Course Structure

for

2-Years M. Sc. in Chemistry

Effective from 2019-2020 Academic Session

Department of Chemistry

National Institute of Technology Sikkim

South Sikkim - 737 139

Sl. No.	Subject Code	Subject Name	L-T-P	Credit
	1st Semester			
		Theory Subjects		
1	CY21101	Organic Chemistry I	4-0-0	4
2	CY21102	Inorganic Chemistry I	4-0-0	4
3	CY21103	Physical Chemistry I	4-0-0	4
4	CY21104	Analytical and Environmental Chemistry	4-0-0	4
5	CY21105	Group Theory and Molecular Spectroscopy	4-0-0	4
		Practical and Sessionals		
6	CY21201	Inorganic Chemistry Laboratory	0-0-6	3
7	CY21202	Physical Chemistry Laboratory	0-0-6	3
		Total Credits	**20-0-12**	**26**
	2nd Semester			
		Theory Subjects		
1	CY22101	Organic Chemistry II	4-0-0	4
2	CY22102	Inorganic Chemistry II	4-0-0	4
3	CY22103	Physical Chemistry II	4-0-0	4
4	CY22104	Instrumental Techniques in Analytical Chemistry	4-0-0	4
5	CY22105	Biochemistry and Medicinal Chemistry	4-0-0	4
		Practical and Sessionals		
6	CY22201	Organic Chemistry Laboratory	0-0-6	3
7	CY22202	Analytical & Environmental Chemistry Laboratory	0-0-6	3
8	CY22203	Seminar	0-0-2	1
		Total Credits	**20-0-14**	**27**
	3rd Semester			
		Theory Subjects		
1	CY23101	Organic Chemistry III	4-0-0	4
2	CY23102	Inorganic Chemistry III	4-0-0	4
3	CY23103	Physical Chemistry III	4-0-0	4

4	CY23104	Spectroscopic Methods of Analysis	3-1-0	4
5	CY2*1XX	Elective I	3-0-0	3
		Practical and Sessionals		
6	CY23201	Computational Chemistry Laboratory	0-0-6	3
7	CY23202	Major Project Part I	0-0-6	3
8	CY23203	Practical Training Evaluation	0-0-4	2
		Total Credits	**18-4-13**	**27**
	4th Semester			
		Theory Subjects		
1	CY2*1YY	Elective II	3-0-0	3
2	CY2*1ZZ	Elective III	3-0-0	3
		Practical and Sessionals		
3	CY24201	Major Project Part II	0-3-18	7
4	CY24202	Industrial Visit	0-0-2	1
		Total Credits	**6-3-18**	**14**
			Grand Total Credits	**94**

L: Lecture hour per week; **T**: tutorial hour per week; **P**: Practical hour per week.

List of Elective Subjects			
CY2*1XX	Elective I	3-0-0	3
CY2*1YY	Elective II	3-0-0	3
CY2*1ZZ	Elective III	3-0-0	3

- For all Elective subjects, the course can be selected from the approved list of electives courses.
- For Elective II & III in 4th Semester, the students doing internships outside the Institute will be permitted to opt these courses on the online platform, if available. Otherwise, they may select the equivalent subject from the subjects available on the online platform with the permission of the department. The Project Supervisor has to assign these two courses and the same should bear the approval of the department committee constituted by the Head. The committee must consist of three faculty members. The examination and evaluation will be done by the Project Supervisor. It is desirable that the concern supervisor selects the courses available on the online platform as approved by the department.

- Project Part I must be carried out in the Institute and evaluation will be done by a committee constituted by the Head for this purpose consisting of not less than three internal faculty members, including the Head.
- Project Part II in 4th Semester can be carried out under joint supervision of Major Project Supervisor and other faulty/scientist in any reputed academic institution/R&D organization/industry as assigned/collaborated by the Major Project Supevisor. The evaluation of the same will be done by a committee constituted by the Head for this purpose consisting of not less than four faculty members, including the Head and preferably an external expert.
- Practical Training shall be carried out after the completion of the 2nd semester and during the summer vacation. The evaluation of the same will be done in the 3rd semester by a committee of not less than three faculty members, including the Head, constituted by the Head for this purpose. The internship includes laboratory trainings / research work carried out in reputed academic institutions/R&D organizations/industries for duration not less than 04 weeks. Any practical training/internship done before the 2nd semester shall not be counted against the above.
- Industrial Visits shall be arranged the department to reputed industries after the completion of the 3rd semester and during the winter vacation or 4th semester. The evaluation of the same will be done in the 4th semester by a committee of not less than three faculty members, including the Head, constituted by the Head for this purpose.

Grand Total Credits: 94						
Sl.	**Course**	**Credit**	**No. of subjects**	**Total credits**	**% of course**	**% of Theory & Practical**
01.	Core Theory	04	14	56	59%	69%
02.	Elective Theory	03	03	09	10%	
03.	Core Laboratory	03	05	15	16%	31%
04.	Major Project Part I	03	01	03	12%	
05.	Major Project Part II	07	01	07		
06.	Seminar	01	01	01		
07.	Practical Training	02	01	02	3%	
08.	Industrial Visit	01	01	01		

SEMESTER I

CY21101: ORGANIC CHEMISTRY I

L	T	P	C
4	0	0	4

Module 1: Mechanisms, Selective Organic Reactions & Rearrangements

Recapitulations of Basics: Reactivities of carbocations, carbanions, radicals, Nucleophilic substitutions, eliminations, nucleophilic additions, conjugate additions, common named reactions, common rearrangements, Green chemistry concepts, PTC, Solid phase synthesis.

Module 2: Stereochemistry

Symmetry and point groups, Topicity, Newman, Sawhorse, Fisher projections, D,L- and R,S, Re-Si nomenclatures, Acyclic systems up to 4 chiral centres:, conformational analysis of cyclopropanes, cyclobutane, cyclopentane, cyclohexene, etc. (C3 to C10 systems), variously substituted cyclohxanes, decalins, perhydro anthracene and perhydro phenanthrene, atropisomerism, Allenes, Biphenyl system, fluxional compounds, Additions to carbonyls: Cram's rules, Felkin-Anh model, Prelog's rule, Allylic strain, helicity, CD, ORD, principles and application, stereochemical aspects of important reactions.

Module 3 Pericyclic Reactions

Classification and stereochemical modes, Thermal and Photo reactions, Selection rules, electrocyclic, cycloaddition, sigmatropic rearrangements, chelotropic, Ene reaction, carbine addition, rationalization by FMO, Zimmerman, Mobius-Huckel methods, metal catalyzed cycloaddions, radical cation reactions.

Module 4 Photochemistry & Radicals

Basic principles, Jablownski diagram, photochemistry of olefinic and carbonyl compounds, cis- / trans- photoisomerism, stereomutation, Norrish Type I and II reactions, Di-Pi-Methane (DPM), rearrangement, Aza-DPM, Paterno-Buchi reaction, photochemistry of arenes, photoreductions of ketones, method of generation and dection (ESR) of radicals, radical cyclisations, Baldwin's rules, substitution, addition and insertion reactions involving radicals, allylic halogenation, autooxidation, Barton reaction.

