesis; Laszlo Kurti Barbara Czako; Academic Press; 2005
6. Name Reactions and Reagents in Organic Synthesis, Second Edition; Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, Jr; John Wiley & Sons, Inc., 2013
7. C-H Bond Activation in Organic Synthesis; Jie Jack Li; CRC Press 2015
8. Photoredox Catalysis in Organic Chemistry, Megan H. Shaw, Jack Twilton, and David W. C. MacMillan J. Org. Chem., 2016, 81 (16), pp 6898–6926
9. Stereochemistry of Organic Compounds,.Eliel E.L. and Wilen, S.H., Wiley Interscience, New York, 1994
10. Classics in Stereoselective Synthesis, Wiley, Erick M. Carreira, Lisbet Kvaerno 2008
11. Green Chemistry: An Introductory Text:, Lancaster, M. Royal Society of Chemistry; 2002

12. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 4th Ed. Cengage Learning, 20082. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, David Kiemle, David L. Bryce; 8th Ed. John Wiley and Sons. 2014
13. A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, Wiley, 1997
14. High-Resolution NMR Techniques in Organic Chemistry 3rd Edition Timothy D.W. Claridge Elsevier Science, 2016
15. Solving Problems with NMR Spectroscopy, 2nd Edition; Atta-ur-Rahman Muhammad Choudhary Atia-tul- Wahab; Academic Press, 2015
16. Organic Structures from Spectra, Fifth Edition, L D Field, S Sternhell, J R Kalman John Wiley and Sons Ltd. 2015
17. Organic Structure Determination Using 2-D NMR Spectroscopy, A Problem-Based Approach Jeff rey H. Simpson, Academic Press, 2008
18. Mass Spectrometry in Medicinal Chemistry; Klaus T. Wanner, Georg Ho¨fner, Wiley, 2007

Course Name Bio-Inorganic Chemistry **Code:** CHE-E-706

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 **=** 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcome (CLOs): Upon completion of this course, students will be able to:

1. Understand the storage and transport mechanisms of essential metals in biological systems.
2. Explain the role of metals in biomineralization and their significance in biological processes.
3. Analyze the redox components involved in energy storage and release, and understand the principles of electron transfer rates and cross reactions.
4. Explain the mechanisms of long-range electron transfer in proteins and the modification of metalloproteins.
5. Understand the transport processes through biological membranes, including anion and cation carriers, electron-coupled transport, proton-coupled transport, and light-driven transport.
6. Analyze the chemistry and biological functions of biological oxygen carriers and

Course Description:

Students will delve into various topics, including the storage and transport of essential metals, biological redox components, oxygen carriers, coordination and intercalation with nucleic acids, and the impact of metal deficiency and toxicity on human health.

Course Outline:

Unit 1: The storage of iron, zinc, copper, vanadium, chromium, molybdenum, cobalt, nickel, and manganese. Transport of Iron, Zinc, copper, vanadium, chromium, molybdenum, and cobalt. Iron Biomineralization

Unit 2: Biological Redox Components. Energy Storage and Release, Coupling Electron Transfers and Substrate Activation. Electron- transfer rates: Self-Exchange and Cross Reactions, Marcus Theory, Cross reactions of blue copper proteins. Long-range electron transfer in proteins. Modified Metalloproteins Transport through membranes, Anion and cation carriers; Coupled transport processes; Electron coupled transport; Proton coupled transport; Light driven transport; Transport via transmembrane channels.

Unit 3: Biological Oxygen Carriers. Haemoglobin, hemocyanin, and hemerythrin. Redox chemistry of free molecular dioxygen. Geometry and electronic structure of coordinated dioxygen. General aspects of chemistry of dioxygenwith iron, copper and cobalt. Other Ligands for Biological Oxygen Carriers: carbon monoxide, nitric oxide, Isocyanide and nitroso species, Iron-sulfur proteins and models. Multi-site redox enzymes: Hydrogenase and Nitrogenase. Biological nitrogen fixation. FeMo cofactor

Unit 4: Coordination, Intercalation and hydrogen bonding.Fundamental Reactions with Nucleic Acids: redox and hydrolytic chemistry. A case study: tris(phenanthroline) metal complexes. Binding Interactions with DNA. Techniques to Monitor binding. Applications of different metal complexes that bind nucleic acids Nature's use of metal/nucleic-acid interactions. Metal deficiency and disease. Toxic effects of metals, Metals used in diagnosis and chemotherapy. A case study of cis-Platin.

