J. C. Bose University of Science and Technology, YMCA, Faridabad

(Established by Haryana State Legislative Act No. 21 of 2009 & Recognized by UGC Act 1956 u/s 22)

Accredited 'A+' Grade by NAAC

Doctor of Philosophy - Chemistry

Ph. D. Chemistry (901)

Program Introduced in 2017

Pre-Registration Course Work (Revised) w.e.f. 2026-2027

Department of Chemistry, Faculty of Sciences

J. C. Bose University of Science and Technology, YMCA, Faridabad

Sector-6, NH-2, Faridabad-121006 Haryana (India)

Program Vision and Mission

Vision:

To advance transformative chemical research that drives scientific excellence, innovation, and sustainable societal development.

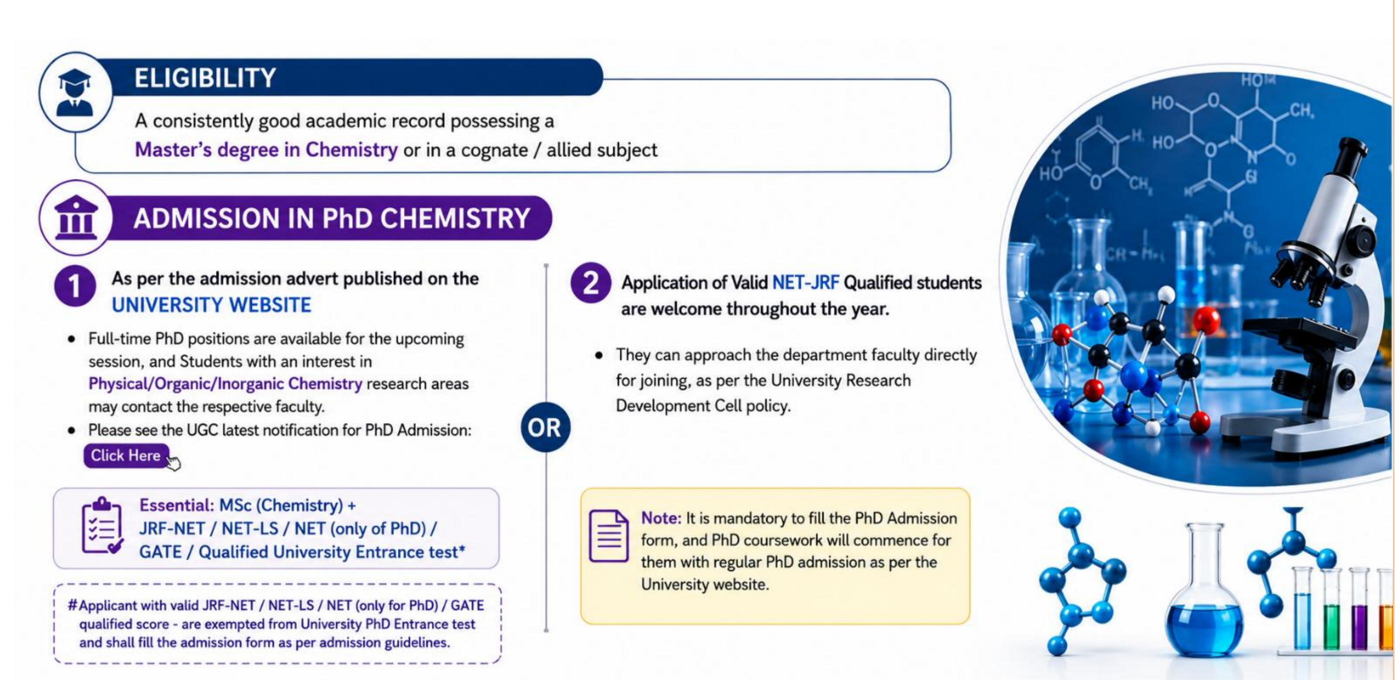
Mission:

To nurture globally competent researchers through interdisciplinary education, cutting-edge research, ethical scientific practices, and impactful innovations addressing emerging challenges in health, energy, materials, and the environment.

Program Objectives

1. To cultivate high-quality doctoral research in frontier areas of chemistry through rigorous scientific inquiry and innovation.
2. To promote interdisciplinary collaborations integrating chemistry with materials science, energy, health, environment, and computational sciences.
3. To develop skilled researchers and academic leaders equipped with advanced experimental, computational, and analytical expertise.
4. To encourage translational research, entrepreneurship, and industry engagement for sustainable technological solutions.
5. To uphold the highest standards of research ethics, scientific integrity, and societal responsibility.

Admission in PhD Chemistry




RESEARCH PROFILE SUMMARY
An interdisciplinary research portfolio spanning materials chemistry, nanotechnology, environmental remediation, corrosion science, and synthetic organic chemistry with a strong focus on sustainable solutions and real-world applications.
RESEARCH EXPERTISE
Advanced Functional Materials
Ion-exchange membranes, ionic liquids, COFs, electrolytes & ion transport studies for energy applications.
Nanomaterials & Photocatalysis
Green synthesis of carbon dots, metal oxides & heterojunctions for efficient dye degradation and environmental remediation.
Corrosion Science & Inhibition
Development of eco-friendly corrosion inhibitors, polymer & nanocomposite coatings with experimental and computational insights.
Analytical & Environmental Chemistry
Pesticide residue analysis, monitoring of environmental pollutants, and risk assessment studies.
Organic Synthesis & Catalysis
Design and synthesis of heterocycles, hypervalent iodine chemistry, and catalytic transformations.
Sensors & Advanced Applications
Nanomaterials for electrochemical sensing, food safety, biomedical applications, and wound-healing materials.
RESEARCH THEMES
Energy Materials & Ion Transport
Green Synthesis of Nanomaterials
Photocatalysis for Environmental Remediation
Corrosion Inhibition & Surface Protection
Sustainable Chemistry & Catalysis
Environmental Monitoring & Analysis
KEY RESEARCH HIGHLIGHTS
Molecular insights into ion-exchange membranes, ionic liquids and viologen-based COFs for hydroxide ion conduction.
Green synthesis of carbon dots and metal oxide nanocomposites for efficient photocatalytic degradation of hazardous dyes.
Comprehensive studies on corrosion inhibition using organic inhibitors, plant extracts, polymers and nano-composite coatings.
Monitoring and risk assessment of pesticide residues in vegetables, soil and water.
Synthesis of biologically active heterocycles and hypervalent iodine reagents for organic transformations.
Development of nanomaterials for electrochemical sensors and wound-healing applications.
APPROACH & STRENGTHS
Integrated Experimental & Computational Approach
Advanced Synthesis & Characterization Techniques
Theoretical Modeling & Molecular Simulations
Structure–Property–Performance Correlation
Sustainability & Environmentally Benign Solutions
APPLICATION AREAS
Clean Energy & Fuel Cells
Water & Wastewater Treatment
Corrosion Protection in Industry
Environmental Sustainability
Sensing & Food Safety
Biomedical & Healthcare Applications
IMPACT
Development of sustainable materials and green technologies.
Addressing environmental challenges through innovative remediation solutions.
Bridging fundamental science with real-world applications.
Contributing to energy, environment, health and industrial sustainability.
Committed to advancing science through innovation, sustainability, and interdisciplinary collaboration for a better and cleaner future.

