Proposed 3rd year Syllabus (Academic year 2021 - 2022)

B. Sc. Blended – Chemistry Stream

SEM V		
Subject Code	**Title of the Subject**	**Credits**
CHM 501	Chemical kinetics, Thermodynamics & Quantum chemistry	3
CHM 502	Catalysis and Industrial processes	3
CHM 503	Design and Synthesis of Organic Molecules	3
CHM 504	Introduction to analytical chemistry	3
CHM 505	Elective Course - 1	2
CHM 506	Elective Course - 2	2
CHM 507	Physical/Analytical Chemistry - LAB	2
CHM 508	Inorganic/Organic Chemistry - LAB	2
CHM 509	Project/ Dissertation	2
Total Credits		**22**

Elective Courses SEM V		
Subject Code	**Title of the Subject**	**Credits**
Elective Course - 1	Molecular Modelling in Chemistry	2
Elective Course - 2	Introduction to forensic Science and technology	2

Students can choose electives from other streams viz. Physics, Environmental Science or Earth Science. They also can choose electives from B. A. Liberal Arts.

SEM VI		
Subject Code	**Title of the Subject**	**Credits**
CHM 601	Solid State chemistry & its Applications	3
CHM 602	Bioinorganic and Coordination chemistry	3
CHM 603	Natural product and Heterocyclic Chemistry	3
CHM 604	Separation Techniques and Advanced Analytical Techniques	3
CHM 605	Elective Course - 3	2
CHM 606	Elective Course - 4	2
CHM 607	Physical/Analytical Chemistry - LAB	2
CHM 608	Inorganic/Organic Chemistry - LAB	2
CHM 609	Project/ Dissertation	2
Total Credits		**22**

Elective Courses SEM VI		
Subject Code	**Title of the Subject**	**Credits**
Elective Course - 3	Materials chemistry	2
Elective Course - 4	Supramolecular chemistry	2

Students can choose electives from other streams viz. Physics, Environmental Science or Earth Science. They also can choose electives from B. A. Liberal Arts.

Syllabus Details

SEMESTER V

CHM 501- Chemical kinetics, Thermodynamics & Quantum chemistry	
Topic Details	**No. of Lectures**
Chemical Kinetics • Order, molecularity, • rate laws – 1^{st}, 2^{nd} order kinetics • Half-life of reactions	2
Kinetics of Complex system • 2nd order reactions (Unequal concentration), • 3rd order reactions (equal concentration)	4
Photochemistry • Photochemical process • The primary quantum yield • Mechanism of decay of excited singlet state • Quenching • FRET • Effect of Temperature	6
Thermodynamics • Thermodynamics of transition • Phase Diagram • Phase Rule	8

Statistical thermodynamics • Macrostate, • Microstate, • Partition functions • Thermodynamic quantities from partition function	8
Quantum chemistry • Black body radiation • Heisenberg uncertainty principle • Wave particle duality, Schrödinger equation, Operators, • Particle in 1D/3D- Box • Postulates of quantum mechanics / Eigen functions, Values • Application to ¶ electrons linear conjugated hydrocarbons	8
Student work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Reading:

1. Peter Atkins & Juliode Paula,"*Atkins'PhysicalChemistry*"(10thedition). Chapters 16 *&*20
2. Atkins & de Paula "*Physical Chemistry*" 7^{th}-10^{th} ed
3. Principles of Chemical kinetics J E House
4. Physical Chemistry, A molecular approach by Donald A McQuarrie, John D. Simon
5. Elements of Physical Chemistry by Atkins
6. Physical Chemistry for Chemical and Biological Sciences by Raymond Chang
7. Physical Chemistry by Atkins, International Edition

CHM 502 - Catalysis and Industrial processes	
Topic Details	**Lectures**
Fundamental aspects of catalysis Homogeneous and Heterogeneous catalysis. The role of catalytic processes in modern chemical manufacturing - organometallic catalysts - catalysis in organic polymer chemistry - catalysis in petroleum industry - catalysis in environmental control.	4

Homogeneous catalysis Steam reformation, natural gas (methane), reformation of hydrocarbons, Monsanto acetic acid synthesis, alkene polymerization, Carbonylation, hydrogenation, hydroformylation, hydrogenation vs hydroformylation, Monoelectronic transfer, Shell process, Wacker acetaldehyde synthesis, photoactivated catalysis and metal cluster catalysts, Asymmetric catalysis using chiral phosphoric acids, CPA (e.g. BINOL-phosphoric acid), e.g. asymmetric hydrogenation, epoxidation, hydroformylation.	12
Heterogeneous Catalyst Ruhrchemie/Rhone-Poulenc Oxo process using aqueous biphasic catalysis, Zeolites, their structure and properties, natural vs synthetic zeolites, zeolytes as catalysts, mesoporous materials in heterogeneous catalysis, The flue gas depollution, Energy and CO2, Hydrogenation, Oxidation, Refining technology etc.	8
Applied Biocatalysts Introduction to enzymes and enzyme catalysed reactions. Classification and mechanism of reaction. Purification and characterization of enzymes. Michelis Menten kinetics, Industrial enzymes. Applications of enzymes in diagnostics, analysis, biosensors and other industrial processes and bio-transformations. Enzyme structure determination, stability and stabilisation. Enzyme immobilization and concept of enzyme engineering. Nanobiocatalysis.	6
Photocatalysis Porphyrins -phthalocyanines and semiconductor as photo catalysts in photolysis reactions - generation of hydrogen by photo catalysts - photocatalytic break down of water andharnessing solar energy - photocatalytic degradation of dyes - environmental applications.	6
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Readings:

1. Weller et al. (IC), 6th ed, Ch 21, 22 & 25, Housecroft and Sharpe (HS), 4th ed, Ch 26, 24.2, 24.7, 25
2. Cotton, F.A. and Wilkinson, G. "Advanced Inorganic Chemistry", 4th Ed. John Wiley & Sons, New York.
3. Huheey, J.E.,Keiter, E.A. andKeiter, R.L. "Inorganic Chemistry: PrinciplesofStructuresandReactivity",4thEd.,LowPrintEdition,Pearson Education Ltd, Asia, Reprint in India.
4. Pecoraro, V.L. "Manganese Redox Enzymes", VCH: New York.
5. Concise Inorganic Chemistry by J.D. Lee - 5th Edition.
6. Inorganic Chemistry, - D.F. Shiver & P.W. Atkins- C.H. Longford ELBS 2nd Edition.
7. Basic Inorganic Chemistry, - F.A. Cotton and G. Wilkinson, Wiely Eastern
8. Industrial Catalysis: A practical approach by Jens Hagen Wiley (2006)
9. Industrial Catalysis: Optimizing catalysts and processes by R. I. Wijngaarden, K. R. Westerterp, and A. Kronberg
10. Handbook of Industrial Catalysts by L. Lloyd 4. Fundamentals of Industrial Catalytic Processes by C. H. Bartholomew
11. Rothenberg, G., Catalysis: Concepts and green applications, Wiley VCH, 2008
12. Gupta, B. D, Elias, A. J., Basic Oranometallic chemistry: Concepts syntheses and applications, 2nd edition, Orient Blackswan, 2013
13. Price and Stevens, Fundamentals of enzymology, Oxford University Press 2000
14. Buchholz, Kasche and Bornscheuer, Biocatalysts and Enzyme Technology, Wiley-VCH 2012
15. Polaina and MacCabe, Industrial Enzymes: Structure, Function and Applications, Springer 2007
16. B. Viswanathan, S. Kannan, R.C. Deka, Catalysts and Surfaces: Characterization Techniques, , New Delhi, 2010.
17. M. Kaneko, I. Okura, Photocatalysis: Science and Technology, Springer, 2003.

CHM 503 - Design and Synthesis of Organic Molecules	
Topics	**Lectures**
Selectivity in organic synthesis Chemo-selectivity, Regioselectivity, Stereo- and enantioselectivity	2
Introduction of Pericyclic reaction Electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, photochemical cycloaddition reactions, Diels-Alder reaction, Dipolar cycloadditions, retrocycloadditions, electrocyclic reactions.	6
C-C single/ double bond formation reactions	8

Mechanism of Knoevenagel, Perkin, Stobbe, Darzen, Acyloin condensations, epoxidations (Prilezhaev, Sharpless, Jacobsen), Metal catalyzed C-C bond formations (Ullmann, Buchwald-Hartwig, Heck, Suzuki, Stille reactions). Phospohorus, nitrogen and sulfur ylids, Wittig reaction, Wittig-Horner reaction, Mannich reaction, Peterson olefination, McMurry reaction, β-eliminations (Hoffman & ester pyrolysis), Cope elimination, mreduction of acetylenes.	
Oxidation and reduction reactions Oxidations of hydrocarbons (alkanes, alkenes and aromatic), alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, alkenes to diols (Manganese, Osmium- based), Sharpless asymmetric dihydroxylation, alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based-ozonolysis), alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, chromium based allylic oxidation), ketones to α-hydroxy ketones, α,β-unsaturated ketones, Hydride reducing agents, Birch reduction, Catalytic Hydrogenation reaction, Carbonyl reduction reaction.	8
Target oriented synthesis Designing organic synthesis, Retrosynthetic analysis, disconnection approach, linear and convergent synthesis. Diversity-oriented synthesis: concept of forward-synthetic analysis, appendage diversity, skeletal diversity, stereochemical diversity, complexity and diversity.	6
Asymmetric Synthesis Use of chiral auxiliaries, chiron approach. Principles and use of enzymes in the syntheis of industrially important sugar / fatty acid esters, sugar nucleotide derivatives; enantiomeric pure compounds and biobased platform chemicals.	6
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Reading:

1. *OrganicChemistry*byJ.McMurray,7thEd.,Thomson,2008.*PrinciplesofOrganicSynthesis*byR. Norman

and J.M. Coxon, 3rd Ed., Chapman and Hall, 1993. *Organic* Chemistry by J. Clayden, N. Greeves, S. Warren and P. Wothers, 2nd Ed, Oxford Press,2012.
2. Carey, F. A. and Sundberg, R. J., "Advanced Organic Chemistry, Part B: Reactions and Synthesis", 5th Ed., Springer.
3. Clayden, J., Greeves, N. and Warren, S., "Organic Chemistry", Oxford University Press.
4. Smith, M.B., "Organic Synthesis", 3rd Ed., Academic Press.
5. Bruckner, R., "Organic Mechanisms: Reactions, Stereochemistry and Synthesis", Springer.