Suggested-teaching learning strategy

5. Lecture with interactive discussions and problem-solving activities.
6. Assignments and individual presentations.
7. Student-led classroom teaching.
8. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home	Oral Test, Viva-Voce, Seminar	Presentation, Seminars

	Assignment		
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings

1. Hughes, M. N. 1981, Inorganic Chemistry of Biological Processes, 2nd Ed.John-Wiley & Sons, New York
2. Kaim, W. and Schwederski, B. 1995 Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York
3. Lippard, S. J. and Berg, J. M. 1994 Principles of Bioinorganic Chemistry, University Science Books,
4. Bertini, I., Grey, H. B., Lippard, S. J. and Valentine, J. S. 1998 Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi
5. Mukherjee, G. N. and Das, A. Elements of Bioinorganic Chemistry

Course Name: Computational Chemistry **Code:** CHE-E-707

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs): Upon completion of this course, students will be able to:

1. Apply Monte Carlo and Molecular Dynamics simulations to understand physical and chemical transformations.
2. Utilize quantum chemistry methods and software for calculating properties and understanding molecular interactions.
3. Understand basic principles of molecular biology and apply computational modeling in drug design.
4. Use simulation software for performing classical simulations and visualize simulation results.
5. Write computer programs in C++, FORTRAN, and Python for solving chemistry problems.
6. Apply parallel programming techniques for efficient computational tasks.

Course Description:

Students will learn various simulation techniques, including Monte Carlo and Molecular Dynamics simulations, and their applications in understanding physical and chemical transformations. The course also covers quantum chemistry methods, molecular biology principles, and computer programming languages commonly used in computational chemistry.

Course Outline:

Unit 1: Monte Carlo, Molecular Dynamics simulations and its applications to understanding of physical and chemical transformations Methods based on Hartree-Fock, Configuration Interaction, Deriving one and two electron properties, Semi-empirical methods, Coupled Cluster theory, Density functional theory, TDDFT. QM/MM methods

Unit 2: Basic molecular biology: Basic principles of biochemistry, energy conversion, enzymatic catalysis, and active transport, enzyme models, drug design, computational modeling.

Unit 3: Introduction to Classical Monte Carlo Molecular Dynamics Simulation and Softwares - DLPOLY, GROMACS, TOWHEE, NAMD.Introduction to Quantum chemistry softwares – NwChem, Gaussian.Visualization softwares – VMD, Povray.

Unit 4: Computer programming languages: C++, FORTRAN. Python, Shell scripting. Writing Monte Carlo, Molecular Dynamics codes for chemistry problems. Parallel programming techniques like Open MP, MPI

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings

1. Pople, J.A. and Beveridge, D.L. 1971 Approximate Molecular Orbital Theory, McGraw Hill, New York
2. Parr, R.G. and Yang, W. 1989 Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford Longman, A. L. 1996 Molecular Modelling, London.
3. Hunt, R. and Shelley 1998 Computers and Common Sense, Prentice Hall, New Delhi
4. Rajaraman, V 1990 Computer Programming in Fortran-90 Prentice Hall, New Delhi
5. Dickson, T. R. 1968 Computer and Chemistry: introduction to programming and numerical methods
6. Detar, D. F. Benjamin, W. A. Computer programs for chemistry 1968-1969 New York Vol. 1-3
7. Jensen, F. 1999 Introduction to Computational Chemistry, John Wiley, New York.
8. Cramer, D. Wiley, J. 2002 Computational Chemistry (Theories and Models), New York.
9. Frenkel, D. and Smit, B. Understanding Molecular Simulation: From Algorithms to Applications
10. Allen, M. P. and Tildsley, D. J. Computer Simulation of Liquids

Course Name: Nanomaterials and Nanotechnology **Code:** CHE-E-708

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learniong Outcomes (CLOs): Upon completion of this course, students will be able to:

1. Understand the fundamental properties of nanomaterials, including their surface to volume ratio, crystal structures, and size-dependent electrical, magnetic, and optical properties.
2. Explain the synthetic approaches for preparing nanomaterials, including top-down and bottom-up methods, colloidal growth, and functionalization techniques.
3. Demonstrate knowledge of characterization techniques used for nanomaterials, including basic characterization methods and specialized techniques for specific nanomaterials.
4. Analyze the properties and applications of different nanomaterials, including metal, metal oxide, semiconductor nanoparticles, carbon nanotubes, graphene, and fullerene.

