SHIV NADAR UNIVERSITY
Chemistry

Department of Chemistry

Chemistry forms the link between the fundamental principles governing the nature of the universe and the science of life. Chemistry education at SNU provides focus on a variety of inter-disciplinary areas, spanning different scientific disciplines as well as non-traditional areas in the arts and humanities, *e.g.* a Major in Chemistry can be combined with a Minor in Bioinformatics at SNU. Or you can pursue a Major in Chemistry with a specialization in either Chemical Physics or Chemical Biology.

Our research programs reach across the campus and beyond, linking together departments, schools, inter-disciplinary centers and internship opportunities in the chemical industry and national labs. University-wide elective courses in the curriculum allow students unprecedented freedom to explore subjects outside their chosen major, in some depth. This flexible and broad curriculum prepares students not just for a career in chemistry upon graduation, but for a leadership role in the world as well.

The Undergraduate Chemistry Experience

The chemistry curriculum at SNU provides both a broad background in chemical principles and in-depth study of chemistry or chemistry-related areas that build on this background. The chemistry curriculum is divided into three categories: introductory general chemistry, foundation courses providing breadth across sub-disciplines, and rigorous in-depth courses that build upon these foundations and develop critical thinking and problem-solving skills. Since chemistry is an experimental science, substantial laboratory work is an integral part of almost all our courses. The introductory general chemistry course provides a common grounding in basic chemical concepts for students with diverse backgrounds, develops basic mathematical and laboratory skills, and prepares students for the foundation courses. Foundation courses in analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry provide breadth and lay the groundwork for more in-depth course work.

Laboratory Experience: The chemistry laboratory experience at SNU includes synthesis of molecules; measurement of chemical properties, structures, and phenomena; hands-on experience with modern analytical instrumentation; and computational data analysis and modeling. All laboratory programs are conducted in a safe environment that includes adherence to national and state regulations regarding hazardous waste management and laboratory safety including, facilities for chemical waste disposal, safety information and reference materials, and personal protective equipment available to all students and faculty. The chemistry laboratories at SNU are equipped with functioning fume hoods, safety showers, eyewashes, first aid kits, and fire extinguishers must be readily available. Students are trained in modern chemical safety, to understand responsible disposal techniques, understand and comply with safety regulations, understand and use material safety data sheets (MSDS), recognize and minimize potential chemical and physical hazards in the laboratory, and know how to handle laboratory emergencies effectively.

Problem-Solving Skills: As part of the SNU experience, students will be expected to develop the ability to define problems, develop testable hypotheses, design and execute experiments, analyze data using statistical methods, and draw appropriate conclusions. The chemistry curriculum provides ample opportunities for developing both written and oral communication skills, as well as team skills. Our instructional programs incorporate team experiences in classroom and laboratory components of the chemistry curriculum.

Careers in Chemistry

Chemistry forms the scientific basis for a wide variety of career options, ranging from traditional areas such as academics, pharmaceuticals, chemical analysis and synthesis, quality control and quality assurance, to inter-disciplinary fields such as molecular biology, materials science and biophysics, and non-traditional areas such as medicine, patent or environmental law, forensic science, technical writing, art conservation, environmental studies, *etc*.

Undergraduate Research in Chemistry

Research activities are not confined to post-graduate level, but are integrated into the under-graduate program at SNU through our REAL (Research Experiential & Applied Learning) courses. Undergraduate research allows students to integrate and reinforce chemistry knowledge from their formal course work, develop their scientific and professional skills, and create new scientific knowledge. Original research culminating in a comprehensive written report provides an effective means for integrating undergraduate learning experiences, and allows students to participate directly in the process of science. Opportunities for research in chemistry at SNU are available in the following broad areas:

- Catalysis
- Chemical biology
- Cheminformatics
- Chemistry of nanomaterials
- Computational quantum chemistry
- Coordination Chemistry
- Green chemistry
- Medicinal chemistry
- Molecular Toxicology
- Polymer chemistry
- Structural Chemistry and Crystallography
- Supramolecular Chemistry
- Synthetic Organic Chemistry

Major in Chemistry

The basic undergraduate degree program offered by the Department of Chemistry is the Bachelor of Science (B.Sc. (Research)) in Chemistry.