CHM 504 - Introduction to analytical chemistry	
Topics	**Lectures**
Fundamentals of Analytical Methods Statistics and chemometrics: statistical calculations, confidence limits, tests of significance, correlation coefficient, propagation of error; sampling methods: representative samples, automation of sampling and sample treatment; experimental design; quality control and assurance, volumetric and gravimetric methods; quantitative aspects of colorimetry; theory of different types of titrations: acid-base, precipitation, redox, complexometric, nonaqueous, etc.; Introduction to analytical sensors; automated method of analysis; continuous flow methods; flow injection analysis; kinetic methods of analysis; miscellaneous methods: turbidimetry, refractometry, polarimetry, optical rotatory dispersion and circular dichroism.	6
Electroanalytical methods Introduction, electrochemical cells, types of electrodes, classifications of electroanalytical methods. Analytical applications of two-electrode systems: conductometry and potentiometry; controlled potential techniques: constant potential (e.g., amperometry), potential step (e.g., pulse techniques), and potential sweep methods (e.g., cyclic voltammetry); electrogravimetry, electrophoresis, electrosynthesis, coulometry, flow electrolysis, thin-layer electrochemistry; electrochemical sensors; electrochemical technology.	8
Environmental Analytical Chemistry Sampling of air, water and soil for chemical analysis; monitoring techniques of air pollutants, air quality standards, pollutants standards index (PSI), monitoring of volatile	6

organic compounds; water pollution: water quality parameters and their determination, algal blooms and algal toxins, monitoring pesticide residues in water and soil, water treatment: municipal water treatment, waste water treatment methods.	
ANALYTICAL BIOCHEMISTRY **Body fluids** Composition of body fluids and detection of abnormal levels of certain constituents leading to diagnosis of disease., Physiological and nutritional significance of water and fat soluble vitamins and minerals. Analysis for constituents of physiological fluids, viz., urine, blood, serum. Analytical techniques for vitamins including microbiological techniques.	3
IMMUNOLOGICAL METHODS General processes of immune response, Antigen-antibody reactions, precipitation reactions, radio, enzyme, and fluoro-immuno assays. Human nutrition : Biological values and estimation of enzymes, carbohydrates, essential amino acids, proteins, and lipids	3
SPECTRAL METHODS Infra-red spectroscopy, NMR, Mass spectroscopy, Raman spectroscopy, Isotope dilution method and activation analysis, radiometric and radio-release methods Auto, X-ray and gamma radiography, Principle, Instrumentation and applications of: Differential Thermal Analysis, Differential Scanning Calorimetry, Thermometric titrations, Evolved gas analysis, HYPHENATED TECHNIQUES : Need for hyphenation, Interfacing devices and applications of GC - MS, GC - IR, MS-MS, HPLC - MS, ICP -MS, ICP - OES.	10
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Readings:

6. D.A.Skoog, D.M.West, F.J.Holler and S.R.Crouch, Fundamentals of Analytical Chemistry 9E, 9th Ed., Brooks/Cole, 2014
7. D.A.Skoog, F.J.Holler and T.A.Nieman, Principles of Instrumental Analysis, 5th Ed., Thomson,1998.
8. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986)

9. Fundamentals of Analytical Chemistry, D .A. Skoog and D. M. West and F. J. Holler Holt- Saunders (1992)
10. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 5th Edition (1998)
11. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt, Jr. J. A.Dean 6th Ed CBS (1986)
12. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean 7th Ed CBS (1986)
13. Introduction to instrumental analysis, R. D. Braun, Mc Graw Hill (1987)
14. General, organic and biological chemistry, H. Stephen Stoker, Cengage Learning.
15. Advance dairy chemistry, vol 3, P. F. Fox, P. L. H. McSweeney Springer.
16. Physiological fluid dynamics vol 3, Nanjanagud Venkatanarayanasastry Chandrasekhara Swamy Narosa 1992
17. Molecular Biological and Immunological Techniques and Applications for food, edited by Bert Popping, Carmen Diaz-Amigo, Katrin Hoenicke, John Wiley & sons.
18. Analytical Chemistry, G. D. Christian, 4 th Ed. John Wiley, New York (1986)
19. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J .Holler Holt- Saunders 6th Edition (1992)
20. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th Edition (1998)
21. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt, Jr J. A. Dean and F. A. Settle Jr 6th Ed CBS (1986)
22. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr 7th Ed CBS (1986)