5. Evaluate the electrochemical behavior of colloidal nanoparticles and understand band gap engineering in semiconductor nanocrystals.
6. Explore the applications of nanomaterials in various fields, such as drug delivery, catalysis, imaging, photovoltaics, and nanotoxicology.
7. Apply quantum mechanical principles to model problems related to quantum wells, wires, and dots, including density of states and interband transitions.
8. Critically analyze recent advances in the synthesis of new nanomaterials and their synthetic strategies.

Course Description: The course provides an in-depth exploration of nanomaterials and their applications in various fields. Students will learn about the fundamental properties of nanomaterials, synthetic approaches for their preparation, characterization techniques, and their wide range of applications. The course covers topics such as surface to volume ratio, crystal structures, synthetic approaches (top-down and bottom-up), functionalization, and properties of different nanomaterials including metal, metal oxide, semiconductor nanoparticles, carbon nanotubes, graphene, and fullerene. Students will also explore the electrochemistry of colloidal nanoparticles, band gap engineering, self-assembled nanostructures, and the applications of nanoparticles in drug delivery, catalysis, imaging, photovoltaics, and more. Additionally, the course introduces students to quantum wells, wires, and dots, density of states, and interband transitions.

Course Outline:

Unit 1: Introduction, Surface to volume ratio, crystal structures, basic properties. Length scale: de Broglie wavelength, Bohr radius, excitons, confinement regimes, The Fermi Energy, Kubo Gap, the mean free path in metals, charging energy. Size and shape-dependent electrical, magnetic and optical properties of metal, metal oxide and semiconductor nanoparticles. Quantum size effect, Superparamagnetism, Surface Plasmon resonance.

Unit 2: Synthetic approaches: Top down and bottom up. Colloidal growth. Chemical synthesis, Classical Theory, Monodispersity, Lamer Plot, Ostwald ripening, Digestive Ripening Homogeneous vs. heterogeneous nucleation and applications of nanomaterials, Anisotropic growth and shape control, Catalyzed (seeded) growth, Nanocrystal doping, solid solutions and Vegard's rule. Non-classical growth. Effect of precursor reactivity and stability on size. Unusual precursor kinetics in III-V semiconductor nanocrystal formation. Functionalisation and basic characterisation of metal, metal oxide and semiconductor nanoparticles. Core-shell / multishell nanoparticles. Properties and synthesis of Carbon nanotubes, grapheme, fullerene. Recent advances in synthesis of new materials and their synthetic strategies. Characterization of nanomaterials.

Unit 3: Properties and Application Electrochemistry of colloidal nanoparticles.Band gap engineering in semiconductor nanocrystals, Carbon based nanoparticles, self assembled nanostructures. Atom and molecule manipulation. Application of nanoparticles in drug delivery, biological imaging of cellular and subcellular structures, catalysis, sensor, tracer, cancer treatment, photovoltaics, single molecule detection and LED. Introduction to nanotoxicology.

Unit 4: Model problems for quantum wells, wires and dots Density of states. Quantum mechanical review; wavefunction, Schrodinger equation, Bands; The Kronig-Penny Model, metals, semiconductor, insulators; Interband transition.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings

1. Kuno, M. Introductory Nanoscience, 2011, Taylor & Francis Group.
2. Rigach, A. L. (Editor), Semiconductor nanocrystal quantum dots: synthesis, assembly and applications
3. Klimov, V. I. Semiconductor and Metal Nanocrystals: Synthesis and Electronic and Optical Properties (Optical Science and Engineering)