Every chemistry undergraduate student of the University is required to take a number of credits from courses broken up into the following categories:

a) CCC (Common Core Curriculum courses offered by the university)
b) UWE (University Wide Electives; courses so designated and offered by departments other than Chemistry)
c) Introductory Chemistry courses (CHY100 – 199)
d) Foundation Chemistry courses (CHY200 – 299)
e) In-Depth Chemistry courses (CHY300 – 499)

The credit requirements for **B.Sc (Research) Chemistry** are:

105 credits = 51 credits in compulsory Chemistry courses (10 Introductory + 21 Foundation + 20 In-Depth) + 36 required Physics/Maths/Life Sci/CS + 6 credits Chemistry electives + 12 credits Senior Project.

+ 24 credits CCC courses + 18 credits UWE courses.

Minor in Chemistry

Undergraduate students of the university who are not majoring in Chemistry have the option to take a Minor in Chemistry. **Academic Requirements for Chemistry Minor:**

29 credits = 21 credits in compulsory courses (10 Introductory + 11 Foundation) + 8 credits chosen from the Chemistry electives.

Chemistry Course Catalog

The chemistry program at SNU provides both a broad background in chemical principles and in-depth study of chemistry or chemistry-related areas that build on this background. The chemistry curriculum is divided into three parts: (1) the introductory chemistry experience, (2) foundation course work that provides breadth, and (3) rigorous in-depth course work that builds on the foundation. Because chemistry is an experimental science, substantial laboratory work is an integral part of this experience.

Introductory or General Chemistry: The introductory or general chemistry experience plays a vital role in educating all students. The introductory courses provide a common background for students with a wide range of high school experiences, and allow a period for consolidation of chemical concepts, as well as mathematical and laboratory skills. For students pursuing a chemistry major, the introductory chemistry courses provide preparation for the foundation course work, ensuring that students know basic chemical concepts such as stoichiometry, states of matter, atomic structure, molecular structure and bonding, thermodynamics, equilibria, and kinetics. Students also need to be competent in basic laboratory skills such as safe practices, keeping a notebook, use of electronic balances and volumetric glassware, preparation of solutions, chemical measurements using pH.

CHY101: **Applied Chemistry** (5 credits: 3 Lectures+ 1 Tutorial + 3-hour Lab) Monsoon

This course will focus on applying principles of chemistry to engineering problems. The principles taught in the course will enable the conceptualization of engineering models. Topics include the problems associated with using untreated water in industries; selecting appropriate methods of treating water for industrial and domestic purposes; understanding the properties of polymers; applications of engineering plastics and relation to properties; constructing electrochemical cells; determining the chloride and iron content in electrolytes; corrosion related problems which occurs due to improper design / selection of materials / incompatible environment; selecting an appropriate method of corrosion prevention; manufacture of coke, cracking, and production of water gas and producer gas; methods of coal analysis.

COURSE CONTENT:

1: Atomic structure, Periodic table, Quantum Chemistry, Spectroscopy

2: Thermodynamics, Energy, Chemical Kinetics, Photosystems

3: Nanomaterials, Organic Chemistry, Polymers

4: Water Corrosion and Biochemistry

Prerequisite: None.

CHY111: **Chemical Principles** (5 credits: 4 Lectures/Tutorial + 3-hour Lab) Monsoon

This course will focus on introductory chemical principles, including periodicity, chemical bonding, molecular structure, organic functional groups, equilibrium and the relationship between structure and properties. Students will explore stoichiometric relationships in solution and gas systems which are the basis for quantifying the results of chemical reactions. Understanding chemical reactivity leads directly into discussion of equilibrium and thermodynamics, two of the most important ideas in chemistry. Equilibrium, especially acid/base applications, explores the extent of reactions while thermodynamics helps us understand if a reaction will happen. The aim of the laboratory will be to develop your experimental skills, especially your ability to perform meaningful experiments, analyze data, and interpret observations. This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

COURSE CONTENT:

1. **The Principles of Periodicity and Chemical Bonding:**
   - Introduction of statistical concepts in physics
   - The statistics of electrons
   - The Born-Oppenheimer approximation and molecular structure
   - Atomic and molecular orbitals; Chemical bonding
   - Chemical periodicity & electronic structure
   - Inter-molecular forces; Spectroscopy
2. **The Principles of Chemical Equilibrium:**
   - Heat & Work; State Functions

- Laws of thermodynamics
- Probability and Entropy
- Ionization Equilibria; pH; Acid-Base Titration
- Activation Energy; Arrhenius equation
- Thermodynamic and Kinetic Stability
- Free Energy, Chemical Potential, Electronegativity
- Phase Rule
- Electrochemistry
- Renewable sources of energy; Photosystem II.

