Punyashlok Ahilyadevi Holkar Solapur University, Solapur

NAAC Accredited-2022
'B++'Grade (CGPA2.96)

Faculty of Science & Technology

(As per New Education Policy 2020)

Syllabus: **Physical Chemistry**

Name of the Course: M.Sc. II (Sem. III &IV)

(Syllabus to be implemented from June 2024)

Punyashlok Ahilyadevi Holkar Solapur University, Solapur
Faculty of Science & Technology
Nep 2020 Compliant Curriculum
M. Sc. II Physical Chemistry
Program Preamble

The Master of Science (MSc) in Physical Chemistry is a comprehensive and dynamic program designed to provide students with a deep understanding of the fundamental principles of Physical Chemistry, along with the practical skills required to apply this knowledge in various scientific and technological contexts. Aligned with the vision of the National Education Policy (NEP) 2020, the program offers a flexible, multidisciplinary, and learner-centric curriculum that encourages critical thinking, innovation, and holistic development. The MSc Physical Chemistry program spans two years, with each year offering a progressively advanced curriculum designed to build a strong foundation in Physical Chemistry while allowing for specialization and interdisciplinary learning. The curriculum is structured around several key components:

1. **Discipline Specific Core Courses:** These core courses form the backbone of the program, providing in-depth knowledge and understanding of essential physical chemistry concepts, theories, and methodologies. Students will engage with topics ranging from Quantum mechanics, electrochemistry, Chemical Kinetics, Spectroscopy, Photochemistry, Solid State Chemistry, Surface Chemistry and Molecular spectroscopy ensuring a robust and comprehensive education in the discipline.
2. **Discipline Specific Elective Courses:** The program encourages intellectual exploration beyond the core discipline by offering a wide range of elective courses. These electives enable students to pursue their interests in diverse subjects, fostering creativity, critical thinking, and a well-rounded educational experience.
3. **Field Projects/Internships/Apprenticeships/Community Engagement Projects/On-Job Training:** To bridge the gap between theoretical knowledge and real-world applications, the program includes opportunities for field projects, internships, apprenticeships, and community engagement. These experiences provide students with practical insights, problem-solving abilities, and exposure to professional environments, enhancing their readiness for careers in Chemistry and related fields.
4. **Research Methodology and Research Projects:** Research is a critical component of the MSc Physical Chemistry program, with students acquiring skills in research methodology, data collection, analysis, and scientific inquiry. By engaging in independent research projects, students are encouraged to develop innovative solutions to complex scientific problems, preparing them for advanced studies and research-oriented careers.

Multiple Entry and Multiple Exit Options

In accordance with the NEP 2020, the MSc Physical Chemistry program incorporates a Multiple Entry and Multiple Exit framework, offering students the flexibility to enter or exit the program at various stages. This approach ensures that students can tailor their educational journey according to their personal and professional goals, with options to earn certificates, diplomas, or degrees based on the duration of study completed.

- **Year 1:**
  Upon completion of the first year, students may exit with a **Certificate in Physical Chemistry**.
- **Year 2:**
  After two years, students may choose to exit with a **MSc Degree in Physical Chemistry**

Eligibility for MSc Physical Chemistry: The candidate having B. Sc. with Chemistry as a principal subject / Chemistry at subsidiary level

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MSc (Physical Chemistry)
Program Outcomes (PO)

Students graduating from the Master of Science in Physical Chemistry program will be able to:

Major Courses:

- **PO1**: Demonstrate in-depth knowledge and understanding of core concepts, theories, and methodologies in the chosen major discipline.
- **PO2**: Apply disciplinary knowledge to solve complex problems, analyze data, and make informed decisions in professional and research contexts.
- **PO3**: Acquire complementary knowledge and skills from a related or distinct discipline, enhancing interdisciplinary understanding and versatility.
- **PO4:** Understanding fundamental principles and laws of physical chemistry
- **PO5:** Development of abilities to study and understand properties of materials

Elective Courses:

- **PO6**: Explore diverse subjects beyond the core discipline, fostering a broad-based education and cultivating critical thinking and creativity.

Research Methodology and Research Project:

- **PO7**: Acquire research skills, including data collection, analysis, and interpretation, fostering a scientific approach to problem-solving to develop independent research projects handling capabilities.
- **PO8:** Empowering the students to do independent research of high caliber

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MSc (Physical Chemistry)
Program Specific Outcomes (PSOs)

Students graduating from MSc (Physical Chemistry) will able to :

PSO1: Mastery of Core Physical Chemistry Concepts: demonstrate understanding of fundamental physical Chemistry principles, including Quantum mechanics, Chemical Kinetics, Electrochemistry, thermodynamics, statistical thermodynamics, surface chemistry, solid state chemistry, molecular spectroscopy etc, allowing them to analyze and solve complex physical problems.

PSO2: Experimental and Analytical Skills: demonstrate proficiency in designing and conducting experiments, using modern laboratory equipment, and employing analytical techniques to interpret and present scientific data effectively.

PSO3: Application of Physical Chemistry knowledge in Technology and Research: apply their knowledge to develop innovative solutions in technology, engineering, and applied sciences, contributing to research and development in both academic and industrial settings.

Proposed structure for Two Year PG Program (M.Sc.) Degree

Level/ Difficulty	Sem.	Major		Minor	Open Elective OE	Vocational and Skill Enhancement Courses (SEC/VSC)	Ability Enhancement Course (AEC), IKS, VEC	Field Project/ RP/CC/Internship/Apprenticeship/ Community Engagement & Services	Credits	Cumulative Credits
		Mandatory	Elective							
6.0/400	I	DSC1-1 (4+2) DSC1-2 (4+2) DSC1-3 (4+2)	DSE1-1 (4+2)	Research Methodology (4)	------	----	----	----	22	44 PG Diploma in Discipline
	II	DSC1-4 (4+2)	DSE1-2 (4+2)	- —	----	------	----	OJT/In-house Project/ Internship/ Apprenticeship (4)	22	
	Total 1 Yrs	24	12	04				04	44	
Exit option: Award of PG Diploma in Discipline with 44 credits OR Continue with Discipline										
6.5/400	III	DSC1-5 (4+2) DSC1-6 (4+2)	DSE1-3 (4+2)	----	------	----	----	RP (4)	22	88 PG Degree in Discipline
	IV	DSC1-7 (4+2) DSC1-8 (4)	DSE1-4 (4+2)	- —	----	------	----	RP (6)	22	

General Structure of the Course:

Sem.	Code with course code	Title of the paper	Semester Examination			L	P	Credit
			UA	CA	Total			
SEM-III		**Major**						
	DSC-5 2302301	Quantum Chemistry	60	40	100	4	-	4
	DSC-6 2302302	Electrochemistry and Chemical Kinetics	60	40	100	4	-	4
		Elective						
	DSE-3 2302306	Solid State Chemistry OR	60	40	100	4	-	4
	DSE-3 2302307	Biophysical Chemistry OR						
	DSE-3 2302308	Radiation and Photochemistry						
		Practical						
	DSC-5 P 2302304	Practical of DSC-5	30	20	50		4	2
	DSC-6 P 2302305	Practical of DSC-6	30	20	50		4	2
	DSE-3 P 2302309 or 2302310 or 2302311	Practical of DSE-3A Practical of DSE-3B Practical of DSE-3C	30	20	50		4	2
		Research Project						
	RP 2302303	Research Project	60	40	100	-	-	4
			330	**220**	**550**			**22**
SEM-IV		**Major**						
	DSC-7 2302401	Statistical Mechanics and Irreversible Thermodynamics	60	40	100	4	-	4
	DSC-8 2302402	Molecular Structure	60	40	100	4	-	4
		Elective						
	DSE-4 2302405	Surface Chemistry OR	60	40	100	4	-	4
	DSE-4 2302406	Chemistry of Materials OR						
	DSE-4 2302407	Nuclear and Radiation Chemistry						
		Practical						
	DSC-7 P 2302404	Practical of DSC-7	30	20	50	-	4	2

	DSE-4 P **2302408** **2302409** **2302410**	Practical of DSE-4A Practical of DSE-4B Practical of DSE-4C	30	20	50	-	4	2
		Research Project						
	RP **2302403**	Research Project	90	60	150	-	-	6
		Total for semester IV	**330**	**220**	**550**	**--**	**---**	**22**

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-III** **Vertical : DSC** **Course Code: 2302301** **Course Name: Quantum Mechanics**
***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: The course consists of two parts. The essential quantum mechanics that is required later is covered in the first part. The basic quantum mechanical principles and their applications to model systems once mentioned in the basic course are discussed in detail. Approximative methods are introduced. The interaction between electromagnetic radiation and molecules is discussed which then leads to the basic principles of various optical (such as infrared and Raman) spectroscopies.