CY21102: INORGANIC CHEMISTRY I

L	T	P	C
4	0	0	4

Module 1: Molecular Structure & Bonding

LCAO-MO methods in homo and heteronuclear diatomic molecules, bonding in triatomic molecules, VSEPR theory, hybridization, Walsh diagram, Bent's rule, structure and reactivity of covalently bonded molecules Atomic and ionic radii–bond length, bond strength. Hydrogen bonding interactions, effect of hydrogen bonding and other chemical forces on melting, boiling and solubility.

Module 2: Non-transition Metal Chemistry

Synthesis, Properties, Structure and Bonding of: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions. Redox Reactions: Latimer diagram, Electrochemical Series. Acids and Bases: Lewis acids and bases; HSAB concept.

Module 3: Transition Metal Chemistry I

Bonding in Coordination Complexes: Crystal-Field theory, d-orbital Splitting in Octahedral, Tetrahedral, Square Planar geometries; Molecular Orbital Theory, □-bonding; Jahn-Teller effect, Spectrochemical series, nephelauxetic series. Electronic Spectra: Selection Rules, d-d transitions, charge-transfer spectra.

Module 4: Symmetry & Group Theory

Group Theory: Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator. Application of symmetry, the symmetries of molecular orbitals (symmetry-adapted linear combinations, construction of MOs, the vibrational analogy).

CY21103: PHYSICAL CHEMISTRY I

L	T	P	C
4	0	0	4

Module 1: Chemical Thermodynamics

Brief review of 1^{st}, 2^{nd} and 3^{rd} laws of thermodynamics, Nernst heat theorem and the third law of thermodynamics, calculation of entropy changes in chemical reactions. Mathematical and thermodynamic probability, Entropy and probability, the free energy of a mixture, Partial molal quantities, Analytical form of the chemical potential in ideal solutions, Chemical potential of a solute in a binary solution, Application of Gibbs-Duhem equation, Nonideal solutions, concept of activity: experimental determination of activity coefficients of non-electrolytes.

Module 2: Chemical Kinetics I

Basics of chemical kinetics, Rate law equations, Arrhenius equation, Composite Reactions – types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state concepts, rate determining steps, microscopic reversibility and detailed balance, Hammet Equation, Hammond postulate, Curtin-Hammett principle, Enzyme kinetics and Michalis-Menten equation, Kinetics of photochemical and photophysical processes, chain reactions (H_2-Br_2 reaction, decomposition of ethane and acetaldehyde) and oscillatory reactions (Belousov-Zhabotinskii reaction).

Module 3: Quantum Chemistry I

Basic postulates and theorems, Physical interpretation of wave function, stationary states, operator formation, atomic unit system, Heisenberg's equation of motion, Schrödinger equation, Solution of Schrödinger equation using Particle in a box problem, Finite barrier problem and tunneling, Linear harmonic oscillator, Introduction to Angular momentum problem and Ladder operators, Rigid rotor, Hydrogen atom problem and its implications.

Module 4: Macromolecules

Polymers-definition, types of polymers, Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, viscosity, light scattering methods, Gel Permeation chromatography). Plastics, elastomers and fibers, kinetics of polymerization, Synthesis and properties of different types of Gel and their applications.

CY21104: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

L	T	P	C
4	0	0	4

Module 1: Measurement Basics and Statistical Concept

Signal and noise, Sensitivity and detection, Accuracy and instrument calibration, Error analysis, Regression plots, Criteria for rejection of data, Q-test, T- test, F-test, ANOVA, Control chart, Use of spreadsheet.

Module 2: Separation Methods

Solvent Extraction: Partition law and its limitations, Distribution ratio, Percent extraction and separation factor, Factors influencing extraction, Multiple extractions.

Chromatography: Introduction, Classification, Theories of column chromatography, Retention Time, Retention value, Capacity factor, Separation factor, Concept of plate and rate theory, Resolution column performance, Planer chromatography-paper and thin layer chromatography, Ion exchangers.

Module 3: Electroanalytical, Thermal and Nuclear Methods

Electroanalytical Methods: Polarography- principle, instrumentation, limitations & applications to qualitative & quantitative analysis, Amperometric & biamperometric titrations.

Thermal Methods of Analysis: Principle, Instrumentation and applications of thermogravimetry, different thermal analysis, thermometric titrations.

Nuclear Methods: Fundamentals of radioactivity and decay, Preparation of radioisotopes for tracers, Applications with radiotracers, Radiometric titrations, Radioactivity measurements by gas filled scintillating detectors.

Module 4: Use of Analytical Chemistry in Environment

Analysis of Air and Water Pollution: Objectives of chemical analysis of air and water, Analysis of Water: colour, turbidity, total solid, conductivity, acidity, alkalinity, hardness, chloride, sulfate, fluoride, phosphates, and different forms of nitrogen, Heavy metal analysis with respect to health significance. Measurement of DO, BOD & COD. Pesticides as water pollutants analysis

Monitoring and analysis of air: Monitoring technique through high volume sample, SPM and RPM sampler, Measurement and analysis of SPM,RPM,SOX,NOX, Air and water pollution laws and standards.

CY22105: GROUP THEORY AND MOLECULAR SPECTROSCOPY

L	T	P	C
4	0	0	4

Module 1: Microwave Spectroscopy

The Electromagnetic radiation, Absorption and emission spectra, Effect of radiation on atoms and molecules, Subdivisions of spectroscopy. Rigid rotor model and rotational spectra, diatomic and polyatomic molecules, chemical analysis by microwave spectroscopy. Non-rigid rotator model. Instrumentation techniques for Microwave spectroscopy.

Module 2: Infrared and Raman Spectroscopy

Basics of molecular vibration and Harmonic oscillator, Anharmonicity, Ro-vibrational spectra. Polarization of light and and scattering. The Raman Effect, pure rotational Raman, vibrational Raman spectra, ro-virbational Raman spectra structure determination from combined Raman and IR spectroscopy. Rotational fine structure of electronic-vibration transitions. Instrumentation of Infra red and Raman spectroscopy.

Module 3: Electronic Spectroscopy of Atoms and Molecules

Atomic structure and spectroscopy: term symbols; many-electron systems and antisymmetry principle. electronic spectra of diatomic molecules, vibrational coarse structure, progressions, intensity of vibrational-electronic spectra: the Franck-Condon Principle, oscillator strengths, spectroscopic and equilibrium dissociation energies, Molecular term symbol, $n \rightarrow \pi$, $\pi \rightarrow \pi$ transition. Kasha's rule, photophysics of radiative and non-radiative transitions, energy transfer processes, Excimers and exciplexes, Fluorescence and phosphorescence, Quantum yield, life time and anisotropy, static and dynamic quenching, Stern-Volmer analysis.

Module 4: Photoluminescence Spectroscopy

Steady state Fluorescence: Principles**,** Jablonski diagram, application of fluorescene spectroscopy, Basic instrumentation, Effect of solvents on fluorescence spectra (general and specific), Chemical and biochemical applications of anisotropy measurements. Flash photolysis, laser flash photolysis.