Scheme and Syllabus for PhD Chemistry (901) Coursework

Course Code	Course Name	Year of Introduction	Credit	Hrs.	Internal	End-Term	Max Marks	Relevant Link
Compulsory Courses								
IDD-104-V	Research and Publication Ethics	2019-20, Revised 2026	2	2	40 %	60 %	100*	Link
IDD-105-V	Research Methodology	2010-11 & 2016-17, Revised in 2026	4	4	40 %	60 %	100*	Link Link
*Subject to change as decided by Research and Development Cell of University being common course in all department								
Elective	Choose anyone from the below listed elective courses **(Total 8 credits required from elective subjects)**							

List of approved Electives Courses
(At least one course from below elective course, one course may be opted from MOOC through approval of DRC)

Course Code	Course Name	Year of Introduction	Credit	Hrs.	Internal	End-Term	Max Marks	Relevant Link
PHAS-11	Spectroscopic Methods in Research	2018-19 (Discontinued)	4	4	25	75	100	Link-1
CHD-101-V	Advanced Computational Chemistry	2020-21; Revised in 2026	4	4	40	60	100	Link-2
CHD-102-V	Advances in Synthetic Organic Chemistry	2021-22; Revised 2026	4	4	40	60	100	Link-3
CHD-103-V	Advanced Nanochemistry	2021-22; Revised 2026	4	4	40	60	100	Link-3
CHD-104-V	Chemistry of Materials	2020-21 Revised 2026	4	4	40	60	100	Link-2
CHD-105-V	Frontiers in Radical Inorganic Chemistry	2021-22; Revised 2026	4	4	40	60	100	Link-3
CHD-106-V	Principles of Fluorescence Spectroscopy and Solvent Effects	2021-22; Revised 2026	4	4	40	60	100	Link-4
CHD-107-V	Spectroscopic Methods in Research	2020-21	4	4	40	60	100	Link-2
CHD-108-V	Supramolecular Systems and their Diverse Applications	2021-22; Revised 2026	4	4	40	60	100	Link-3

Initiative towards Indian Knowledge Systems (IKS)

Indian Knowledge Systems (IKS) offer a rich scientific heritage that complements modern research in chemistry, materials science, and environmental sustainability. Traditional Indian practices in metallurgy, natural product chemistry, water purification, corrosion protection, and herbal formulations demonstrate principles of green chemistry, resource conservation, and sustainable technologies. Integrating IKS with contemporary advancements in nanotechnology, functional materials, environmental remediation, and analytical sciences promotes interdisciplinary learning while fostering innovation rooted in indigenous knowledge. This approach enables students to appreciate India's scientific contributions and develop sustainable solutions for present-day societal and environmental challenges.

Based on Research Profile (materials chemistry, green synthesis, nanotechnology, environmental remediation, corrosion science, sustainable chemistry, sensors, and environmental analysis etc.), the department encourages PhD scholars to strengthen the following IKS aligned areas:

Foundations of Indian Knowledge Systems in Natural Sciences

- Philosophy of Indian scientific traditions.
- Concepts of Panchamahabhuta (5-Elements) and their relevance to material properties.
- Ancient Indian contributions to chemistry, metallurgy, medicine, and environmental management.

Traditional Materials and Advanced Functional Materials

- Ancient Indian metallurgy: Iron Pillar of Delhi, zinc extraction at Zawar, Wootz steel.
- Corrosion resistance mechanisms in historical Indian artifacts.
- Natural polymers, bio-based materials, and traditional composites.

Nanotechnology in Indian Traditional Knowledge

- Conceptual parallels between ancient formulations and modern nanoscience.
- Ayurvedic Bhasmas as examples of nano-structured materials.
- Characterization and applications of traditional nano-formulations.

Green Synthesis and Catalysis

- Plant extracts and natural products as reducing and stabilizing agents.
- Bio-inspired synthesis routes for nanoparticles.
- Traditional catalytic processes in food, medicine, and material preparation.

Corrosion Science and Protective Coatings

- Traditional methods of preservation of metals and monuments.
- Organic inhibitors derived from medicinal plants.
- Natural coatings, oils, and bio-based protective materials.

Healthcare, and Sustainable Technologies

- Traditional diagnostic approaches in Ayurveda.
- Herbal indicators and natural sensing materials.
- Nanomaterials for healthcare and environmental monitoring.

PhD Chemistry (901) Coursework
Semester-I

विश्वविद्यालय अनुदान आयोग
University Grants Commission
(मानव संसाधन विकास मंत्रालय, भारत सरकार)
(Ministry of Human Resource Development, Govt. of India)

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E-mail : secy.ugc@nic.in

ज्ञान–विज्ञान विमुक्तये

सत्यमेव जयते

प्रो. रजनीश जैन
सचिव
Prof. Rajnish Jain
Secretary

D.O.No.F.1-1/2018(Journal/CARE) December, 2019

Respected Sir/Madam,

University Grants Commission in its 543rd meeting held on 9th August, 2019 approved two Credit Courses for awareness about publication ethics and publication misconducts entitled **"Research and Publication Ethics (RPE)"** to be made compulsory for all Ph.D. students for pre-registration course work **(attached as Annexure)**.

In view of the above, you are requested to ensure that the above two Credit courses may be made compulsory for all Ph.D. students for pre-registration course work undertaken in your University from the forthcoming academic session.

With regards,

Yours sincerely,

(Rajnish Jain)

Course	Name of Courses	Internal + End Sem = Max Marks	Hrs. Per Week	Credit
IDD-104-V	Research and Publication Ethics (RPE)	40 % + 60 % = 100 %	2	2
		L - 4	T - 0	P - 0

Course Objectives:

- Course for awareness about the publication ethics and publication misconducts.