Methods of quantum chemical calculations and their applications in chemistry are treated in the second part of the course. The Hartree-Fock method, its theoretical background and implementation but also post-Hartree-Fock methods and the density functional theory are described and discussed. Their application for calculating molecular properties such as energies, molecular geometries, vibrational spectra and features of chemical reactions is introduced and illustrated. This part of the course includes quantum-chemical calculation assignments where a modern quantum chemical software package is used for computing molecular properties and chemical reactions.

Course Objectives:

- Describe in detail the formalism of quantum mechanics, relate to and summarize the concepts of quantum mechanics in order to define, calculate and explain the behaviour of quantum mechanical model systems.
- Describe, explain and apply basic quantum chemical theory for atomic and molecular many-electron systems to the computation of molecular properties, chemical reactivity and molecular spectroscopy.

Course Outcomes:

CO1: Students will learn basics of quantum mechanics.

CO2: Learn concepts of atomic orbitals and their shapes, spectroscopic selection ules, ionization potentials, etc.

CO3: Able to understand selection rules and to predict the electronic spectra of conjugated organic molecules.

CO4: Will familiarize in understanding and choosing the appropriate basis sets for

electronic structure calculations with appropriate corrections through use of electron correlation methods

CO5: Students can predict all the properties of materials at molecular level even for nanostructures, drugs, solids oxides, composites, solid electrolytes, electrode materials used in batteries and other electronic devices, etc.

CO6: For larger molecules like macrocycles, polymers, peptides etc., learners will be capable of replace or modify computationally demanding two electron integrals through use semiempirical methods and parameterization tools used in these methods.

CO7: Knowledge of this course will make learners a potential candidate to work independently in any R&D laboratory or research laboratory or academic institutes of international repute.

Unit – I Formalism of Quantum Mechanics:

Hrs: (15) Weightage: 20 Marks

Recapitulation of quantum mechanics, Postulates of Quantum Mechanics, Eigen function and Eigen values, Acceptability of wave functions, Normalized and orthogonal wave functions, Operators and operator algebra, Schmidt Orthogonalization, Hermitian operators, properties of Hermitian operators, Theorems related to commutator operations. Free particle, particle in a box; One / two / Three-dimensional Box. Degeneracy in multidimensional box. Quantum Tunneling effect Concept of angular momentum, angular momentum operators, Ladder operators.

Unit – II Quantum Mechanics of some simple systems:

Hrs: (15) Weightage: 20 Marks

Rigid rotator, Linear harmonic oscillator, the formal solutions, energy levels, degeneracy, properties of wave functions and selection rules. The hydrogen and hydrogen like atoms: Schrodinger equation for hydrogen atom (in polar coordinates) and its complete solution. The radial distribution function and its significance, shapes of atomic orbitals. Application to hydrogen like atoms and molecules (e.g He^{+}, Li^{2+}etc.

Unit – III. Hückel molecular Orbital Theory

Hrs: (15) Weightage: 20 Marks

Variation principle, Secular equations and secular determinants. Formalism of Hückel molecular Orbital Theory, origin of aromatic stability and calculation of delocalization energy. HMO calculations for organic molecules (e.g. ethylene, cyclopropyl, allyl, butadiene,

cyclobutadiene, trimethylene methane etc.), free valence index and prediction of chemical reactivity, Use of symmetry based linear combination to simplify the problem of Hückel theory calculations for larger aromatic molecules (like butadiene).

Unit – IV: Advanced quantum chemistry

Hrs: (15) Weightage: 20 Marks

Schrödinger wave equation and Hamiltonian for Multi-electron systems. An introduction to ab initio methods: Self–consistent field (SCF) theory, Hertree-Fock (HF) method, Basis sets, Slater type orbitals (STOs) and Gaussian type atomic orbitals (GTO's), HF-SCF procedure post HF-methods: Configuration Interaction, Perturbation theory and Coupled cluster method.

REFERENCE BOOKS

1) Introductory Quantum Chemistry by A. K. Chandra. TataMcGraw-Hill.1988.
2) Quantum Chemistry by Donald A McQuerrie, Viva Books, 2003
3) Molecular Quantum Chemistry, by P. Atkins and R. Friedman, Oxford University Press, 2005.
4) Quantum Chemistry, W. Kauzmann, Academic press.
5) Quantum Chemistry by Levine, Prentice Hall.
6) Quantum Chemistry by R. K. Prasad, New Age International.
7) Modern Quantum Chemistry, N. S. Ostlund & A Szabo, McGraw Hill.
8) Density Functional Theory of atoms and molecules, R. G. Parr and W. Yang, Oxford Press.
9) Semiempirical MO Theory, J. Pople and D. L. Beveridge.
10) Theoretical Chemistry by S. Glasstone.
11) Huckel Molecular Orbital Theory by Keith Yates

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-III** **Vertical : DSC** **Course Code: 2302302** **Course Name: Electrochemistry and Chemical Kinetics**

***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: Electrochemistry and Chemical Kinetics course is designed for understanding the basic concepts of both these areas of physical Chemistry. The first two units are devoted to electrochemistry while remaining two units allotted for Chemical Kinetics. The course consists of ion-solvent interactions and interface electrodics, advanced theories of chemical reactions and homogeneous and heterogeneous catalysis.

Course Objectives:

- To study chemistry of ions in solution
- To understand Electrode-electrolyte interface and different electrochemical processes.
- To get knowledge of Chemical kinetics of simple and complex reactions
- To acquire skills in Analysis techniques for fast reactions
- To study the Kinetics of reactions in solution phase

Course Outcomes (Cos):

Students will be able to

CO1: understand basic principles of electrochemistry

CO2: Study of electrochemical charge transfer properties of materials and designing of applied experiments for electroanalytical testing of materials.

CO3: quantify the charge of the material and used for testing of electrokinetic phenomenon.

CO4: Learn the principles and techniques to understand adsorptions and desorption from the electrode interface in the electrolyte solution

CO5: give fundamental equation of electrodics to study the reversible charge transfer behavior in the materials electrolyte interfaces.

CO6: understand the basic principles of Kinetics

CO7: learn different theories of rates of reaction

CO8: Learn from fundamental to advanced theories and applications of chemical kinetics

CO9: apply different methods of study of dynamics of fast reaction mechanism

CO10: learn effect different equations expressions expressing reaction constant and substitution constant.

Unit – I Equilibrium electrochemistry and ion-solvent interactions

Hrs: (15) Weightage: 20 Marks

Debye–Hückel Theory of inter-ionic attraction, Ionic atmosphere, Time of relaxation, Relaxation and Electrophoretic effects, Debye – Hückel Onsager equation and its validity, Debye – Falkenhagen effect, Wein effect, Debye Hückel limiting law, Qualitative and quantitative test of Debye Hückel limiting equation, Debye-Hückel Bronsted equations, osmotic coefficient, Bjerrum theory, association constant. The Born Model and expression for the free energy of ion solvent interactions. Thermodynamic parameters for ion solvent interactions. Calculations of heats of hydration of ions and the concept of hydration number (Van Arkel, de Boer's, and Bernal- Fowler methods). Numerical problems.

