Centurion
UNIVERSITY
Shaping Lives...
Empowering Communities...

M.Sc.
Applied Chemistry Syllabus

(Two Years Programme)

School of Applied Sciences

Centurion University of Technology & Management

2025-26

DEPARTMENT OF CHEMISTRY

M.Sc. Chemistry

Two Year Programme

Course Structure 2025-26

Basket I - Core Courses					
Sl. No.	Code	Subject Name	T-P-P	Credits	Level
SEMESTER – I					
1.	CUTM4528	Material Synthesis and Applications	3-1-0	**4**	**6**
2.	CUTM 4529	Industrial Pollution and Management	3-1-0	**4**	**6**
3.	CUTM 4530	Energy Reaction Dynamics	3-1-0	**4**	**6**
4.	CUTM 4532	Stereochemistry and Organic Reaction Mechanism	3-1-0	**4**	**6**
5.	CUTM 4538	Advanced Polymeric Materials	3-1-0	**4**	**6**
SEMESTER – II					
6.	CUTM 4526	Instrumentation Techniques	2-2-0	**4**	**6**
7.	CUTM 4531	Energy Storage Devices and Thermodynamics	3-0-1	**4**	**6**
8.	CUTM 4533	Modern Reagents in Organic Synthesis	3-0-1	**4**	**6**
9.	CUTM 4534	Organometallic and Supramolecular Chemistry	3-0-1	**4**	**6**
10.	CUTM 4537	Symmetry and Group Theory	3-0-1	**4**	**6**
SEMESTER – III					
11.	CUTM4527	Scientific Computing using MATLAB	1-2-1	**4**	**6.5**
12.	CUTM 4535	Nano Pharmaceuticals	3-0-1	**4**	**6.5**
SEMESTER – IV					
13.	CUTM 4536	Green and Sustainable Chemistry	3-1-0	**4**	**6.5**
14.	CUTM 1409	Computational materials science	2-2-0	**4**	**6.5**
		Total	**14*4=56**		
			Basket II (Specialization)	24	
			Basket III (Research Methodology and IPR)	04	
			Skill	04	
			Grand Total	**88**	

Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM4526	Instrumentation Techniques	2-2-0	

Contact Hours: 40 (Theory: 20 hours, Practical: 20 hours)

1. Course Objectives:

This course is designed for postgraduate students from diverse science backgrounds. The primary objective is to provide a comprehensive understanding of the principles, instrumentation, and applications of modern analytical techniques. It aims to equip students with the necessary skills to select and apply appropriate instrumental methods for qualitative and quantitative analysis in their respective research areas.

2. Course Outcomes (COs):

Upon successful completion of this course, students will be able to:

COs	Course outcomes
CO1	Understand the fundamental principles,components,and performance characteristics of modern analytical instruments
CO2	Explain the theory and instrumentation of various spectroscopic, chromatographic, microscopic, and surface analysis techniques
CO3	Choose an appropriate instrumental technique for a specific analytical problem in Physics, Chemistry, or Biology
CO4	Interpret and analyze data obtained from instruments like UV-Vis, FTIR, GC- MS, HPLC, SEM, and XRD.
CO5	Demonstrate hands-onskillsinoperatingbasiclaboratoryinstrumentsand performing data analysis.

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	2		1	3	2	2			3	2	3	2	
CO2	2	3	3	2		3	2	2	2		2	2	3	3	2
CO3	3	2	3		2	2	3	3	2		3	2	3	2	3
CO4	2	3	3	2		2	2	2	2		2	1	3	3	2
CO5	3	2	3	3	2	2	3	1	3		2	2	3	3	3

Part A: Theory (20Hours)

ModuleI: Fundamentals of Instrumentation& Data Analysis (3 Hours)

- Introduction: Classification of instrumental methods.
- Basic Components & Performance: Transducers, detectors, signal processors. Accuracy, precision, sensitivity, resolution.
- Errors & Data Handling: Systematic and random errors, statistical analysis.
- SignalsandNoise:Sourcesofnoise,signal-to-noiseenhancementtechniques.

Module II: UV-Visible & Luminescence Spectroscopy **(4 Hours)**

- UV-VisibleSpectroscopy:Principles(Beer-LambertLaw),instrumentation,and applications.
- Fluorescence & Phosphorescence Spectroscopy: Theory of molecular luminescence, instrumentation, and applications.
- Photoluminescence (PL) Spectroscopy: Principles of luminescence in semiconductors and nanomaterials, instrumentation, and applications in materials characterization.

ModuleIII: Vibrational & RamanSpectroscopy **(3Hours)**

- Infrared (IR/FTIR) Spectroscopy: Principles of molecular vibrations, instrumentation, sample handling, and applications in functional group identification.
- RamanSpectroscopy:TheoryofRamanscattering,instrumentation(lasers,filters, detectors), and applications, including comparison with IR spectroscopy.

ModuleIV:ChromatographicSeparationTechniques **(3Hours)**

- Principles: Adsorption, partition,ion-exchange,andsize-exclusionmechanisms.
- Gas Chromatography (GC):Principle, instrumentation(columns, detectors).
- High-PerformanceLiquidChromatography(HPLC):Principle,instrumentation(pumps, columns, detectors).

ModuleV:MassSpectrometry(MS) **(3Hours)**

- Principles:Ionization,fragmentation,mass-to-chargeratio.
- Instrumentation:Ionsources(EI,CI),massanalyzers(quadrupole,time-of-flight).
- HyphenatedTechniques:IntroductiontoGC-MSandLC-MSforstructuralelucidation.

Module VI: Electron Microscopy Techniques (2 Hours)

- Principles, instrumentation, and applications:Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM).
- ElementalAnalysis:EnergyDispersiveX-raySpectroscopy(EDS)coupledwithSEM/TEM.

ModuleVII:X-rayBasedAnalyticalTechniques(2Hours)

- X-rayDiffraction(XRD):Bragg'sLaw,principlesofpowderXRD,andapplicationsin crystal structure identification.
- X-rayFluorescence(XRF):Principles,instrumentation,andapplicationsinnon-destructive elemental analysis.
- X-rayPhotoelectronSpectroscopy(XPS):Principles,instrumentation,andapplications for determining surface elemental composition and chemical states.

PartB: Practicals (20Hours)

A total of 10experiments (2 hours each)is to be performed.

1. Performerroranalysisonagivendataset,includingcalculationofabsolute,relative, and percentage errors.
2. Calculatethemean,standarddeviation,andvarianceforasetofexperimental measurements.
3. Determine the λ_max of $KMnO_4$ and verify the Beer-Lambert Law using a UV-VisSpectrophotometer.
4. IdentifythefunctionalgroupsinagivenorganicsampleusingFTIRspectroscopy.
5. Determinetheelementalcompositionofasolid/liquidsampleusingX-rayFluorescence (XRF) spectroscopy (data analysis).
6. Separate a mixture of amino acids or plant pigments (any material) using Paper/Thin Layer Chromatography and determine their $R_f$values.
7. Analyzethevibrationalmodesofamaterial(e.g.,carbonnanotubes,siliconwafer)from a given Raman spectrum (data analysis).
8. Determine the elemental composition and chemical states of a surface from a givenXPS spectrum (data analysis).
9. DemonstrationofGasChromatography(GC)fortheseparationofamixtureofvolatile compounds (data analysis).

10. DemonstrationofHigh-PerformanceLiquidChromatography(HPLC)(dataanalysis).
11. Analyzethe surfacemorphology of agiven sampleusingprovided SEMmicrographs.
12. Determine the crystal structure and lattice parameters from a given powder XRD pattern.

3. RecommendedBooks:

Textbooks:

1. Singh, D.K., Pradhan, M. and Materny, A. eds., 2021. *Modern techniques of spectroscopy: basics, instrumentation, and applications*. Singapore: Springer.
2. Hawkes,P.W.andSpence,J.C.eds.,2019.*Springerhandbookofmicroscopy*.Springer Nature.
3. Kumar, C.S., Singh, M.M. and Krishna, R., 2023. *Advanced Materials Characterization: Basic Principles, Novel Applications, and Future Directions*. CRC Press.

References:

1. Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. R. (2014). *Introduction toSpectroscopy*. Cengage Learning.
2. Goldstein,J.I.,etal.(2017).*ScanningElectronMicroscopyandX-rayMicroanalysis*. Springer.
3. Briggs,D.,&Seah,M.P.(1990).*PracticalSurfaceAnalysis,AugerandX-rayPhotoelectron Spectroscopy*. Wiley.

Course Outline

Code	**Course Title**	**T-P-Pj (Credit)**	**Prerequisite**
CUTM4527	Scientific Computing using MATLAB	1-2-1	Undergraduate-level knowledge of mathematics, particularly linear algebra and calculus

Target Audience: M.Sc.(Physics, Chemistry, Mathematics)

ContactHours:12 Theory, 22Practice, 11Project Sessions

- Course Objectives

This course aims to equip postgraduate students in the physical and mathematical sciences with essential computational skills using the MATLAB environment. The primary objective is to empower students to apply numerical methods and data analysis techniques to solve complex scientific problems, visualize results effectively, and automate research tasks.By the end of the course, students will be proficient in using MATLAB as a powerful tool for computation, modeling, and analysis, including an introduction to its machine learning capabilities.

- 2.LearningOutcomes

Upon successful completion of this course, students will be able to:

.

COs	Course outcomes
CO1	Navigate and utilize the MATLAB Integrated Development Environment (IDE) with confidence.
CO2	Develop and debug structured programs using MATLAB scripts and functions
CO3	Implement fundamentalnumericalalgorithmstosolvescientificproblems(e.g.,solving systems of equations, ODEs, and data interpolation).
CO4	Process,analyze,and visualizescientificdatatoextractmeaningfulinsightsandcreate publication-quality graphics
CO5	Apply basic signal, image, and machine learning techniques to relevant datasets using MATLAB toolboxes to design and execute a computational project from problem formulation to final presentation.