Elective Course 1 CHM 505 - Molecular Modelling in Chemistry	
Topic Details	**Lectures**
Brief Review of the basic Principles of quantum mechanics of atoms and molecules. Potential energy surfaces and intermolecular interactions: Quantum mechanical ab initio calculations within Born-Oppenheimer approximation and modelling of calculated energies by model potentials for simple atoms, molecules and ions. Energy calculations using molecular mechanics.	10
Simple applications of molecular modelling: Study of an assembly of atoms or molecules (clusters and/or bulk phases). Approximation of the total potential energy as the sum of pair potentials. Concept of large number of microstates, averages and basic principles of simulations. Study of cluster and bulk properties through simulations.	6
Modelling of water and small organic molecules: Nonpolarizable and polarizable rigid models. Flexible models and calculation of force constants. Structural, dielectric and dynamical properties of a polar medium: Continuum models versus molecular models. Calculation of free energy using molecular models.	6

Modelling of macromolecules: Study of self-organized assemblies, biomolecules like peptides, proteins, membranes and ion channels. Concept of hydrophobic and hydrophilic interactions. Use of molecular modelling in drug design, QSAR	2
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Readings

1. A.R. Leach, Molecular Modeling : Principles and Applications, Longman (1996).
2. J. H. Jensen, Molecular Modeling Basics, CRC Press (2010).
3. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed., Wiley (2004).
4. J. Israelachvili, Intermolecular and surface Forces, Academic (1991)
5. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Clarendon Press (1987)
6. D. Frenkel and B. Smit, Understanding Molecular Simulation : From algorithms to Applications, Academic Press (1996)
7. P.W. Atkins, Molecular Quantum Mechanics, Oxford (1997)
8. W. Koch & M. C. Holthausen, A Chemist's Guide to Density Functional Theory, Wiley
9. Szabo, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications (1996).

Elective Course 2 - Introduction to forensic science & technology	
Topic Details	**Lectures**
History and development of Forensic Science Historical aspects of forensic science, Definitions and concepts of forensic science, Need of Forensic Science, Basic Principles of Forensic Science, Scope of development of forensic science. Functions of Forensic Science, Different branches of Forensic Science. Frye case and Daubert standard. Scope and development of forensic science.	6

Legal aspects of crime: Crime – Introduction Natures, causes and consequences of crime, Broad concepts of criminal Justice system, Procedures involved in the detection of crime, Filing of criminal charges, Indian police system – The Police Act, Human rights and criminal justice system in India. Set up of INTERPOL. Duties and qualification of forensic science.	3
Organizational set up of FSL in India Hierarchical set up of central forensic science laboratory, Hierarchical set up state forensic science laboratory, Government examiners of questioned documents. Chemical examiners laboratory, Finger print bureaus, National crime records bureau, Bureau of police research and development, Mobile crime laboratory, Duties of forensic scientist, code of conduct of forensic scientists. Drug enforcement administrator. Defense research and development organization.	3
Forensic Chemistry **Petroleum and Petroleum Products**: Distillation and fractionation of petroleum. Commercial uses of different petroleum fractions. Analysis of petroleum products. Analysis of traces of petroleum products in forensic exhibits. Comparison of petroleum products. Adulteration of petroleum products. **Cases Involving Arson**: Chemistry of fire. Conditions for fire. Fire scene patterns. Location of point of ignition. Recognition of type of fire. Searching the fire scene. Collection and preservation of arson evidence. Analysis of fire debris. Analysis of ignitable liquid residue. Post-flashover burning. Scientific investigation and evaluation of clue materials. Information from smoke staining. **Explosives: Classification of explosives** – low explosives and high explosives. Homemade explosives. Military explosives. Blasting agents. Synthesis and characteristics of TNT, PETN and RDX. Explosion process. Blast waves. Bomb scene management. Searching the scene of explosion. Mechanism of explosion. Post blast residue collection and analysis. Blast injuries. Detection of hidden explosives	8

Forensic Biology Nature and importance of biological evidence. Significance of hair evidence. Transfer, persistence and recovery of hair evidence. Structure of human hair. Comparison of hair samples. Morphology and biochemistry of human hair. Comparison of human and animal hair. Types and identification of microbial organisms of forensic significance. Identification of wood, leaves, pollens and juices as botanical evidence. Diatoms and their forensic significance	4
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	6

Suggested readings:

1. B.B. Nanda and R.K. Tiwari, Forensic Science in India: A Vision for the Twenty First Century, Select Publishers, New Delhi (2001).
2. M.K.BhasinandS.Nath,RoleofForensicScienceintheNewMillennium,UniversityofDelhi, Delhi(2002).
3. S.H. James and J.J. Nordby, Forensic Science: An Introduction to Scientific and Investigative Techniques, 2nd Edition, CRC Press, Boca Raton (2005)
4. 4.W.J. Tilstone, M.L. Hastrup and C. Hald, Fisher's Techniques of Crime Scene Investigation, CRC Press, Boca Raton (2013).