Unit – II Interface Electrochemistry and It's Applications

Hrs: (15) Weightage: 20 Marks

Electrical double layer and it's theories. Exchange current density, over potentials, Butler-Volmer equation, high field and low field approximations, Tafel equations,

Fuel cell: Introduction, Hydrogen – oxygen fuel cells, hydrocarbon - air fuel cell, alkaline fuel cells. **Corrosion**: Introduction, Classification, mechanism, and kinetics of corrosion, Pourbaix diagrams. Factors affecting corrosion: Nature of the metal, Nature of the corroding environment, Prevention of corrosion: Material selection & Design, protective coatings, corrosion inhibitors. **Bioelectrochemistry**: Nerve impulses, Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, electrochemical impedance spectroscopy.

Unit – III Theories of reaction rates

Hrs: (15) Weightage: 20 Marks

Equilibrium and rate of reaction, Partition functions and activated complex, Transition state theory (Thermodynamic and partition function approach), Reaction between polyatomic molecules, calculation of activation parameters of a reaction. Collision theory, energy factor, orientation factor, rate of reaction, Lindemann's mechanism of unimolecular reaction, weakness of the collision theory.

Unit – IV Homogeneous Catalysis and Kinetics of Fast Reactions

Hrs: (15) Weightage: 20 Marks

Homogeneous Catalysis: general catalytic mechanism, equilibrium and steady- state treatment, activation energies for catalyzed reactions. General acid-base catalysis, mechanisms of acid-base catalysis (Arrhenius and van't Hoff intermediates), catalytic activity and acid base strength, Acidity functions, autocatalysis, and oscillatory reactions. Mechanism of enzyme catalyzed reactions and rate law for single substrate, Lineweaver-Burk plot, effect of pH and temperature.

Fast Reactions: Relaxation techniques, pressure jump and temperature jump methods, NMR relaxation, flash photolysis and molecular beam methods

REFERENCE BOOKS

1) An Introduction to Electrochemistry by S. Glasstone, Tata McGraw Hill Ind. Pvt.Ltd.
2) Modern electrochemistry Vol I & II by J. O. M. Bockris and A. K. N.Reddy.
3) Physical chemistry by S. Glasstone, Tata McGraw Hill Pvt.Ltd.
4) Electrolytic Solutions by R. A. Robinson and R. H.Stokes
5) Physical Chemistry by P. W. Atkins.ELBS.
6) Theoretical electrochemistry by L. I. Antropov, MIRPublishers.
7) Chemical and electrochemical energy systems by R. Narayan and B. Viswanathan, Universities press
8) Handbook of fuel cell technology by Maget HJR, prentice-Hall, NewJersey.
9) Electroforming: A comprehensive survey of theory, practice and commercial applications by P. Spiro, London1971.
10) Electrotyping by McMillan Walter George
11) Electrotyping and Stereotyping by B. Harris and S. Alexander.

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-III** **Vertical : RP** **Course Code: 2302303** **Course Name: Research Project-I**
***Teaching Scheme** **Practicals:08 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: The research project for M. Sc. Physical Chemistry is introduced to get familiarize with literature survey of the work done in the field of interest

- It is expected that project should provide hands on training to the students on various instruments.
- They should learn independent working on a short research project.

Course Outcomes:

CO1: They should learn independent working on a short research project

CO2: Students must do a literature review in their subject of interest and choose a project topic in consultation with their supervisor.

CO3: The students will get idea of A survey of literature, The work schedule, Using Chem Draw program to draw structures, Writing the synopsis

CO4: Project work involving organic synthesis/evaluation of biological studies or in-plant training in any of the pharmaceutical or chemical industry

In Semester III, there is a Research Project of 4 credits. Students have to carry out project either at college laboratory or university laboratory or in any recognized R & D laboratory (Public/Private/Government) or Industry or Institute of national repute across the country under the guidance of scientist or a post-graduate faculty member.

Students are expected to work on assigned research project and submit the results at the end of the semester in the form a dissertation. Open defense of the student on his/her dissertation shall be arranged. This defense shall be in front of the panel of examiners. This will be valued for 40 marks. Students are required to work for a specific project under supervision of concerned faculty member. Project should be completed under the guidance of a faculty member in the same Department or Industry or research organization. In case of Industry/ research organization one member of that body can also be included as project guide.

Guidelines for Assessment

- Quality of literature survey and novelty in the problem

- Clarity of problem definition and feasibility of problem solution
- Clarity of objective and scope
- Quality of work attempted
- Presentation skills

पुण्यश्लोक अहिल्यादेवी होळकर सोलापूर विद्यापीठ ॥ विद्यया संपन्नता ॥ NAAC Accredited-2022 'B++' Grade (CGPA-2.96)	**Punyashlok Ahilyadevi Holkar Solapur University, Solapur** **M.Sc. (Physical Chemistry) Semester-III** **Vertical : DSC** **Course Code: 2302304 and 2302305** **Course Name: Practical I and II** **&** **Vertical : DSE** **Course Code: 2302309/2302310/2302311** **Course Name: Practical III Based on DSE3A/3B/3C**
***Teaching Scheme** **Practicals:04 Hours/week, 02 Credits**	***Examination Scheme** **UA:30 Marks** **CA: 20 Marks**

Course Preamble: The practical course is designed in such a way that students will get an experiential learning. The practicals are set on the core papers as well as elective courses. Some practicals on quantum chemistry are also designed. The practicals based on pHmetry, Potentiometry, Spectrophotometry, Thermochemistry, Polarography, Conductometry and Chemical Kinetics are included in the course. These practicals are further divided into short and long experiments.

A Physical chemistry practical course aims to provide students with hands-on experience in the laboratory, reinforcing theoretical concepts and developing essential laboratory skills.

Couse Objectives

- **Experimental Techniques:**
  - Master fundamental laboratory techniques such as weighing, measuring, titration, filtration, and crystallization.
  - Develop proficiency in using laboratory equipment, including balances, glassware, burners, and heating devices.
- **Observation and Data Collection:**
  - Observe chemical reactions and record accurate observations, measurements, and data.
  - Develop skills in data analysis, including graphing, calculations, and interpretation of results.

- **Problem-Solving and Critical Thinking:**
  - Apply theoretical knowledge to solve practical problems and design experiments.
  - Develop critical thinking skills to analyze experimental results and draw conclusions.
- **Laboratory Safety:**
  - Understand and adhere to laboratory safety procedures and regulations.
  - Handle chemicals and equipment safely and responsibly.

Course Outcomes (COs)

CO1: In-depth training on laboratory solution preparations on all concentration scales

CO2: Training on laboratory safety and lab ethics in scientific work

CO3: Training on planning, design and execution of experiments

CO4: Training on scientific literature search, defining the objective of the work, research skills, data representation in tabular and graphical form etc.

CO5: Training on experimental verification of fundamental theories, comparison of data with literature and scientific discussion on any deviation of data from expected theoretical values or reported literature.

CO6: Training on electrochemical analysis of different physicochemical aspects of materials

CO7: Training on different techniques needed to characterize the detergents

CO8: Application of theoretical and practical knowledge for research training through mandatory research/industrial projects

1. Potentiometry

2. Determination of standard electrode potential (E_o) value of Ag / AgI electrode and the solubility product of AgI and PbI_2.
3. Determination of dissociation constants of dibasic acid potentiometrically.

2. Conductometry

1. To determine equivalent conductance at infinite dilution of strong electrolytes and weak acid by using Kohlrausch Law and dissociation constant for weak acid conductometrically.
2. Kinetic study of hydrolysis of ethyl acetate in presence of OH^- ions.

3. pH – Metry

1. Determination of hydrolysis constant and degree of hydrolysis of aniline hydrochloridep Hmetrically.
2. Determination of acid- base dissociation constants of amino acids.