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	–	–	–	1			2	2	3	1	3	–	2
CO2	3	3	2	2	–	2			3	2	2	–	3	2	3
CO3	3	3	2	2	2	2			3	2	2	2	3	3	2
CO4	3	2	1	–	–	–			2	1	3	2	2	3	2
CO5	3	3	3	3	2	2			3	3	3	2	3	3	2

Course Structure and Session Distribution

Module	ModuleTitle	Theory Sessions	Practice Sessions	Project Sessions
1	IntroductiontotheMATLAB Environment	2	4	0
2	ProgrammingFundamentalsin MATLAB	2	4	0
3	DataHandling,Analysis,and Visualization	1	4	0
4	NumericalMethodsforScientists	3	4	0
5	Introduction to Signal and Image Processing	1	3	0
6	Machine Learning using MATLAB	3	3	1
7	Project Work and Advanced Topics	0	0	10
	Total	12	22	11

Content

Module1:Introduction to the MATLAB Environment

- Theory:MATLABIDE(CommandWindow,Workspace,Editor,HelpBrowser),basic syntax, defining variables. [2 Hours]
- Practice Sessions(1-4):
    1. Aim: To familiarize with the MATLAB IDE by calculating the energy of a photon using Planck's equation (E=hν). [1 Hour]
    2. Aim:To create and manipulate vectors representing position in 3Dspace (Physics) and matrices for linear transformations. [1 Hour]
    3. Aim: To understand element-wise operations for stoichiometric calculations in a chemical reaction. [1 Hour]
    4. Aim: To generate and customize a2D plot of a projectile's trajectory.[1Hour]

Module 2: Programming Fundamentals in MATLAB

- Theory: Script files vs.functions, function definition and calling, control flow(if-else if- else, switch), loops (for, while), logical operators. [2 Hours]
- Practice Sessions(5-8):

  5.Aim:Towriteauser-definedfunctiontocalculatethepHfromagivenhydrogenion concentration. [1 Hour]

  6.Aim:To implement control flow to determine the phase of water (solid, liquid, gas) based on temperature and pressure inputs. [1 Hour]

  7. Aim:TouseaforlooptocalculatethetermsofaTaylorseriesexpansionfora function like sin(x) [1 Hour]

  8.Aim: To use a struct to store properties of chemical elements (e.g., name, symbol, atomic number, mass) [1 Hour].

Module3:Data Handling, Analysis, and Visualization

- Theory: Importing and exporting data(CSV,TXT,Excel),datatypes,descriptive statistics. [1 Hour]
- Practice Sessions(9-12):

  9. Aim:Toimportexperimentaldatafromaspectrometer(.csvfile)intotheMATLAB workspace. [1 Hour]

  10. Aim:Toperformdescriptivestatisticalanalysis(mean,median,standarddeviation) on a set of experimental measurements. [1 Hour]

  11. Aim:To create a semi-log plotto analyze first-order reaction kinetics(Chemistry). [1 Hour]

  12. Aim: To generate a 3D surface plot to visualize an electric potential field or a mathematical function z = f(x,y) [1 Hour].

Module4: Numerical Methods for Scientists

- Theory: Solving systems of linear equations, polynomial interpolation and curve fitting, concepts of numerical integration and differentiation, introduction to Ordinary Differential Equations (ODEs). [3 Hours]
- Practice Sessions(13-16):

  13. Aim: To solve a system of linear equations representing Kirchhoff's laws for an electrical circuit. [1 Hour]

  14.Aim: To perform a polynomial curve fit for a Beer-Lambert law calibration curve. [1 Hour]

15. Aim: TocomputethenumericalintegralofaGaussianfunctiontofindthearea under the curve. [1 Hour]

16.Aim:TosolvetheODEforradioactivedecayofanisotopeusingode45[1Hour]. Module 5:

Module-5. Introduction to Signal and Image Processing

- Theory: Concepts of frequency domain, Fast Fourier Transform (FFT), basic digitalfiltering. Fundamentals of digital images. [2 Hours]
- PracticeSessions(17-19):

17.Aim: To analyze a noisy signal from an instrument by computing its Fast Fourier Transform (FFT) to identify primary frequencies [1 Hour].

18.Aim:Toread,display,andcropamicrographimage(e.g.,fromSEMorAFM)ofa nanostructured surface. [1 Hour]

19.Aim:Toenhanceamicrographimagebyapplyingspatialfiltersfornoisereduction and edge detection to better visualize surface features. [1 Hour]

Module6: Machine Learning using MATLAB

- Theory: Overview of Machine Learning (ML), supervised vs. unsupervised learning, concepts of classification, regression, and clustering. [3 Hours]
- PracticeSessions(20-22):

20.Aim:TousetheClassificationLearnerAppto classifychemical compounds based on their spectroscopic data. [1 Hour]

21.Aim: To use k-means clustering to group particles based on size and shape fromimage analysis data. [1 Hour]

22.Aim: To build a regression model to predict a material's property (e.g., band gap) based on experimental parameters. [1 Hour]

Module7:ProjectWorkandAdvancedTopics

- Theory: Introduction to Symbolic Math Toolbox, principles of parallel computing in MATLAB (parfor). [1 Hour]
- Practice & Project: Students will work on a semester-long project relevant to their domain.Sessionswillbededicatedtoprojectbrainstorming,development,debugging, and final presentations. [10 Hour Sessions]

Recommended Books and Resources

1. Textbooks:

- *Turk,Irfan.PracticalMATLAB.Berkeley,CA,USA:Apress,2019.*
- *Xue, D. and Chen, Y., 2018.Scientific computing with MATLAB. Chapman and Hall/CRC.*
- *Paluszek,M.andThomas,S.,2016.MATLABmachinelearning.Apress.*

2. Online Resources:

   - Math WorksOfficialDocumentation: https://www.mathworks.com/help/matlab/
   - Math Works On ramp(Free interactive tutorial).
   - Coursera/edX courses on MATLAB.

Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM4528	Material Synthesis and Applications	3-1-0	

Objective

- To provide students with a comprehensive understanding of the synthesis, properties, and applications of nanomaterials and composite systems.
- Students will gain practical experience in synthesizing and characterizing nanomaterials, while exploring their potential in various industrial and technological applications.

Learning outcome

COs	Course outcomes
CO1	Understand the fundamental principles, types, and properties of nanomaterials and nanocomposites.
CO2	Describe and compare various synthesis techniques for nanomaterials and composite systems.
CO3	Apply appropriate synthesis methods to prepare nanomaterials and composite materials in

	the laboratory.
CO4	Analyze the relationship between synthesis method and material properties.
CO5	Evaluate materials for real-world applications (electronics, catalysis, biomedical, etc.).

CO,PO, PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	-	2	3	-	-	-	-	-	-	2	3	2	2
CO2	3	3	2	3	3	-	-	-	-	-	-	2	3	3	2
CO3	2	2	1	3	3	-	-	-	-	-	-	2	3	2	1
CO4	2	3	2	3	2	-	-	-	-	-	-	3	2	3	2
CO5	2	3	3	2	2	2	2	-	-	1	1	3	2	3	1

<u>Course content</u>

Module-I **(5hrs)**

Introduction to Nanomaterials and Composite Systems

Introduction to nanomaterials, Properties of materials and nanomaterials, role of size in Nanomaterial, Types of nanomaterials (0D, 1D, 2D, 3D) based on morphology and quantum confinement effect, Overview of composite materials (matrix and reinforcement), Definition of nanocomposite, Properties of composite and nanocomposite.Types of nanocomposite (i.e. metal oxide, ceramic,polymer and carbon based); Core-Shell structured nanocomposites

Module-II: **(5hrs)**

Synthesis Approaches of Nanomaterials

Bottom-up approach and Top-down approach, Importance of synthesis methods in tailoring nanomaterials properties, Thermodynamics and kinetics in nanoparticle formation, Factors affecting synthesis: temperature, pH, concentration, surfactants, stabilizing agents.

Module -III: **(6hrs)**

Physical Methods of Synthesis

Mechanical milling (ball milling, high-energy attrition), Physical vapor deposition (PVD), sputtering, Laser ablation, thermal evaporation, Arc discharge and electron beam evaporation,Advantages and limitations of physical techniques

Practice-1: Preparation of metal nano powder using Ball milling method.

Module - IV: **(6hrs)**

Chemical Methods of Synthesis

Sol-gel method, Co-precipitation, microemulsion, Hydrothermal and solvothermal techniques, Chemical vapor deposition (CVD) and atomic layer deposition (ALD), Synthesis of carbon based nanomaterials: Graphene, Graphene oxide and Carbon nanotubes (CNTs), Synthesis of quantum dots (QDs)

Practice-2: Sol-Gel Synthesis of ZnO Nanomaterial

Practice-3: Co-Precipitation Synthesis of Fe_3O_4 Magnetic Nanomaterials

Practice-4: Synthesis of graphene oxide using modified Hummer's method.

Module-V: **(5hrs)**

Fabrication of composite and nanocomposites

Synthesis of composite: Filament Winding, Injection and compression molding, Pultrusion Process, Synthesis of nanocomposite: In-situ and ex-situ synthesis techniques, Polymer, metal, and ceramic matrix nanocomposites.Processing methods: melt mixing, solution casting, electrospinning

Practice-5: Fabrication of Polymer Nanocomposites

Practice-6: Preparation of natural fibers reinforced composite materials

Module VI: **(5hrs)**

Properties of Composites

Geometrical aspects: volume and weight fraction, Unidirectional continuous fiber, Determination of stiffness and strengths of unidirectional composites, tension, compression, flexure and shear.

Module VII: **(6hrs)**

Applications of Nanomaterials and Composites

Aerospace and automotive components, Electronics and sensors, Biomedical applications (drug delivery, tissue engineering), Energy storage and conversion (batteries, fuel cells, supercapacitors), Environmental remediation (water purification, air filters)

Practice-7: Electrical Conductivity Test of Carbon-based Nanocomposites

Practice-8: Water purification test of synthesized nanomaterials

Text Books:

1. Inorganic Materials Synthesis and Fabrication by J.N. Lalena, D.A. Cleary, E.E. Carpenter, N.F. Dean, John Wiley & Sons Inc.
2. Introduction to Nanoscience and Nanotechnology" – K.K. Chattopadhyay & A.N. Banerjee.
3. The Chemistry of nanomaterials: Synthesis, Properties and Applications, Vol-I by C.N.R. Rao, A. Muller and A.K. Cheetham.
4. Polymer Nanocomposites: Processing, Characterization, and Applications" – Joseph H. Koo.
5. Introduction to Nanocomposite Materials: Synthesis, Properties and Applications" – Thomas E. Twardowski

Reference Books:

1. Encyclopedia of Nanotechnology by M.Balakrishna Rao and K.Krishna Reddy, Vol I to X,
2. Encyclopedia of Nanotechnology by H.S. Nalwa
3. Nano: The Essentials – Understanding Nano Scinece and Nanotechnology – by T.Pradeep; Tata Mc.Graw Hill
4. Handbook of chemical Vapor deposition (cvd), Principles, technology, and applications, By Hugh o. Pierson, Second edition, Noyes publications, William Andrew Publishing, LLC.
5. Mohr - SPIE Handbook of Technology and Engineering of Reinforced Plastics/Composites – (Van Nostrand, 1998

Course Outline

Code	**Course Title**	**T-P-Pj (Credit)**	**Prerequisite**
CUTM 4529	Industrial Pollution and Management	3-1-0	

Introduction:
This course provides an

Course Objective:
Theobjectives ofthe courseare

- To encourage understanding of basic and advanced concepts in Industrial pollution aspects
- and waste water treatment technologies.
- To expose the students for different processes used in industries and in research field.
- To grow skills required in various industries, research labs and in the field of human health.
- To develop the students to accept the challenges in industrial sectors.