Eligibility: M.Phil., Ph.D. students and interested faculty members (It will be made available to post graduate students at later date)

Course Content: (30 hrs.)

Unit-I	RPE Overview

• This course has total 6 units focusing on basics of philosophy of science and ethics, research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

Unit-II	Pedagogy

• Class room teaching, guest lectures, group discussions, and practical sessions.

Unit-III	Evaluation

• Continuous assessment will be done through tutorials, assignments, quizzes, and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

PhD Chemistry (901) Coursework				
Semester-I				
Course	**Name of Courses**	**Internal + Theory Exam = Max Marks**	**Hrs. Per Week**	**Credit**
IDD-105-V	**Research Methodology**	**40 + 60 = 100**	**4**	**4**
		L - 4	**T - 0**	**P - 0**

Course Objectives:

- Understand research process in order to plan a research proposal
- Learn methods to devise and design a research set-up
- Plan and perform data collection methods and its analysis
- Conclude research in report writing

Course Outcomes:

The research scholar shall be able to:

- CO1 Plan a research proposal and design the research.
- CO2 Collect data through experiments or surveys as per research requirement.
- CO3 Understand and apply sampling and sampling distributions.
- CO4 Understand and perform quantitative and qualitative data analysis.
- CO5 Write research report with proper citations.

Course Content:

Unit 1

Introduction to Research: Definition, need and purpose of research, types of research, research process, approaches to research, planning a research proposal, literature review.

Unit 2

Measurement Scales: Indexes vs. Scales, Types of Scale, construction of Scale, Bogardus social distance scale, Thurstone Scale, Likert Scale, Semantic Differential Scale, Guttmann Scale.

Unit 3

Data Collection Methods: Experiments and Surveys, Experiments: Classical Experiments, Independent & Dependent Variables, Pre-Testing & Post Testing, Double Blind Experiment, Subject Selection, Variation on Experiment Design.

Survey Research: Topics appropriate for survey research, Guidelines for asking questions, Questionnaire Construction, Strengths & Weakness of Survey Research, Types of Surveys.

Unit 4

Sampling: Types of sampling methods: Non-Probability Sampling, Probability Sampling, Theory & Logic of Probability Sampling, Sampling Distributions & Estimates of Sampling Error.

Unit 5

Data Analysis: Qualitative v/s Quantitative data analysis, Qualitative Data Analysis: Discovering Patterns, Grounded Theory Method, Semiotics, Conversation Analysis, Qualitative Data Processing. Quantitative Data Analysis: Quantification of Data, Univariate Analysis, Bivariate Analysis, Multivariate Analysis, Regression Analysis, Description Analysis. Hypothesis. Multiple Attribute Decision Making.

Unit 6

Report Writing, Ethical Issues and Outcomes: Report Preparation, Structure of Report, Report Writing Skills, Citations, Research Papers, Intellectual Property Rights, Plagiarism, Patent, Commercialization, Ethical Issues.

Suggested Books/Reading:

1.	Research Methodology by R. Panneerselvam, PHI.
2.	Research Methodology by C.R. Kothari & Gaurav Garg, New Age Publishers.
3.	Research Methodology by Deepak Chawla and Neena Sondhi, Vikas Publishing.
4.	The practice of social research by Earl Babbie, Cengage.
5.	Multiple Attribute Decision Making, Gwo-Hshiung Tzeng and Jih-Jeng Huang, CRC Press
6.	Research Methodology by Ranjit Kumar, Sage Publications.

PhD Chemistry (901) Coursework				
Semester-I				
Course	Name of Courses	Internal + End Sem = Max Marks	Hrs. Per Week	Credit
PHAS 11	Spectroscopic methods in research	25 + 75 = 100	4	4

This course of AY 2018-2019 discontinued in 2026	L - 4	T - 0	P - 0

Course Objectives:

- To learn the spectroscopic techniques being used as a tool for structural elucidation of organic compounds.
- To also understand the basic techniques for isolation and purification of organic compounds.

Course Content:

Unit-I **Separation and purification**

Separation techniques for the organic compounds, solvent extraction and chromatographic techniques- including principle, theories, types, experimentation(sample loading, development and detection of chromatogram in common chromatography; paper, TLC, column , GC-MS, HPLC) and applications of various adsorption and partition chromatography.

Unit-II **Nuclear Magnetic Resonance Spectroscopy- I**

General introduction and definition, chemical shift, spin -spin interaction, shielding mechanism, mechanism of mea surement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), complex spin-spin interaction between two, three, four and five nuclei (first order spectra), spin system -Pople notation, virtual coupling.

Unit-III **Nuclear Magnetic Resonance Spectroscopy- II**

Stereochemistry, concept of topicity, effect of enantiomeric and diastereomeric protons, hindered rotation, Karplus curve - variation of coupling constant with dihedral angle. Fourier transform technique and its advantages. Resonance of other nuclei-F, P.Tools for simplification of complex NMR spectrum (chemical and instrumental) :-Deuteration, changing solvent, trifluoroacetylation, basification and acidification, lanthanide shift reagents, increased magnetic field strength, double resonance and nuclear overhauser effect (NOE), variable temperature probe. Concept of 2D-NMR spectroscopy.

Carbon- 13 NMR Spectroscopy: General considerations, Comparison of 1H-NMR and 13C-NMR, Proton coupled and proton decoupled 13C-NMR, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Nuclear Overhauser effect.

Unit-IV **Infrared Spectroscopy and Mass Spectrometry**

Infrared Spectroscopy: Principle and Theory, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines.Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.FT-IR.

Mass Spectrometry: Introduction, ion production - EI, CI, FD and FAB, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, Nitrogen rule, molecular weight determination molecular formula from isotopic ratio data, is otope profile of halogen compounds, fragmentation pattern - simple cleavage, retro-Diels Alder, Hydrogen transfer rearrangement like scrambling, ortho effect, McLafferty rearrangement, fragmentation patterns of hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amines, nitro, amides, nitriles.

Composite Problems

Problems involving the application of the above spectroscopic techniques (UV/Visible, IR, NMR and Mass) for structural elucidation of organic molecules.