4. Polarography

1. To determine half wave potential of a given ion using half height method, differential method and wave equationmethod

5. Chemical Kinetics

1. To determine the order of reaction between acetone and iodine catalyzed by acid.

6. Spectrophotometry

1. To determine pKa value of methyl red indicator at roomtemperature.
2. Determination of indicator constant and isosbestic point of an indicator (bromocresol purple).
3. Determination of stability constant of ferric thiocyanate complex by Ostwald method.

7. Latent heat of Fusion:

1. Determination of latent heat of fusion of a given solid.

8. Quantum Plots

1. Graph plotting of mathematical functions-linear, exponential, trigonometry and identify whether they are acceptable or non acceptable as wave functions.
2. Polar plots of atomic orbitals such as 1s, $2p_x$ and $3d_z^2$ orbitals by using angular part of hydrogen atom wave functions.

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-III** **Vertical : DSE** **Course Code: 2302306** **Course Name: Solid State Chemistry**
***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: The course contains basic solid state chemistry principles, crystals structure, Bragg's diffraction equation, different types of solid state reactions, their mechanisms, preparation of materials and their purification techniques.one unit is devoted to the nanomaterials. This unit includes different methods of preparation of nanomaterials and latest nanomaterial characterization techniques.

Course Outcomes (COs)

CO1: Students can be able to provide an introduction to the concepts underlying solid state chemistry.

CO2: Describe specific crystal structures by applying basic crystallographic concepts

CO3: Understand generation of X-ray radiation and its effects of on matter as well Bragg's diffraction equation to find out structural information of solid materials

CO4: Understand the atomic and electronic structure, electric conductivity, optical property, magnetism of solid materials.

CO5: Understand the physical and optical properties of metal, semiconductor, and insulator using free electron theory and band theory

Unit I: The Solid State: **Hrs: (15) Weightage: 20 Marks**

Types of solids, crystal structure, crystal symmetry, symmetry element, crystal defects and non-stoichiometry, Miller indices, lattice constants, Bravis lattice, and crystal structure determination by X-ray diffraction – Bragg's single crystal and powder diffraction method. Debye-Sherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-Ray intensities, structure

factor and its relation to intensity and electron density,

Unit II : Solid State Reactions: **Hrs: (15) Weightage: 20 Marks**

General principle, types of reactions: Additive, structure sensitive, decomposition and phase transition reactions, material transport in solid state reactions, Kirkendall effect, kinetics of solid state reactions, factors affecting the reactivity of solid state reactions.

Unit III : Preparation of materials: **Hrs: (15) Weightage: 20 Marks**

Purification: Crystallization, sublimation and zone refining. Preparation of single crystal: Theory of nucleation, crystal growth, methods of preparation of single crystal, single crystal growth from solution, growth from melt. Doped organic and inorganic crystalline materials for device application.

Unit IV :Synthesis and Characterization of Nanomaterials

Hrs: (15) Weightage: 20 Marks

General Introduction to Nanomaterials, Nanoscience and nanotechnology, History. Chemical Methods: Metal nanoparticles: Reduction method, Semiconducting or composite nanomaterials: Hydrothermal and Solvothermal method, Sol-gel, Arrested Precipitation, and other methods include Langmuir-Blodgett, Micelles-Microemulsions. Characterization Tools: Electron Microscopy (TEM & SEM), Probe Microscopy (STM & AFM), Diffraction Technique (XRD), UV-Visible-NIR spectroscopy, BET.

REFFERENCE BOOKS :

1) Principals of solid state, H. V. Keer, WileyEastern.
2) Solid state chemistry, N. B.Hannay
3) Solid state chemistry, D. K. Chakrabarty, New AgeInternational
4) An Introduction to Crystallography : F. G.Philips
5) Crystal Structure Analysis : M.J.Buerger
6) New Directions in Solid State Chemistry (Second Eds.), C.N.R.Rao and G. Gopalkrishnan, Cambridge Oxford Press.
7) A basic course in crystallography, JAK Tareen, TRN Kutty, Universities press.
8) Essentials of crystallography, M.A. Wahab, Narosa Publications.
9) Solid State Chemistry: Lasley E. Smart, Elaine A. Moore.
10) Introduction to Solid State Physics: Charles Kittel
11) Wilcox : Preparation and Properties of Solid State Materials: Vol I & II, Dekker
12) Hagenmuller, Preparative Methods in Solis State Chemistry
13) Lohn Wulff, The Structure and Properties of Materials Vol. IV, Electronic Properties (Wily Eastern)

14) Chemistry of Imprefect Crystals (Holland) E.A. Kroger

15) The Structure and properties of materials: Vol.III Electronic properties by John Wulff.

16) Electronic processes in materials: L. V. Azroff and J. J.Brophy

17) Chemistry of imperfect crystal : F. A.Krogen

18) Elements of X-ray Diffraction by B. D. Cullity, AddisonWeily.

19) Solid state Chemistry and its applications, A. R.West, Plenum.

20) Solid state Chemistry: An Introduction, 3rd Ed., L. E. Smart and

E. A. Moore, Taylor and Francis,2005.

21) Introduction to solids, L. V. Azaroff, Tata McGraw Hill.,1977.

22) Ludovico Cademartiri and Geoffrey A.Ozin, Concepts of Nano chemistry, Wiley–VCHVerlagGmbH&co,2009

23) C.Bréchignac, P.Houdy, Marcel Lahmani, Nano materials and Nano chemistry, Springer,2007

24) C.N.R.Rao, Achim Müller, Anthony K. Cheetham, Nano materials Chemistry ,John Wiley & Sons, 2007

25) Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri, Nano chemistry: A Chemical Approach to Nano materials, Royal Society of Chemistry (Great Britain)

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-III** **Vertical : DSE** **Course Code: 2302307** **Course Name: Biophysical Chemistry**
***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: This course consists of four units. Unit I contain the study of building blocks of living organisms like amino acids, proteins, nucleic acids, enzymes and their chemistry. The consequent units comprise biopolymer chemistry, biological processes and their details. The last unit is devoted for muscle mechanism, nerve system mechanism and thermodynamics involved in them.

Course Outcomes (COs)

CO1: students will know about Amino acids, proteins, enzymes , DNA & RNA in living systems , electrolytes, the chirality of biological molecules , the biochemical process , weak and strong interactions, macromolecules and rubber elasticity , polyelectrolytes biopolymers.

CO2: Students will learn the applications of optical and thermodynamic technique to study the interactions of biomolecules with water

CO3: Learn about the photo-biological processes

CO4: Study about different mechanic hemical processes in the body.

CO5: Kinetic properties of muscle and molecular mechanism of receptor

Unit – I : Chemistry and Biology: **Hrs: (15) Weightage: 20 Marks**

Amino acids, proteins, enzymes, DNA & RNA in living systems, electrolytes, the chirality of biological molecules, the biochemical process, weak and strong interactions, macromolecules and rubber elasticity, polyelectrolytes, biopolymers.

Unit-II: Physical aspects of biopolymers: **Hrs: (15) Weightage: 20 Marks**

X-ray diffraction, electronic absorption & luminescence Spectroscopy, optical activity, magnetic activity, magnetic optical activity. Osmosis, hydrophobic hydration and interactions. The properties of amino acids and their aqueous solutions.

Unit – III : Photobiological Process: **Hrs: (15) Weightage: 20 Marks**

Photosynthesis, mechanism of vision, the molecular mechanism of photoreceptor.

Unit – IV : Mechano-chemical processes: Hrs: (15) Weightage: 20 Marks

Introduction, thermodynamics, nerve conduction and membrane equilibria, muscle and muscle proteins, their chemistry and physics, kinetic properties of muscle, mechano- chemical systems, biomechanics.