4. Thanh, N.T. K. and Sayed, M. A. 2012 El Magnetic Nanoparticles: From Fabrication to Clinical Applications
5. Huck, W. T. and Huck, Wilhelm T. S. (Editor) Nanoscale Assembly: Chemical Techniques
6. Dresselhaus, M. S, Dresselhaus, G. and Avouris, P. Springer-Verlag. Carbon Nanotubes : Synthesis, Structure, Properties, and Applications
7. Acklin, B. and Lautens, E. Magnetic Nanoparticles: Properties, Synthesis and Applications
8. Taurozzi, J. S 2011 Nanoparticle-polymer composite membranes: Synthesis, characterization, and environmental applications.
9. Karn, B. Colvin, V. and Alivasatos, P. 2004 Nanotechnology and the Environment.
10. Zhou, B. Hermans, S., Somorjai, G. A. (Editors)Nanotechnology in Catalysis Volumes 1 and 2

Course Name: Strategies in Organic Synthesis **Code:** CHE-E-709

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs): Upon completion of the course students will be able to:

1. Demonstrate a comprehensive understanding of advanced synthetic methods, reagents, and intermediates in organic synthesis.
2. Apply the knowledge and principles learned to design efficient synthetic routes and execute complex organic transformations.
3. Analyze and predict the outcomes of reactions based on mechanistic understanding and stereochemical considerations.
4. Apply retrosynthetic analysis to plan and execute the synthesis of complex molecules.
5. Critically evaluate and select appropriate synthetic strategies based on considerations such as yield, availability of synthones, and reaction mildness.
6. Design and carry out total syntheses of natural products using the principles of retrosynthetic analysis and synthetic strategies.

Course Description:

Strategies in Organic Synthesis is a comprehensive course that explores advanced techniques and principles in organic synthesis. With a focus on designing efficient synthetic routes and executing complex transformations, students will delve into topics such as C-C bond formation, advanced reagents and intermediates, stereochemistry, asymmetric synthesis, and retrosynthetic analysis. Through 60 lectures, students will gain expertise in applying various strategies, evaluating synthetic pathways, and conducting total syntheses of natural products. This course provides a solid foundation for students pursuing research careers in synthetic organic chemistry and related fields.

Course Outline:

Unit 1: Advances in C-C bond formation: Reaction by Organometallic Reagents, Sigmatropic Rearrangements, Pericyclic reactions, reactions of carbenes, Benzyne, Coupling reactions – Heck, Suzuki, and related, Wittig, Tebbes, Petasis, Grubbs, Peterson reactions, Simmon-smith reactions, radical reaction, Umpolung reactions

Unit 2: Advance reagents and intermediates in organic synthesis: Hetero-atom alkylation or acylation, Nucleophilc substitution or addition by hereoatom nucleophiles, Mitsunobu reaction, pericyclic reactions, nitrenes. Reagents for Oxidation, Reduction, elimination, addition, organo silicon, organotin reagents, organo boron, organo-phosprus, organosulfur, organoselenium, Titanium, Fluorinating agents, Important starting materials and intermediates.

Unit3: Advanced stereochemistry and asymmetric synthesis:Methods of determination atropisomerism of biphenyls, quasiracemates, dynamic stereochemistry, Axial chirality, planar chirality, helical chirality, determination of absolute configuration, Conformational analysis based on physical properties and chemical reactivity, shape of small and medium ring,Steroselectivity Asymmetric synthesis using chiral pool, chiral auxiliaries, chiral reagents and chiral catalysts.