COs	Course outcomes
CO1	To **Describe** the types of pollution, environmental legislation, and water quality management practices
CO2	To **Analyze** water and air quality by determining physical and chemical parameters
CO3	To **Evaluate** the efficiency of different treatment methods for wastewater treatment
CO4	To **Apply** pollution control strategies for industrial wastewater treatment and air quality management.
CO5	To **Design and recommend** suitable treatment methods for industrial and municipal wastewater

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	-	-	-	2	3	-	-	-	-	2	3	2	-
CO2	3	3	2		2	-	3	-	-	-	-		3	2	-
CO3	3	3	3	2	2	-	2	-	-	-	-	2	3	3	-
CO4	2	3	2	-	-	3	3	3	-	1	2	2	3	3	-
CO5	2	2	2		2	-	3	2	-	-	1	3	3	3	-

Course Outline

Module-1: Fundamentals of pollution **(5Hrs)**

Types of Pollution, Pollution control aspects, Industrial Emissions-Liquids, Gases, Environmental Legislation, Water quality management in India, Air (Prevention & Control of Pollution) Act

Module 2 Water quality standard **(6 Hrs)**

Drinking Water quality standard, Introduction to Irrigation Water Treatments, Stream standard and effluent standard, Characterization of Municipal waste water.

Practice 1: Water Analysis-**Determination of Chemical Parameters of Water** (Hardness, Alkalinity, Acidity, COD, or BOD)

Practice 2: Water Analysis-**Determination of Physical Parameters of Water** (Temperature, Colour, Odour, Taste, Conductivity)

Practice 3: Measurement of Turbidity of a given water sample using Nephelometric or Turbidimetric method

Module 3 Methods of treatment of waste water **(6 Hrs)**

Water treatment sewage plant, process with primary treatment aeration settling tank to chlorination and filtration, Basics of water filtration, softening, desalination and disinfection for small to medium sized water supplies. Secondary treatment, Tertiary treatment methods for waste water treatment

Practice 4: Determination of Dissolved oxygen in water sample

Practice 5: Determining the chloride content in given water sample using mohr's method

Practice 6: Analyzing water samples for total phosphorous

Module 4 Air pollution and its Permissible limit **(5 Hrs)**

National Ambient Air Quality Standards for Ozone, Air Pollution Control Devices, Measuring Particulate Matter in Air.

Practice 7:**Determination of Chloride content in a water sample using Mohr's method**.

Practice 8:**Measurement of Particulate Matter (PM10 / PM2.5) in Air using Gravimetric or Filter Paper Method**.

Module 5 Management and treatments of Waste chemicals **(6Hrs)**

Hazardous Waste Regulations and Hazardous Materials, Fertilizers and Pesticides Minimization of VOC emission, Segregation of waste water stream, Characterization of Municipal waste water and Chemical sector waste water

Practice 9:Characterization of Municipal Wastewaterfrom a local municipal area

Module 6 Industrial Waste Water Treatment **(5 Hrs)**

Water and Wastewater Treatment Engineering, Water Quality Control, Pollution control in Chemical Industries, General considerations

Practice 10: Characterization of Industrial Wastewater (pH, COD, BOD, Total Solids) from a local industry or simulated sample

Module 7 Industrial Waste Water Treatment **(7 Hrs)**

Pollution control aspects of Fertilizer industries, Pollution control in Petroleum Refineries, Pollution control in Pulp and Paper Industries.

Text Books

1. Pollution control in Process Industries, S.P .Mahajan, Tata McGraw Hill Publishing Company Ltd, New Delhi

Reference Books:

1. Industrial Pollution and Management, Arvind Kumar, Aph Publishing Corporation.
2. Environmental Pollution by Chemicals - Walker, Hulchiason.
3. Biochemistry and Microbiology of Pollution - Higgins and Burns.
4. Environmental Pollution - Laurent Hodge, Holt.
5. Waste Water Treatment - Datta and Rao (Oxford and IBH).
6. Sewage and waste treatment – Hammer
7. Environment and Metal Pollution - Khan (ABD Pub. Jaipur).
8. Environment Pollution - Timmy Katyal (Satke Anmol Pub. New Delhi).

Code	**CourseTitle**	**T-P-Pro (Credit)**	**Prerequisite**
CUTM 4530	**Energy Reaction Dynamics**	3-1-0	

Course objective

- **To understand concepts of thermodynamics**
- **To have proper understanding of chemical kinetics**
- **To apply the knowledge to solve the problems in research.**

Course Outcomes. After the completion of the course the students will be able to

COs	Course outcomes
CO1	Recall on the basic to advanced concepts of chemical thermodynamics
CO2	Describe the laws of statistical thermodynamics and its applications
CO3	Interpret the order of different chemical reactions.
CO4	Analyze the behavior photocatalytic reactions.
CO5	Evaluate the rate constant and compare the kinetics of different chemical reactions.

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	1	2		2	1		3	2	2	3	3	2	1
CO2	2	3	1	3		3	1		2	3	3	2	2	3	2
CO3	3	2	2	2		2	1		3	2	2	3	3	2	1
CO4	2	3	1	3		3	1		2	3	3	2	2	3	2

CO5	3	2	2	2		2	1		3	2	2	3	3	2	1

Module I: **(5 hours)**

Basic concepts of thermodynamics: state and path functions and their applications; thermodynamic description of various types of processes;

Module II: **(7 hours)**

Concept of entropy, reversible and irreversible processes, Clausius inequality, Free energies, Criteria of spontaneity. Fundamental equations for open systems, Partial molar quantities and chemical potential, Gibbs-Duhem equation, Real gases Concepts of fugacity and activity. Entropy changes in chemical reactions, The Gibbs energy of real gases.

Module III **(5 hours)**

Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities - calculations for model systems.

Module IV: **(6 hours)**

Basics of chemical kinetics, Rate law equations, Arrhenius equation, Composite Reactions – types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state concepts, rate determining steps, microscopic reversibility

Module **V**: **(5 hours)**

Hammet Equation, Hammond postulate, Curtin-Hammett principle, Enzyme kinetics and Michalis-Menten equation.

Module VI: **(6 hours)**

Kinetics of photochemical and photophysical processes, chain reactions (H2-Br2 reaction, decomposition of ethane and acetaldehyde), and oscillatory reactions (Belousov-Zhabotinskii reaction).

Module VII: **(5 hours)**

Kinetics of Complex reactions, parallel and consecutive reactions, salt effects.

Practices

1. Determine the Enthalpy Change for the dissolution of salts like NaOH or KNO_3.

2. Compare Heat of Neutralization for strong acid–strong base vs. weak acid–strong base.
3. Study Endothermic and Exothermic Reactions: dissolving NH_4Cl in water vs. $CaCl_2$ in water).
4. Rate of Reaction using Sodium Thiosulfate and Hydrochloric Acid (disappearance of cloudiness).
5. Effect of Temperature on Reaction Rate using the reaction between vinegar and baking soda.
6. Study Effect of Concentration on Reaction Rate using the iodine clock reaction (simple version).
7. Study the kinetics of Photodecomposition of Silver Chloride (exposure to sunlight).
8. Study of Photosynthesis Rate in pondweed under varying light (bubble counting method).
9. Effect of Temperature and pH on Catalase Activity from potato or liver (foam height with H_2O_2).
10. Investigate the Rate of Starch Breakdown by salivary amylase (iodine test).
11. Color Change Reactions for visual understanding of kinetics (e.g., methylene blue oxidation in glucose solution).
12. Specific Heat Capacity of Water – simple calorimetry using a heater and thermometer.

Reference Books:

1. Engel, T. and Reid, P. *Physical Chemistry 3rd Ed.,* Prentice Hall, 2012
2. McQuarrie, D. A. and Simon, J. D. *Molecular Thermodynamics* Viva Books, 2004.
3. Roy, B. N. Fundamentals of Classical and Statistical Thermodynamics Wiley, 2001
4. Levine, I .N. *Physical Chemistry* 6th Ed. Tata McGraw Hill, 2010.
5. Atkins P. and De Paula, J. *Physical Chemistry* Tenth Ed.*,* OUP, 2014.
6. Castellan, G. W. *Physical Chemistry 4th Ed.,* Narosa, 2004.

Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM 4531	Energy Storage Devices and Thermodynamics	**3+0+1**	

Course Objectives : By the end of this course, students should be able to

- **Understand the fundamental** Thermodynamics Principles and their relevance to energy systems.
- **Analyze**thermodynamic processes used in battery operation
- Evaluate energy conversion efficiency in various systems..
- **Evaluate performance characteristics** such as energy conversion efficiency, energy density, power density, cycle life, efficiency, and safety.
- Describe the working principles of different energy storage devices including batteries, capacitors, fuel cells.
- Apply thermodynamic principles to model and assess the performance of energy storage devices.
- Calculate energy efficiency, exergy efficiency, and losses in various storage systems.

Course Outcomes

CO1	**Apply the laws of thermodynamics** to analyze and solve problems related to energy systems and cycles.
CO2	**Evaluate the performance of thermodynamic systems**, including efficiency and work potential using concepts of enthalpy, entropy, and exergy.
CO3	**Classify and compare various energy storage technologies**, including electrochemical, thermal, mechanical, and chemical storage systems
CO4	**Analyze the energy and exergy efficiency** of energy storage devices using thermodynamic principles
CO5	**Design and simulate simple energy storage systems** for practical applications, considering thermodynamic constraints and operational parameters.

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2				2	3					2	2	1	
CO2	3	3			2								3	2	
CO3	3	3	2	3	2							2	3	3	
CO4	2	3	3	2	3		2				1	2	3	3	
CO5	2	2		2	3		2	2				3	2	3	

Module-1.Energy storage systems overview **(5hrs)**

Scope of energy storage, needs and opportunities in energy storage, Technology overview and key disciplines, comparison of time scale of storages and applications, Energy storage in the power and transportation sectors. Importance of energy storage systems in electric vehicles, Current electric vehicle market.

Module-2:Thermal storage system **(6hrs)**

-heat pumps, hot water storage tank, solar thermal collector, application of phase change materials for heat storage-organic and inorganic materials, efficiencies, and economic evaluation of thermal energy storage systems.