REFERENCE BOOKS :

1) Biophysics by M.V.Volhenshfein.
2) Natural products : Chemistry & Biological Significance, J.Mann, R.S. Davidson, J.B. Hobb's, D.V. Banthrope and J.B. Harborne, Longmar Essex
3) Elements of Inorganic Photochemistry, G.J. Ferrandi, wiley
4) Principals of bioinorganic chemistry, S.J. Lippard and J.M. Beng, University Science Books,
5) Principals of biochemistry, A.L. Lechinger, worth publisher
6) Biochemistry, J.David Rawn, Neil Patterson
7) Hydrophobic interactions byBen-Naim,Plenum.

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-III** **Vertical : DSE** **Course Code: 2302308** **Course Name: Radiation and Photochemistry**
***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: This open elective course helps students to learn the concepts involved in radiation and photochemistry. The first two units are of radiation chemistry and LASERS respectively. The last two units devoted to photochemistry. These units give the basic principles involved in photochemistry and also various photophysical pathways. The last unit consists of some exemplary photochemical reactions involved in atmospheric chemistry as well as organic chemistry.

Course Outcomes (COs)

CO1: student will learn basic principles and advanced radio-chemical processes

CO2: Student will be familiar with lases and their wide applications

CO3: Students will learn basic principles of photochemistry

CO4: They may do the data interpretation of rates of radiative process for the obtained data from the electrochemical transient and flash photolysis.

CO5: Applications of photochemistry for degradation of polymers and other smog, singlet molecular oxygen generation etc.

Unit-I :Radiation Chemistry: **Hrs: (15) Weightage: 20 Marks**

Introduction, Radiation Types, their characteristics, Radiation in chemical processes.

Unit-II Lasers and Lasers in Chemistry: **Hrs: (15) Weightage: 20 Marks**

Introduction, characteristics of laser, uses of lasers in chemical process, laser induced chemical reactions, organic photochemistry, lasers as a photochemical tool, laser induced selective bond chemistry, overview, bond selective chemistry of light atom molecules.

Unit-III : Basics of photochemistry: **Hrs: (15) Weightage: 20 Marks**

Electrochemistry of excited states, life time measurements, flash photolysis, energy dissipation by radiative and non radiative processes, properties of excited states, structure, dipole moment, acid-base strength, reactivity, photochemical kinetics, calculations of rates of radiative process, bimolecular quenching, Luminescence for sensors and switches, charge transfer excited state,

photoinduced electron transfer reactions.

Unit-IV : Miscellaneous Photochemical reactions:

Hrs: (15) Weightage: 20 Marks

Photo-fries reaction of anilides, photo-fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog, photodegradation of polymers, photochemistry of vision.

REFRENCE BOOKS :

1) Molecular Photochemistry, N.J.Turro,W.A.Benjamin
2) Fundaments of Photochemistry, K.K.Rohatagi – Mukherji, Weiley –Eastern
3) Elements of Inorganic Photochemistry : G.S.Ferraudi,Wiley
4) Concepts of Inorganic Photochemistry, A.W.Adamson& P.J. Fleischauer,Wiley
5) A Guide To lasers in chemistry, Gerald R. Van Hecke& KerryK.Karukstis.
6) Photochemistry, R.P.Kundall, A Gilbert, ThomsonNelson

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-IV** **Vertical : DSC** **Course Code: 2302401** **Course Name: Statistical Mechanics and Irreversible Thermodynamics**
***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: This theoretical course consists of four units each of 15 theory hours. This course includes basic understanding of statistical mechanics, the mathematical formalism required for understanding it. The third unit is devoted to the quantum statistics viz; Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics and their applications. The fourth unit entirely designed for irreversible thermodynamics. The core concepts of irreversible thermodynamics followed by some important phenomena.

Course Outcomes (Cos)

CO1: Students with weaker background in mathematical principles will learn how to explore the scientific findings with mathematical models and advance it further.

CO2: Learn principles of statistics to understand and estimate bulk thermodynamic properties of materials.

CO3: Understand how microscopic properties where quantum effects are predominant can be correlated to macroscopic properties where classical thermodynamics is important through an ensemble theories and statistical distribution laws.

CO4: Through these studies, students will be able to evaluate the thermodynamic properties of systems of quantum particles such as bosons and fermions.

CO5: Knowledge can be used to utilize the classical and statistical thermodynamic principles for computer simulation of real life processes through molecular dynamic simulations.

Unit – I Modern Theoretical principals:

Hrs:(15) Weightage: 20 Marks

Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and minima. Integrating Factors, Pfaff differential equations, Caratheodory's theory. Legendre transformations. Derivation of thermodynamic identities. The second law of thermodynamics, classical formulations, mathematical consequences of second law. Entropy changes, Clausius inequality. Free energy concept. General condition of equilibrium.

Unit – II Classical Statistical Mechanics:

Hrs:(15) Weightage: 20 Marks

Probability and distribution, Stirling's Approximation, Weights and configurations, the most probable configuration, Ensembles, ensemble average and time average of property. Ergodic hypothesis. Statistical equilibrium, thermodynamic probability, Boltzmann – Planck equation. Maxwell-Boltzmann (MB) distribution law. Molecular Partition function and its significance. Rotational, translational, vibrational, and electronic partition functions. Relationship between partition function and thermodynamic properties. Thermodynamic probability and entropy: Partition function and third law of thermodynamics, Application to monoatomic gases - Sackur tetrode equation, applications to diatomic molecules, Statistical expression for equilibrium constant, Limitations of Maxwell-Boltzmann statistics, Numerical Problems.

Unit – III. Quantum Statistical Mechanics

Hrs:(15) Weightage: 20 Marks

Bose-Einstein and Fermi-Dirac statistics, bosons and fermions, characteristic Bose- and Fermi-temperatures, thermodynamic properties of phonon and photon gas, use of quantum statistics for evaluation of absolute entropies, condensation of helium, Fermi energy, electron gas in metals. Heat capacity of solids. Einstein and Debye specific heat equations. Characteristic temperatures. Quantum solids, Debye T^3 law.

Unit – IV: Thermodynamics of Irreversible Processes

Hrs:(15) Weightage: 20 Marks

Conservation of mass in closed and open systems, conservation of energy in closed and open systems. Law of increasing entropy. Non-adiabatic processes and Clausius inequality, steady state. Thermodynamic equations of motions. Entropy production in closed and open systems. Entropy production due to heat flow, Chemical and electrochemical affinities. Coupling reactions. Rates and affinities. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients. Concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Diffusion, electromotive force, electro-osmosis, thermoelectric effects, and other reactions involving cross relations. Saxen's relations.

REFERENCE BOOKS

1) S. N. Blinder, Advanced physical Chemistry, The Macmilan Company, 1967.
2) L. K. Nash, Elements of statistical thermodynamics, 2nd Edition, Addison Wesley, 1974.
3) T.L. Hill, An Introduction to Statistical Thermodynamics, Addison-Wesley, 1960.
4) S. Glasstone, Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists, D. Van Nostrand Company, Inc., 1944.

5) Statistical thermodynamics by B.J. McCelland, Chapman and Hall.
6) D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva Books, New Delhi, 1998.
7) An Introduction to Statistical Thermodynamics, R. P. H. Gasser and W. G.Richards, World Scientific Pub. Co. Pvt. Ltd.,1995.
8) Statistical Mechanics, Donald A. McQuarrie, Viva Books, New Delhi, 2000.
9) An Introduction to Statistical Thermodynamics, M. Dole, Dover, New York,1986
10) I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Wiley, New York, 1968.
11) R.P. Rastogi, Introduction to Non-equilibrium Physical Chemistry: Towards Complexity and Non-linear Science, Elsevier, Oxford, 2008.

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***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: The study of interaction of electromagnetic radiation with matter is of prime importance in chemistry. This helps chemists in understanding the structure of the chemical compound, its behaviour and also the properties associated with them. This course designed to learn rotational, vibrational, Raman spectroscopy and Electronic spectroscopy of atoms and molecules. The group theory plays a vital role in understanding the structure of the molecules. Symmetry, types, elements and the concepts like character table formulation and its application is included in this unit.