Unit 4: Retrosynthetic analysis and selected total synthesis: Retrosynthetic strategies: Transform-Based Strategies, Structure-Goal Strategies, Topological Strategies, Stereochemical Strategies, Functional Group-Based Strategies. Choosing one path over other: Consideration of yield, availability of synthone, mildness of any reaction, Retrosynthesis and total synthesis of various natural products.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Advanced Organic Chemistry, Fourth Edition, Part A and B by F.A.Carey and R.J.Sundberg
2. Organic Chemistry by Clayden, Greeves,Warren and Wothers
3. Advanced organic chemistry by J. March, 6th Ed.
4. Some modern methods of organic synthesis – W. Carruthers (Cambridge) Stereochemistry of carbon compounds - E. L. Eliel
5. Stereochemistry of Organic compounds – D. Nasipuri
6. Organic Synthesis: Concepts and Methods, 3rd Edition,Jürgen-Hinrich Fuhrhop, Guangtao Li, E. J. Corey
7. Organic Synthesis: Concepts, Methods, Starting Materials, 2nd Edition, Jürgen-Hinrich Fuhrhop, Gustav Penzlin
8. Workbook for Organic Synthesis: The Disconnection Approach, Paul Wyatt, Stuart Warren
9. Organic Synthesis: Strategy and Control, Paul Wyatt, Stuart Warren
10. Classics in Stereoselective Synthesis, Erick M. Carreira Lisbet Kvaerno
11. Main Group metals in organic synthesis, Hisashi Yamamoto and Koichiro Oshima
12. Modern Fluoro-organic Chemistry Synthesis, Reactivity, Applications by Peer Kirsch
13. Fluorine Chemistry for Organic Chemists: Problems and Solutions MILOS HUDLICKY
14. The Total Synthesis of Natural Products (Vol 1-9) -- John ApSimon
15. Reagents, auxiliaries, and catalysts for C-C bond formation, Hand book of Reagents for Organic Synthesis by Robert M. Coates, Scott E. Denmark
16. Oxidising and reducing agents, Hand book of Reagents for Organic Synthesis by Steven D. Burke, Rick L. Danheiser

17. Acidic and basic reagents, Hand book of Reagents for Organic Synthesis by Hans J. Reich, James H. Rigby
18. Activating agents and protecting groups, Hand book of Reagents for Organic Synthesis by Anthony J. Pearson, William R. Roush
19. Chiral Reagents for Asymmetric Synthesis, Hand book of Reagents for Organic Synthesis by A. Leo Paquette.
20. Organic synthesis by M. B. Smith
21. The Logic of Chemical Synthesis by E. J. Corey and X.-M. Cheng.
22. The Molecules that change the world by K.C. N

Course Name: Supramolecular Chemistry **Code:** CHE-E-710

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs): Upon completion of the course students will be able to:

1. Demonstrate understanding of various forces involved in construction of supramolecular assemble
2. demonstrate understanding of concepts of self-assembly use for construction of various class of supramolecules and apply for generating new supramolecular assemblies
3. Describe synthesis of various class of supramolecules.
4. Demonstrate understanding of concepts of supramolecular catalysts and its advantages
5. demonstrate understanding of porphyrin chemistry and its applications
6. Explain importance of supramolecular chemistry in biological systems
7. Demonstrate understanding of various classes of solid state host-guest systems
8. Construct new supramolecular assemblies and demonstrate understanding of applications of various supramolecular systems in diverse fields

Course Description

This course provides a comprehensive understanding of supramolecular chemistry, focusing on the construction and applications of various supramolecular assemblies. Students will explore the forces involved, self-assembly concepts, synthesis methods, supramolecular catalysts, porphyrin chemistry, biological systems, solid-state host-guest systems, and the construction of new supramolecular assemblies. Through a combination of theoretical knowledge and practical skills, students will gain the ability to apply supramolecular chemistry principles in diverse fields.

Course Outline

Unit 1: Quantification of non-covalent forces and medium effects Host design; Preorganization; Enthalpy and entropic contributions; Cooperativity and allosteric effects; Induced fit; Complexation selectivity. Introduction, Proteins and Foldamers: Single Molecule Self-Assembly, Biochemical Self- Assembly, Self-Assembly in Synthetic Systems: Kinetic and Thermodynamic Considerations, Self-Assembling Coordination Compounds, Self-Assembly of Closed Complexes by Hydrogen Bonding, Catenanes and Rotaxanes, Helicates and Helical Assemblies, Molecular Knots

Unit 2: Lariat ethers and podands, Crown ethers, cryptands, calyx[n]arenes, cucurbit[n]urils, spherands; Selectivity of Cationc omplexation; Macrocyclic, macrobicyclic and template effects Concepts in anion host design; Guanidinium-based receptors; Organometallic receptors; Neutral receptors; Hydride sponge; Anticrowns; Biological Anion receptors Binding by cavitands, cyclodextrins, cucurbit[n]urils, dendrimers, molecular clefts and tweezers, cyclophane Hosts

Unit 3: Catalysis by cation, anion and neutral receptors. Supramolecular metallocatalysis; Cocatalysis; Biomolecular and abiotic catalysis. Biological Inspiration for Supramolecular Chemistry, Alkali Metal Cations in Biochemistry, Porphyrins and TetrapyrroleMacrocycles, Supramolecular Features of Plant Photosynthesis. Uptake and Transport of Oxygen by Haemoglobin, Enzymes and Coenzymes, Neurotransmitters and Hormones, DNA.