Module-3:Chemical storage system **(5hrs)**

Chemical storage system such as hydrogen, methane etc., concept of chemical storage of solar energy, application of chemical energy storage system, advantages and limitations of chemical energy storage, challenges, and future prospects of chemical storage systems.

Module-4:Electromagnetic storage systems **(5hrs)**

-double layer capacitors with electrostatically charge storage, superconducting magnetic energy storage (SMES), concepts, advantages and limitations of electromagnetic energy storage systems, and future prospects of electrochemical storage systems.

Module-5:Electrochemical storage Devices-1 **(5hrs)**

Batteries-Working principle of battery, primary and secondary (flow) batteries, battery performance evaluation methods, major battery chemistries and their voltages- Li-ion battery& Metal hydride battery vs lead-acid battery.

Module-6:Electrochemical storage Devices-2 **(6hrs)**

Supercapacitors- Working principle of supercapacitor, types of supercapacitors, cycling and performance characteristics, difference between battery and supercapacitors, Introduction to Hybrid electrochemical supercapacitors .**Fuel cell:** Operational principle of a fuel cell, types of fuel cells, hybrid fuel cell-battery systems, hybrid fuel cell-supercapacitor systems.

Module-7:Battery design for transportation: **(7hrs)**

Mechanical Design and Packaging of Battery Packs for Electric Vehicles, Advanced Battery-Assisted Quick Charger for Electric Vehicles, Charging Optimization Methods for Lithium-Ion Batteries, Thermal run-away for battery systems, Thermal management of battery systems, Recycling of Batteries from Electric Vehicles

Project Topics

1. Design and performance analysis of a lithium-ion battery pack for electric vehicles.

2. Comparative study of lithium-ion vs. sodium-ion batteries: Efficiency, safety, and cost.
3. Simulation of a hybrid energy storage system for a microgrid using MATLAB/Simulink
4. Integration of solar PV with thermal and electrochemical storage for off-grid applications.
5. Simulation of thermal runaway in battery packs using COMSOL or ANSYS.
6. Lab-scale testing and analysis of a TES system using wax or salt hydrates.
7. Techno-economic analysis of hydrogen-based energy storage.
8. Development of a sustainable energy storage model using biomass and thermal energy.

Recommended Textbooks

- Allen J. Bard & Larry R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd edition, Wiley
- Frank S. Barnes and Jonah G. Levine, Large Energy Storage Systems Handbook (Mechanical and Aerospace Engineering Series), CRC press (2011)
- Ralph Zito, Energy storage: A new approach, Wiley (2010)
- A Text Book of Battery Science. by Dr. R. Hemalatha, Dr. M.Alagar , Dr. R. HepziPramilaDevamani , Dr. P. Ramesh Babu, 2022 edtn,Royal Book Publishing.
- Thomas B Reddy, Linden's Handbook of Batteries(4th edition), cGraw-Hill Education
- Pistoia, Gianfranco, and Boryann Liaw. Behaviour of Lithium-Ion Batteries in Electric Vehicles: Battery Health, Performance, Safety, and Cost. Springer International Publishing AG, 2018.
- Robert A. Huggins, Energy storage, Springer Science & Business Media (2010)

Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM 4532	Stereochemistry and reaction mechanism	3-1-0	

Objective

- To understand and focus on the dependency of reaction outcomes on stereochemical relationship of the molecules.
- To be able to visualize complex molecules in three dimension.
- To learn different aspects of stereoselective and stereospecific reactions.
- Study of reaction mechanism and nature of transition states.

Learning outcome

COs	Course outcomes
CO1	Understand the principles of stereochemistry, including chirality, optical activity, and stereoisomerism.
CO2	Predict stereochemical outcomes of organic reactions.
CO3	Explain and analyze various types of reaction mechanisms (SN1, SN2, E1, E2, etc.)
CO4	Apply reaction mechanism knowledge to predict products and intermediates.
CO5	Correlate stereochemistry and reaction pathways with applications in drug design, synthesis, and catalysis.

CO,PO, PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	-	2	-	-	-	-	-	-	-	2	3	2	2
CO2	3	3	2	3	-	-	-	-	-	-	-	2	3	3	1
CO3	2	3	2	3	-	-	-	-	-	-	-	3	3	3	1
CO4	2	3	2	3	-	-	-	-	-	-	-	3	3	3	1
CO5	2	3	3	2	2	2	2	2	1	1	1	3	3	3	1

Course content

Module-I:

Principles of stereochemistry

IUPAC nomenclature of organic molecules including regio- and stereoisomers, Configurational and conformational isomerism inacyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity,diastereoselectivity and asymmetricinduction.

Practice-1: Measure the optical rotation of a chiral compound (e.g., glucose, lactic acid) using a polarimeter

Module-II:

Dynamic stereochemistry

Stereoselective Reactions, Asymmetric Induction in synthetic reactions, Acyclic Stereoselection–Considerations to Carbonyl additions- 4membered and 6-membered transition states, Cram and FelkinModels.

Practice-2: Synthesis and Resolution of Racemic Mixtures

Parctice-3: Thin Layer Chromatography (TLC) of Stereoisomers

Parctice-4: Identify meso compounds via melting point comparison and optical rotation.

Module - III:

Aromaticity and Organic reactive intermediates

Aromaticity of Benzenoid and non-benzenoid compounds – generation andreactions.Organic reactive intermediates: Generation, stability and reactivity ofcarbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

Practice-5: Preparation of p-nitrobenzoic acid from p-nitrotoluene (Oxidation)

Module-IV:

Types of organic reactions

Substitution Reactions: SN1, SN2, SNi, SN1', SN2' reactions, reactivity, solvent effect, nature of bases, effects of leaving groups.Aromatic electrophilic substitution reaction, Aromatic nucleophilic substitution reaction. Addition Reactions: Addition to carbon-carbon multiple bonds. Addition to carbon-hetero multiple bonds. Elimination reactions: E2, E1 and E1cB

Practice-6: Preparation of benzhydrol from benzophenone (Reduction)

Practice-7: Perform a reaction prone to rearrangement (e.g., alcohol to alkene via H^+) and analyze rearranged products

Module V:

Reaction Mechanism

Methods of determining reaction mechanisms, Prediction of Probable Products – Kinetic vs Thermodynamic Control, Hammond postulate, Curtin Hammett principle. Kinetic isotope effect, Baldwin rules for ring closure. Effect of structure and medium on reactivity, Substituent Effects, Hammett Plots and Linear Free Energy Relationships, Other Linear Free Energy Relationship, Acid-Base Related Effects

Practice-8: Bromination of Alkenes Using NBS (N-Bromosuccinimide)

Module VI:

Pericyclic reactions-I

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, allylsystem, classfication of pericyclic reactions FMO approach, Woodwrd- Hoffman correlationdiagram method and perturbation of molecular (PMO) approach for the explanation of pericyclicreactions under thermal and photochemical conditions.

Practice-9: Photochemical Electrocyclic Reaction of Hexatriene to Cyclohexadiene

Module VII

Pericyclic reactions-II

Electrocyclic Reactions: Conrotatory and disotatory motions (4n) and (4n+2), allyl systems and secondary effects. Cycloadditions: Antarafacial and suprafacial additions, notation of cycloadditions, (4n) and (4n+2) systems. Sigmatropic reaction under thermal and photochemical conditions. suprafacial and antarafacialshifts of H. Sigmatropic shift involving carbon moieties, retention and inversion ofconfigurations, (3.3) and (5.5) sigmatropic rearrangements.

Practice-10: Thermal Diels–Alder Cycloaddition

Text Books:

6. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International Publishers.
7. E.L.Eliel, Stereochemistry of Organic Compounds, Wiley
8. Subrata Sengupta, Stereochemistry of Organic Molecules, Book Syndicate Pvt. Ltd.
9. M M Smith, Organic Synthesis, Mc Graw Hill.
10. B. Mahapatra, A. Ghoshal, A. K. Nad, An Advanced Course in Practical Chemistry, NEW CENTRAL BOOK AGENCY, 2011
11. Advanced Organic Chemistry: Reactions Mechani;sms and Structure by Jerry March, Mc.Graw H
12. Pericyclic reactions by S.N. Mukharji, Mcmilan

Reference Books:

6. Stereochemistry of Organic Compounds" – Ernest L. Eliel, Samuel H. Wilen
7. Advanced Organic Chemistry: Part A – Structure and Mechanisms" – Francis A. Carey, Richard J. Sundberg
8. Organic Chemistry" – Jonathan Clayden, Nick Greeves, Stuart Warren
9. Organic Chemistry: Structure and Function" – K. P. C. Vollhardt, Neil E. Schore.
10. Principles of Organic Synthesis" – R.O.C. Norman & J.M. Coxon
11. Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Richgardso

Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM4533	Modern Reagents in Organic Synthesis	3-1-0	

Objective

- To gain knowledge on reagents that are used in organic synthesis.
- To gain confidence in deriving the mechanism of an organic transformation.
- To gain a thorough understanding of the mechanisms of various organic transformations towards the target molecule.
- To know retrosynthetic analysis towards the synthesis of target molecules.

Learning outcome

COs	Course outcomes
CO1	Understand the properties and reactivity of modern organic reagents.
CO2	Classify reagents based on their functions (oxidizing, reducing, protecting, etc.).
CO3	Select appropriate reagents for specific synthetic transformations.
CO4	Analyze the mechanisms of reagent-based organic reactions.
CO5	Apply knowledge of modern reagents in multistep organic synthesis relevant to pharmaceuticals and materials.

CO,PO, PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	-	2	2	-	-	-	-	-	-	2	3	2	2
CO2	3	2	-	2	2	-	-	-	-	-	-	2	3	2	2
CO3	3	3	2	3	3	-	-	-	-	-	-	3	3	3	1
CO4	2	3	2	3	3	-	-	-	-	-	-	3	3	3	1
CO5	2	3	3	3	3	2	2	2	1	1	1	3	3	3	1

Course content

Module-I:

Carbocation (Pinacol-Pinacolone Rearrangement, Wagner-Meerwein Rearrangement, Demjanov reaction, Favorski Rearrangement, Fries Rearrangement, Benzil-Benzilic Acid Rearrangement)

Practice-1: Formation of Grignard reagent (RMgX) from alkyl or aryl halides, which reacts with carbonyl compounds to form alcohols.