Prerequisite: None.

CHY112: **Structure and Bonding** (5 credits: 3 Lectures+ 1 Tutorial + 3-hour Lab) Spring

This course will introduce atomic theory, classical and quantum bonding concepts, and chemical kinetics. Students will be introduced to new lab techniques and ways to measure progress of reactions. Kinetics (rates of reaction) provides information about how reactions work and, along with thermodynamics, provides the basis for evaluating the viability of a reaction. This concept will be explored particularly with respect to substitution reactions. The class will have reading assignments and lecture/discussion meetings at which we will critically examine the major concepts, discuss articles, and review some of the current developments in the field. Taking Chemical Principles and Structure and Bonding provides a good background for students interested in environmental applications. This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

<u>Unit-1</u>: Chemical periodicity

Chemical periodicity: Periodic table, group trends and periodic trends in physical properties. Classification of elements on the basis of electronic configuration. Modern IUPAC Periodic table. General characteristic of s, p, d and f block elements. Position of hydrogen and noble gases in the periodic table. Effective nuclear charges, screening effects, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii. Ionization potential, electron affinity and electronegativity (Pauling's, Mulliken's and Allred-Rochow's scales) and factors influencing these properties. Inert pair effect. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements.

<u>Unit 2</u>: Chemical Bonding and structure and acid-base reactions

Ionic bonding: Size effects, radius ratio rules and their limitations. Packing of ions in crystals, lattice energy, Born-lande equation and its applications, Born-Haber cycle and its applications. Solvation energy, polarizing power and polarizability, ionic potential, Fazan's rules.

Covalent bonding: Lewis structures, formal charge. Valence Bond Theory, directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, VSEPR theory, Bonding, inductive effect, Hyperconjugation effect, mesomeric effect shapes of molecules and ions containing lone pairs and bond pairs (examples from main groups chemistry), Partial ionic Character of covalent bonds, bond moment, dipole moment and electronegativity differences. Concept of resonance, resonance energy, resonance structures

Acid-Base reactions : Acid-Base concept; Arrhenius concept, theory of solvent system (in H_2O, NH_3, SO2 and HF), Bronsted-Lowry's concept, relative strength of acids, Pauling rules. Amphoterism. Lux-Flood concept, Lewis concept. Superacids, HSAB principle. Acid-base equilibria in aqueous solution and p_H. Acid-base neutralisation curves; indicator, choice of indicators.

Unit 3: An Introduction to Coordination Compounds

Group theory, Bonding in coordination compounds, d-orbitals, t_{2g}-e_g splitting, structures of coordination complexes, octahedral and tetrahedral complexes, square planar complexes

Unit 4: Basics of Organic Chemistry

Homolytic and heterolytic bond fission; Hybridization, Bonding, inductive effect, Hyperconjugation effect, mesomeric effect, acidity and basicity of organic molecules, pKa,. Organic reactions; nucleophilic substitution, elimination, addition and electrophilic aromatic substitution reactions. Basic concept for characterization of organic molecules.

Reaction intermediates: Carbocations, carbanions, free radicals,carbenes, Benzynes - their shape and stability.

Electron displacements Inductive, electromeric, resonance, hyperconjugation.

Electrophiles and nucleophiles. Nucleophilicity and Basicity

Intermolecular forces of attraction: van der Waals forces, ion-dipole, dipole-dipole and hydrogen bonding.

Aromaticity and Tautomerism

Acidity/Basicity: Alkanes/Alkenes, Alcohols/Phenols/Carboxylic acids, Amines

Molecular chirality and Isomerism: Cycloalkanes (C3 to C8): Relative stability, Baeyer strain theory and Sachse Mohr theory.

Stereochemistry: Structural- and Stereo-isomerism.

Molecular representations: Newman, Sawhorse, Wedge & Dash, Fischer projections and their inter conversions.

Conformations and Conformational analysis: Ethane, n-butane, ethane derivatives,

cyclohexane, monosubstituted and disubstituted cyclohexanes and their relative stabilities.