Course Outcomes (Cos)

CO1: Students will learn basics principles and laws of spectroscopy.

CO2: From this course student will learn symmetry operations and groups theory for probing the detail spectral detail of molecule

CO3: Understand the fundamental modes of oscillations of molecules based on the properties like dipole movement of the molecules

CO4: Applications of rotational and vibrational spectroscopy

CO5: Fundamental of polarizability of molecules and Raman active modes

CO6: Structural investigations of the material based on the microwave, IR and Raman spectra and various theories of peak splitting

CO7: Basic Principles of Electronic spectroscopy, progression, sequencing and Birje Spooner plots

CO8: Instrumentation and applications of the Electronic spectroscopy for structural elucidation.

CO9: Structural investigations of the material based on the NMR radiations and various theories of peak splitting

Unit – I Rovibrational Spectroscopy Hrs:(15) Weightage: 20 Marks

Classification of molecules according to their moment of inertia. Rotational spectra of rigid and non-rigid diatomic molecules. Selection rules. The intensities of spectral lines. The effect of isotopic substitution. Polyatomic molecules. The Stark effect. Morse potential energy function and vibrational spectrum, fundamental vibrational frequencies. Force constant, zero-point energy. The Anharmonic oscillator, the diatomic vibrating rotator, the interactions of rotations and vibrations. Selection rules. Molecular properties calculations from rovibrational analysis for diatomic molecules CO, HCl, NO etc. Isotope effect (e.g. rovibrational spectra of HCl and DCl). Polyatomic molecules: Fundamental vibrations and their symmetry, overtone and combination bands. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Instrumentation for rovibrational spectroscopy.

Unit – II Raman Spectroscopy and Group Theory

Hrs:(15) Weightage: 20 Marks

Raman Spectroscopy: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Polarization of light and the Raman effect. Structure determination from Raman and Infra-red spectroscopy. Selection rules. Mutual exclusion principle.

Group Theory: Symmetry elements, symmetry operations and point groups. Properties of group, symmetry operations as a group, multiplication table. Reducible and irreducible representations, orthogonality theorem, Properties of irreducible representations. Constructions of character table for point groups. Use of group theory in IR and Raman spectral analysis.

Unit – III Electronic Spectroscopy Hrs:(15) Weightage: 20 Marks

General nature of band spectra. Beer-Lambert Law, integrated absorption coefficient and oscillator strength. Term symbols for atoms and molecules. The hydrogen atom and hydrogen like species spectrum. Sequences and progressions, the vibrational course structure and rotational fine structure of electronic band. The Franck- Condon principle, dissociation energy and dissociation products. Birje-Sponer extrapolation. The fortrat diagram. Predissociation, classification of electronic states. The spectrum of molecular hydrogen. Electronic spectra of polyatomic molecules.

Unit – IV NMR and ESR spectroscopy Hrs:(15) Weightage: 20 Marks

Nuclear Magnetic Resonance (NMR): The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels and signal to noise ratio, The Larmor precession, relaxation times, the meaning of resonance, selection rules and the resonance condition. NMR experiment and instrumentation, significance of shielding constants and chemical shift, the origin and effect of spin – spin coupling, factors affecting chemical shift, chemical analysis by NMR. Simple and complex splitting patterns. Fourier Transform and FT NMR. Exchange phenomena, ^{13}C NMR spectroscopy.

Electron Spin Resonance (ESR): Basic Principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities, selection rules and McConnell relationship. Bonding parameters from 'g' value and coupling constants. Measurement techniques, instrumentation, and applications.

REFERENCE BOOKS

1) Fundamentals of molecular spectroscopy by C.N. Banwell.
2) Physical chemistry by P.W. Atkins. ELBS.1986
3) Introduction to molecular spectroscopy by G.M. Barrow.
4) Molecular spectroscopy by I.N. Levins, Wiley Interscience.
5) Nuclear magnetic Resonance by J.D. Roberts, McGraw Hill.
6) Introduction to Magnetic resonance by A. Carrington and A.D. McLachlan. Harper and Row.
7) Electron Spin Resonance: Elementary theory and practical applications by J.E. Wetz and J.R. Boulton, McGraw-Hill.

	Punyashlok Ahilyadevi Holkar Solapur University, Solapur **MSc (Physical Chemistry) Semester-IV** **Vertical : RP** **Course Code: 2302403** **Course Name: Research Project-II**
***Teaching Scheme** **Practicals:12 Hours/week, 06 Credits**	***Examination Scheme** **UA:90 Marks** **CA: 60 Marks**

Course Preamble: The research project for M. Sc. Physical Chemistry is introduced to get familiarize with literature survey of the work done in the field of interest

- It is expected that project should provide hands on training to the students on various instruments.
- They should learn independent working on a short research project.

In Semester IV, there is a Research Project of 6 credits. Students have to carry out project either at college laboratory or university laboratory or in any recognized R & D laboratory (Public/Private/Government) or Industry or Institute of national repute across the country under the guidance of scientist or a post-graduate faculty member. It is expected from the students detailed study of the chosen topic of research.

Course Outcomes:

CO1: They should learn independent working on a short research project

CO2: Students must do a literature review in their subject of interest and choose a project topic in consultation with their supervisor.

CO3: The students will get idea of A survey of literature, The work schedule, Using Chem Draw program to draw structures, Writing the synopsis

CO4: Project work involving organic synthesis/evaluation of biological studies or in-plant training in any of the pharmaceutical or chemical industry

In Semester III, there is a Research Project of 4 credits. Students have to carry out project either at college laboratory or university laboratory or in any recognized R & D laboratory (Public/Private/Government) or Industry or Institute of national repute across the country under the guidance of scientist or a post-graduate faculty member.

Students are expected to work on assigned research project and submit the results at the end of the semester in the form a dissertation. Open defense of the student on his/her dissertation shall be arranged. This defense shall be in front of the panel of examiners. This will be valued for 60 marks. Students are required to work for a specific project under supervision of concerned faculty member.

Project should be completed under the guidance of a faculty member in the same Department or Industry or research organization. In case of Industry/ research organization one member of that body can also be included as project guide.

Guidelines for Assessment

- Quality of literature survey and novelty in the problem
- Clarity of problem definition and feasibility of problem solution
- Clarity of objective and scope
- Quality of work attempted
- Presentation skills

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***Teaching Scheme** **Practicals:04 Hours/week, 02 Credits**	***Examination Scheme** **UA:30 Marks** **CA: 20 Marks**

Course Preamble: The practical course is designed in such a way that students will get an experiential learning. The practicals are set on the core papers as well as elective courses. Some practicals on quantum chemistry are also designed. The practicals based on pHmetry, Potentiometry, Spectrophotometry, Thermochemistry, Polarography, Conductometry and Chemical Kinetics are included in the course. These practicals are further divided into short and long experiments.

Couse Objectives

- **Experimental Techniques:**
  - Master fundamental laboratory techniques such as weighing, measuring, titration, filtration, and crystallization.
  - Develop proficiency in using laboratory equipment, including balances, glassware, burners, and heating devices.

- **Observation and Data Collection:**
  - Observe chemical reactions and record accurate observations, measurements, and data.
  - Develop skills in data analysis, including graphing, calculations, and interpretation of results.
- **Problem-Solving and Critical Thinking:**
  - Apply theoretical knowledge to solve practical problems and design experiments.
  - Develop critical thinking skills to analyze experimental results and draw conclusions.
- **Laboratory Safety:**
  - Understand and adhere to laboratory safety procedures and regulations.
  - Handle chemicals and equipment safely and responsibly.

Course Outcomes (COs)

CO1: In-depth training on laboratory solution preparations on all concentration scales

CO2: Training on laboratory safety and lab ethics in scientific work

CO3: Training on planning, design and execution of experiments

CO4: Training on scientific literature search, defining the objective of the work, research skills, data representation in tabular and graphical form etc.