Suggested Books/Reading:

1.	Introduction to Spectroscopy- A Guide for Students of Organic Chemistry, 2 nd Edn. By Donald L. Pavia, Gary M. Lampman and George S. Kriz. Saunders Golden Sunburst Series. Harcourt Brace College Publishers, New York.
2.	Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.
3.	Application of Spectroscopy of Organic Compounds, J. R. Dye r, Prentice Hall.
4.	Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, Tata McGraw-Hill.
5.	Spectroscopy of Organic Compounds by P.S. Kalsi, Wiley Estern, New Delhi.
6.	Organic Spectgroscopy by William Kemp, John Wiley.
7.	Organic Mass Spectrometry by K.G. Das & E.P. James, Oxford & IBH Publishing Co.

PhD Chemistry (901) Coursework				
Semester-I				
Course	**Name of Courses**	**Internal + Theory Exam = Max Marks**	**Hrs. Per Week**	**Credit**
CHD-101-V	**Advanced Computational Chemistry**	**40 + 60 = 100**	**4**	**4**
		L - 4	**T - 0**	**P - 0**

Course Objectives:

- This course will introduce theoretical concepts of Molecular Dynamics and quantum mechanics. Experiments based on the theory will be part of the course. Research Scholars interested in computational chemistry will be benefit from the course.

Course Outcomes:

- Knowledge of basis set selection and quantum calculation methods to tackle simple/complex molecular system.
- Adapt in principles of molecular dynamics simulations method to learn molecular analysis of liquid systems.
- Enhancement in understating of molecular methods in terms of computing.
- Advancement in learning of plotting methods and data analysis.

Course Content:

Unit-I **Introduction to Quantum Computational Chemistry (L-15 hrs.)**

Topics: Scope of computational chemistry, Restricted and Unrestricted Hartree-Fock, Basis Sets: Slater and Gaussian Type Orbitals, Polarization and Diffuse Functions, Split-valence Sets, Core-valence Sets; Potential energy surfaces: Geometry optimization, local and global minima, transition state theory, and pair potentials.

Unit-II **Fundamentals of Molecular Dynamics (MD) simulations (L-15 hrs.)**

Topics: Introduction to Computer Simulation –Visual Representation of Molecular Systems, Lennard Jones potentials -- Potentials and Force-Fields, Phase Space, Periodic Boundary Conditions, Minimum Image convention. Propagation of Newton's Equation, Time Step and Energy Minimization; Monte Carlo simulations–introduction and Metropolis algorithm

Unit-III **MD Algorithms & applications (L-15 hrs.)**

MD algorithms, Thermostats - types and temperature fluctuations, Treatment of Statistical Mechanical Ensembles – Averages – Fluctuations – Time Correlation Function – Radial Distribution Function, Mean Square Displacement - Diffusion coefficient.

Unit-IV **Hands on exercises (L- 15 hrs.)**

Introduction and Use of MD Program, Visualization using Visual Molecular Dynamics (VMD), Simulations of water molecules. Computations of Single Point Energy, Optimization, and Transition States of Polyatomic Molecules; Plotting with GRACE. Course Outcome: This course will enable a research scholar to acquaint with computational chemistry skills and basics to independently tackle various research problems in the field of physical chemistry and enhance his/her understanding of a chemical system at molecular level.

Suggested Books/Reading:

1.	Computer Programming in Fortran 90 And 95, V Rajaraman
2.	Computer Simulations of Liquids, M. P. Allen and D. J. Tildesley.
3.	Molecular Modeling: Principles and Applications, Andrew R. Leach, Addison Wesley Publishing Company, 1997.
4.	Introduction to Computational Chemistry, Frank Jensen, John Wiley & Sons, 2007.
5.	Electronic Structure: Basic Theory & Practical Methods, by Richard M. Martin, Cambridge University Press
6.	Introduction to the Theory and Applications of Molecular and Quantum Mechanics, by Errol Lewars, Kluwer Academic Publishers, New York, Boston, Dordrecht, London, Moscow, 2004

PhD Chemistry (901) Coursework				
Semester-I				
Course	Name of Courses	Internal + Theory Exam = Max Marks	Hrs. Per Week	Credit
CHD-102-V	Advances in Synthetic Organic Chemistry	40 + 60 = 100	4	4
		L - 4	T - 0	P - 0

Course Objectives:

Course Outcomes:

Course Content:

Unit-I | **Advance Heterocyclic Chemistry – I (L-15 hrs.)**

Common approaches to heterocyclic synthesis: cyclisation and cycloaddition routes. Heterocycles in organic synthesis: masked functionalities, umpolung, Stork annulation reaction and applications in the synthesis of Lansoprazole, Clopidogrel, Ritonavir, Dasatinib, Remdesivir, Galantamine, Doxorubicin, Celecoxib and/or recently discovered molecules, along with their retrosynthetic analysis.

Unit-II | **Advance Heterocyclic Chemistry – II (L-15 hrs.)**

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Six-membered heterocycles: Pyridazine, Pyrazine, Oxazine, Thiazine, Seven-membered heterocycles: Azepins, Oxepins, Thiepins, Fused heterocycles: Benzimidazole, Benzoxazole and Benzthiazole, Biologically important heterocycles: Pyrimidines and Purines; Synthesis of heterocycles using binucleophiles: Thiosemicarbazide, Thiocarboxamide Hydroxylamine, Hydrazines; ANRORC and vicarious nucleophilic substitutions in heterocycles.

Unit-III | **C–H Activation – I (L-15 hrs.)**

Mechanisms of C–H bond activation with transition metals: Oxidative addition, Sigma bond metathesis, Electrophilic activation, Metalloradical activation, Organic synthesis involving: Chelation-assisted C–H activation, Ortho-C–H activation, Meta-selective C–H functionalization, C–H activation in heterocycles, Base-assisted C–H activation, C–H, C=C and C≡C activated annulation reactions.

Unit-IV | **C–H Activation – II (L- 15 hrs.)**

Important synthetic approaches via C–X bond activation (X = C, N, O, S, etc.).
Topics include: Role of non-metallic activation of bonds in organic synthesis, Asymmetric C–H activation, Shilov system, Carbon–Heteroatom bond-forming reactions, Carbon–Carbon bond-forming reactions, Glazer–Eglinton coupling, Buchwald reaction with examples

Suggested Books/Reading:

1. T. Gilchrist, Heterocyclic Chemistry, Prentice Hall, 3rd Edition, 1997.
2. J. A. Joule & K. Mills, Heterocyclic Chemistry, Wiley-Blackwell, 2010.
3. A. R. Katritzky, Handbook of Heterocyclic Chemistry, Academic Press, 2nd Edition, 2000.
4. Yu, Jin-Quan; Shi, Zhangjie, C–H Activation
5. K. I. Goldberg & A. S. Goldman, Activation and Functionalization of C–H Bonds, 2004.
6. Xiao-Feng Wu, Transition Metal-Catalyzed Heterocycle Synthesis via C–H Activation, Wiley-VCH Verlag GmbH & Co. KGaA, 2016.
7. Debabrata Maiti & Srimanta Guin, Remote C–H Bond Functionalizations, Wiley-VCH, Weinheim, 2021.