Practice-2: Rearrangement of Pinacol to Pinacolone under Acidic Conditions

Module-II:

carbanion (Alkylation, Aldol condensation (asymmetric reaction), Robbinson annulation, Claisen condensation, Dieckmann condensation Reaction, Perkin Reaction, Stobbe Condensation Reaction, Moritas-Baylis-Hilmann reaction, Bamford-Steven, Shapiro reaction)

Practice-3: Aromatic compounds undergo electrophilic aromatic substitution with an alkyl halide, in the presence of a Lewis acid catalyst

Practice-4: The reaction of α,β-unsaturated carbonyl compounds or aldehydes/ketones to form β-hydroxy carbonyl compounds followed by dehydration to produce α,β-unsaturated carbonyl compounds.

Module -III:

Free radicals (Allylic halogenations, acyloin condensation, McMurry coupling, Hunsdiecker reaction, Bouveault-Blanc reduction), carbenes (Wolff Rearrangement, Reimer-Tiemann), nitrenes (Hofmann, Beckmann, Curtius, Schmidt, Lossen Rearrangement), arynes, phosphorous ylides (Wittig Reaction), sulfur ylides.

Parctice-5: Formation of alkenes by reacting an ylide (phosphorus ylides) with carbonyl compounds.

Practice-6: Allylic Bromination of Alkenes (Allylic Halogenation)

Module - IV:

Oxidizing reagents: Chromium reagents, manganese reagents, Ruthenium tetroxide, TPAP, Lead tetraacetate, Osmium tetroxide, Hypervalent Iodine reagents [Dess-Martin periodinane (DMP), o-iodoxybenzoicacid (IBX)], Cerric ammonium nitrate, DDQ, Selenium dioxide, DMSO based oxidizing reagents, Aluminiumalkoxides (Oppenauer Oxidation), peroxyacids.

Practice-7: Oxidation of aldehydes to carboxylic acids (e.g., oxidation of benzylic alcohol to benzoic acid)

Practice-8: Manganese Reagents: $KMnO_4$ Oxidation

Module-V:

Reducing reagents: Heterogeneous catalytic hydrogenation, Homogeneous Catalytic hydrogenation (Wilkinson's Catalyst), Dissolving metal reduction (Clemmesen Reduction Reaction, Birch Reduction)Reduction with hydride-transfer reagents (Aluminiumalkoxides, Lithium aluminium hydride, sodium borohydride, DIBAL-H, Tinhydrides, Silanes, diimide, Borane and derivatives.

Practice-9: Reduction of aldehydes and ketones to primary and secondary alcohols.

Module VI:

C-C bond forming reactions: Main Group Chemistry – Organometallic reagents in Organic synthesis: Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details: Organozinc (Reformatsky Reaction), Organoaluminium, Organosilicon, Organocerium, Organoborane (Hydroboration of alkenes, Allyl boranes, CBS reaction), Organocadmium, Organomercury, Organotin (Reduction with tri n-Butyltinhydride) compounds. Transition–metal Chemistry: Organotitanium, Organochromium, Organoiron, Organocopper, Organopalladium compounds.

Practice-10: Reaction between an α-halo ester and a zinc enolate to form a β-hydroxy ester.

Module VII:

Illustration of protection and deprotection in synthesis. The Disconnection Approach: One-group and two-group disconnections, control in carbonyl condensations, Umpolung, radical reactions in synthesis, use of acetylenes, ring annulation strategies. Cross-coupling C-C reactions involving boron, tin, silicon reagents and aryl/alkenyl/alkynyl and alky halides. Metathesis and Grubb's Catalyst. Organocatalysis: Introduction to organo-catalyzed reactions, Classifications (HOMO, LUMO, SOMO catalysis), Enamine, Iminium, H-bonding catalysis and asymmetric organocatalysis (Michael, aldol, Mannich etc).

Text Books:

13. J. Clayden, N. Greeves, and S. warren, Organic Chemistry, Oxford University Press , Second edition, 2012.
14. E.L.Eliel, Stereochemistry of Organic Compounds, Wiley
15. R. K. Kar, Name Reactions and Rearrangements in Organic Chemistry, New India Book Agency.
16. William Carruthers and Iain Coldham, Modern Methods of Organic Synthesis, Cambridge University Press , Fourth Edition.

Reference Books:

12. A. R. Parikh, H. Parikh and K. Parikh, Name reactions in Organic Synthesis, Foundation Books
13. Advanced Organic Chemistry: Part A – Structure and Mechanisms" – Francis A. Carey, Richard J. Sundberg
14. Michael B. Smith, Organic Synthesis, McGraw Hill International Editions , Fourth Edition
15. V. K. Ahluwalia and R. K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House , Fourth Edition

Code	Course Title	T-P-Tut (Credit)	Prerequisite
CUTM 4534	**Organometallic and Supramolecular Chemistry**	3-0-1	

Objective

- To explain the synthesis, bonding, structure, and properties of organometallic compounds
- To comprehend the application of organometallic compounds as a catalyst in various synthesis and their function in various biological systems involving metals.
- To design and develop novel functional systems by joining multiple chemical components through non-covalent interactions.

Course outcome

COs	Course outcomes
CO1	Recall the synthesis, structure, bonding, and reactivity of both main group and transition metal organyls
CO2	Understand the basic structure of different supramolecular system
CO3	Analyze the stability and properties of metal organyls and supramolecular assemblies
CO4	Evaluating the important roles of organometallic compounds in catalysis
CO5	Able to create new ideas for advanced research, publish articles as well,and develop products.

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2		2		2	1		3	2	2	3	3	2	3
CO2	2	3		3		3	1		2	3	3	2	2	3	2

CO3	3	2		2		2	1		3	2	2	3	3	2	3
CO4	2	3		3		3	1		2	3	3	2	2	3	2
CO5	3	2		2		2	1		3	2	2	3	3	2	3

Module I:Organometallic compounds: synthesis, bonding and structure, and reactivity.

Transition Metal π-Complexes Transition Metal π- Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene, and trienyl complexes, preparations, properties, nature of bonding and structural features. Transition Metal Compounds with Bonds to Hydrogen Transition metal hydrides: Synthesis, properties and reactivity. Transition metal dihydrogen compound: Preparation, properties and reactivity**.** **(6 hours)**

Module II: **Organometallics in homogeneous catalysis.**

Coordinative unsaturation, oxidative addition and reductive elimination reactions. Insertion reactions (insertion of CO, SO_2 and alkenes). Reactions of coordinated CO in metal carbonyls. Homogenous hydrogenation of alkenes, hydroformylation of alkenes, isomerisation of olefins, Wacker's process, Zeigler-Natta Polymerization of ethylene, Monsanto acetic acid, Reduction of CO by hydrogen (Fischer-Tropsch reaction).

(6 hours)

Module III:Cages and metal clusters

Metal cluster compounds. Preparative methods for metal cluster compounds. Various types of reactions of metal cluster compounds, Cluster of borane and higher boranes compounds**.** **(4 hours)**

Module IV: **Application of Organometallic Compounds**

Organometallic precursors for nanomaterials, Organometallic-derived catalysts and their applications in materials science, Synthesis and properties of organometallic polymers, Application of Organometallic compounds in catalysis, drug delivery, and sensors.

(4 hours)

Module V: **Introduction to Supramolecular Chemistry**

Molecules and Supramolecules,Large Molecules Classification, Nomenclature, Thermodynamic and Kinetic selectivity, Supramolecular interactions, Supramolecular host design, Macrocyclic versus acyclic hosts, Chelate Macrocyclic and macrobicyclic hosts, High dilution synthesis, Template synthesis. **(6hours)**

Module VI: **Molecular Recognition**

Receptors, design and synthesis of co-receptors multiple recognition, Hydrogen bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.**(6 hours)**

Module VII: **Supramolecular Reactivity**

Cation binding hosts (Crown Ether, Cryptand, Spherand; Nomenclature, Selectivity and Solution Behaviours), binding of anions (Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts), binding of neutral molecules (Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers).

(7 hours)

Reference Books:

1. Basic Organometallic Chemistry: Concepts, Syntheses and Applications. B D Gupta, A J Elias, 2004.
2. "Organometallic Chemistry" edited by E. W. Abel, F. G. A. Stone, and G. Wilkinson
3. Supramolecular Chemistry by J. W. Steed & J. L. Atwood, 2nd Edn, John Wiley, 2009.
4. J. M. Lehn, Supramolecular Chemistry, VCH, Weinheim, 1995
5. Christian, G. D., Analytical Chemistry, 6th Ed., John Wiley & Sons, Inc. (2004).
6. Khopkar, S.M., Basic Concepts of Analytical Chemistry, 3rd Edition, Publisher: New Age International Publishers (2008), ISBN: 9788122420920, 8122420923.

Suggestive List of Projects

1. Synthesis of Cu (II)-N, N-Diethylethylenediamine and Tetrammine cupric sulphate [Cu $(NH_3)_4$] $SO_4.H_2O$ complexes and their applications.
2. Synthesis of Sodium cobaltinitrite, $Na_3[Co(NO_2)_6]$ complex and its applications.
3. Synthesis of Potassium trioxalato chromate (III) ($K_3[Cr(C_2O_4)_3]$. $3H_2O$) and its applications.
4. Preparation and Reactivity of Grignard Reagents.
5. Study of the Catalytic Activity of Transition Metal Complexes in Simple Organic Reactions

6. Study of organometallic compounds in asymmetric catalysis.
7. Synthesis and properties of new supramolecular structures.
8. Structural investigation of bioactive organic molecules and their metal complexes
9. Self-assembly of nanostructures using supramolecular chemistry
10. Molecular recognition in drug delivery systems
11. Supramolecular polymers: synthesis and applications
12. Molecular cages and their use in encapsulation
13. Design of supramolecular hydrogels for biomedical applications
14. Coordination-driven self-assembly of supramolecular structures
15. Development of supramolecular sensors for chemical detection

Code	CourseTitle	T-P-Tut (Credit)	Prerequisite
CUTM 4535	**Nano Phytopharmaceuticals**	3-1-0	

Course Objective:
The objectives of the course are

- To know the techniques of isolation, purification and identification of phytomolecules
- Understand the principles of phytochemistry, including the extraction, isolation, and Characterization of bioactive plant compounds.
- Explore modern analytical techniques for the identification and quantification of

Phytoconstituents such as alkaloids, glycosides, terpenoids, and resins.

- Examine the applications of nanotechnology in pharmaceuticals, food, and agriculture, with a focus on drug delivery, regenerative medicine, and smart agrochemicals.
- Assess the safety, efficacy and environmental impact of nanomaterials used in biomedical and Industrial applications.