Module 5: Group Theory

Reducible and irreducible representations, classes and characters, Great Orthogonality and related theorems, Projection operator, Direct product representation Applications: SALC, Spectroscopic selection rules, Polyatomic vibration and normal modes.

CY21201: INORGANIC CHEMISTRY LABORATORY

L	T	P	C
0	0	6	3

1. Qualitative analysis of radicals in a given mixture comprising of less common metals (Be, Mo, W, Ti, Zr, Th, V, U, Cr and all the radicals included in B.Sc. (Honours) Chemistry syllabus.
2. Simple experiments will be conducted to elucidate the working principles, instrumentation and handling of Gas Chromatograph, UV-Vis spectrometer, IR spectrometer, Oxygraph (Measurement of gaseous oxygen by Clark type electrode), conductivity meter, pH meter and Nephlometer

Preparation of Inorganic compounds/complexes and their physico-chemical characterization by different spectroscopic (IR, UV-Visible, NMR *etc.*) & magnetic susceptibility measurements. Depending on the availability of reagents/instruments compounds/complexes will be selected from the list given below:

(i) Transition metal acetylacetonates

(ii) *Cis*- and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride

(iii) *Tris*(ethylenediamine)cobalt(III) chloride

(iv) Nitropentaminocobalt(III) chloride

(v) *Cis*- and *trans*-bis(glycinato)copper(II)

(vi) Ru(II/III) complexes of bipy

(vii) Sodium tetrathionate

L	T	P	C
0	0	6	3

CY22202: PHYSICAL CHEMISTRY LABORATORY

1. Studies on the kinetics of iodination of acetone.
2. Determination of coordination number of Cu^{++} (partition method).
3. Ion exchange capacity of resin.
4. Verification of Beer's law and studies on the kinetics of alkaline hydrolysis of crystal violet.
5. Estimation of acid potentiometrically.
6. Estimation of acid pH metrically.
7. Determination of pK_1 and pK_2 of phosphoric acid potentiometrically.
8. Studies on the kinetics of reaction between $K_2S_2O_8$ and KI spectrophotometrically.
9. (A) Binary phase diagram (H_2O-Phenol)

(B) Ternary phase diagram of H_2O-C_6H_6-CH_2COOH.

10. Determination of CMC and micellization parameters of an ionic surfactant conductometrically.
11. Determination of the activation energy of the reaction between $KBrO_3$ and KBr.
12. Estimation of Cl^-, Br^- and I^- in a mixture potentiometrically.
13. Determination of composition of Fe^{2+}- salicylate complex by Job's method.
14. Synthesis of silver nano particle
15. Synthesis of polymer

SEMESTER II

CY21101: ORGANIC CHEMISTRY II

L	T	P	C
4	0	0	4

Module 1: Oxidations and Reductions

Oxidations: Cr(VI), Mn, Se-, Pb-, transition metal, DMSO-based, Hypervalent iodine based, functionalization of C=C (hydroboration-oxidations, epoxidatiions, aziridinations, etc.) and C≡C, oxidation of allylic-CH, CH-activation, enzymatic oxidations (Baker;s yeast)

Reductions: Metal (Pd, Fe, etc.) catalyzed Heterogeneous hydrogenations, homogeneous reductions, reductions by hydride transfer ($LiAlH_4$, $NaBH_4$, DIBAL, $LiBH_4$, $NaCNBH_4$, Bu_3SnH, etc.), alkali metals in liquid ammonia, W-K, diimide, electroreductions of carbonyl, alkyl halides and nitro, enzymatic reductions

Module 2: Reagents and Protective groups

Chemistry, reagents and applications of organolithium, organoborane, organophospohouros, organo sulphur, and organosilicon compounds, emphasis on ylides chemistry.

Selective protection/deprotection of common functional groups like hydroxyl, carboxyl, carbonyl, amino groups. Umpolung.

Amino acids and Peptides: structures, N- and C-terminal sequencing, peptide syntheses (DCC, etc couplers).

Module 3: Synthetic Applications of Organometallic Reagents

Reagents and Applications of Organotransition element reagents (viz. Pd-coupling reactions, Pauson-Khand, Rh-cyclopropanation, olefin metathesis, Tebbe's, Ziegler-Natta, McMurry, Wilkinson, Schrock, other reductions, etc.), Organo-Sn, Organo-Ti, Grignard, Organo-Pb, etc., Carbenes.

Module 4: Heterocycles

Aromaticity of heterocyclic compounds, Synthesis of Heterocyclic ring containing oxygen, nitrogen, Sulphur and reactions. Furan, Pyrrole, Thiophene, 1,2-, 1,3-, 1,4-azoles, pyridine, quinolone, isoquinoline, Indoles, pyrimidines, pyrazidines, pyrazines, purines, pteridines, biosynthesis of nucleotides, DNA, RNA, Role of heterocycles in biological systems.

Module 5: Natural Products - Terpenoids, Alkaloid, Flavonoids

Familiarity with methods of structure elucidation (chemical & spectroscopic), synthesis, biosynthesis, biogenesis of representative examples of acyclic, monocyclic and bicyclic mono- / di-terpenes, like carvone, camphor, citral, pinenes, abietane, aebietic acid, Gutta-Percha, vulcanized rubber, etc. of alkaloids – nicotine, atropine, conine, papaverine, cinchona group, isoquinoline alkaloids – morphine, ephedrine, thibein; Steroids: occurrence, nomenclature, basic skeleton, synthesis and stereochemistry, biosynthesis of flavonoids, lignans.

L	T	P	C
4	0	0	4

CY22102: INORGANIC CHEMISTRY II

Module 1: Organometallic Chemistry I

18-electron rule, metal carbonyls, nitrosyls, cabonyl hydrides, dioxygen and dinitrogen compounds. Metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes. Hydrides, Metallocenes, Metal arene complexes. Carbonylate anions, Oxidative addition and reductive elimination, insertion and elimination reactions. Fluxional molecules. Isolobal analogy and metal clusters.

Module 2: Reactivity of Transition Metal Complexes

Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution reactions, nucleophilicity parameters, *etc*.

Redox reactions-complementary and non-complementary reactions, mechanisms of outer sphere and inner sphere electron transfer reactions, theory of outer sphere processes, the Marcus cross relation.

Module 3: Magnetochemistry and Inner Transition Metal Chemistry

Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Curie equation, Russell-sander's terms, determination of magnetic susceptibility, magnetic properties of first transition series metal ions and lanthanides. CFT and its limitations, Orgel and Tanabe-Sugano diagrams and spectra, calculations of Dq, B and b-parameters, charge transfer spectra, anomalous magnetic moment, magnetic exchange coupling and spin crossover.

Inner Transition Elements: Comparison of characteristics of Inner Transition and Transition metals. Magnetic properties and absorption spectra of Lanthanides and Actinides. Lower oxidation state compounds. General chemistry of Actinides.

Module 4: Bioinorganic Chemistry I

Role of alkali and alkaline earth metal ions in biology; Na^+ -K^+-Pump, ionophores and crown ethers. Metal site structure, function. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein. Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins. Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin.