PhD Chemistry (901) Coursework				
Semester-I				
Course	**Name of Courses**	**Internal + Theory Exam = Max Marks**	**Hrs. Per Week**	**Credit**
CHD-103-V	**Advanced Nanochemistry**	**40 + 60 = 100**	**4**	**4**
		L - 4	**T - 0**	**P - 0**

Course Content:

Unit-I	**Synthesis Methods: (L-15 hrs.)**

Nanotechnology, Top down and Bottom up techniques, Nanomaterials, Preparation of nanomaterials- solid state reaction method, sol-gel method, hydrothermal, Coprecipitation method, Chemical Vapor Deposition, Ball Milling, Electrodeposition, Green synthesis, Microemulsion synthesis, Quantum Dot synthesis, sonochemical assisted synthesis, core-shell nanostructures, Organic-Inorganic hybrid nanocomposites.

Unit-II	**X-ray and Spectroscopic Techniques (L-15 hrs.)**

X-ray and Spectroscopic Techniques: X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), X-ray emission spectroscopy, Raman spectroscopy, Beer's Lambert Law, UV-Vis spectroscopic technique, Fourier transform infrared spectroscopy, Fluorescence and Photoluminescence Spectroscopy, Mass spectroscopy, Nuclear magnetic resonance spectroscopy, Electron spin resonance spectroscopy, Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA).

Unit-III	**Microscopy Techniques (L-15 hrs.)**

Microscopy Techniques: Interaction of electrons with solids, Optical microscopes, Electron microscope, Types of electron microscopes, Scanning electron microscope, Transmission electron microscope, Dark and bright field imaging, Analysis of SAED pattern, High resolution Transmission electron microscope, Scanning Tunnelling Microscope, Scanning transmission electron microscope, atomic force microscope.

Unit-IV	**Application of Nanotechnology (L- 15 hrs.)**

Application of Nanotechnology: For remediation of pollutants, waste-water treatment, photocatalysis, electrocatalysis, adsorption, heavy-metal removal, optical and electrochemical sensing of harmful analyte in aqueous media, EMI shielding, nanomaterials in textile and cosmetic, electrical and electronic industries.

Suggested Books/Reading:

1.	Poole Jr., C.P., Owens, F.J. "Introduction to Nanotechnology", Wiley (2003).
2.	Roco, M.C.; Bainbridge, W.S. (eds.): 2001, Societal implications of nanoscience and nanotechnology, (Proceedings of a workshop organized by the National Science Foundation, September 28-29, 2000), Kluwer, Dordrecht.
3.	Zander, C., Enderlein, J. & Keller, R.A. 2002 Single Molecule Detection in Solution. Wiley-VCH Verlag.
4.	Ferziger, J. H., Numerical Methods for Engineering Applications, 2nd ed., Wiley Interscience (1998).
5.	Nanomaterials: synthesis, Properties and Applications by Edelstein A S and Cammarata R C,Taylor and Francis, 2012.
6.	Nanochemistry: A Chemical Approach to Nanomaterials by G. A. Ozin, A.C. Arsenault, and L. Cademartiri, The Royal Society of Chemistry, Cambridge, 2nd Ed., 2009.
7.	Nanostructures & Nanomaterials: Synthesis, Properties, and Applications by Guozhong Cao, Imperial College Press, London, 2004.
8.	Nanoscale Science and Technology, edited by R. W. Kelsall, I. W. Hamley, and M. Geoghegan, Wiley, West Sussex, 2005.

PhD Chemistry (901) Coursework				
Semester-I				
Course	**Name of Courses**	**Internal + Theory Exam = Max Marks**	**Hrs. Per Week**	**Credit**
CHD-104-V	**Chemistry of Materials**	**40 + 60 = 100**	**4**	**4**
		L - 4	**T - 0**	**P - 0**

Course Objectives:

- The objective of this course is to provide the basic understanding of different type of materials, their behavior, analysis and degradation

Course Outcomes:

After the successful completion of the course the learner would be able to

- understand nature of different type of materials and their response mechanism to local atmosphere
- understand chemistry of corrosion and its prevention
- learn about important techniques to analyze and characterize the materials at various stages
- learn and understand different characterization techniques.

Course Content:

Unit-I	**Materials, and their behavior (L-15 hrs.)**

Carbon steels and irons; stainless steel; aluminium, copper, tin and their alloys; refractory metals; natural and synthetic rubbers; thermoplastics; thermosetters; ceramics; carbon and graphite; wood

Unit-II	**Corrosion (L-15 hrs.)**

Thermodynamics of corrosion; mechanism and kinetics of corrosion; forms of corrosion; factors affecting and preventive measures for corrosion; corrosion testing; mechanism of corrosion inhibitor action; inhibitor efficiency; application of inhibitors for boiler corrosion, cooling water system, reinforced concrete and cement, chemical and petrochemical industries.

Unit-III	**Electro-chemical methods of Analysis (L-15 hrs.)**

Electrogravimetry; Polarographic analysis; Coulometric analysis and coulometric titrations; Amperometric titrations; anodic stripping voltammetry and cyclic voltammetry; Electrochemical Impedance Spectroscopy; Polarization studies (Tafel polarization & Linear poraization technique). Chronoamperometry, chronopotentiometry, electrochemical impedance spectroscopy (EIS)

Unit-IV	**Characterization Techniques (L- 15 hrs.)**

Surface analysis: Electron spectroscopy for chemical analysis (ESCA), X-Ray Diffraction, Fourier Transform Infra Red (FTIR) Spectroscopy, AFM and Scanning Electron Microscopy (SEM), SEM-EDX, Transmission Electron Microscopy (TEM), Atomic Absorption Spectroscopy (AAS), Energy-dispersive X-ray spectroscopy (EDX, EDS)

Suggested Books/Reading:

1.	M.G. Fontana, Corrosion Engineering, McGraw Hill International Book Co. London.
2.	J. C. Scully, Fundamental of Corrosion, Pergamon Press Inc. New York USA.
3.	Corrosion Inhibitors, Principles & Applications, V.S. Sastry, John Wiley & Sons
4.	Introduction to Atmospheric Science, J M Wallace and P V Hobbs, Academic Press

PhD Chemistry (901) Coursework				
Semester-I				
Course	**Name of Courses**	**Internal + Theory Exam = Max Marks**	**Hrs. Per Week**	**Credit**
CHD-105-V	**Frontiers in Radical Inorganic Chemistry**	**40 + 60 = 100**	**4**	**4**
		L - 4	**T - 0**	**P - 0**

Course Objectives:

- This course will introduce basic and advanced concepts of coordination chemistry with respect to non-innocent (redox-active) ligands and their transition metal complexes. Experimental part based on theory will be part of this course. Research scholars interested in coordination chemistry will be benefitted.

