Shivaji University, Kolhapur

Name of Department: Chemistry

Name of Programme: M.Sc Physical Chemistry

Vision: Engender Human Resource to Lead the Competitive Science World for Nation Building
Mission : Impart most advanced scientific knowledge and training to the students so that genuine researchers and skilled scientists of world standard will be made available for the advancement of national science and technology programs as well as to cater the needs of industrial and pharma sectors
Program Outcomes PO1: Understanding fundamental principles and laws of physical chemistry PO2: Development of abilities to study and understand properties of materials PO3: Design and testing of electrochemical cells and electrochemical properties of materials PO4: Understanding forces responsible for various types of structure property correlations PO5: Studies of physicochemical properties of novel materials including nanomaterials PO6: Studies of protein-ligand binding interactions PO7: Solid material design, property measurements, structural analysis and application testing PO8: Empowering the students to do independent research of high cali

Program Specific Outcomes
PSO1: Electronic structure calculation and property analysis or prediction

PSO2: Understanding kinetics and dynamics of materials in gas and condensed phases PSO3: Structure elucidation and estimation of molecular properties PSO4: Independently perform a computer simulation to predict structures, reaction paths, molecular/material properties, etc.		
Course Outcomes		
Part-I Semester-I		
CH-1.1	**(Inorganic Chemistry – I)**	1. CO1: Students will be able to explain the basic chemistry of transition metals and its compounds, spectroscopic characteristics of such compounds, nomenclature, reactions and applications. CO2: Students will obtain knowledge about Preparation, structure, physical and chemical properties of metal carbonyls of transition metals. CO3: Students will be able to understand the all aspects of synthesis, bonding, structure and reactivity of organometallic compounds and their applications in homogenous catalysis. CO4: Student will be able determine the stability of the complexes and will be able to explain the nuclear stability and reactions.
CH-1.2	**(Organic Chemistry – I)**	CO1: Students will able to differentiate between various organic reactive intermediates. CO2: Students can recognize, classify, explain, and apply fundamental organic reactions. CO3: Students will have ability to distinguish between

		different kinds of isomers. CO4: Course will develop interest in writing and finding mechanisms of new reactions. . .
CH-1.3	**(Physical Chemistry – I)**	CO1: Students will be able to understand basic principles of thermodynamics and statistical mechanics CO2: Able to learn advanced topics like quantum statistics and molecular dynamic simulation methods. CO3: Develop abilities to understand how to estimate and analyze the physicochemical properties of condensed and gas phase materials. CO4: Able to utilize spectral data to estimate molecular thermodynamic properties through partition function calculations. CO5: Understand properties of detergents and colloidal materials CO6: Learns the principles and techniques to understand gas and liquid adsorptions on solid surfaces CO7: Can learn spectral techniques to study surface adsorption phenomena. CO8: Learn principles and techniques for estimation of average molecular weight of a polymer or biological macromolecules CO9: Develop abilities to characterize polymers through understanding theories of virial coefficients, concepts of glass transition temperatures, etc.

CH.1.4:	**Analytical Chemistry-I**	CO1: Students would acquire the knowledge about the fundamentals of Analytical Chemistry including the sampling, sample pretreatment, basic techniques, methods and data handling, processing and statistical analysis of the same. CO2: Students would acquire the knowledge and understand the scope of Analytical Chemistry spanning various fields. The students will learn fundamentals of qualitative analysis using conventional techniques CO3: Students will learn the chromatographic techniques, choice of chromatographic techniques and tuning of the chromatographic technique as per the need based on the samples to deal with, learn electroanalytical techniques and computation chemistry which would groom them for alternative analytical strategies which form one of the important components of analytical chemistry. CO4: Students will learn about referring to the standard reference books and infer information from the same. Analytical case study problems would be discussed to familiarize with the scope and advantages of Analytical Chemistry.
PCH-1.1	**(Practical – I)**	CO1: Ability in professional sampling and sample treatment before actual analysis CO2: Ability to treat and evaluate the results of analysis CO3: Understanding and capability of performing basic chemical processes in a chemical laboratory CO4: Capability of performing measurements on basic

		analytical instruments (photometers, spectrometers, chromatographs, ion-selective electrodes)
PCH-1.2	**(Practical – II)**	CO1: Students can be able to prepare various concentration solutions like molar, normal, ppm, etc. CO2: Determine the rate constants of various first order and second order reactions CO3: Determine the redox potential of a system, relative strength of acid etc using potentiometer, conductometer CO4: Know the formation of alloys like Brass, Bronze, phase diagram for binary and ternary systems studied in details like a composition, critical temperature, etc CO5: Validity of Freundlich adsorption isotherms to remove toxic material such as dye, acetic acid, and other industrial effluents
Part-I Semester-II		
CH-2.1	**(Inorganic Chemistry – II)**	CO1: Students will get the knowledge of the basic chemistry of non-transition elements and their compounds, synthesis and structural features, and applications. CO2: To be able to explain the structures of inorganic compounds based on different theories. Student will understand the chemistry of various types of solvents. CO3: Be well versed with the knowledge about the chemistry of Lanthanides and Actinides with respect to occurrence, separation, compounds and applications. CO4**:** To understand the three dimensional structures