CY22103: PHYSICAL CHEMISTRY II

L	T	P	C
4	0	0	4

Module 1: Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translational, rotational vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions, Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions. Introduction to Fermi-Dirac and Bose-Einstein Statistics.

Module 2: Quantum Chemistry II

Approximation methods in quantum chemistry: The variational method, Linear variational method, Perturbation theory (time independent), Time dependent perturbation theory: Harmonic perturbation and Fermi golden rule, Einstein's coefficients of induced emission and absorption. Application of variational method and nondegenerate perturbation theory to the helium atom problem. Electron spin, Anti symmetry principle, Degenerate perturbation theory and its application to Zeeman and anomalous Zeeman effect, Stark effect. Hückel M.O. theory for conjugated systems, bond order and charge density calculations, Slater determinant.

Module 3: Chemical Kinetics II

Methods of determining rate laws, collision theory of reaction rates, Arrhenius equation and activated complex theory. Potential energy surfaces. Unimolecular reactions and their treatments (Lindemann-Hinshelwood, Rice-Ramsperger-Kassel [RRK], and Rice-Ramsperger-Kassel-Marcus [RRKM] theory). Experimental Methods: Enzyme kinetics, studies of fast reactions by flow method, relaxation method, flash photolysis and NMR.

Module 4: Surfaces and Interfaces

Physisorption and chemisorption. Langmuir, Freundlich and BET isotherms. Adsorption on surface: BET equation, Hysterisis, Harkinss & Jura equation. Surface catalysis: Langmuir-Hinshelwood mechanism. Self-assembly, heterogeneous catalysis.

L	T	P	C
4	0	0	4

CY22104: INSTRUMENTAL TECHNIQUES IN ANALYTICAL CHEMISTRY

Module 1: Chromatographic Techniques

Ion exchangers; Process leading to non-ideal chromatography, extended from Van Deemeter equation, Gas Chromatography- instrumentation , types of column, stationary and mobile phases, detectors, Kovat's index, High performance liquid chromatography(HPLC)- instrumentation, stationary and bonded-stationary phases, detectors, Ion chromatography, Size exclusion chromatography, Supercritical fluid chromatography, Affinity chromatography, Electrophoresis.

Module 2: Electroanalytical Methods

Instrumentation, Theory & applications, Polarography- normal DC, pulse & differential pulse polarography, AC polarography, Lineaar & cyclic voltammetry, Square wave voltammetry, Coulometry at controlled potential, Chronopotentiometry, Anodic stripping voltammetry, Sensors- different types of solid and liquid sensors, nano material and chemically modified sensors, Applications in environmental biological sample analysis.

Module 3: Nuclear and X-ray Methods

Radiotracers- Choice & synthesis of radiotracers, isotope dilution methods, neutron activation analysis, Material science studies using positron emitters & Mossbauer source, Principles of X-ray spectra, X-ray absorption, Emission fluorescence and diffraction methods and applications, Ion beam analysis, Proton induced X-ray emission, Rutherford backscattering spectrometry, Elastic recoil detection analysis for hydrogen measurement, Nuclear microprobe.

Module 4: Mass spectroscopy

Different types of ion sources, Mass analyzer and detectors, Resolution and resolving power, Interpretation of mass spectra , Hyphenated systems like LS-MS, GC-MS MS-MS, ICP-MS

CY21105: BIOCHEMISTRY AND MEDICINAL CHEMISTRY

L	T	P	C
4	0	0	4

Module 1: Amino acids, Proteins, Nucleic acids

Structure and functions of amino acids, Proteins, Nucleic acids. Base stacking, Stabilized forms of DNA-A, B and Z forms, Melting of DNA double helix, Replication, Transciption, Translations.

Module 2: Metabolisms and Electron Transport

Glycolysis, TCA cycle, Glyoxylate cycle, Gluconeogenesis, β-Oxidation of fatty acids, Omega oxidation, Ketone bodies, Biosynthesis and degradation of amino acids, Oxidative phosphorylation, Role of membrane-bound carriers in electron transfer, Synthesis of ATP, Regulation of oxidative phosphorylation, Uncouplers, Biological transport, structure and properties of biological membranes, passive transport and active transport, glucose, Na^+ and K^+ transport.

Module 3: Pharmacodynamics and Pharmacokinetics

Receptors as drug targets: Enzymes, ion-channels, G-proetin-coupled receptors, kinase linked receptors, nucleic acids, signal transduction, agonists, antagonists,

Pharmacokinetics: drug absorption, distribution, metabolism, excretion, administration, dosing.

Module 4: Drug Action

Mode of actions of various: Antibacterial agents, Antiviral agents, Anticancer agents, Opiod analgesics, Cholinergics, anticholinergics anticholinesterases, anti-ulcer agents. NSAIDS. Hypoglycaemic agents.

Module 5: Drug Discovery

Finding a lead, optimization, QSAR, molecular docking studies.

CY22201: ORGANIC CHEMISTRY LABORATORY

L	T	P	C
0	0	6	3

Preparations / Extraction / Chromatography

Estimation of amines / phenols using bromate – bromide solution / acetylation method. Determination of iodine and sponification values of an oil sample.

Single step reactions like nitration of aromatics; reduction of nitro to amine; protection of alcohol, amine; LAH, $NaBH_4$ reductions of ester / ketone / aldehydes; Diels-Alder reaction with Anthracene and Maleic anhydride; etc.

Multistep Synthesis: Cannizzaro reaction: 4-chlorobenzaldehyde as substrate. Benzilic Acid Rearrangement:

Benzaldehyde $\rightarrow$ Benzoin $\rightarrow$ Benzil $\rightarrow$ Benzilic acid.

Hofmann bromamide Rearrangement: Phthalic anhydride-Phthalimide $\rightarrow$ Anthranilic acid

Beckmann Rearrangement: Benzene $\rightarrow$ Benzophenone $\rightarrow$ Benzophenone oxime $\rightarrow$ Benzanilide.

Skraup Synthesis: Preparation of quinoline from aniline.

Synthesis using Phase Transfer Catalysis: Alkylation of diethyl malonate or ethyl acetoacetate and an alkyl halide.

Peckmann Condensation for Coumarin

Three-component synthesis: Dihydropyrimidinone

L	T	P	C
0	0	6	3

CY22202: ANALYTICAL AND ENVIRONMNTAL CHEMISTRY LABORATORY

1. Determination of DO, BOD and COD of water.
2. Estimation of ions in mixture.
3. Paper chromatography and Ion-exchange chromatography
4. Gas chromatography
5. Spectroscopic determination of iron in cement
6. Determination of Ni in steel (Gravimetrically)

CY22203: SEMINAR

Report writing and delivering seminar based on literature survey of cutting recent research topics in chemistry.

SEMESTER III

CY23101: ORGANIC CHEMISTRY III

L	T	P	C
4	0	0	4

Module 1: Asymmetric Synthesis

Principles and methods of asymmetric syntheses, organometallic reagents and organocatalysts for aldol, epoxidations, dihydroxylation, aminohydroxylation, hydroboration, cylopropanation, cyycloadditions, D-A. reaction, nucleophilic and conjugate additions, electrophile induced cyclisations, iodolactonisations, reduction of C=C bonds.