CHM 507 - Physical/Analytical Chemistry – LAB

1. Kinetics of Alcohol Dehydrogenase-Catalysed Oxidation of Ethanol
2. To study the phase diagram of a binary system (Phenol + water) and the effect of impurities (e.g. NaCl). Photolysis of Ethanal.
3. To determine the energy of activation for the acid catalysed hydrolysis of methyl acetate
4. Determination of specific rotation of lactic acid/sucrose by polarimeter.
5. Determination of Na, K in a soil sample by flame photometry.
6. Determination of glucose from food sample by glucose oxidase method.
7. Use of fluorescence to do "presumptive tests" to identify blood or other body fluids
8. To study the kinetics of saponification of ester by conductometric method

CHM 508 - Inorganic/Organic Chemistry – LAB

1. Oxo synthesis: - hydroformylation of propene with [HRh(CO)(PPh3)3]
2. Oligomerization of Ethylene (SHOP Process)
3. L-Amino Acids by Aminoacylase Process
4. Catalytic hydrogenations with metal catalysts based on Ni, Co, Pd, or Pt.
5. Knoevenagel condensation between aldehyde (4-diethylaminobenzaldehyde) and malonic acid, cyanoacetic acid or malononitrile.
6. Preparation of pyridinium dichromate and its use in oxidation of benzyl alcohol
7. Synthesis of trans-9-(2-Phenylethenyl)anthracene
8. Asymmetric reduction of EAA by using Bakers yeast

CHM 509 – Project/ Dissertation

Project-based learning offers an opportunity to the students to work independently under guidance of a supervisor. Students will be assigned to the on campus faculty/ research scientists from various national research institutes such as NCL/ IISER/ working in chemistry research; under whose guidance he or she would work on a problem keeping the focus to enhance their own ability to critical thinking, identification of research problems and research gaps, formulate research objectives, formulation of research plan, and problem solving via execution of specific experiments, and develop specialized skills to handle specific problems. This would train the students to nurture their creativity and innovative ideas, collaboration/teamwork and leadership, communications, learning self-reliance and project management.

Adequate assessment requirements for individual marking are presentations with discussions and seminars on the working process and the results.

Syllabus Details – Semester VI

CHM 601 - Solid State chemistry & its Applications	
Topic Details	**Lectures**
Fundamentals Types of solids - close packing of atoms and ions - bcc, fcc and hcp voids –Gold schmidt radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluroite - antifluorite - diamond and graphite-spinel - normal and inverse spinels and perovskite - lattice energy of ionic crystals -Madelung constant - Born-Haber cycle and its applications.	5
Theories Band theory of solids. Free electron Theory, zone theory, MO theory of Solids dislocation in solids: Schottky and Frenkel defects. Line defects and plane defects – nonstoichiometric compounds. Electrical properties: Energy bands, insulators, semiconductors and conductors- super conductors-dielectric properties, piezo-electricity, ferro electricity- conductivity in pure metals. Superconductivity: Occurrence, BCS theory, high temperature super conductors- introduction to nanoparticles- metal nanoparticles- particle size determination.	5
X- Ray diffraction Theory- the crystal systems and Bravais lattices - Miller indices and labelling of planes - symmetry properties - crystallographic point groups and space groups - X-ray diffraction - powder and rotating crystal methods - systematic absences and determination of lattice types - analysis of X-ray data for cubic system - structure factor and Fourier synthesis -Fundamentals of electron and neutron diffraction.	4
Chemistry of Nanostructure Materials Introduction; fundamentals of nanomaterials science, surface science for nanomaterials, colloidal chemistry; Synthesis, preparation and fabrication: chemical routes, self-assembly methods, biomimetic and electrochemical approaches; Size controls properties (optical, electronic and magnetic properties of materials) - Applications (carbon nanotubes and nanoporous zeolites; Quantum Dots, basic ideas of nanodevices)	4

Introduction to nanoscience and nanotechnology Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything.* fundamental physicochemical principles - size dependence of the properties of nanostructured matter -quantum confinement, single electron charging, the central importance of nanoscale morphology. Societal aspects of nanotechnology: Health, environment, hype and reality. The advent of the nanomaterial. Top down and bottom up approaches to building materials. Properties of nanomaterials such as nanoparticles, carbon nanotubes. Overview of self-assembly. Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, ball milling, molecular beam epitaxy, chemical vapour deposition method and electro deposition.	5
The basic tools of nanotechnology Scanning electron microscopy (SEM), TEM and EDAX analysis and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM) and an introduction to its basic principles& applications. Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-Vis-IR spectrophotometers, Principle of operation and application for band gap measurement.	5
Metal nanoparticles Size control of metal nanoparticles and their characterization, study of their properties, optical, electronic, magnetic. Surface plasmon band and its applications, role in catalysis, alloy nano particles, stabilization in sol, glass, and other media, change of bandgap, blueshift, colour change in sol, glass, and composites, Plasmon resonance	4
Carbon nanostructures Introduction. Fullerenes, C60, C80 and C240 nanostructures. Properties & applications (mechanical, optical and electrical). Functionalization of carbon nanotubes, reactivity of carbon nanotubes. Nano-sensors: Temperature sensors, smoke sensors, sensors for aerospace and defence. Accelerometer, pressure sensor, night vision system, nano tweezers, nano-cutting tools, integration of sensor with actuators and electronic circuitry biosensors.	4
Student Work • Assignments, Tutorials	9