		of solid-state materials of industrial importance and to get the knowledge of bio-inorganic Chemistry.
CH-2.2	**(Organic Chemistry – II)**	**Course Outcomes (COs)** CO1: Illustration of modern synthetic methods and applications of reagents. CO2: Provide knowledge of different organometallic compounds and various coupling reactions. CO3: Understand principle and applications of protection and deprotection of various functional groups. CO4: It will elaborate to understand the concept of chemoselectivity, regioselectivity and enantioselectivity.
CH2.3	**(Physical Chemistry – II)**	CO1: Students will learn basics of quantum mechanics. CO2: Knowledge of the course will form the basis or essential requirement for the course "Advanced Quantum Chemistry" CO3: Able to understand selection rules and to predict the electronic spectra of conjugated organic molecules. CO4: Able to study photochemical and photophysical phenomena CO5: Capable of qualitative and quantitative analysis of various ingredients from industrial, food and pharma samples using techniques of emission spectroscopy. CO6: Capable of understand the electrochemical aspects of materials, ionic processes and

		electrochemical sensors, battery materials and characterizations etc. CO7: Able to study electrokinetic effects and their applications in the field of protein separation, characterization etc. CO8: Understanding the molecular dynamics through kinetic studies. Applications to explore reaction pathways, protein-ligand binding rates, etc. will help to understand life governing processes.
CH.2.4:	**Analytical Chemistry-II**	CO1: Students will acquire the knowledge of spectroscopic tools/instruments used in chemical analysis and interpretation of the data. The scope and limitations of the spectroscopic tools would be discussed so that the students learn about the type of samples which could be analyzed by these tools offering choices among the spectroscopic tools. CO2: Students will learn about the simple and advanced instruments used for analysis like NMR, MS, AAS, ICP and thermal analysis (TGA, DTA, DSC etc.) techniques spanning wide variety of samples to be considered for analysis. CO3: Students will learn about the instrumentation, sample preparation and handling of sample, analysis and data interpretation and structural elucidation. CO4: Learning about different instruments will give them idea about appropriate choice of the instrument for analysis based on the source and type of analyte(s) in the sample under consideration.
PCH-2.1	**(Practical – III)**	CO1: Students developed for precise sample solution preparation and sample treatment before actual

		analysis. CO2: Students can be able to perform the calculations and error analysis CO3: Develop understanding of basic chemical processes and deciding methods of analysis. CO4: Capability of performing measurements on basic analytical instruments (photometers, spectrometers, chromatographs, high end thermometers, refractometer, pH meter etc.)
PCH-2.2	**(Practical – IV)**	CO1: Students can be able to prepare various concentration solutions like molar, normal, ppm, etc. CO2: Determine the unknown concentration and thermodynamic parameters using conductometer CO3: Student will explore how to estimate order of reaction and the catalysis CO4: students can estimate refractive index and molecular weights of species. CO5: Students can understand the estimation of equilibrium properties like redox potential, phase diagram etc
Part-II Semester-III		
PCH-3.1	**(Advanced Quantum Chemistry)**	CO1: Learn concepts of atomic orbitals and their shapes, spectroscopic selection rules, ionization potentials, etc. CO2: Learn advanced quantum methods such HF-SCF theory and post-HF methods and learners will be able to do accurate electronic energy and molecular structure calculations

		CO3: Knowledge of the course will be used to do computer simulations to calculate molecular properties, nmr shift, IR and Raman spectra etc. for small to medium sized molecules or molecular assemblies. 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 will learn most advanced method of quantum mechanics i.e Density Function Theory for electron structure calculations CO6: Learners will be capable of calculate the transition states, potential energy surfaces and reactions paths for chemical reactions using DFT method CO7: 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. CO8: 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. CO9: 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.

PCH-3.2	**(Electrochemistry)**	CO1: Students will be able to 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: Charge of the material can be quantified and used for testing of electrokinetic phenomenon. CO4: Study of electrode electrolyte interfaces based on the properties of material shows the energetically viability of electron transfer CO5: Learn the principles and techniques to understand adsorptions and desorption from the electrode interface in the electrolyte solution CO6: Fundamental equation of electrodics to study the reversible charge transfer behavior in the materials electrolyte interfaces. CO7: Learn principles and techniques for estimation of charge transfer behaviors in semiconductor materials CO8: Develop abilities to characterize materials through understanding theories electrode reaction.
PCH- 3.3:	**Molecular Structure - I**	CO1: Students will learn basics principles and laws ofspectroscopy. 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.