Module 2: Retrosynthesis and Strategies in Total Syntheses

Retrosynthetic analysis, synthetic equivalents, convergent and divergent syntheses, functional group interconversions, one group C-X, two groups C-X disconnections, one and two groups C-C disconnections,

Few classic total syntheses: Reserpine (Woodward), Strychnine, Taxol, Tetracyclines.

Module 3: Carbohydrate Chemistry

Basic structure and type of sugars, Protection / deprotection strategies, orthogonality, glycosylation methods, armed-disarmed concept, glycals, deoxy-sugars, aminosugars, cyclitols, polysaccharide synthesis, polysaccharides as vaccines, importance of carbohydrates as chiral pool.

Module 4: Supramolecular Chemistry

From molecular to supramolecular chemistry, factors leading to strong binding (non-covalent interactions), new molecular receptors, crown ethers, siderophores, cyclophanes, cyclodextrin and their applications in specific recognitions, supramolecular reactivity and catalysis, switching devices, self-assembly of aggregates, crystal engineering, importance of molecular recognitions in life processes.

Module 5: Bioorganic Chemistry

Molecular models of biological receptors, biomimetic chemistry, design synthesis and binding studies of synthetic receptors, Enzyme models, micelles, biopolymers, catalytic antibodies, principle of gene synthesis, gene delivery, gene therapy, antisense therapy.

L	T	P	C
4	0	0	4

CY23102: INORGANIC CHEMISTRY III

Module I: Organometallic Chemistry II

Definition, classifications and bonding in organometallic compounds. Structural methods of Organometallics. Preparative methods. Fundamental processes in reactions of organo-transition metal complexes. Applications of transition metal complexes to catalysis, organometallics directed towards organic synthesis. Bio-organometallics, Organometallics in environmental chemistry. Metal clusters and models for heterogeneous catalysis. Application of Organometallics in Industry.

Module 2: Inorganic Chains, Rings, Cages, Clusters & Framework

Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Phosphorus-Oxygen, Phosphorus-Sulfur, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions, Framework structures, Inorganic clusters, organic-inorganic hybrid materials, Porous materials, molecular clusters to materials. Inorganic materials for energy storage, Hydrogen economy, CO_2 sequestration applications Application in industry, Hydrides & hydrogen-storage and other relevant examples from the recent literature. Synthesis of materials, Defects and ion transport, Metal oxides, nitrides & fluorides, Chalcogenides, Intercalation compounds & metal-rich phases, Framework structures, Hydrides & hydrogen-storage materials, Semiconductor Chemistry, Molecular materials (Single molecular magnets, 1-D metals, Liquid crystals).

Module 3: Metals in Biology

Dioxygen activation by heme and non-heme metalloenzymes: Cytochrome P450, Methane Monooxygenases (pMMO & sMMO), *Rieske dioxygenase*, □-ketoglutarate-dependent hydroxylases. Other metal containing enzymes: Hydogenases, Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, Nitrogenase etc. Solar energy capture during Photosynthesis: Photosystem I and II, Oxygen Evolving Complex.

Module 4: Chemical Toxicity and Metallotherapy

Toxic chemicals in the environment; toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens; metal containing drugs in therapy; platinum complexes as anticancer drugs, Pt-DNA binding, tetrathiomolybdate (MoS_4^{2-}) as Cu-chelation therapy in Wilson diseases (WD) and cancer. Other metallo-drug (As, Au, Cu etc), interaction of heavy metal ions with DNA; DNA cleavage; structure-activity relationship and mode of action.

L	T	P	C
4	0	0	4

CY23103: PHYSICAL CHEMISTRY III

Module 1: Electrochemistry

Theory of electrolytes, Ion-electron theory; Debye Hückel Limiting law, Activity Coefficients, Debye-Huckel-Onsagar theory of inter-ionic interaction, Theory of electrified interfaces, Guoy-Chapman, Stern, Tobin etc. models; overpotential, exchange current density, Bulter volmer equation, Tafel plot. Polarizable and non-polarizable interfaces, Electrocapillarity (EC), nature of EC curves, Lipmann equation, Electrical double layer theory.

Module 2: Electrochemical Cell and Corrosion

Electrochemical cell: Basic idea about Electrode Potentials and Cells, Galvanic vs. Electrolytic Cell, Nernst Equation, Primary Cell, secondary cell (Lead acid battery, Nickel-cadmium battery, Nickel-Metal hydride battery, Zinc-air battery, Lithium battery, Lithium ion battery). Fuel Cells- hydrogen-oxygen fuel cell.

Corrosion*:* Introduction to corrosion, Classification of corrosion, Electrochemical theory of corrosion. corrosion monitoring and prevention methods.

Module 3: Solid-State

Bragg-Miller indices, X-ray structural analysis of crystals, identification of unit cells, structure of simple lattices and X-ray intensities, Defects in solids: point, line and plane defects, Determination of equilibrium concentration of Scottky and Frenkel defects, F-centres/color-centres in ionic crystals, Band theory of solids, Semiconductors (extrinsic and intrinsic), Organic conducting solids, solid state reactions.

Module 4: Nanoscience

Introduction to Nanoscience, unique properties of nanomaterials, classifications of nanomaterial. band gaps, exciton, quantum confinement. General methods of synthesis of nanomaterials and nanostructures: top down, bottom up approach. Characterizations techniques of nanomaterials. Applications of nanomaterials.

CY23104: SPECTROSCOPIC METHODS OF ANALYSIS

L	T	P	C
3	1	0	4

Module 1: NMR

Principle, instrumentation and different techniques (CW & FT)of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J), spin dcoupling, spin tickling, first and second order spectra, classification of ABX, AMX, ABC, A_2B_2 in proton NMR; relaxation time and their importance, determination of relaxation times, Introduction to ^{13}C NMR, rules for 13C calculations, principles of decoupling, gated and inverse gated decoupling, selective polarization technique, NOE, DEPT, Elementary ideas on 2D NMR spectroscopy (^{1}H-^{1}HCOSY, NOESY, HMQC, HSQC, HMBC), Extension to other nuclei (^{19}F, ^{31}P etc), Chemical shift reagents, Temperature dependent NMR and molecular dynamics.

Module 2: Mass Spectrometry

Principle, instrumentation, applications and applications of mass spectrometry. Methods of generation of ions in EI, CI, FD, FAB, ESI, MALDI and other techniques. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotopes, ion-molecule interaction and analysis of fragmentation patterns of various functional groups. Application of mass spectrometry to simple structural and mechanistic problems. Tandem MS/MS, protein structure analysis, microarray, concepts in bioinformatics.

Structure elucidation of Organic Compounds: Use of combined spectroscopic techniques (UV, IR, NMR, MS) for structure determination and other applications.

Module 3: Photoelectron and Mössbauer Spectroscopy

Photoelectron spectroscopy, EXAFS, The influence of nuclear spin and the Zeeman effect. Spin resonance Spectroscopy: Basic Concepts, Nuclear spin states, mechanism of absorption, population densities of nuclear spin states, NMR Spectrometer. Electron Paramagnetic Resonance: Underlying principle, presentation of spectra, instrumentation, hyperfine splitting (applications to radicals). **Mössbauer Spectroscopy:** Basic principles, spectral parameter Applications – oxidation states of iron compound. Mass spectral techniques.