• Reviews of various research papers, reports, books • Presentations	

Suggested Reading:

1. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.
2. G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.
3. C. N. R.Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials, Volume Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004, Chapter 4.
4. Nanoparticles- Theory and Applications by Schmid
5. Carbon Nanomaterials by Challa
6. Nanomaterials- Synthesis, properties and applications by Rao CNR, Miller A, Cheetham AK.
7. Solid State Chemistry and it's Applications by West/ Nanoscale materials in Chemistry by Klabunde
8. Carbon Nanotubes- Basic Concepts and Physical Properties by Reich S, Thomsen C, Maultzsch

CHM 602 - Bioinorganic and Coordination chemistry	
Topic Details	**Lectures**
Metal ligands in biological system • Amino acid side chains, specialized ligands, porphyrins, enterobactin, etc. • availability of Fe, Cu and Zn • uptake of Fe, gut, transferrin and ferritin • oxygen transport • Zn-source of nucleophilic –OH, Cu-essential but toxic • photosynthesis-chlorophyll reaction center and oxygen evolving center.	6
Theories of coordination compounds VB theory - CFT - splitting of d orbitals in ligand fields and different symmetries - CFSE - factors affecting the magnitude of 10 Dq – evidence for crystal field stabilization - spectrochemical series - site selection in spinels – tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - Nephelauxetic effect – MO theory - octahedral - tetrahedral and square planar complexes-bonding and molecular orbital theory - experimental evidence for -bonding.	6

Reactions Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution - ligand field effects and reaction rates - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases - racemization and isomerization - mechanisms of redox reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms - mixed valent complexes.	6
Electronic spectra and magnetism Microstates, terms and energy levels for d1 – d9 ions in cubic and square fields - selection rules - band intensities and band widths - Orgel and Tanabe-Sugano diagrams - evaluation of 10 Dq and β for octahedral complexes of cobalt and nickel - charge transfer spectra - magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena.	5
Structure Structure of coordination compounds with reference to the existence of various coordination numbers (2, 3, 4, 5 & 6) - site preferences - isomerism - trigonal prism - absolute configuration of complexes - stereo selectivity and conformation of chelate rings - coordination number seven and eight. Spectral and magnetic properties of lanthanide and actinide complexes.	5
IR and Raman spectroscopy Structural elucidation of simple molecules like N2O, ClF3, NO3-, ClO4- - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and DMSO - effect of isotopic substitution on the vibrational spectra of molecules - applications of Raman spectroscopy.	5
EPR theory and instrumentation, spin Hamiltonian, isotropic and anisotropic EPR spectra, magic pentagon rule, applications of EPR spectroscopy (i) in structure determination of coordination complexes and (ii) metalloproteins (Fe and Cu)	3

Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Reading:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, 4thEdition, Harper Collin College Publishers, 1993.
2. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 4th& 5thEdns, Wiley Interscience, New York, 1998.
3. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Edition, Wiley Eastern, 1992.
4. J. Lewis, R.G. Wilkins, Modern Coordination Chemistry, Inter Science Publisher, 1960.
5. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford University Press, Oxford, l994.
6. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A &Part B, 2ndEdn, Wiley. 2009.
7. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson Prentice Hall, 2005
8. J.E. House, Inorganic Chemistry, Elsevier, 2008.
9. Housecroft and Sharpe, 3rd ed, Chap 29; Weller et al, 6th ed, Chap 26.
10. Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons
11. Douglas, B.E., McDaniel,D.H. and Alexander, J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons
12. Figgis, B.N., and Hitchman, M.A "Ligand Field Theory and Its Applications", Wiley Eastern Ltd
13. Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education, Inc.