CO5: Training on experimental verification of fundamental theories, comparison of data with literature and scientific discussion on any deviation of data from expected theoretical values or reported literature.

CO6: Training on electrochemical analysis of different physicochemical aspects of materials

CO7: Training on different techniques needed to characterize the detergents

CO8: Application of theoretical and practical knowledge for research training through mandatory research/industrial projects

1. **Potentiometry**

2. To determine instability constant & stoichiometry of silver ammonia complex potentimetrically.

3. Determination of Thermodynamic Parameters for electrochemical reactions. (To determine ΔG^o, ΔH^o and ΔS^o for the formation of 1 mole cadmium in 1 wt.% amalgam at 25^0C and activity coefficient of solution).

2. Conductometry

1. Determination of the critical micelle concentration of sodium lauryl sulphate in aqueous solution.

2. To determine the hydrolysis constant and degree of hydrolysis of aniline

hydrochloride.

3. pH – Metry

1. To determine the dissociation constants of dibasic acids pHmetrically.

4. Chemical Kinetics

1. Study of the effect of ionic strength on the reaction between persulphate and iodide by visual method.

5. Spectrophotometry

1. To determine stoichiometry & stability constant of ferric- Sulphosalicylic acid/salicylic acid complex by Job's Method and mole ratio method spectrophotometrically.

2. Determination of concentration of Cr and Mn simultaneously spectrophotometrically.

6. Spectroscopy:

1. Characterization of the complexes by electronic and IR spectral data.
2. Analysis of an ESR spectrum of an organic/inorganic radicals.
3. Interpretation of TGA curve.
4. Interpretation of X-ray diffractogram.
5. Analysis of rotational-vibrational spectra of simple molecules like HCl and DCl.

***** Any other relevant experiment may be added.

Reference books:

1. Practical physical chemistry by Friendly and kitchner-logmann, Green and Co.
2. Senior Practical physical chemistry by B.D. Khosala and V.S. Gerg-R chand andCo.
3. Systematic experimental physical chemistry by Rajboj and Chondhekar-Anjali pub.
4. Advanced Practical physical chemistry by JB Yadhav – Goelpub.
5. Experimental physical chemistry by Das and Behra, Tata McGraw Hill.
6. Practical physical chemistry by Athawale and Mathur
7. Experimental physical chemistry by Daniel, Mathews and Williams.
8. A textbook of qualitative and quantitative inorganic analysis by A I Vogl.
9. Selected Experiments in physical Chemistry, N. G. Mukherrjee, J. N. Ghosh andSons.
10. Experiments in Physical Chemistry, J. C. Ghosh, Bharati Bhavan.
11. Practical Physical Chemistry, B. Vishwanathan and P. S. Raghvan, Viva Books, 2005.

12. A Laboratory manual of experiments in physical chemistry, C. D. Brennan & C.F. H. Tipper, McGraw Hill, 1967.

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***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course Preamble: **Surface chemistry** is a branch of physical chemistry that focuses on the behavior of substances at interfaces, particularly between solids, liquids, and gases. It is a vital field with applications ranging from materials science and catalysis to environmental chemistry and biology. This course designed to learn the followings

- **Interfaces are ubiquitous:** Interfaces are present in numerous natural and technological processes, from the adsorption of gases on solid surfaces to the formation of emulsions and foams.
- **Technological importance:** Understanding surface chemistry is crucial for developing new materials with tailored properties, improving catalytic processes, and addressing environmental challenges.
- **Fundamental knowledge:** Surface chemistry provides insights into the interactions between molecules at surfaces, which can be applied to a wide range of fields.

In this course, the students will explore the followings

- **Adsorption and desorption:** The processes of molecules adhering to and detaching from surfaces.
- **Surface thermodynamics:** The energetic aspects of surface phenomena, including surface tension and interfacial energy.
- **Surface kinetics:** The rates of surface reactions, including heterogeneous catalysis.
- **Colloids and dispersions:** Systems containing particles dispersed in a continuous medium, such as emulsions and foams.
- **Characterization techniques:** The methods used to study surfaces and interfaces, including surface spectroscopy and microscopy.
- **Applications of surface chemistry:** The use of surface chemistry in various fields, such as materials science, catalysis, and environmental chemistry.

Course Outcomes (COs)

CO1: Students can be able to understand the surface phenomenon's like adsorption, mechanism of adsorption, factors affecting adsorption. The utilization of adsorption mechanism for removal of industrial effluents and purification of materials studied in detail.

CO2: Explain the link between liquid surface tension and contact angle, and demonstrate how certain experimental techniques can be used for the assessment of liquid surface tension

CO3: Apply knowledge on thermodynamics of micellization in surfactant solutions describe the influence of physical variables such as temperature, molecular structure of surfactant, and solvent characteristics on parameters such as critical micellization concentration (CMC), association number, micelle structure etc.

CO4: Describe and explain different types of colloidal systems and interactions between colloidal particles

CO5: Instrumentation of BET surface area and adsorption isotherms to determine surface area of catalysts which is one of the important criteria to select catalyst in industries

Unit-I : Adsorption and surface phenomenon: Hrs:(15) Weightage: 20 Marks

Introduction, types of adsorption and isotherms, Langmuir and B.E.T. adsorption isotherms, BET instrumentation, measurement of surface area of solids, Catalysis: types, heterogenesis catalysis, turnover number, activity and selectivity. Surface activity, surfactants and their classification, surface excess concentration, surface pressure, concept of positive and negative adsorption, Derivation of Gibb's adsorption equation, significance and experimental verification, micelle and reverse micelle, Kraft Temperature methods for the determination of critical micelle concentration, energetics of micellization and applications.

Unit II : Liquid-Gas interfaces Hrs:(15) Weightage: 20 Marks

Types of interfaces, Surface and interfacial tension, Young and Laplace equation for vapor pressure at curved , plane and spherical interfaces , Kelvin equation for Vapor Pressure inside and outside the liquid droplet, methods of determination of surface tension.

Unit III: Liquid-Liquid interfaces: Hrs:(15) Weightage: 20 Marks

Surface spreading, spreading coefficient, cohesion and adhesion energy, surface energy and spreading coefficient, Langmuir–Adam surface pressure balance, formation of insoluble monomolecular films, Langmuir-Blodget films, physical states of film, π-A isotherm and its comparison with P-V isotherm, derivation πA = kT equation, gaseous, liquid expanded and condensed films. Emulsion, identification of emulsion, types of emulsion, emulsion stability, emulsifier, theories of emulsification, preparation of nanoparticles by using reprecipitation and emulsion method.

Unit IV : Solid –Liquid and Solid-Solid interfaces Hrs:(15) Weightage: 20 Marks

Contact angle and wetting of solids, methods of determination of contact angle, contact angle hysteresis, detergency, surface energy of solids, adhesion and adsorption, sintering and sintering mechanism, Tammann temperature and its

importance, surface structure and surface composition solid lubricants

REFERENCE BOOKS :

1. Physical chemistry of surfaces: A.W. Adamson.
2. Theory of adsorption and catalysis by Alrfed Clark,
3. Chemisorption by B.M.W. Trapnell and H.O. Hayward.
4. Introduction to colloids and surface Chemstry by D.J.Shaw.
5. Solid state chemistry Chakraborty
6. Surface chemistry by J.J. Bikermann
7. Colloidal and Surface chemistry by Satake, Hayashi and Sethi, Discovery Pub.House
8. Surface chemistry by K. R. Desai, Oxford BookCo.