Module 4: X-ray Diffraction

Basics of X-ray Diffraction. Crystal Growth: Crystallization techniques, Evaluation of crystals. Data Collection: Crystal selection, Operation of instrument, Data collection methods. Data Solving and Refining, X-ray structure determination.

L	T	P	C
0	0	6	3

CY23201: COMPUTATIONAL LABORATORY

1. Study on the effect of ionic strength on the kinetics of $KBrO_3$ + KBr reaction.
2. Study the kinetics of inversion of cane sugar by polarimetry.
3. Conformation energy plot of ethane
4. Conformation energy plot of 1-fluoroethanol.
5. Potential Energy surface of a diatomic molecule
6. Geometry optimization of water molecules and IR frequency calculation
7. Why nitrogen molecule is inert, but CO is active. Insight from quantum chemical phenomena and effect of correlation.
10. Computation of Absorption spectra of a fluorophore
11. Transition state search of a reaction
12. Determination of structural features such as bond lengths, bond angles, dihedral anges of molecules extracted from Cambridge Crystallographic database.

CY23202: MAJOR PROJECT PART I

CY23203: PRACTICAL TRAINING EVALUATION

ELECTIVE SUBJECTS

CY2*111: Pharmaceutical Chemistry

Module 1: Pharmacology

General Pharmacology: Introduction, Routes of Administration of Drugs, Mechanism of action of Drugs

(Absorption, Distribution, Metabolism and Excretion of Drugs), Basic idea of mechanism of Drug action, Drug Toxicity, Pharmacology of ANS - Neurohumoral transmission, Drug acting on Sympathetic and Parasympathetic, Drugs acting on CNS - Sedative and Hypnotic agents, Hypoglycemic agents, Respiratory pharmacology: Drugs used in the treatment of various disorders of the respiratory tract, Antiviral drugs, Cancer chemotherapy,

Module 2: Pharmacokinetics

Principles of Pharmacokinetics: first order, zero order, Biological half life; Pharmacokinetics of Multiple; Dosing; Dosage regimen design based on mean average; minimum and maximum plasma concentrations;

Concept of Steady state plasma concentration and Renal clearance; One compartmental open model and calculation; Basic idea of two compartmental model and its use, concept of AUC, Cmax , Tmax , Absorption and Elimination rate constants, lag time, onset of action, duration of action, termination of action, Flip-flop phenomena. Non-Linear Kinetics: Special reference to Michaelis-Menten equation.

Module 3 Medicinal Chemistry II

Physicochemical aspects (Optical, geometric and bioisosterism) of drug molecules and biological action, drug receptor interaction including transduction mechanisms.

ACTIVITY RELATIONSHIP INCLUDING PHYTOCHEMICAL PROPERTIES OF THE FOLLOWING CLASSES OF DRUGS:

A) Drugs acting at synaptic and neuroeffector junction sites:

1) Cholinergics and anticholineesterases; 2) Adrenergic drugs; 3) Antispasmodic and antiulcer drugs; 4) Neuromuscular blocking agents; 5) Eicosanoids; 6) Analgesic, Antipyretics, Antiinflammatory (Non steroidal) agents.; 7) DIURETICS, ANTICOAGULANT AND ANTIPLATELET DRUGS AND CARDIOVASCULAR DRUGS Oxytocics (including Oxytocin, ergot alkaloids and prostaglandins), Biochemical approaches in drug

designing wherever applicable should be discussed.

CY2*112: Spectroscopy and Computational Applications in Modern Chemistry

Module 1:

Details of UV-vis and IR spectroscopy. Principle and application in interpretation of organic functional groups, Woodward-Hoffman rule. ^{1}H NMR Spectroscopy: Basic theory – phenomenon of energy absorptions (resonance) and relaxation, chemical shift, shielding and de-shielding mechanisms, equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry - Karplus equation. 13C NMR Spectroscopy: Principles; broadband decoupling, DEPT.

Module 2:

Mass Spectrometry: Types of ionization techniques, basic principles of EI. Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS and MS/MS techniques, fragmentation pattern of small molecules and interpretation of spectroscopic (NMR, IR and mass) data, as applied to organic, inorganic and biological systems

Module 3:

Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE, INDOR, INEPT for simple compounds and problems. Applications of multinuclear NMR in inorganic compounds – Examples from 1H, 11B, 13C, 19F, 15P NMR of paramagnetic molecules – Lanthanide shift.

Module 4:

Concept of vector space, matrix representation of operators, Hermitian operators and matrices, solutions of eigenvalue equation. Comparison between Schrodinger and Heisenberg pictures. Born-Oppenheimer approximation, theories of valence, the MO and VB methods for H2 molecule – their relative merits, dissociation curve, excited state, configuration interaction. Many electron systems – its characteristics, independent particle model (IPM), Hartree and Hartree- Fock methods for closed shell (elementary ideas).

CY2*113: Synthetic Methodologies & Applications in Chemistry

Module I: Development of Methodology

Advance reagents used as catalyst, oxidizing agent, reducing agent, Application to chemical transformation.

Module II: Supramolecular Chemistry

Host guest chemistry, Design and synthesis of supramolecular architecture, Practical application of supra molecular chemistry.

Module III: Asymmetric synthesis

Introduction of chirality, Stereo selective & Stereospecific Synthesis, carbohydrate chemistry and functional group transformation.

Module IV: Organocatalyst in organic synthesis

Design of organocatalyst and application to develop new asymmetric transformations.

CY2*114: MOLECULAR CATALYSTS FOR WATER OXIDATION

Module 1

Role of water oxidation in Energy Storage; Natural Photosynthetic Water Oxidation; Water Electrolysis.

Module 2

Heterogeneous oxide-based catalysts. Molecular Catalysts for Water Oxidation;

Module 3

Mechanistic investigation regarding O-O bond formation pathways (Water Nucleophilic Attack, WNA mechanism; Interaction of two M-O units, 12M etc). Deactivation pathways.

Module 4

Selected examples of Manganese based catalysts; Ruthenium based catalysts; Iridium based catalysts; Iron based catalysts; Cobalt based catalysts; other catalysts; Challenges and future direction.

CY2*115: Inorganic Photochemistry

Module 1

Introduction to inorganic photochemistry. Photochemical laws and photochemical kinetics. Photophysical processes.

Module 2

The electronic absorption spectra of inorganic compounds. Characteristics of the electronically excited states of inorganic compounds. Photoelectochemistry of excicted state redox reactions.

Module 3

Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions.

Module 4

Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies.

Text/References

G. L.Geoffrey and M. S. Wrighton, Organometallic Photochemistry, Academic Press, 1979.
K. K. Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1978.
M. S. Wrighton, Inorganic and Organometallic Photochemistry, ACS Pub.,1978.
V. Balzani and V. Carasiti, Photochemistry of Co-ordination compounds, Academic Press, 1970.