Course Outcomes:

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

- Understand the behaviour of redox-active ligands and transition-metal complexes.
- Define basic principles involved in Coordination Chemistry and Metal–Ligand Interactions.
- Illustrate the spectroscopic methods in redox-active transition-metal complexes.
- Interpret valence tautomeric behaviour with various techniques.

Course Content:

Unit-I	**Introduction of Non-Innocent Ligands (L-15 hrs.)**

Difference between innocent (redox-inactive) and non-innocent ligands (redox-active). Classification of Non-Innocent Ligands: o-Dioxolene, o-Phenylenediamine, o-Aminophenol, o-Dithiolene; General trends in bond-length behaviour in o-dioxolene, o-phenylenediamine, o-aminophenol ligands and redox-active transition-metal complexes.

Unit-II	**Coordination Chemistry and Metal–Ligand Interactions (L-15 hrs.)**

A brief view of reported transition-metal complexes with non-innocent ligands in literature: Synthesis, structure and magnetism of mono-o-iminobenzoquinonato complexes, Synthesis, structure and magnetism of pentacoordinate bis-o-iminobenzoquinonato complexes, Synthesis, structure and magnetism of hexacoordinate bis-o-iminobenzoquinonato complexes, Synthesis, structure and magnetism of homoleptic transition-metal complexes with bidentate N-aryl-o-iminoquinone ligands, Comparison with o-quinone analogues, Coordination compounds of other o-iminobenzoquinone derivatives.

Unit-III	**Spectroscopic Methods (L-15 hrs.)**

Characterization of synthesized ligands by: CHN Analysis, NMR Spectroscopy, Mass Spectrometry, IR Spectroscopy. Characterization of synthesized transition-metal complexes by: CHN Analysis, NMR Spectroscopy (for diamagnetic complexes), Mass Spectrometry, Infrared Spectroscopy, Electron Spin Resonance (ESR) Spectroscopy, Absorption Spectroscopy, Spectro-electrochemistry, Temperature-dependent Mössbauer Spectroscopy. Investigation of redox behaviour by electrochemical methods: Cyclic Voltammetry, Coulometry.

Unit-IV	**Valence Tautomerism (L- 15 hrs.)**

Difference between valence tautomerism and electron delocalization, Basic requirements for valence tautomerism and electron delocalization, Valence tautomerism in Fe and Co complexes, Temperature-dependent Mössbauer spectroscopy in iron complexes, Temperature-dependent ESR studies in Fe and Co complexes, Temperature-dependent ^1H NMR studies in Co complexes.

Suggested Books/Reading:

1.	F. O. Rice, *Review of the Properties and Reactions of Some Inorganic Free Radicals*.
2.	Andrew F. Parson, *An Introduction to Free Radical Chemistry*, ISBN: 9780632052929.
3.	*Inorganic Free Radicals in Solution*, Chemical Reviews, 1952, **50**, 3375–454.
4.	*Coordination Chemistry Reviews*, 2020, **414**, 213240 and references therein.
5.	*Coordination Chemistry Reviews*, 2009, **253**, 291–324 and references therein.
6.	F. A. Cotton and Wilkinson, *Advanced Inorganic Chemistry*, John Wiley.
7.	J. E. Huheey, *Inorganic Chemistry*, Harper & Row.
8.	A. B. P. Lever, *Inorganic Electronic Spectroscopy*, Elsevier.

Suggested Web Sources

- https://nptel.ac.in/courses/103106162/
- https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=14

Mode of Transaction

- Lecture, demonstration, e-tutoring, discussion, assignments, quizzes, case study, PowerPoint presentations.
- LMS/ICT Tools: Digital Classrooms, DLMS, Zoom, G-Suite, MS PowerPoint, Online Resources.

PhD Chemistry (901) Coursework				
Semester-I				
Course	Name of Courses	Internal + Theory Exam = Max Marks	Hrs. Per Week	Credit
CHD-106-V	Principles of Fluorescence Spectroscopy and Solvent Effects	40 + 60 = 100	4	4
		L - 4	T - 0	P - 0

Course Objectives:

- To learn about Steady State Fluorescence Spectroscopy, Time Resolved Fluorescence Spectroscopy, Fluorescence Spectroscopy Principle, instrumentation and various applications.
- To learn about Solvent and Environmental Effects on Fluorophores

Course Outcomes:

After the successful completion of the course the learner would be able to

- To use Steady State Fluorescence Spectroscopy, Time Resolved Fluorescence Spectroscopy.
- Understand the Solvent and Environmental Effects on probe molecules
- To understand various factors that Affect Emission Spectra
- To understand how to collect and interpret fluorescence emission and excitation spectra

Course Content:

Unit-I **Introduction to Fluorescence (L-15 hrs.)**

Phenomena of Fluorescence, Jablonski Diagram, Characteristics of Fluorescence Emission, The Stokes Shift, Emission Spectra Are Typically Independent of the Excitation Wavelength, Exceptions to the Mirror- Image Rule, Fluorescence Lifetimes and Quantum Yields, Fluorescence Quenching. Timescale of Molecular Processes in Solution, Fluorescence Anisotropy, Resonance Energy Transfer, Steady-State and Time- Resolved Fluorescence, Why Time-Resolved Measurements? Information from Fluorescence, Emission Spectra and the Stokes Shift, Quenching of Fluorescence, Fluorescence Polarization or Anisotropy, Resonance Energy Transfer, New Fluorescence Technologies, Fluorescence Correlation Spectroscopy.