9) Physical chemistry Gurdeep Raj

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***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks** **CA: 40 Marks**

Course preamble: Chemistry of Materials is a multidisciplinary field that explores the relationship between the chemical composition and structure of materials with their physical and mechanical properties. It bridges the gap between chemistry and materials science, providing a fundamental understanding of how materials are designed, synthesized, and characterized for specific applications. In this course, the students will explore: Structure-property relationships: The correlation between the atomic and molecular structure of materials and their physical properties, such as strength, conductivity, and magnetism. Material synthesis: The methods used to prepare materials, including chemical reactions, physical processes, and self-assembly. Characterization techniques: The tools and methods used to analyze the composition, structure, and properties of materials, such as X-ray diffraction, spectroscopy, and microscopy. Material classes: The different types of materials, including metals, ceramics, polymers, and composites. Material applications: The use of materials in various industries, such as electronics, energy, and healthcare. The design and synthesis of materials with tailored properties for specific purposes, such as lightweight materials for aerospace, and high-temperature materials for energy applications.

Course Outcomes (COs)

CO1: Students can differentiate between the Glasses, Ceramics, Composite and Nanomaterials

CO2: Students will understand the synthesis characterization and application of igh Tc materials

CO3: Students will adopt the different methodology of synthesis of polymers, morphology of of polymers and based on the morphologies their applications

CO4: Different mythologies of film formation and their applications

CO5: Learn to fabrications of solid state electronic devices.

Unit I : Glasses, Ceramics, Composite and Nanomaterials:

Hrs: (15) Weightage: 20 Marks

Glassy state, glass formers and glass modifiers, applications, Ceramic structures, mechanical properties, clay products. Reformatories, characterizations, properties and applications. Microscopic composites; dispersion- strengthened and particle– reinforced, fibre – reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, and applications.

Unit II : High Tc Materials: Hrs: (15) Weightage: 20 Marks

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3

and 2-1-4 materials, and normal state properties: anisotropy; temperature dependence of electrical resistance; optical photon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption – pairing and multigap structure in high Tc materials, applications of high Tc materials.

Unit III: Polymeric Materials: Hrs: (15) Weightage: 20 Marks

Molecular shape, structure and configuration, crystallinity, stress- strain behavior, thermal behavior, polymer types and their applications, conducting and ferro- electric polymers.

Unit IV : (A)Thin films and Langmuir- Blodgett Films:

Hrs: (08) Weightage: 11 Marks

Preparation techniques: evaporation/ sputtering, chemical processes, MOCVD, sol – gel etc. Langmuir- Blodgett (LB) film, growth techniques, photolithography, properties and application of thin and LB films.

(B) Materials of Solid State Devices: Hrs: (07) Weightage: 09 Marks

Rectifiers, transistors, capacitors IV-V compounds, low dimensional quantum structure; optical properties.

REFERENCE BOOKS :

1. Solid State physics, N.W. Ashcrott and N.D. Mermin, Saunders College

2.Material Science and Engineering, An introduction, W.D. Callister, Willey.

3.Principals of Solid State, H.V.Keer, Willey Eastorn.

4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS

5. Thermotropic Liquid Crystals, Ed, G.W. Gray, John Willey.
6. Text book of liquid crystals, Kelkar and Halz, Chemie Verlag

पुण्यश्लोक अहिल्यादेवी होळकर सोलापूर विद्यापीठ ।। विद्यया संपन्नता ।। NAAC Accredited-2022 'B++' Grade (CGPA-2.96)	**Punyashlok Ahilyadevi Holkar Solapur University, Solapur** **MSc (Physical Chemistry) Semester-IV** **Vertical : DSE** **Course Code: 2302407** **Course Name: Nuclear and Radiation Chemistry**
***Teaching Scheme** **Lectures:04 Hours/week, 04 Credits**	***Examination Scheme** **UA:60 Marks**

	CA: 40 Marks

Course preamble: Nuclear and Radiation Chemistry is a specialized field that deals with the properties and behaviour of atomic nuclei, as well as the effects of radiation on matter. This course delves into the fundamental principles of nuclear chemistry, including nuclear reactions, radioactive decay, and the applications of nuclear energy and radiation. In this course, students will explore: Nuclear reactions: The processes that involve the transformation of atomic nuclei, including nuclear fission and fusion. Radioactive decay: The spontaneous transformation of unstable nuclei into more stable nuclei, accompanied by the emission of radiation. Nuclear energy: The production and use of energy from nuclear reactions, including nuclear power plants. Radiation effects: The interaction of radiation with matter, including ionization, excitation, and biological effects. Radioactive materials: The properties, handling, and storage of radioactive substances. Nuclear applications: The use of nuclear technology in various fields, such as medicine, agriculture, and industry. Nuclear safety and security: The measures taken to prevent accidents and ensure the safe use of nuclear materials. The students will explore the accelerator technology.

Course Outcomes (COs)

CO1: To familiar with Radiation hazards and safety

CO2: Students can differentiate between various types of nuclear reactions

CO3: To know about the accelerators technology, types of accelerators

CO4: To understand the principle of radioisotope and their applications in various fields

CO5: To study radiolysis, kinetics of radiolysis

Unit I: **Hrs: [15] Weightage: 20 Marks**

Nuclear reactions: Bethe's notation, types of nuclear reactions, conservation in nuclear reactions, compound nucleus theory, experimental evidence, specific nuclear reactions, photonuclear and thermonuclear reactions.

Accelerators: Basic components, Cockroft-Walton accelerator Van de Graaff accelerator, Linear accelerators, cyclotrons, synchrotrons.

Unit II: **Hrs: [15] Weightage: 20 Marks** Radiation hazards and safety ; Natural and manmade sources of radiations, internal and external radiation hazards, safe handling methods, personal dosimetry, reactor safety, the effects of Three miles and Chernobyl accidents, radiation protecting materials.

Biological effects of radiations : The interaction of radiations with biological cells, various stages, somatic and genetic effects, maximum permissible dose ICRP recommendations

Unit III. **Hrs: [15] Weightage: 20 Marks**

Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization

The origin of chemical elements, cosmology, premordial nucleosynthesis, stellar evolution and stellar nucleosynthesis, solar nutrino problem, Synthesis of Be, B, Li in cosmos Management of radioactive waste: liquids, solids and gases

Unit IV. **Hrs: [15] Weightage: 20 Marks**

Radiolysis of organic systems : Alkanes, aromatic hydrocarbons, alcohols

Radiolysis kinetics : Empirical rate studies, molecular kinetics, non-homogeneous kinetics, effect of solute concentrations on the molecular yields from water, radical scavenging, chain reactions, pulse radiolysis

References

1. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).

2. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).

3. Essentials of Nuclear Chemistry: H. J. Arnikar. New Age Publication Ltd. (1995).

4. Radiation chemistry and Nuclear Methods of Analysis W. D. Ehmann, D. E. Vance. John Wiley (1991).

5. Nuclear and Radiochemistry G. Friedelander, J. W. Kennedy, E.. S. Macias, J. M. Miller John Wiley (1981).

6. Source Book of Atomic Energy, S. Glasstone, D. Van Nostrand (1967)

Nature of question paper (M. Sc. II):

Time: 2 ½ hours Maximum Marks: 60

Instructions

1. All questions are compulsory
2. All questions carry equal marks.
3. Figures to the right indicate full marks.
4. Use of log tables and calculators is allowed.

Q 1. A) Choose correct alternative **Marks 8 (1 x 8)**
Sub-questions (i) to (viii)

B) Fill in the blanks **Marks 4 (1 x 4)**
Sub questions (i) to (iv)

Q 2. Answer the following (any six) **Marks 12 (2 x 6)**
Sub-questions (a) to (h)

Q 3. Answer the following (any three) **Marks 12 (3 x 4)**
Sub-questions (a) to (d)

Q 4. Answer the following (any two) **Marks 12 (6 x 2)**
Sub-questions (a) to (c)

Q 5. Answer the following (any two) **Marks 12 (6 x 2)**

Sub-questions (a) to (c)

At least 25 % questions should be problem oriented, where-ever possible, in view to train students for the SET/NET/GATE and other competitive examinations. These questions should test the understanding of candidate rather than the memory. The question paper should cover all the Units included in the syllabus of the respective paper and the weightage of the questions should correspond to the number of lectures allotted to the respective Units / Topics.