Geometrical isomerism in unsaturated and cyclic systems: cis–trans and, syn-anti isomerism, E/Z notations. Geometrical isomerism in dienes- Isolated and conjugated systems, determination of configurations.

Chirality and optical isomerism: Configurational isomers. Molecules with one or two chiral centres- constitutionally symmetrical and unsymmetrical molecules; Enantiomers and Diastereomers. Optical activity, Disymmetry, Meso compounds, racemic modifications and methods of their resolution;

stereochemical nomenclature: erythro/threo, D/L and R/S nomenclature in acyclic systems. Measurement of optical activity: specific rotation.

Substitution reactions: Free radical- Halogenation, relative reactivity and selectivity; Allylic and benzylic bromination; Nucleophilic Subsititution (S_N1, S_N2, S_N1', S_N2' S_Ni) ;Electrophilic Substitution (S_NAr, Addition Elimination vs. Elimination addition); Organometallic reagents.

Prerequisite: Chemical Principles.

CHY120: **Molecules and Medicines** (3 credits: 3 Lectures) Spring [UWE]

Since the time of Hippocrates until modern days, human being has explored several means of alleviating pain and curing disease. There have been pathbreaking discoveries resulting in the development of medicines of immense benefit. Present day research of inventing novel molecules constantly adds to the repertoire of drugs available to counter ill-health.

We will begin with a short introduction (which discusses fundamental organic chemistry followed by development and testing of drugs). Next we will explore the discovery and development of a range of drugs and medicines that relieve pain, effect cures and reduce the symptoms of ill-health. We will discuss how drugs interact with and affect their target areas in the human body. There are online videos to help you to understand the three-dimensional structures and shapes of the molecules concerned and to develop an understanding of how the drugs work.

Prerequisite: CHY101.

CHY140: **Chemistry of Color and Art** (3 credits: 2 Lectures+ 2-hour Lab) Spring [REAL, UWE]

This inter-disciplinary course will introduce students to the basic principles of optics, and the chemical principles behind the colors of gemstones and pigments. Absorption and scattering of light, emission of light from gases and generation of light from electricity, chemical reactions and thermal radiation will be discussed. Students will have the opportunity to discover for themselves the fundamentals of chemical and digital photography, color vision and art. Field trips to natural locations, art galleries and museums will be included to provide opportunities for creating individual works of art.

Prerequisite: None.

Foundation Courses: Foundation courses provides breadth and lays the groundwork for the in-depth course work in each of the five major areas of chemistry: analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry. The chemistry laboratory experience at SNU includes synthesis of molecules; measurement of chemical properties, structures, and phenomena; hands-on experience with modern instrumentation; and computational data analysis and modeling. Students get hands-on experience with a variety of analytical instruments, including spectrometers, and are expected to understand the operation and theory of modern instruments and use them to solve chemical problems as part of their laboratory experience.

CHY211: **Chemical Equilibrium** (5 credits: 3 Lectures+ 1 Tutorial + 3-hour Lab) Monsoon

In this we will adopt a case studies approach to understanding thermodynamic principles already familiar to students from earlier courses. The culmination of the course will be a capstone project developed by each student. The student will develop a question, research background, develop an experimental plan, carry it out and present the results to the class. In class we will explore real chemical questions involving equilibrium, acid base chemistry, electrochemistry, surface phenomena and solution chemistry by reading and discussing research papers.

Prerequisites: Chemical Principles.

CHY213: **Chemical Analysis lab** (3 credits: 1 Lecture + 3-hour Lab) Monsoon

Analyses of compounds are an integral aspect of chemistry. We get to know the structure, spatial orientation and purity of compounds we synthesize through analysis which helps us to advance in our investigation. To address this purpose a bevy of instruments ranging from UV spectroscopy, IR spectroscopy to High Pressure Liquid Chromatography are available. However accurately understanding the output from these instruments is an essential attribute for a successful chemist. In this course we will learn to interpret and understand working of various types of analytical instruments commonly used for analysis in a chemistry lab.

1. Introduction-Infra Red Spectroscopy (1 experiment and 2 lectures)
2. Ultra Violet Spectroscopy (2 experiments and 4 lectures)
3. Fluorescence Spectroscopy (3 experiments and 6 lectures)
4. Nuclear Magnetic Resonance Spectroscopy (4 experiments and 8 lectures)
5. Liquid chromatograph mass spectrometry and high performance liquid chromatography (3 experiments and 6 lectures)
6. X-Ray crystallography (3 experiments and 6 lectures)

Prerequisites: Chemical Principles, Structure & Bonding.