Unit 4: Solid-State Host-Guest Compounds. Clathrate Hydrates, Urea and ThioureaClathrates, Other Channel Clathrates, Hydroquinone, Phenol, Dianin's ompound and the Hexahost Strategy, Tri-o-thymotide, Cyclotriveratrylene, Inclusion Compounds of the Calixarenes, Solid-Gas and Solid-Liquid Reactions in Molecular Crystals. Introduction, Supramolecular Photochemistry, Information and Signals: Semiochemistry and Sensing, Molecule-Based Electronics, Molecular Analogues of Mechanical Machines, Nonlinear Optical Materials.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Steed, J. W. and Atwood, J. L. Supramolecular Chemistry John Wiley and Sons, Ltd.
2. Lehn, J.–M. Supramolecular Chemistry-Concepts and Perspectives, VCH.
3. Schnider. H.-J. and Yatsimirsky, A.K. Principles and Methods in Supramolecular Chemistry John Wiley and Sons, Ltd.
4. Bianchi, A., James, K. B. and Garcia-Espana, E. Supramolecular Chemistry of anions, Wiley-VCH.
5. Teikink, E. R. T. and Vittal, J. J. Frontiers in Crystal Engineering.
6. Steed, J. W. and Atwood, J. L. Encyclopedia of Supramolecular Chemistry.
7. Cragg, P. J. A Practical Guide to Supramolecular Chemistry.

Course Name: Material Chemistry **Code:** CHE-E-711

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 **= 4** Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Outcomes (CLOs):

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

1. Apply knowledge of solid-state chemistry principles to analyze and identify the nature of bonding in solid state compounds.
2. Classify compounds based on binary and tertiary composition and characterize defect in solids.
3. Compare and differentiate different reaction methods and their correct application for synthesis of divergent solid materials.
4. Recognize reactivity difference and phase transformation in materials.

Course Description:

Chemistry of materials provides an in-depth exploration of the chemistry of inorganic materials, with a focus on solid-state chemistry. Students will gain a comprehensive understanding of the principles, preparation technique, reactivity and applications of inorganic materials .

Course Outline:

Unit I. Introduction to Materials chemistry: Metallic, covalent and ionic solids; structural classification of binary and tertiary compounds. Non-stoichiometry in material solids: Oxygen deficient oxides, metal deficient oxides and classification of non-stoichiometry. Crystal defects: Types of defects: Point defects; Dislocations: Line defects and Plane defects.

Unit II. Materials preparation techniques: Ceramic method, Different wet chemical methods: For Powder materials: Co-precipitation, Precursor, Combustion, Sol-gel, Spray roasting, Freeze drying. For Single crystals: i) Growth from melt ii) Flux method iii) Epitaxial growth of single crystal thin films: Chemical and Physical methods iv) Chemical vapour transport v) Hydrothermal method vi) Dry high pressure method. Amorphous Materials & Nanomaterials.

Unit III. Reactivity of Solid Materials: Tarnish reactions, decomposition reaction, solid-solid reactions, addition reactions, double decompositions reaction, electron transfer reaction, solid-gas reactions, intering, factors influencing reactivity of solids.

Unit IV. Phase Transformations in Solid Materials: Thermodynamic consideration, structural change in phase transformation, Martensite transformation, temperature and pressure induced transformations, order- disorder transitions, electronic transition, transformation with a change in composition.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings

1. D. K. Chakraborty, Solid State Chemistry, New Age International Publisher, New-Delhi, 2010, 2nd Ed.

2. H. V. Keer, Principles of the Solid State, New Age International (P) Ltd., New-Delhi, (Wiley Eastern Ltd, New-Delhi), 1993, 1st Ed. (Reprint 2005).