Course Outcomes:
After completion of the course students will be able to:

CO1	Understand the fundamental principles of phytochemistry including extraction, isolation, purification, and identification of phytoconstituents such as alkaloids,

	glycosides, terpenoids, and resins.
CO2	Apply modern analytical and spectroscopic techniques (e.g., TLC, GC-MS, UV-Vis) to qualitatively and quantitatively analyze phytochemicals from natural sources.
CO3	Demonstrate knowledge of the industrial production and utilization of key phytoconstituents like curcumin, taxol, vinblastine, and others in pharmaceuticals
CO4	Analyze and evaluate the application of nanotechnology in drug delivery, food packaging, and agriculture, including understanding of nanocomposites and nanofertilizers.
CO5	Develop critical insights into the safety, efficacy, and environmental implications of nanomaterials and explore their role in early disease detection and regenerative medicine.

CO,PO,PSO MappingMatrix

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	2	1	3										3	2	
CO2	3	2	3										3	3	
CO3	3	2	3										3	3	
CO4	2	2	3										2	3	
CO5	3	2	3										3	3	

Course Content

Module-I (Basics of Phytochemistry) (3hrs)

Basics of Phytochemistry, isolation, purification and identification techniques of phytomolecules.

Module-II (methods of extraction) (3hrs)

Modern methods of extraction, application in the Isolation, Identification and Analysis of Phytoconstituents like
a) Terpenoids: Menthol, Citral, Artemisin
b) Glycosides: Glycyrhetinic acid &Rutin
c) Alkaloids: Atropine, Quinine, Reserpine, Caffeine

d) Resins: Podophyllotoxin,

CurcuminModule-III (Industrial production) (3hrs)

Industrial production, estimation and utilization of the following phytoconstituents: Curcumin, Atropine, Podophyllotoxin, Caffeine, Taxol, Vincristine and Vinblastine

Module-IV (Nanotechnology in Food and pharmaceutical industry) (6hrs)

Nanotechnology in Food and pharmaceutical industry: Nano particle-based drug delivery systems,

Regenerative medicine, nano-immuno conjugates, Bioavailability and delivery of nutraceuticals and

functional foods using nanotechnology, Polymer-based nanocomposites for food packaging,

nanocomposites for food packaging, Toxicity and environmental risks of nanomaterials.

Module-V (Nanotechnology in Biomedical and Pharmaceutical Industry) (6hrs)

Nanotechnology in Biomedical and Pharmaceutical Industry:Tissue engineering/regenerative medicine,

Nanorobotics in surgery, Nano-tools for early detection diseases, Nano-medicine for cancer treatment

Module-VI (Nanotechnology in Agriculture) (6hrs)

Nanotechnology in Agriculture: Introduction of Nanotechnology in agriculture, Potential of nanofertilizers,

Precision farming, smart delivery system, Insecticides using nanotechnology.

Module-VII (Molecular Cell Biologyy) (6hrs)

Molecular Cell Biology: Cell- Structure & Function of Cell Membrane, Different cell types and their. Functions, Sub-cellular Organelles and their Functions, Nucleotide- Structure and Functions of DNA &RNA. Biologically important nucleotide, protein synthesis, unnatural amino acid, Mechanistic understanding of various diseases and target identification for early detection

PRACTICE

Practice 1:
Thin Layer Chromatography (TLC) of plant extracts to separate and preliminarily identify phytochemicals like alkaloids, flavonoids, and terpenoids.

Practice 2:
Soxhlet extraction of a selected plant (e.g., peppermint for menthol), followed by Gas Chromatography-Mass Spectrometry (GC-MS) analysis to identify constituents like menthol or citral.

Practice 3:
Quantitative UV-Visible Spectrophotometric estimation of curcumin or caffeine from formulated products or plant sources, following standard protocols.

Practice 4:
Prepare a simple polymer-based nanocomposite film (e.g., starch-chitosan-based) for food

packaging and evaluate its barrier properties.

Practice 5:
Model a nano-drug delivery system using software (e.g., NanoDDS simulation or molecular docking tools) to understand drug loading and release behavior.

Practice 6:
Formulate and characterize a model nano-fertilizer using zinc oxide nanoparticles and test its release profile in soil or water medium.

Practice 7:
Isolate genomic DNA from plant cells (e.g., banana) and visualize using gel electrophoresis,followed by a brief discussion on DNA structure and function.

References Recommended:

Text Books:

1. Berg, J.M., Tymoczko, J. L. and Stryer, L. (2006) Biochemistry. VIth Edition. W.H. Freeman and
2. Co.
3. Nelson, D. L., Cox, M. M. and Lehninger, A. L. (2009) Principles of Biochemistry. IV Edition.
4. W.H. Freeman and Co.
5. 3. Murray, R. K., Granner, D. K., Mayes, P. A. and Rodwell, V.W. (2009) Harper's Illustrated
6. Biochemistry. XXVIII edition. Lange Medical Books/ McGraw-Hill.
7. 4. Thomas L Lamke, David A Williams, Victoria F. Roche, S. William Zito. "Foy's principle
8. of medicinal chemistry",7th edition.
9. 5. *Pharmacognosy and Phytochemistry* by Vinod D. Rangari, Edition: Latest (typically 3rd
10. or 4th edition), Publisher: Career Publications, ISBN: 9788188739642
11. 6. *Textbook of Nanotechnology in Drug Delivery* – **Eds. Melgardt M. de Villiers,**
12. **PornanongAramwit, Glen S. Kwon, Publisher:** Springer / CRC Press, **ISBN:**
13. 9781441999216
14. 7. *Molecular Biology Techniques: A Classroom Laboratory Manual* by Heather Miller, D.
15. Scott Witherow, Sue Carson, 3rd Edition, Academic Press, **ISBN:** 9780123855442

Journals:

- Journal of Nanobiotechnology
- International Journal of Nanomedicine
- Phytomedicine
- Current Nanomedicine
- Drug Delivery and Translational Research

CourseOutline

Code	**CourseTitle**	**T-P-P**	**Prerequisite**
CUTM4536	Green and Sustainable Chemistry	3-1-0	

Course Objectives

- Tolearnthefundamentalphilosophyandthelatestdevelopmentsinsustainablechemistry.
- Tofamiliarizewithdifferentgreenreactionalternativesofconventionalreactionsprocedures with real world applications.
- To understand importance of recycling and its application in circular economy.
- To assess the toxicity level in a substance.

Course Outcomes

COs	Course outcomes
CO1	Will gain knowledge about the responsibility of a chemist towards the solution of various environmental issues
CO2	Able to observe and differentiate the environmental friendly chemicals to fulfill our requirements in life
CO3	Able to judge in every step of life to select sustainably viable options starting from personal to professional front
CO4	Will be equipped to be part of problem-solving endeavor related to environmental issues
CO5	To assess the toxicity level in a substance

CO, PO, PSO Mapping Matrix

CO/PO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**	**PO11**	**PO12**	**PSO1**	**PSO2**	**PSO3**
CO1	3	2	3	2		2	2		3	2	2	2	3	3	2
CO2	2	3	2	3		3	2		2	2	3	3	2	2	2
CO3	2	2	2	3		2	2		2	3	2	3	2	2	3
CO4	3	2	2	2		3	3		2	3	3	2	3	2	3
CO5	3	3	3	3		3	2		3	3	2	3	3	3	2

CourseContent

ModuleI : Fundamental: (5Hrs.)

Brief idea about sustainability and SDGs; Basic Concepts of Sustainable Chemistry; Sustainability assessment; Need of sustainable chemistry; Role of chemistry in sustainability.

ModuleII (7Hrs.)

Green Chemistry:

Principles of green chemistry; Designing safer chemicals; Toxicokinetic and Toxicodynamic, predict the properties and environmental aspects before synthesis; Use of catalysts, to reduce time and energy demands, minimize waste; Design for energy efficiency, least energy intensive route for synthesis.

ModuleIII (4Hrs.)

Green Solvents:

Atom economy, metathesis; Ionic liquids, classification, synthesis & applications; Deep eutecticsolvents, classification, synthesis & applications; Supercritical fluids, preparation and variousapplications.

Practice1: Ionic liquidsynthesis

Practice2: Deepeutecticsolventspreparation

Practice3: Diels Alder reaction in water: Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

ModuleIV (6Hrs.)

Green Synthetic Methods:

Green alternative of conventional synthetic methods; Green catalysis (Phase Transfer Catalysts, Chitosan, enzymes), solvent freereactions, Microwave assisted reactions,ExamplesofGreenSynthesis-Ibuprofen.IndustrialGreenImprovements of Consumer Products; Vitamin C Synthesis using enzymes (Hoffman La Roche),Zoloft -Presidential Chemistry Award Winning Innovation (Pfizer), Methyl Methacrylate syngasprocess(EastmanChemicals).Realworldapplicationsofgreenchemistry:Awardwinning discoveries.

Practice4: Greensynthesisofnanoparticles(Au/Ag/Cu)usingleafextracts.

Practice5: Photoreduction of benzophenone to benzopinacole in the presence of light.

Practice 6: Esterification Reaction – A Greener Alternative.

Practice 7: Oxidation of benzyl alcohol to benzaldehyde via greener approach.

Practice 8: Solvent free aldol condensation reaction.

Practice 9: Solvent free wittig reaction.

Practice 10: Substitution (SN2) Reaction.

ModuleV (6Hrs.)

Sustainable materials:

Renewable Feed stocks and applicationofRenewable feed stocks (rawmaterials)inorganicsynthesis:Alizarine, Indigo, Coniine synthesis, (±)-Usnic acid from lignin, tetracyclin antibiotics from Chitin derived L-Rednose,(−)-Bissetone and (−)-palythazine from cellulose derived glucose. Biodegradable polymers (PEF,PLA,PBSandPHA): Synthesis and theirapplications.

Practice11: Vitamin C clock reaction using vitamin C tablets, tincture of iodine, hydrogen peroxide, and liquid laundry starch. Effect of concentration on clock reaction.

ModuleVI (5Hrs.)

Recyclingandcirculareconomy:

Plastic recycling in circular economy. Sustainable packaging. Life Cycle Analysis (LCA), CradletograveandCradleto Cradledesign.Circulareconomy:Examples andsuccess stories.

Practice12: Biodegradable plastics for sustainable packaging.

ModuleVII (5Hrs.)

Toxicity:

Introduction to toxicology, Subdisciplines of toxicology, Acute, Sub acute and chronic toxicology;Toxicity Pathways, Mechanism of toxicology, Adverse Outcome Pathways, Dose response relationship.