CHM 603 - Natural Product and Heterocyclic chemistry	
Topic	**Lectures**
Classification of natural products Chemical structure, classification, structure elucidation based on degradative reactions- Isolation and structural elucidation of selected alkaloids and terpenes- quinine, morphine, and reserpine, citral, juvabione and logiofolene –Insect pheromones.	5

Amino Acids, Peptides and Proteins Classification of Amino Acids, Zwitterion structure and Isoelectric point. Synthesis of amino acids-reactions - properties- Amino Acids in Nature: - Amino Acids and their Metabolites in Nature –Structure of proteins- Peptides.	5
Steroids classification- Synthesis and structure elucidation of cholesterol, conversion of cholesterol to progesterone- androsterone and testosterone-cortisone- Vitamin D – Nucleic Acids- structure of nucleosides and nucleotides-RNA and DNA, Watsons and Crick model DNA-drug interaction	5
Carbohydrates Classification of carbohydrates, reducing and non-reducing sugars, General properties of glucose and fructose, their open chain structure. Epimers, muta-rotation and anomers. Determination of configuration- Hudsons rules-Structure of sugars transformation of sugars, Preparation of alditols, glycosides, deoxysugars. Synthesis of vitamin C from glucose.	5
Heterocycles Synthesis, Properties and uses of Five membered heterocyclic ring systems with one or two hetero atoms-Furan, pyrrole, thiophene and thiazole: six membered heterocyclic ring system-Pyridine. Fused heterocyclic ring systems- Indole, quinoline. Biologically important heterocycles: Pyrimidines and purines.	8
New materials derived from heterocycles Syntheses of cyanines and related dyes. Organic sensitizers for DSSC, electron donors and acceptors for organic solar cells, optical chemo-sensors and organic semiconductors for thin-film transistors.	8
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Reading:

1. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education, 6thedn.
2. F. A. Carey and R. J. Sundberg, (Eds) 3rd Edition, Part B. Plenum/Rosetta, 1990.
3. I. Fleming, Selected Organic Synthesis, John Wiley and sons, 1982.
4. Atta-ur-Rahman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.
5. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press.
6. R. J. Simmonds: Chemistry of Biomolecules: An Introduction, RSC.

7. Designing organic Synthesis by Stuart Warren1983.
8. Organic Chemistry by Cram andHammond.
9. Organic Chemistry by Clayden, Greeves, Warren andWothers

CHM 604 - Separation Techniques and Advanced Analytical Techniques	
Topic	**Lectures**
Extractionstechniques Partition law and its limitations, distribution ratio, separation factor, factors influencing extraction, multiple extractions. Extraction of metal. Technique of extraction: batch, continuous and counter current extractions. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non- aqueous media.	8
Chromatography Introduction and classification, theory of column chromatography, retention time, retention volume, capacity factor, concept of plate and rate theory, resolution, column performance, normal and reverse phase chromatography, paper and thin layer chromatography, ion-exchangers.	6
GC principle, instrumentation, Application Introduction, Theory, Principle, GSC and GLC, Seperation mechanism involve in GSC and GLC, Instrumentation of Gas chromatography, working of gas chromatography, gas chromatogram and qualitative –quantitative analysis. Application of Gas chromatography	4
HPLC principle, instrumentation, Application Introduction, Need of liquid chromatography, Seperation mechanism involved in adsorption and partition HPLC, Instrumentation and working of HPLC, Applications of HPLC, Introduction to supercritical fluid chromatography.	4
Mass spectrometry	6
GCMS/LCMS	2
Data Analysis	2

Quantitative chemical analysis; calculation of analytical results (calibration curve method, standard addition method, internal standards method) Significant figures: confidence and interval; Student's T-test; F-test; Q-test	
Sensor Introduction, Classifications of sensors, Sensitivity and Limit of detection, Types of Sensors- Optical, Electrochemical & Biosensor. Application of Sensor in environmental and biological samples.	4
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	9

Suggested Readings

1. Textbook of Quantitative Chemical Analysis- 3rd Edition, A. I.Vogel
2. Principles of Physical Chemistry 4th edition – Prutton andMarron
3. Instrumental Methods of Chemical Analysis- Chatwal andAnand
4. Basic Concept of Analytical Chemistry-2nd edition S.M.Khopkar
5. Vogel's textbook of Quantitative Inorganic Analysis-4th edition Besset Denney, Jaffrey,Mendham
6. Instrumental Methods of Chemical Analysis- 6th edition Willard, Merritt, Dean andSettle
7. Analytical Chemistry bySkoog
8. Introduction to Instrumental Analysis- R.D. Braun
9. Instrumental methods of Chemical Analysis-Willard, Dean &Merrit- 6th Edition

Elective Course 3 - Materials Chemistry	
Topic Details	**Lectures**
Basics of crystalline solids Crystalline solids, crystal systems, Bravais lattices, coordination number, packing factors – cubic, hexagonal, diamond structures, lattice planes, Miller indices, interplanar distances, directions, types of bonding , lattice energy, Madelung constants, Born Haber cycle, cohesiveenergy,Symmetryelements,operations,translationalsymmetriespointgroups,spacegroups,equivalent positions, close packed structures, voids, crystal structures, Pauling rules, defects in crystals, polymorphism,twinning.	8

Silica based materials Introduction to Zeolites, metallosilicates, silicalites and related microporous materials, Mesoporous silica, metal oxides and related functionalized mesoporous materials: Covalent organic frameworks, Organic-Inorganic hybrid materials, periodic mesoporous organo silica, metal organic frameworks: H_2 /CO_2 gas storage and catalytic applications	8
Composite materials Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.	8
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	6