PCH-3. 4)	**(A) (Solid State Chemistry**	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
PCH-3.4)	**(B) (Advanced Chemical Kinetics**	CO1: Students can understand the basic principles of kinetics, proton transfer and effect of proton ion on the rates of reaction CO2: Various electron transfer process like inner sphere and outer sphere reactions CO3: Different models to study catalysis and reaction mechanisms CO4: Different methods of catalysis like micellization and pseudo ion exchange CO5: students can learn the advanced theories of chromium ion reduction
PCH-3.4	**(C) Radiation and Photochemistry**	CO1: student will learn basic principles and advanced radicochemical 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 obtaioned data from the electrochemical transient and flash photloysis. CO5: Applications of photochemistry for degradation of polymers and other smog, singlet molecular oxygen generation etc.
PCHP – V	**Practical -V**	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 uncertainty estimations for experimentally measured and derived properties of solutions CO5: Training on buffer preparations, equilibrium studies and spectral analysis.

PCHP – VI	**Practical-VI**	CO1: Training on scientific literature search, defining the objective of the work, research skills, data representation in tabular and graphical form etc. CO2: 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. CO3: Experimental spectral measurements and analysis for understanding binding equilibria CO4: Training on evaluation of bulk thermodynamic properties of condensed states CO5: Computer lab training to perform *ab initio* and DFT electronic structure calculation through computer simulations
Part-II semester-IV		
PCH4.1	**(Thermodynamics and Molecular Modelling)**	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. CO5: Learn techniques of MD simulations to evaluate the molecular properties and structural features for understanding the functions of biopolymers and it's applications in drug design, material design, protein chemistry, polymer industry, etc. CO6: Training to do the simulations independently through this advanced course will make learners a trained potential candidate for placement in world class research laboratories, institutes, R and D sectors of pharma industries, etc. CO7: Students will learn applicability of principles of thermodynamics where irreversible effects or near equilibrium phenomena exists. CO8: Students will gain knowledge about science behind the industrially important phenomena like production of electricity from thermal sources, Peltier effects,

		electrophoresis, osmosis, thermos-diffusion, thermos-conductivity etc. CO9: Knowledge gained on entropy production and entropy flow in chemical and biological systems will help learners to understand coupling reactions mostly existing in living organisms.
PCH-4.2	**(Chemical Kinetics)**	CO1: Students can understand the basic principles of Kinetics CO2: Students can learn different theories of rates of reaction CO3: Learn from fundamental to advanced theories and applications of chemical kinetics CO4: Different methods of study of dynamics of fast reaction mechanism CO5: Different mechanistic aspects of surface reaction and industrial applications CO6: Reaction mechanism and photocatalytic applications of materials CO7: Linear free energy equation and substitutions on aromatic group CO8: Students learn effect different equations expressions expressing reaction constant and substitution constant.
PCH-4.3	**(Molecular Structure – II)**	CO1: Students will learn basics principles and laws ofelectronic structure and spectroscopy. CO2: This course studies the electronic properties of materials CO3: The molecular property dipole movement correlation with electronic structure of a molecule CO4: Applications of Magnetic properties measurements to the coordination complexes the CO5: Brief study of magnetic properties of materials. CO6: Structural investigations of the material based on the NMR radiations and various theories of peak splitting CO7: Basic Principles of Mossbauer

		spectroscopy w.r.t fine and hyperfine electron energy splitting CO8: Instrumentation and applications of the Mossbauer spectroscopy.
PCH-4.4	**(A) (Surface Chemistry)**	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
PCH-4.4	**(B) (Chemistry of Materials)**	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.
PCH-4.4 (C)	**(Biophysical Chemistry)**	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 iopolymers. 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
PCHP – VII	**Practical-VII**	CO1: Training on electrochemical analysis of different physicochemical aspects of materials CO2: Training on different techniques needed to characterize the detergents CO3: Training on Modeling properties of materials CO4: Training on estimation of protonation states of acidic, neutral and basic natural amino acids CO5: Understanding principles of thermodynamics through enthalpy dilution experiments
PCHP – VIII	**Practical-VIII**	CO1: Application of theoretical and practical knowledge for research training through

		mandatory research/industrial projects CO2: Training to estimate properties of ionic and non-ionic detergents. CO3: Computer lab training to perform molecular dynamic simulations to estimate molecular properties of biomacromolecules in aqueous or mixed aqueous solutions. CO4: Making well trained experimentalist to handle any experimentally and theoretically challenging scientific problems for advancement science and technology.