CY2*116: Determination of Molecular Structure by X-ray Diffraction

Module 1

Generation of X-rays, monochromators, safety; Concept of direct and reciprocal lattices, Bragg's law of X-ray diffraction in direct and reciprocal lattice, crystal systems, point groups

Module 2

Bravais lattices; Rotational axes of symmetry, screw axes, glide planes, equivalent points, systematic absences, space groups

Module 3

Argand diagram, intensity data collection and quantitative aspects of X-ray diffraction, temperature factor and scaling of data.

Module 4

The phase problem, direct method of solving structures; Patterson method, isomorphous replacement method; Structure refinement and their critical evaluation.

CY2*117: Frontiers in Bioinorganic Chemistry

Module 1

Developing facets of Inorganic Chemistry; Oxidative generation of molecular oxygen from water during photosynthesis; Its importance from the standpoint of non-conventional energy research;

Module 2

Reductive cleavage of the dioxygen bond; Reductive cleavage of dioxygen bond and novel organic transformations including methane to methanol performed by a large number of Fe containing metalloenzymes;

Module 3

Reductive cleavage of dioxygen bond and novel organic transformations performed by a large number of Cu containing metalloenzymes and synthetic catalysts.

CY2*118: The Chemistry of Metal-Carbon Bond: Structure Reactivity & Applications

Module 1

Introduction to Organometallics: Bonding, Types of Ligands, and some basics concepts like isoelectronic and isolobal analogy; Characterization techniques of Organometallic compounds (NMR and IR spectroscopy and Mass spectrometry);

Module 2

Representative chemistry of main group Organometallics; Organometallic chemistry of lithium and magnesium: synthesis, structures, fluxionality and reactivity; Chemistry of Aluminum: Aluminum alkyls. Use of aluminum alkyls in polymerization of olefins;

Module 3

Organometallic chemistry of transition metals σ – bondedligands: Metal alkyls, aryls and hydrides. Stability, preparation and reactivity; Metal- carbonyls / Metal- phosphines / metal- nitrosyls / metal isocyanide: structures, reactivity and bonding; Metal- carbenes, metal-carbynes, Fischer carbenes, Schrock, carbenes, complexes with N-heterocyclic carbenes (NHCs), π - bonded ligand:

Module 4: Metal-olefins, alkyls metal alkynes, dienes, Cp and Cp*, structure, bonding and reactivity. Reactions in Organometallic Chemistry: Oxidative addition, reductive elimination, insertion, elimination, and migration; Applications of organometallics in organic synthesis; C-C bond coupling reactions (Heck, sangoshira, Suzuki); Reduction using transition metal hydrides, asymmetric hydrogenation. Olefin metathesis

CY2*119: Solid-State Chemistry

Basic Principles and applications Solid State Reactions: General Principles, Experimental procedure, Kinetics of solid-state reactions, Synthesis of Single Crystals, Phase transitions, electronic and magnetic properties Factors that influence kinetics of phase transition. Electronic Properties and Band Theory: Electronic structure of solids- band theory. Magnetic Properties: Classification of materials. Magnetism: Types, determination of magnetic susceptibility. Quantum theory of paramagnetism. Cooperative phenomena. Magnetic domains. Hysteresis.

Diffractions Techniques X-ray Diffraction: Diffraction of X-rays by crystals: The Laue equations and Bragg's law. X-ray diffraction experiments: The powder method and the single crystal method. Electron diffraction: Scattering intensity versus scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cells.

High-Tc Oxide Superconductors Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Non-linear materials: Second and third order non-linear effects; molecular rectifiers. Photochromic materials; optical data storage, memory and switches.

CY2*120: Advanced Physical Chemistry

Tunnelling Phenomena: Principles and selected problems. Ab initio and Semi-empirical Methods for Closed Shell Systems: The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem. Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations). Density functional theory. Semiempirical Molecular Orbital Methods I - PI Electron Systems: The Hückel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method. Semiempirical Molecular Orbital Methods II - All valence - Electron systems: The Extended Hückel Method, The CNDO Method.

Electronic Structure of Linear and non linear Molecule The MO - LCAO Approximation, The Hydrogen Molecule Ion, H_2^+ , The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations. Electronic Structure of AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

CY2*121: Nanoscience

Introduction Surface to volume ratio, crystal structures, basic properties. Length scale: de Broglie wavelength, Bohr radius, excitons, confinement regimes, The Fermi Energy, Kubo Gap, the mean free path in metals, charging energy. Size and shape-dependent electrical, magnetic and optical properties of metal, metal oxide and semiconductor nanoparticles. Quantum size effect, Superparamagnetism, Surface Plasmon resonance.

Synthetic approaches Top down and bottom up. Colloidal growth. Chemical synthesis, functionalisation and basic characterisation of metal, metal oxide and semiconductor nanoparticles. Core-shell / multishell nanoparticles. Properties and synthesis of Carbon nanotubes, grapheme, fullerene. Recent advances in synthesis of new materials and their synthetic strategies. Characterization of nanomaterials.

Polymer-nanoparticle composite. Band gap engineering in semiconductor nanocrystals, Carbon based nanoparticles, self assembled nanostructures. Atom and molecule manipulation. Application of nanoparticles in drug delivery, biological imaging of cellular and subcellular structures, catalysis, sensor, tracer, cancer treatment, photovoltaics, single molecule detection and LED. Introduction to nanotoxicology. Model problems for quantum wells, wires and dots Density of states.

CY2*122: Advanced Materials

Glasses, ceramics, composites and Nano materials. Glasy state, glass formers and modifiers, applications, ceramic structures, mechanical properties, clay products, refractories, characterization, property and application. Preparation, characterization, properties, applications of nanomaterials.

Thin Films and Langmuir – Blagett films: Preparator techniques, chemical, MOCVD, sol-gel etc. CB films, growth technique, Properties and applications. Liquid Crystals: Mesomorphic behavior, different phases in liquid crystals order parameters, textures, twisted and chiral nematics, chiral nematics, application of liquid crystals.

Fullerenes, Graphene, Carbon Nanotubes, Metal Organic Frameworks.

CY2*123: Computational Chemistry

Monte Carlo, Molecular Dynamics simulations and its applications to understanding of physical and chemical transformations Methods based on Hartree-Fock, Configuration Interaction, Deriving one and two electron properties, Semi-empirical methods, Coupled Cluster theory, Density functional theory, TDDFT. QM/MM methods. Basic molecular biology Basic principles of biochemistry, energy

conversion, enzymatic catalysis, and active transport, enzyme models, drug design, computational modeling. Introduction to Classical Monte Carlo Molecular Dynamics Simulation and Softwares - DLPOLY, GROMACS, TOWHEE, NAMD. Introduction to Quantum chemistry softwares – NwChem, Gaussian.Visualization softwares – VMD, Povray. Computer programming languages C++, FORTRAN. Python, Shell scripting. Writing Monte Carlo, Molecular Dynamics codes for chemistry problems. Parallel programming techniques like Open MP, MPI

CY2*124: Organometallic Chemistry of Main Group Elements

Module 1: Group 1 and Group 2

Energy, Polarity, and Reactivity of M-C bonds; Stability and Lability of Main Group Organometallic compounds. Overview on the preparation of organometallic compounds; Organolithium compounds – Synthesis, Structures and Application; organometallic compounds of the heavier alkali metals – Reactivity comparison with alkyl lithium compounds; organometallic compounds of the alkaline earth metals – application of Group 2 metal alkyls and hydrides – special emphasis on Magnesium hydride.