CHY221: **Organic Reactions and Mechanisms** (4 credits: 3 Lectures + 3-hour Lab) Monsoon

Fundamental Reaction Types, Electrophiles, nucleophiles, reaction intermediates (carbocation, carbanion, carbene, nitrene etc), concept of transition state, Acid base chemistry, basicity vs nucleophilicity, Nucleophilic substitution reactions (SN1, SN2, SN_{Ar} etc), Elimination reactions, Saytzeff rule, Hoffman rule, Substitution vs elimination, importance of pKa in organic reaction mechanism, addition to double bonds, markonikoff vs anti-markonikoff's rule, reactions at the carbonyl center, tautomerism concept, aromaticity, resonance concept, resonance vs tautomerism, electrophilic aromatic substitution reactions, concept of rate limiting step, Hammett equation and Taft equation, Kinetic isotope effect, Hammond's postulate.
C-C bond forming reactions and their mechanism focusing on Carbanion alkylation, Carbonyl addition and carbonyl substitution reactions, Conjugate addition reactions (1,2-addition & 1,4- addition), Reactions of alkene, alkynes and aromatics. C-N and C-O bond forming reactions and their mechanism.

Glycosylation reactions. Oxidation and reduction reactions, Rearrangement reactions, Free radical reactions. Photochemical reactions and mechanism, Norrish type I and II reactions, Electrophilic substitution reactions. The above reaction will be taught under some name reactions.

Prerequisites: Chemical Principles, Structure & Bonding.

CHY242: **Coordination Chemistry** (4 credits: 3 Lectures + 3-hour Lab) Spring

Metals ions play important role in producing color in so called "coordination complexes". Understanding of the coordination complexes lies at the heart of coordination chemistry. This course will focus on the basic concept of coordination chemistry and their quantification in photophysical and magnetic properties. Students will synthesize interesting color compounds and perform reactions to promote the understanding of common reactions. Intensive use of analytical and spectroscopic techniques to interpret extent of reaction, purity of product and photophysical property particularly color of the coordination complexes will be involved.

Introduction: Meaning of metal coordination and use of metal coordination in formation of color complex

Structures of complexes: Coordination number, bonding of organic ligands to transition metals, coordination number, linage isomerism, electronic effects, steric effects, the chelate effect, Fluxional molecule.

Spectra & bonding: MO diagram: CO, O_2, N_2, $-CN$, H_2O, NH_3, BF_3; Valence bond theory: Application and limitations; Crystal field theory: application and limitation; Molecular orbital theory: Application in ⍰-bonding, electronic spectra including MLCT, LMCT d-d transition, and magnetic properties of complexes.

Reaction and kinetics: Nucleophilic Substitution reaction, rate law, mechanism of reactions, trans effect, ligand field effect, iner sphere and outer sphere reaction.Prerequisites: Chemical Principles, Structure & Bonding.

CHY244: **The Nature of Materials** (3 credits) Spring [REAL]

Students will apply the principles of chemistry to substantive research projects that they will design, execute, and present. Lecture material will focus on the principles behind modern materials such as polymers, semi-conductors, and novel nanostructures.

Prerequisites: Chemical Principles, Structure & Bonding, Organic Reactions & Mechanisms.

CHY252: **Biochemistry** (3 credits: 2 Lectures + 3-hour Lab) Spring [REAL]

Students in this course will apply principles from general and organic chemistry, as well as general biology, to understand the molecular processes that characterize life. The goal of this class will be to give students a solid background with which they can appreciate the chemistry of life. Beginning with fundamental principles, the course will then delve into a detailed look at metabolism - the specific means by which organisms use chemical energy to drive cell functions and how they convert simple molecules to complex biological molecules. Students will have the opportunity for independent work, and will apply the principles of biochemistry to a research project that they will design, execute, and present. Taking Chemical Principles, Structure & Bonding and Biochemistry provides the basic foundation for students interested in a minor in Bioinformatics.

Pre/Co-requisites: Chemical Principles, Structure & Bonding, Essentials of Biology.