Unit-II **Instrumentation for Fluorescence Spectroscopy (L-15 hrs.)**

Spectrofluorometers, An Ideal Spectrofluorometer, Distortions in Excitation and Emission Spectra, Light Sources, LED Light Sources, Laser Diodes, Monochromators, Wavelength Resolution and Emission Spectra, Polarization Characteristics of Monochromators, Stray Light in Monochromators, Calibration of Monochromators, Optical Filters, Colored Filters, Thin-Film Filters, Filter Combinations, Neutral-Density Filters, Optical Filters and Signal Purity, Photomultiplier Tubes, Spectral Response of PMTs, Time Response of Photomultiplier Tubes, Photon Counting versus Analog Detection of Fluorescence Symptoms of PMT Failure, CCD Detectors, Polarizers, Corrected Excitation Spectra, Corrected Excitation Spectra Using a Quantum Counter, Corrected Emission Spectra, Corrections Using a Standard Lamp, Conversion between Wavelength and Wavenumber, Quantum Yield Standards, Common Errors in Sample Preparation, Absorption of Light and Deviation from the Beer-Lambert Law, Deviations from Beer's Law.

Unit-III **Time-Domain Lifetime Measurements (L-15 hrs.)**

Overview of Time-Domain and Frequency Domain Measurements, Meaning of the Lifetime or Decay Time, Phase and Modulation Lifetimes, Examples of Time-Domain and Frequency-Domain Lifetimes, Time- Correlated Single-Photon Counting Principles of TCSPC, Example of TCSPC Data, Convolution Integral, Light Sources for TCSPC, Laser Diodes and Light-Emitting Diodes, Femtosecond Titanium Sapphire Lasers, Picosecond Dye Lasers, Flashlamps, Synchrotron Radiation , Electronics for TCSPC, Constant Fraction Discriminators, Amplifiers, Time-to-Amplitude Converter (TAC) and Analyte-to-Digital Converter (ADC), Multichannel Analyzer, Delay Lines, Pulse Pile-Up, Detectors for TCSPC, Streak Cameras, Upconversion Methods, Data Analysis: Nonlinear Least Squares, Assumptions of Nonlinear Least Squares, Overview of Least-Squares Analysis, Meaning of the Goodness-of-Fit, Autocorrelation Function, Analysis of Multi-Exponential Decays, Comparison of $\chi 2$ Values: Effect of the Number of Photon Counts, Decay Laws, Multi-Exponential Decays, Lifetime Distributions, Applications of TCSPC

Unit-IV **Fluorescence Quenching and Solvent Effects (L- 15 hrs.)**

Quenchers of Fluorescence, Theory of Collisional Quenching, Derivation of the Stern-Volmer Equation, Interpretation of the Bimolecular Quenching Constant, Theory of Static Quenching, Combined Dynamic and Static Quenching, Examples of Static and Dynamic Quenching, Deviations from the Stern-Volmer Equation: Quenching Sphere of Action, Derivation of the Quenching Sphere of Action, Effects of Steric Shielding and Charge on Quenching, Modified Stern-Volmer Plots, Experimental Considerations in Quenching, Applications of Quenching to Proteins, Overview of Solvent Polarity Effects, Effects of Solvent Polarity, Polarity Surrounding a Membrane-Bound Fluorophore, Other Mechanisms for Spectral Shifts, General Solvent Effects: The Lippert-Mataga Equation, Derivation of the Lippert Equation, Application of the Lippert Equation, Specific Solvent Effects, Specific Solvent Effects and Lippert Plots, Temperature Effects, Phase Transitions in Membranes, Additional Factors that Affect Emission Spectra, Locally Excited and Internal Charge-Transfer States, Excited-State Intramolecular Proton Transfer (ESIPT), Changes in the Non-Radiative Decay Rates, Changes in the Rate of Radiative Decay, Effects of Viscosity, Effect of Shear Stress on Membrane Viscosity, Probe–Probe Interactions, Advanced Solvent-Sensitive Probes, Effects of Solvent Mixtures.

Suggested Books/Reading:	
1.	Principles of Fluorescence Spectroscopy by Joseph R. Lakowicz Third Edition Springer, 2006.
2.	Physical Chemistry by Thomas Engel, Philip Reid and Warren Hehre PEARSON 2013, ISBN 978-0- 321-81200-1.
3.	Solvents and Solvent Effects in Organic Chemistry by Christian Reichardt and Thomas Welton Fourth Edition, ISBN:9783527324736, 2010.
4.	Introduction to Fluorescence by David M. Jameson CRC Press; 1st edition (28 Feb. 2014) ISBN-10 : 1439806047.
5.	Molecular Fluorescence: Principles and Applications by Bernard Valeur Wiley-VCH; 2nd edition (26 April 2012) SBN-10 : 3527328378.
6.	Time-Correlated Single Photon Counting by Desmond V. O'Connor Academic Pr , ISBN-10 : 0125241402.
7.	Modern Molecular Photochemistry by Nicholas J. Turro University Science Books,U.S.; New edition (8 July 1991) ISBN-10 : 0935702717.
8.	Principles of Molecular Photochemistry: An Introduction by Nicholas J. Turro, University Science Books; 2009th edition (16 Jan. 2009) ISBN-10 : 1891389572

PhD Chemistry (901) Coursework

Semester-I

Course	Name of Courses	Internal + Theory Exam = Max Marks	Hrs. Per Week	Credit
CHD-107-V	**Spectroscopic Methods in Research**	**40 + 60 = 100**	**4**	**4**
		L - 4	**T - 0**	**P - 0**

Course Objectives:

- To learn the spectroscopic techniques being used as a tool for structural elucidation of organic compounds. To also understand the basic techniques for isolation and purification of organic compounds.

Course Content:

Unit-I **Separation and purification (L-15 hrs.)**

Separation techniques for the organic compounds, solvent extraction and chromatographic techniques- including principle, theories, types, experimentation (sample loading, development and detection of chromatogram in common chromatography; paper, TLC, column, GC- MS, HPLC) and applications of various adsorption and partition chromatography.

Unit-II **Principle and Practice of NMR and Optical Spectroscopy (L-15 hrs.)**

Fundamentals of FT NMR spectroscopy, relation between structure and NMR properties, one-dimensional spectroscopy to two dimensional NMR (COSY, NOESY and HSQC) and their use in structure elucidation. Principles and analytical applications of optical spectroscopic methods including atomic absorption and emission, UV - visible, IR absorption, scattering and luminescence.

