	Course Title	L	T	P	С
Course Code					
	Applied Chemistry	3	0	2	4
Pre-requisite		Syllabus Version			
		1.0			

### **Course Objectives**

- 1. To enable students to learn fundamental concepts in different branches of chemistry
- 2. To be well-versed in analytical and computational skills in chemistry
- 3. To teach practical skills in chemistry and apply knowledge for societal applications

#### **Course Outcomes**

Upon completion of this course, students will be able to

- 1. Explain the fundamental concepts in physical, analytical, and materials chemistry.
- 2. Apply chemical concepts for the advancement of materials in electrical, magnetic, and energy domains
- 3. Demonstrate instrumental techniques in chemistry
- 4. Solve chemical problems by applying computational chemistry
- 5. Experiment to quantify the metal ions, to prepare nanomaterials, and to visualize molecules using computational tools.

## **Module:1** Chemical thermodynamics and kinetics

9 hours

Introduction-Terminologies- Zeroth law- First law of thermodynamics – Enthalpy and heat capacity – Applications of first law of thermodynamics – Second law of thermodynamics – Carnot cycle- Third law of thermodynamics – Gibbs Helmholtz equation. Chemical Kinetics – Rate equation – Order of the reaction – Integral rate equations – Half life time of reactions-Molecularity – Collision theory of reaction rate – Effect of temperature and catalysts on reaction rate -Numericals.

# **Module:2** Energy devices

8 hours

Electrochemical and electrolytic cells —electrode materials with examples (semi-conductors), classifications of batteries - chemistry of Li - ion secondary batteries, Fuel cells: H<sub>2</sub>-O<sub>2</sub> and solid oxide fuel cell (SOFC); Solar cells - photovoltaic cell (silicon based), photoelectrochemical cells and dye-sensitized cells.

### Module:3 Functional materials

10 hours

Electrical materials: Ohm's law, resistivity, classification - metals, semiconductors (intrinsic & extrinsic-Si), insulators, superconductors. Magnetic materials: para, dia, ferro & anti-ferro magnetism, applications in storage devices. Liquid cooling – types of coolants, thermal conductivity, and applications. Nanomaterials: introduction, top-down and bottom-up approaches for synthesis - bulk vs nano (gold), quantum dots.

### **Module:4** Spectroscopic and diffraction techniques

6 hours

Fundamental concepts in spectroscopic and diffraction techniques – Principle, instrumentation, and applications of UV-Visible and powder XRD (determination of crystallite size, numericals)

## **Module:5** Computational Chemistry: Basics to Applications

10 hours

Introduction-Quantum mechanical calculations. Molecular orbital theory: atomic orbitals, molecular orbitals. Orbital interactions- chemical bonding. Potential energy curve/surface, electrostatic potentials, geometry optimization, frequency, reaction mechanism, application of AI to screen semiconductors

Mo	dule:6	Contemporary Topics Industry Expert Lecture	2 hours			
		Total Lecture hours:	45 hours			
Te	xt Books					
1	Theodore	ore E. Brown, H Eugene, LeMay Bruce E. Bursten, Catherine Murphy, Patrick				
	Woodwa	vard, Matthew E. Stoltzfus, Chemistry: The Central Science, 2017, 14th edition,				
	Pearson 1	on Publishers, 2021. UK				
2	Frank Jer	nsen, Introduction to computational chemistry, 2022, 3 <sup>rd</sup> edition, Wiley				
Reference Books						
1.	A.R Wes	West, Solid State Chemistry and its Applications, 2021, 2 <sup>nd</sup> edition, Wiley, UK.				
2.	Lawrence	vrence S. Brown and Thomas Holme, Chemistry for engineering students, 2020, 4 <sup>th</sup>				
	edition.	, , , , , , , , , , , , , , , , , , ,				
Mode of Evaluation: Quiz, Assignment, CAT and FAT						
Recommended by BoS -						
Approved by Academic Council -						

S. No.	Indicative List of Laboratory Experiments				
1	Construction of galvanic cells using waste metal and evaluation of Thermodynam functions (enthalpy, entropy, and free energy) from EMF measurements.				
2	Determination of reaction rate, order and molecularity – ester hydrolysis (ethylacetate).				
3	Colorimetric estimation of Ni <sup>2+</sup> using conventional and smartphone digital-imaging method.				
4	Assessment of the Fe <sup>2+</sup> content using potentiometry.				
5	Preparation of ZnO semiconductor and its characterization.				
6	Estimation of sulfate ion in water by the conductivity method.				
7*	Build atoms and molecules, visualization of atomic orbitals and hybridized orbitals. Calculating the orbital contributions.				
8*	Conformational analysis of cyclohexane and ethane molecules and plotting the potential energy profile.				
9*	Application of AI to screen semiconductors, materials, medicinal compounds - case study.				
10	Size-dependent colour variation of Cu <sub>2</sub> O nanoparticles by spectrophotometer				
11	Synthesis of hydroxyl apatite from biowaste and its use for the removal of heavy metals				
12	Fabrication of DSSC as a renewable energy resource using a natural dye.				
13	Colorimetric estimation of Fe <sup>2+</sup> using conventional and smartphone digital-imaging method				
14.	Determination of reaction rate, order, and molecularity following sucrose hydrolysis by the amylase enzyme.				
	#Concepts of Molarity, Molality and Normality will be discussed appropriately * For experiments 7, 8 & 9, minimum four molecules to be studied.				

Total hours:			30 hours
Mode of Evaluation: CAT, FAT, Quiz			
Recommended by the Board of Studies			
Approved by the Academic Council	No	Date	