3. C. N. R. Rao & K. J. Rao, Phase Transitions in Solid, McGraw Hill, New York, 1977, 1st Ed.

4. W. D. Callister, Material Science and Engineering: An Introduction, John Wiley, New York, 2007, 7th Ed.

5. B. D. Fahlman, Materials Chemistry, Springer, Netherlands, 2011, 2nd Ed. 9. Harry R. Allcock, Introduction to materials Chemistry, John Wiley & Sons, 2011, 1 st Ed.

Course Name: Concepts in Catalysis **Code:** CHE-E-712

Semester: I **Course Level:** 700 **Total Marks:** 100

L+T+P: 3+1+0 **= 4** Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs): Upon completion of this course, students will be able to:

1. Understand the fundamental concepts in catalysis.
2. Explain synthetic approaches for the development of catalytic system both for homogeneous and heterogeneous system.
3. Demonstrate knowledge of characterization techniques used for identifying catalytic process including reaction intermediates.
4. Analyze the properties and applications of different types of catalyst such as nanocatalysts, including metal, metal oxide, metal complexes, zeolites and MOF.
5. Critically analyze recent advances in the development of new catalysts and their synthetic strategies.

Course Description: The course will provide background and current theories in catalysis and the applications of catalyst compounds in chemical reactions and industries. The course would provides an in-depth study of divergent catalytic systems where students would learn about the fundamental concepts in catalysis. The synthetic approaches for the preparation of catalyst, characterization techniques, and their wide range of applications.

Course Outline:

Unit 1: Origin and development of catalysis: Difference between heterogeneous, homogeneous, auto and photocatalysis, Photocatalysis, catalytic polymerizations, phase transfer catalysis and biocatalysis with suitable examples. Importance of heterogeneous and homogeneous catalysts in chemical reactions. Theories of Catalysis: Boundary layer theory, Catalysis by semiconductors, Wolkenstein theory, Balanding's approach. Activity and life of the catalysts, active centers, promoters and poisons, catalyst deactivations.

Unit 2: Heterogeneous Catalysis: Adsorptions: Physical and chemical adsorption, dissociative adsorptions. Types of heterogeneous Catalysts, Preparations of the Catalysts, significance of zeolites and supported catalysts. Characterization of solid catalysts: Surface area, structure and surface morphology, X-ray diffraction, SEM, TEM, X-ray absorption spectroscopy, XPS and Auger spectroscopy to surface studies. Heterogeneous reactions: Thermodynamic consideration in surface reactions, ammonia synthesis, oxidation reduction reactions (selected examples), mechanism of catalytic reactions, method of finding rate of the reactions and the rate determining steps.

Unit 3: Homogeneous Catalysis: Intermediate stages in homogenous Catalysis, energy profile diagram, general scheme for calculating kinetics of reactions, decomposition of hydrogen peroxide, acid-base catalysis.

Unit 4: Catalysts for energy and environmental: Catalytic gasification, steam reforming, auto-industrial emission control and fuel cells.

Suggested-teaching learning strategy

5. Lecture with interactive discussions and problem-solving activities.
6. Assignments and individual presentations.
7. Student-led classroom teaching.
8. Group discussions.
9.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested Readings:

1. Masel, Richard I (2001). *Chemical Kinetics and Catalysis*. New York: Wiley-Interscience.

2. Wei, Hui; Wang, Erkang (June 21, 2013). "Nanomaterials with enzyme-like characteristics (nanozymes): next-generation artificial enzymes". *Chemical Society Reviews*. **42** (14): 6060–6093. 93.

3. B.A. Averill, J.A. Moulijn, R.A. van Santen, P.W.N.M. van Leeuwen, Catalysis: An Integrated Approach, 2nd Edition, Elseiver (1999)

4. Jens K Nørskov & Felix Studt, Fundamental Concepts in Heterogeneous Catalysis, Wiley; 1st edition (2014)

5. M. Albert Vannice, Kinetics of Catalytic Reactions, Springer; (2005)

6. Henry Wise & Jacques Oudar Material Concepts in Surface Reactivity and Catalysis, Dover Publications (2002)
7. S. L. Scott, C. M. Crudden, C. W. Jones, Nanostructured Catalysts, Springer (2003).