Suggested readings:

- Atkins P, Overton T., Rourke J. Weller M. and Armstrong F Shriver and Atkins. Inorganic Chemistry Oxford University Press, Fifth Edition,2012.
- Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry. JohnWiley,1974.
- Poole, C.P. & Owens, F.J. Introduction to Nanotechnology John Wiley2003.
- Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning,

Elective Course 4 - Supramolecular chemistry	
Topic Details	**Lectures**
Introduction-the meaning of supramolecular chemistry, phenomenon of molecular recognition and their quantification	1
Building blocks of supramolecular chemistry- acyclic receptors for neutral and charged guests, macrocycles and crown ethers, macrobicycles and cryptands, macropolycycles, cucurbiturils and cyclodextrins	8
Sensors and information processing, electro-optic phenomena, molecular machines	6
Amphiphilic molecules and their aggregation, Langmuir-Blodgettry, molecular recognition at the air-water interface	2
Discrete and polymeric metal-organic hybrid materials- guest inclusion, catalysis and other applications.	6
Future scopes	1
Student Work • Assignments, Tutorials • Reviews of various research papers, reports, books • Presentations	6

, Suggested Reading:

1. Supramolecular Chemistry: Concepts and Perspectives, J.-M. Lehn, VCH, Weinheim, 1995.
2. Principles and Methods in Supramolecular Chemistry, H. J. Schneider and A. Yatsimirsky, Wiley, New York, 2000.
3. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester, 2009.
4. Steed, J.W. and Aswood, J.L., "Supramolecular Chemistry", Wiley.
5. Dodziuk, H, "Introduction to Supramolecular Chemistry", Springer, ISBN 1402002149.
6. Beer, P.D., Gale, P.A. and Smith, D.K., "Supramolecular Chemistry", Oxford Chemistry Printers, ISBN-10: 0-19-850447-0.
7. Cragg, P., "A Practical Guide to Supramolecular Chemistry", Wiley-VCH, ISBN: 0-470-86654-3.
8. Schneider, H.J. and Yatsimirsky, A., "Principles and Methods in Supramolecular Chemistry", Wiley-VCH, ISBN: 0-471-97253-3.

CHM 607 - Physical/Analytical chemistry Lab

1. Preparation and characterization of MgO nanoparticle.
2. Preparation and characterization of ZnO nanoparticle.
3. Preparation and characterization of Graphene Oxide.
4. Green synthesis of metal and metal oxide nanoparticles from plant leaves extract.
5. Green synthesis of Silver nanoparticles using neem leaves.
6. Determination of Iron by UV-Visible Spectrophotometry
7. Determination of Iron by Atomic Absorption Spectrometry
8. Determination of Caffeine in Soft Drinks by High Performance Liquid Chromatography.
9. Environmental Monitoring of Hydrocarbons: A Chemical Sensor Perspective.

CHM 608 - Inorganic /Organic chemistry Lab

1. Synthesis and spectrophotometric study of copper complexes: (i) synthesis of bis(salicylaldimine)copper(II) and cis-bis(glycinato)copper(II),
2. Study of the complex formation between Fe(III) and thiocyanate/salicylic acid/sulphosalicylic acid or between Ni(II) and *o*-phenanthroline, and (ii) spectrophotometric determination of formation constant of the complex (Job's method and molar ratio method).
3. Synthesis of tetraamminecopper (II) sulfate monohydrate [Cu(NH3)4]SO4•H2O
4. Eucalyptus oil from leaves (Steam distillation)
5. Fisher indole synthesis
6. Separation of Aminoacids/ sugars by paper chromatography and TLC
7. Synthesis of Natural product (any 2)
8. To perform colour tests for carbohydrates for reducing/non-reducing sugars.

EVSB 609 - Project/ Dissertation

Project-based learning offers an opportunity to the students to work independently under guidance of a supervisor. Students will be assigned to the on campus faculty/ research scientists from various national research institutes such as NCL/ IISER/ working in chemistry research; under whose

guidance he or she would work on a problem keeping the focus to enhance their own ability to critical thinking, identification of research problems and research gaps, formulate research objectives, formulation of research plan, and problem solving via execution of specific experiments, and develop specialized skills to handle specific problems. This would train the students to nurture their creativity and innovative ideas, collaboration/teamwork and leadership, communications, learning self-reliance and project management.

Adequate assessment requirements for individual marking are presentations with discussions and seminars on the working process and the results.

Summer training / Internship

Even though summer training/internship is not mandatory and not a part of curriculum; students will be encouraged to work as summer trainee or interns in other institutes/ laboratories/ industries depending upon the scopes and availability during summer/winter recess.

After the period of training, it is expected that students achieve the following:

- Recognize the duties, responsibilities and ethics at a professional position.
- Ability to apply knowledge learned to solve specific problems in relevant domain of science.
- Gain exposure and practical experience in the relevant field.
- Ability to prepare technical reports for the training.
- Ability to communicate effectively in the work environment.