Unit-III **Molecular Modeling and Simulations: Concepts and Techniques (L- 30 hrs.)**

Review of basic concepts: Length and time scales, intermolecular interactions and potential energy surfaces, evaluation of long range in teractions static and dynamic properties of simple and complex liquids molecular dynamics: Microcanonical and other ensembles; Constrained simulations; non - equilibrium approaches Monte Calo methods: Random numbers and random walk, metropolis algorithm in various ensembles, biased montecarlo scheme free energy estimation; mapping phase diagrams, generating free energy landscape, collective variables rare event simulations and reaction dynamics, advanced topics: first principles molecular dynamics, quantum montecarlo methods, coarse - graining and multiscale simulations for nanoscale system

Suggested Books/Reading:

1.	Introduction to Spectroscopy- A Guide for Students of Organic Chemistry, 2nd Edn. By Donald L. Pavia, Gary M. Lampman and George S. Kriz. Saunders Golden Sunburst Series. Harcourt Brace College Publishers, New York.
2.	Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.
3.	Application of Spectroscopy of Organic Compounds, J. R. Dye r, Prentice Hall.
4.	Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, Tata McGraw-Hill.
5.	Spectroscopy of Organic Compounds by P.S. Kalsi, Wiley Estern, New Delhi.
6.	Organic Spectroscopy by William Kemp, John Wiley.
7.	Organic Mass Spectrometry by K.G. Das & E.P. James, Oxford & IBH Publishing Co.
8.	Organic Spectroscopy (Principles & Applications) by Jagmohan.

PhD Chemistry (901) Coursework				
Semester-I				
Course	Name of Courses	Internal + Theory Exam = Max Marks	Hrs. Per Week	Credit
CHD-108-V	Supramolecular Systems and their Diverse Applications	40 + 60 = 100	4	4
		L - 4	T - 0	P - 0

Course Objectives:

- CO1: Learn the diverse categories of supramolecular systems.
- CO2: Explore various types of supramolecular MOFs.
- CO3: Acquire knowledge about supramolecular systems as sensors and catalysts.
- CO4: Gain knowledge about cancer-targeted drug delivery.

Course Content:

Unit-I **Supramolecular Sensors (L-15 hrs.)**

Introduction to supramolecules. Calix[n]arene, pillar-arene and cucurbituril properties and their reactions. Fundamental sensing processes (electrical, chemical, molecular sensors). Transduction processes (PET, ICT, FRET, ESIPT, electrochemical redox process, etc.). Supramolecules as chemosensors for cations, anions, neutral molecules. Different sensing techniques: fluorescence sensors, colorimetric sensors, electrochemical sensors, array-based sensors, molecular switches, and gas sensors.

Unit-II **Supramolecular Metal–Organic Frameworks (L-15 hrs.)**

Classification of metal–organic framework materials (MOFs) (topology and chemical composition). Synthesis methods of MOFs. Properties of MOFs (crystallinity, porosity, chemical and thermal stability). Methods for structural characterization of MOFs (XRD, SEM/EDX, porosity, thermal analysis, etc.). Design and use of supramolecular MOFs for capture, separation, and storage of gases. Design and use of MOFs in catalysis. Other applications of MOFs such as sensors and drug-delivery systems.

Unit-III **Supramolecular Systems as Nano-Catalysts (L-15 hrs.)**

Basic nanomaterials: mesoporous materials, different metal nanoparticles, their synthesis and characterization. Various metals such as Pd, Au, Ag, and Fe-doped nanosurfaces and methods for their characterization (TGA, XPS, etc.). Anchoring of supramolecular systems on these surfaces and their catalytic properties toward organic reactions such as coupling, oxidation, and enzyme-mimic catalysis. Recent examples from the literature.

Unit-IV **Targeted Drug Delivery Vehicles (L- 15 hrs.)**

Different types of tumor drugs. Supramolecules as carriers for cancer drugs. In-vitro and in-vivo drug release and uptake. MTT assay and FACS analysis. Basics of site-specific drug delivery. Design of molecules targeting various organelles of the cell. Nucleus, mitochondrion, lysosomes, and ER-targeting molecules. Basic strategies for designing organelle-specific molecules. Advantages and applications of supramolecules for controlled-release drug-delivery systems.

Suggested Books/Reading:

1.	Gale, P. A. and Steed, J. W. Supramolecular Chemistry: From Molecules to Nanomaterials, 2012.
2.	Diederich, F., Stang, P. J., and Tykwinski, R. R. Modern Supramolecular Chemistry, 2008.
3.	Steed, J. W., Turner, D. R., and Wallace, K. J. Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley & Sons, 2007.
4.	Steed, J. W. and Atwood, J. L. Supramolecular Chemistry, Wiley, Chichester, 2009.
5.	MacGillivray, L. R. Metal-Organic Frameworks: Design and Application, John Wiley & Sons, 2010.

MODE OF TRANSACTION

Lecture, demonstration, e-tutoring, discussion, assignments, quizzes, case studies, PowerPoint presentations.

LMS/ICT Tools: Digital Classrooms, DLMS, Zoom, G-Suite, MS PowerPoint, Online Resources.

Department of Chemistry

Elective Courses for PhD Program in Chemistry (Program Code: 901)

Mapping of the Course w.r.t. Employability / Entrepreneurship / Skill Development						
Course Code	**Course Name**	**Year of Introduction/Revised**	**Employability**	**Entrepreneurship**	**Skill Development**	**Relevant Link**
CHD-101-V	Advanced Computational Chemistry	2020-21; Revised in 2026	Yes (√)	Yes (√)	Yes (√)	Link-2
CHD-102-V	Advances in Synthetic Organic Chemistry	2021-22; Revised 2026	Yes (√)	Yes (√)	Yes (√)	Link-3
CHD-103-V	Advanced Nanochemistry	2021-22; Revised 2026	Yes (√)	Yes (√)	Yes (√)	Link-3
CHD-104-V	Chemistry of Materials	2020-21 Revised 2026	Yes (√)	Yes (√)	Yes (√)	Link-2
CHD-105-V	Frontiers in Radical Inorganic Chemistry	2021-22; Revised 2026	Yes (√)	Yes (√)	Yes (√)	Link-3
CHD-106-V	Principles of Fluorescence Spectroscopy and Solvent Effects	2021-22; Revised 2026	Yes (√)	Yes (√)	Yes (√)	Link-4
CHD-107-V	Spectroscopic Methods in Research	2020-21	Yes (√)	Yes (√)	Yes (√)	Link-2
CHD-108-V	Supramolecular Systems and their Diverse Applications	2021-22; Revised 2026	Yes (√)	Yes (√)	Yes (√)	Link-3

Chairperson
Department of Chemistry