Textbooks:

- ***Newtrendsingreenchemistry:V.K.Ahluwalia,M.KidwaiAnamayaPublishers***
- ***IntroductiontoGreenChemistry:AlbertS.Matlack,2ndedition,CRCPress***
- ***WastetoWealth-Thecirculareconomyadvantage:PeterLacyandJakobRutqvist,MaEditions***

Reference Book

- ***GreenSolvents-IonicLiquids:PaulT.Anastas(SeriesEditor),PeterWasserscheid,AnnegretStark, Wiley-VCH***
- ***Sustainablechemistry:G.Reniers andC.ABrebbia,WITPress***
- ***A text book of modern toxicology: Ernest Hodg, Wiley Interscience.***

Code	**CourseTitle**	**T-P-Pro (Credit)**	**Prerequisite**
CUTM 4537	**Symmetry and Group theory**	3-0-1	

Course Objectives

- To introduce students to fundamental concepts of symmetry and group theory, including symmetry elements, operations, and classification of molecular symmetry through point groups.
- To develop proficiency in applying group theoretical concepts to chemical systems, particularly in constructing and interpreting character tables, and understanding reducible and irreducible representations.
- To enable students to apply symmetry principles in spectroscopy, molecular orbital theory, fostering interdisciplinary understanding and analytical skills using both manual and software-assisted approaches.

Course outcomes

COs	Course Outcomes
CO1	Recall and define key concepts of symmetry and group theory, including types of symmetry elements, operations, and group classifications.
CO2	Explain the mathematical structure of groups (abelian and non-abelian), and describe their application in molecular symmetry and chemical systems.
CO3	Apply group theoretical principles to identify point groups of molecules and construct group multiplication tables and character tables.
CO4	Analyze molecular symmetry to predict vibrational modes and spectroscopic activity (IR and Raman) using character tables.
CO5	Develop symmetry-based models and design interdisciplinary projects involving symmetry in molecular structures, crystallography, or natural patterns using software tools.

CO, PO, PSO Mapping Matrix															
CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	1	2		2	1		3	2	2	3	3	2	1
CO2	2	3	1	3		3	1		2	2	3	2	2	3	2
CO3	3	2	2	1		2	1		2	2	2	3	3	2	1
CO4	2	3	1	3		3	1		2	3	3	2	2	3	2
CO5	3	2	2	2		2	1		2	2	2	3	3	2	1

Module I: **(4 hours)**

Introduction to symmetry, symmetry in nature, elements of symmetry, identity, axis of symmetry, plane of symmetry, point of symmetry, identity operation, symmetry operations.

Module II: **(4 hours)**

Groups, abelian group, non-abelian group, Point Group, generator, axial. Representation of symmetry, matrix methods in symmetry, groups.

Module III: **(4 hours)**

Molecules of low symmetry, molecules of high symmetry, molecules of special symmetry, group multiplication table, point group, non-axial point group, identification of molecular point groups.

Module IV: **(4 hours)**

Isomorphic groups, group generating elements, subgroups, matrix representation of symmetry elements, matrix representation of point groups.

Module V: **(4 hours)**

Character table, Great Orthogonality theorem. Reducible and irreducible representations, character of a representation, properties of irreducible representations,

Module VI: **(4 hours)**

Construction of character table, character table for C_{2V} point group, structure of character tables, the standard reduction formula.

Module VII: **(4 hours)**

Applications of group theory: Application to molecular orbital theory, LCAO-MO pi bonding. Application to simple pi systems (cyclopropene, cyclobutene and benzene)

Projects

1. Molecular Symmetry Explorer (Chart/Model-Based)
   - Objective: Identify and classify point groups of everyday or organic molecules (e.g., H_2O, NH_3, BF_3, CH_4).
   - Deliverables: 3D models, point group justification, and symmetry element identification.

2. Character Table Construction for a Selected Point Group
   - Objective: Derive and interpret the character table for a point group such as C_2v, D_3h, or C_3v.
   - Deliverables: Derivation using the reduction formula and matrix representation, highlighting reducible to irreducible representation conversion.

3. Group Theory in Vibrational Spectroscopy
   - Objective: Predict IR and Raman active modes for simple molecules (e.g., CO_2, H_2O, SO_2).
   - Deliverables: Symmetry analysis, vibrational mode classification, and spectroscopic predictions.

4. Symmetry and Chemical Reactivity
   - Objective: Study the relationship between molecular symmetry and chemical reactivity or stability (e.g., aromaticity in benzene).
   - Deliverables: Theoretical explanation, symmetry-based analysis, diagrams/models.

Reference Books

1. Chemical Applications of Group Theory – F. Albert Cotton
3rd Edition Publisher: Wiley-Interscience, 1990 ISBN: 978-0471510949
2. Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy – Daniel C. Harris & Michael D. Bertolucci 1st Edition Publications, 1989 ISBN: 978-0486661445
3. Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications – Alan Vincent
2nd Edition Wiley, 2001 ISBN: 978-0471489153
4. Group Theory and Chemistry – David M. Bishop Edition: 1st Edition Publisher: Dover Publications, 1993 ISBN: 978-0486673554
5. Group Theory in Chemistry and Spectroscopy: A Simple Guide to Advanced Usage – Boris S. Tsukerblat 1st Edition Dover Publications, 2006 ISBN: 978-0486450353

Code	CourseTitle	T-P-Pro (Credit)	Prerequisite
CUTM4538	Advanced Polymeric Materials	3-1-0	

Objectives

- To understand the importance of the chemical approach to polymers and the subject provides an introduction to polymer science with respect to synthesis, polymerization kinetics and networkformation/gelation of macromolecules formed bystep-growth and chain-growth polymerization.
- To Study the, methods of measuring the molecular weight, polymerization kinetics and Copolymerization and polymer processing technologies.
- To understand about radical and ionic polymerization and techniques of polymer analysis.
- To study mechanical properties and applications of polymers.

Course Outcomes

COs	Course outcomes
CO1	**Identify and classify** various types of advanced polymeric materials based on their structure, properties, and applications.
CO2	**Explain** the synthesis, processing methods, and structure–property relationships of high-performance and functional polymers.
CO3	**Analyze** the behavior and performance of smart polymers (e.g., shape-memory, self-healing, conductive polymers) under different environmental or mechanical stimuli.
CO4	**Evaluate** the role of nanotechnology and polymer composites in enhancing material properties for specific high-end applications.
CO5	**Apply** characterization techniques such as DSC, TGA, FTIR, SEM, and others to investigate polymer morphology, thermal behavior, and mechanical properties.

CO, PO, PSO Mapping Matrix

CO/PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	2	1	3										3	2	
CO2	2	1	3										3	3	
CO3	3	2	3										3	3	
CO4	2	2	3										2	3	
CO5	3	2	3										3	3	

Course content

Module I: Fundamental (5hrs)

Introduction of polymers; Degree of polymerization; Concept of molecular weight, polydispersity; Glass transition temperature (T_g) and melting point T_m; Factors affecting T_g and T_m, Importance of T_g.; polymerization processes.Types of copolymers; Copolymer composition; Methods of determination of reactivity ratios and copolymerization behavior; Kinetics of copolymerization.

Module II: Fundamentals of biopolymers (5hrs)

Definition of biopolymers and types of biopolymers, Definition of bioplastics and types of bioplastics, Description of certain biopolymers like starch, cellulose, chitosan, gelatin, alginate, keratin, fatty acids, lipids, aliphatic polyesters (PLA, PHB), Cellulose derivatives

Module III: Ionic and Radical Polymerization (5hrs)

Comparison of Radical and Ionic Polymerizations; Cationic Polymerization; Anionic Polymerization; Ring Opening Polymerization; End Group Functionalization.Introduction to Radical Polymerization; Kinetics of Radical Polymerization; Ziegler-Natta Catalysis: Stereochemistry of Polymers.

Module IV: Polymer biodegradation and biocomposites (5 hrs)

Natural biodegradable polymer, synthetic biodegradable polymer and modified naturally biodegradable polymer, Testing methods of biodegradability [polymer-Enzyme assays, Plate test, Respiratory test, Gas evolution test (CO_2& CH_4)], Use of biopolymers in composite and bioplastic formation and their application in packaging and medical industries

Module V: Analysis and Applications of Polymers (6hrs)

Introduction and instrumentation; Applications of Differential thermal analysis (DTA); Thermogravimetric analysis (TGA); Differential scanning calorimetry (DSC) and Dynamic Mechanical Analysis (DMA); Determination of Mechanical Properties.Application of polymer in Elctronics; Application of polymer in cosmetics; Application of polymer in Medicine.

Module VI (4 hrs)

Polymers in packaging - Definition, functions of packaging, types and selection of package, Packaging hazards, interaction of package and contents.**Packaging materials:-** Major Plastic packaging materials viz. Polyolefins, Polystyrene, Polyvinylchloride, Polyesters, Polyamides (Nylons), Polycarbonate and newer materials such as High Nitrile Polymers, Polyethylene Napthalate (PEN), Nanomaterials, biodegradable materials – properties and applications, recycling; Wood, Paper, Textile, Glass, Metals – Tin, Steel, aluminum, Labelling materials, Cushioning Materials – properties and areas of application.

Module VII (6hrs)

Product Conversion technology - Extrusion – Blown film, cast film, sheet, multilayer film & sheet, Lamination, Injection molding, Blow molding, Thermoforming; Cartoning Machinery, Bottling, Can former, Form Fill and Seal machines, Corrugated box manufacturing machineries, Drums – types of drums, molded pulp containers, Closures, Application of Robotics in packaging. Surface treatment for printing, Printing processes – offset, flexo, gravure and pad printing.

Practice 1: Determination of Viscosity average molecular weight of a polymer.
Practice 2: Synthesis of Nylon66

Practice 3: Free Radical Polymerization of Styrene
Practice 4: Preparation of Polyvinyl Chloride
Practice 5: Synthesis of polythene
Practice 6: **Investigation of the rate of biodegradation of any sample (biopolymer) through the anaerobic condition**
Practice-7:Extraction of Starch from Patatoes.
Practice 8: Synthesis of PLA
Practice 9: Synthesis of PMMA
Practice 10: Synthesis of PAN
Practice 11:Testing methods of biodegradability [polymer-Enzyme assays, Plate test, Respiratory test, Gas evolution test (CO_2& CH_4)]

Textbooks:

1) *B. Ratner, A. Hoffman, F. Schoen, J Lemons, Biomaterials Science: An introduction to materials in Medicine. 2nd edition, Academic Press, 2004.*
2) *S. Dumitriu, 2nd edition, Polymeric Biomaterials. Marcel Dekker, 2002*
3) Dean, D. A., Evans, E. R., & Hall, I. H. (Eds.). (2005). *Pharmaceutical packaging technology*. CRC Press.
4) Paine, F. A. (1990). *Fundamentals of packaging*. London: Blackie.
5) Athayle, A.S. (1992). *Plastics in Flexible Packaging*. Multi-tech Publishing Co.
6) Kirwar, M.J. (2005). *Paper and Paperboard Packaging Technology*. Blackwell Publishing.
7) Principles of Polymerization, Fourth Edition – George Odian
8) Gedde Ulf. W. Polymer Physics, Chapman & Hall London (1995)
9) Rodriguez, Ferdinand, Principles of Polymer Systems Mc. Craw – Hill, International Book Co. International Student Edn. 1985.