Module 2: Group 13 and Group 14 (14 hours)

Organometallic compounds of Boron Group; Organoboron compounds, Organoaluminum compounds, Gallium, Indium and Thallium Organyls –Syntheses, structure and application. Organosilicon, Orgaogermenium, Organotin and organo-lead compounds –Syntheses and Application.

Module 3: Group 15 and Group 16 (10 hours)

Organometallic compounds of Nitrogen Group; E^{V} – Organyls (As, Sb, Bi); E^{III} – Organyls (As, Sb, Bi); chain and ring containing E-E bonds ; E single bonds; E (P, As, Sb, Bi) as partner of multiple bond. Organometallic compounds of selenium and Tellurium –Syntheses and properties.

Module 4 : Current Trends (4 hours)

Recent advances in Main Group Organometallic compounds; Carbenes (classifications, properties and utilization), Metal –Metal multiple bonded compounds –structure and reactivity.

CY2*125: Electrochemistry: Fundamentals & Applications

Module 1

Nomenclature & classes of Electrochemical methodology, Sign and graphical conventions, Utilization of Electrochemistry for chemical characterization; Dynamics of electron transfer (Kinetics and thermodynamics)

Module 2

Potentiometry Measurements- introduction, principles and applications. Controlled-potential methods- Polarography, Linear Sweep & Cyclic Voltammetry, Chronoamperometry & Chronocoulometry, Controlled-potential bulk electrolysis.

Module 3

Indicator Electrodes- Measurement of electrode potential, Junction potential. Reference electrodes, Voltammetric indicator electrodes. Electrochemical cells and instrumentation (Electrochemical, Voltammetry, Polarography, Spectro-electrochemistry cells.

Module 4

Electrocatalysis- Oxygen evolution reaction (OER), Hydrogen evolution reaction (HER), Oxygen reduction reaction (ORR), CO_2 reduction etc. Some representative case studies

CY2*126: Surface Science and Catalysis

Module 1. Fundamentals of Surface Catalysis:

Catalyst concepts, Classification and types of catalysts, activation energy concept, comparison of homogeneous & heterogeneous catalysis, enzyme catalysis, green catalysis , photocatalysis, nano catalysis, autocatalysis, phase transfer catalysis , catalyst promoters, catalyst poisons, metals as catalysts, metal supported catalysts, solid acid catalysts; Catalyst life cycle: Preparation. Activation, Reconstruction, Deactivation and Regeneration. Active sites and catalyst modifies. Trades Off-Activity, Selectivity, Stability and Accessibility.

Module 2. Kinetics of Surface Reactions:

Heterogeneous Catalysis mechanism, Adsorption- Physisorption and chemisorption, Gibbs adsorption isotherm, types of adsorption isotherms, Langmuir, Freundlich and BET isotherms. Kinetics of Gas-solid reaction- Langmuir-Hinshelwood and Langmuir-Rideal mechanism. Enzyme catalysis - rates of enzyme catalyzed reactions, effect of substrate concentration, pH and temperature, determination of Michael's parameters. Michaelis-Menten equation, lineweaver -burk plot, acid-base catalysis.

Module 3. Synthesis and Characterization of Catalyst:

Synthesis: Co-Precipitation method: Co-Precipitation method: General principles governing precipitation from solutions viz., Physico Chemical considerations, Chemical considerations and Process considerations. Sol-Gel technique: Important parameters in sol-gel preparation- Solution Chemistry, Aging, Drying and Calcination. Preparation of clathrates. **Characterization:** Characterization of catalysts and their surfaces: Methods of surface analysis, surface area, pore size, void fraction, particle size, mechanical strength, surface chemical composition, surface acidity, basicity and reactivity. BET analyser, X-ray diffraction , SEM, TEM, X-rayabsorption spectroscopy, XPS and Auger spectroscopy.

Module 4. Applications:

Water oxidation, Hydrogen Evolutions, Bio-fuel, photocatalytic degradation of dyes - environmental applications. Dehydrogenation, dehydration, Catalytic processes in petroleum industry- reforming, cracking and hydro treating, hydrogenation, hydrodesulphurization, Fischer-Tropsch process, methane decomposition, steam reforming.

CY2*127: Drug Targets and Therapeutics

Module 1: <u>Pathophysiology of common disorders</u>

Introduction to Cancer, Diabetes, and bacteria mediated disorders. Genetic basis of cancer, Signal transduction and regulatory kinases, switches, Tumor suppressor genes, regulatory signaling pathways: Receptor Tyrosine Kinases, growth receptors, cell division / cell cycle proteins. Types of Diabetes and effect on antioxidant machinery. Generation and Role of reactive oxygen species/ reactive nitrogen species in cancer and hyperglycemia. Mode of cell death: apoptosis and autophagy. Role of bacterial biofilm formation in pathogenesis.

Module 2: <u>Drug design and cellular targets</u>

Role of structure–activity relationship (SAR) in drug design and development. Important cellular targets in different disease models : Membrane proteins and receptors, eukaryotic and prokaryotic cell division proteins, metabolic enzymes, DNA and RNA etc. Mode of actions of various: Antibacterial agents, Antiviral agents, Anticancer agents and antidiabetic agents. Biological Assays for Lead Identification and High Throughput Screening: MTT, XTT, FACS based assays.

Module 3: <u>Drug delivery techniques</u>

Objective of drug delivery and optimization, Different routes of drug delivery : oral, intraperitoneal and intravenous. Vehicles used for drug delivery: Liposomes, nanoparticles, micelles etc. Nano based drug delivery systems: recent developments and future prospects.

Module 4: Health safety and Ethical perspective

Drug toxicity: cause and effect, Different types of toxicity: Liver, spleen, and cardiotoxicity. Markers of toxicity. Ethical challenges of drug development.

CY2*128: Bio-Physical Chemistry

Module 1 Thermodynamics and Interactions in Biological System: Covalent and non-covalent interactions in Biological Systems, Protein Folding, Hydrogen Bonding,

Module 2 Bio-Electro Chemistry: Charge transport in Biological System, Application of Sodium-Potassium exchange in cell and neuron. Message passing and Cell signaling in biological systems. Response systems in Biology, Application of electrochemical Cell in Biological System, Pacemaker

Module 3 Kinetics in Biological Processes: Basic Kinetics. Rapid Reaction Techniques, Relaxation Methods, Hydrogen exchange, Enzyme kinetics

Spectroscopic Identification Techniques for Biological Structure Elucidation

UV-Visible and other spectroscopic Techniques involving electronic spectroscopy, NMR, Raman, Infra-Red Spectroscopy, Mass Spectrometry, Atomic Force Spectrometry.

CY2*129: Advanced Heterocyclic Chemistry

CY2*130: Natural Product Chemistry

CY2*131: Chemical Biology

CY2*132: Advanced Stereochemistry

CY2*133: Advanced Quantum Chemistry & Statistical Thermodynamics