Reference Books:

1. Cowie; JMG Polymers: Chemistry & Physics of Modern Materials, Nelson Thornes ltd. Chelterham, 2001
2. Hiemenz; Paul C. Polymer Chemistry- The Basic Concepts; Marcell&Deckker, Inc. New York (1984)
3. Polymer Science by V.R. Gowarikar, N.V. viswanathan and J. Sreedhar, New Age International.
4. Textbook of Polymer science: F.M. Billmeyer, John wiley and sons.

Code	Subject Name	T-P-Pr (Credit)	Pre requisite
CUTM1409	**Computational Materials Science**	**2-2-0**	

Course Objective

- To teach the fundamental definitions, concepts, and tools of Computational Materials Science, and how they are applied to address materials modeling challenges.
- To impart practical skills in developing computational models using Molecular Dynamics (MD), Hartree-Fock (HF), and Density Functional Theory (DFT) approaches for simulating physical and electronic behavior.
- To provide students with hands-on training in open-source and commercial software tools, including Python-based coding, Biovia Materials Studio, and Quantum ESPRESSO, for performing calculations, visualization, and analysis of material systems.

Course outcome

COs	Course outcomes
CO1	Define and explain key concepts of interatomic potentials, cohesive energy, statistical ensembles, and basic principles of Hartree and Hartree-Fock approximations. I, III, IV
CO2	Apply molecular dynamics and Monte Carlo simulation techniques using standard algorithms (e.g., Verlet, Metropolis) to model simple systems and predict material behavior. II, III
CO3	Analyze electronic structures and total energy calculations using Density Functional Theory, identifying the effect of k-points, basis sets, and exchange-correlation functionals. IV, V
CO4	Evaluate the accuracy and limitations of DFT results for vibrational frequencies, magnetic properties, and adsorption behavior on surfaces using slab models. V, VI
CO5	Design and execute a simulation-based mini-project combining MD, Monte Carlo, or DFT techniques to investigate a materials problem such as diffusion, surface adsorption, or phase transition. II to VI

CO, PO, PSO Mapping Matrix

CO/PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	2	1	3										2	2	
CO2	3	1	3										3	3	
CO3	3	2	3										3	3	
CO4	3	2	3										2	3	
CO5	3	3	2										3	2	

Course outline

Module I **(4 Hours)**

Introduction to computational materials science: Cohesive Energy, Modelling & Simulation, Basic forms of interatomic interactions (pair potentials, The Lennard-Jones potential, Morse Potential, Brenner Model, Tersoff Model)

Practice (2 hours sessions):

1. Introduction to Python
2. **Python Experiment:** Model and visualize three common potentials: Lennard-Jones potential (LJ), Morse Potential, Brenner Model, Tersoff Model.

Module II

Molecular Dynamics **(4 Hours)**

Statistical Ensembles used in Molecular Dynamics (NVT, NVE, NPT), Thermostat (Andersen's method, Berendsen thermostat, Nose-Hoover thermostat), Boundary Conditions. MD Methodology (Verlet algorithm, Velocity Verlet algorithm), Force Field, Diffusion

Practice (2 hours sessions):

3. **Simulate water molecules at room temperature using NVT or NPT ensemble and analyze the structural and dynamic properties.** (Build using Amorphous Cell module, choose a suitable force field (e.g., COMPASS or CVFF), Run MD using Forcite module for 100–500 ps)

Module III

Monte Carlo Methods and Hartree Approximation **(5 Hours)**

Monte Carlo Simulations, Metropolis algorithm, 2D Ising Model and its simulation, The Variational Principle, The Hartree Approximation,

Practice (2 hours sessions):

4. Investigate how different guest molecules (e.g., water, methane) adsorb in various sites of a nanoporous host like CNT using Forcite module of BIOVIA MS
5. **Variational Principle – Ground State Energy Approximation**

Compute and compare total ground state energy of molecules H_2, He, or LiH using Hartee mechanism of BIOVIA MS.

Module IV

Density Functional Theory-I **(4 Hours)**

The Hartree-Fock Approximation, Periodic structures, supercells, andlattice parameters, K Points, Energy Cutoffs, Geometry Optimization

Practice: (2 hours sessions)

Prediction of Lattice Parameters of AlAs using CASTEP of BIOVIA Material Studio.

Visualize and compare electron density of atoms like Be, Ne, Ar using $DMol^3$ module of BIOVIA MS.

Module V

Density Functional Theory-II **(4 Hours)**

Density Functional Theory (From Wave Functions to Electron Density), The Hohenberg-Kohn Theorems, The Kohn-Sham Equations, Exchange Correlation Functionals (LDA, GGA, PBE)

Practice: (1 hours sessions)

6. Optical Properties Si, Ge and GaAs

Module VI

Extensions of Density Functional Theory **(4 Hours)**

DFT for Surfaces of Solids (Slab Models, Surface Relaxation, Adsorbates on Surfaces)

Practice: **(2 hours sessions)**

7. Adsorption of CO onto a Pd (110) Surface

Module VII **(3 Hours)**

DFT Calculations of Vibrational Frequencies, Electronic Structure, Magnetic Properties

Practice (4-hour sessions)

8. Predicting the Thermodynamic properties of Ge using BIOVIA MS
9. Band gap prediction of ZnO in DFT using BIOVIA MS
10. Density of States of AlAs using DMol3 using BIOVIA MS.
11. Simulating Electron transport with DFTB+

Total theory 28 hours and total practice 30 hours

Textbook:

1. Introduction to Computational Materials Science, Richard LeSar, (Cambridge University Press, 2016).
2. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory. Attila Szabo, Neil S Ostlund. (Dover Publications Inc. 1996).

Reference Books:

Computational Materials Science: An Introduction. June Gunn Lee, (CRC Press, 2011).

Code	Subject Name	Type of course	T-P-Pr (Credit)
CUTM 2378	**Research Methodology and IPR**	Theory+Project	**(2-0-2)**

Objective

- To develop an appropriate framework for research studies
- To develop an understanding of various research designs and techniques.
- To identify various sources of information for literature review and data collection.
- To develop an understanding of the ethical dimensions of conducting applied research.
- To Demonstrate enhanced Scientific writing skills
- warn the common mistakes in the field of research methodology.
- To make expertise in academic writing, patenting

Course outcome

COs	Course Outcomes
CO1	Search, select and critically analyse research articles and papers
CO2	Formulate and evaluate research questions
CO3	Develop the ability to apply the methods while working on a research project work
CO4	Describe the appropriate statistical methods required for a particular research design
CO5	Choose the appropriate research design and develop appropriate research hypothesis for a research project in research methodology.

CO, PO, PSO Mapping Matrix															
CO/PO/PSO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**	**PO11**	**PO12**	**PSO1**	**PSO2**	**PSO3**
CO1	3	2	2	1									2	1	
CO2	3	2	3	2									3	2	
CO3	3	2	3	2									3	2	
CO4	2	1	2	3									2	3	
CO5	2	2	2	3									1	3	

Module 1:Elementary Research Methodology

Research Concept, Objective, characteristics, Steps and Significance of Research, Arbitrary and Scientific Research, Research approaches. Types of research: Historical, Descriptive, Analytical, Case Study, Quantitative vs. qualitative, Conceptual, Empirical Action Research, Research Methods vs Methodology. Research Problems: Selection and definition of the research problems, formulating a research problem, identifying variables and Constructing hypothesis; Choosing a mentor, lab and research question; maintaining a lab notebook; Selection of problems - stages in the execution of research.

Module II: Academic Writing and Presentation

Technical writing skills - types of reports; layout of a formal report; standard of Journal (Impact Factor, Citation Index), Scientific writing skills - importance of communicating science; problems while writing a scientific document; plagiarism, software for plagiarism; scientific publication writing: elements of a scientific paper including abstract,

introduction, materials & methods, results, discussion, references; drafting titles and framing abstracts; publishing scientific papers - peer review process and problems, recent developments such as open access and non-blind review; characteristics of effective technical communication; scientific presentations; ethical issues; scientific misconduct.

Module III: Scientific communication skills

Concept of effective communication- setting clear goals for communication; determining outcomes and results; barriers to effective communication; non-verbal communication- importance of body language, power of effective listening; Presentation skills - formal presentation skills; preparing and presenting using over-head projector, PowerPoint; defending interrogation; scientific poster preparation &presentation; participating in group discussions; Computing skills for scientific research - web browsing for information search.

Module IV: Introduction to IPR

Introduction to intellectual property; types of IP: patents, trademarks, copyright & related rights, industrial design, traditional knowledge, geographical indications. IP as a factor in R&D; IPs of relevance to biochemistry and few case studies; plant variety protection.

Module V: Types of Patents

Basics of patents: types of patents; Indian Patent Act 1970; recent amendments; WIPO Treaties; Budapest Treaty; Patent Cooperation Treaty (PCT) and implications; filing of a patent application; role of a Country Patent Office; precautions before patenting-disclosure/non-disclosure - patent application- forms and guidelines including those of different regulatory bodies, fee structure, time frames; types of patent applications: provisional and complete specifications.

PROJECTS

1. Write a review article and submit to a journal.
2. Write a book chapter/ book for publishing.
3. Write an original article for a journal.

Books:

1. Geoffrey Marczyk, David DeMatteo, David Festinger (2005) ***Essentials of Research Design and Methodology***, John Wiley & Sons, Inc.
2. Carol Ellison (2010) ***McGraw-Hill's ConcisevGuide to WritingvResearch Papers***, McGraw-Hill
3. Kothari CR (2016) ***Research Methodology: Methods and Techniques***, New Age Pvt Ltd
4. Ganbawale RM, (2017) ***Bioststistics and Research Methodology***, New Central Book Agency
5. Sinha, S.C. and Dhiman, A.K., (2002). ***Research Methodology***, EssEss Publications. 2 volumes.
6. Trochim, W.M.K., (2005). ***Research Methods: the concise knowledge base***, Atomic Dog Publishing. 270p.
7. Wadehra, B.L. (2000). ***Law relating to patents, trademarks, copyright designs and geographical indications***. Universal Law Publishing.
8. Neuman, W.L. (2008). ***Social research methods: Qualitative and quantitative approaches,*** Pearson Education