In-Depth Courses: In-depth courses provide not only advanced instruction, but also development of critical thinking and problem-solving skills. Students are expected to be able to define problems clearly, develop testable hypotheses, design and execute experiments, analyze data using appropriate statistical methods, and draw appropriate conclusions, applying an understanding of all chemistry sub-disciplines. Students are also expected to be able to use the peer-reviewed scientific literature effectively and evaluate technical articles critically, learning how to retrieve specific information from the chemical literature, with the use of online, interactive database-searching tools.

CHY311: **Chemical Binding** (4 credits: 3 Lectures + 2-hour Computer Lab) Monsoon

Quantum mechanics provides the microscopic basis for a fundamental understanding of chemistry, molecular structure, bonding, and reactivity. This course and the associated computer lab provide a comprehensive treatment of valence bond and molecular orbital theories, post Hartree-Fock wave function and density functional methods. Students will learn to compute molecular structures, spectra, and thermochemical parameters for molecules in the gas-phase and for condensed-phase systems.

- Postulates of Quantum Mechanics
- Atomic Orbitals and Basis Sets
- The Born-Oppenheimer approximation and the molecular Hamiltonian
- The Concept of the Potential Energy Surface
- Geometry Optimization techniques
- Semiempirical and *ab initio* Quantum Mechanics
- Variation and Perturbation Theory
- Valence Bond and Molecular Orbital theories
- Independent-Particle Models: the Hartree method
- Spin, statistics and the Pauli principle
- The Hartree-Fock Self-Consistent Field equations
- Electron Correlation, Density Matrices and Natural Orbitals
- Density Functional Theory
- Periodic systems
- Implicit and explicit solvent methods
- QM/MM and ONIOM

Prerequisites: Chemical Principles, Structure & Bonding, Calculus, Linear Algebra, physics, CS.
Co-requisite: Molecular Spectroscopy.

CHY313: **Molecular Spectroscopy** (4 credits: 3 Lectures+ 3-hour Lab) Monsoon

Introduction to spectroscopy and its applications, Application of rotational spectroscopy, vibrational spectroscopy, vibration-rotation spectrum, application of IR spectroscopy in identification of functional groups, Theory of UV-Vis/electronic spectroscopy, Introduction to fluorescence spectroscopy, Introduction to mass spectroscopy, Introduction to Nuclear Magnetic Resonance (NMR).

Introduction: Meaning of spectroscopy and use of different spectroscopic tools to understand diverse applications

Origin of a spectra: Energy and electromagnetic spectrum, factors affecting line broadening and intensity of lines, selection rules, rotational spectroscopy of diatomic molecules, Effect of isotopic substitution, Non-rigid rotator,

Rotational& vibrational spectroscopy: Application of rotational spectroscopy, vibrational spectroscopy, vibration-rotation spectrum, breakdown of Born-Oppenheimer Approximation, vibration of polyatomic molecules, application of IR spectroscopy in identification of functional groups.

UV-vis spectroscopy: Theory of UV-Vis/electronic spectroscopy: Lambert-Beer's Law, Woodward-Fieser Rules, Chemical analysis by electronic spectroscopy;

Fluorescence spectroscopy: Introduction to fluorescence spectroscopy: Jablonski diagram, Frank-Condon principle, Stokes shift, solvent relaxation, solvatochromism, excimer and exciplex formation, quantum yield & life time;

Mass spectroscopy: Introduction to mass spectroscopy: isotope effect, fragmentation patterns;

Nuclear Magnetic Resonance (NMR): Introduction to Nuclear Magnetic Resonance (NMR): Basic principles, NMR active nuclei, shielding-deshielding effect, chemicals shift, coupling between nuclei, identification of chemicals compounds.

Prerequisites: Chemical Analysis lab.

Co-requisite: Chemical Binding.

CHY316: **Electrochemistry** (2 credits) Spring

1. General discussion about oxidation and reduction: electron transfer vs atom transfer
2. Concept of free energy
3. Definition: Electrochemical cell, electrodes etc.; types of cell: Electrolytic cell vs Galvanic cell; concentration cell vs chemical cell.
4. Types of electrodes: (i) metal electrode, advantage of amalgam electrode; (ii) non-metal electrode, e.g. hydrogen gas electrode, glassy carbon electrode. What is glassy carbon electrode? What is the difference between glassy carbon and graphite electrode?
5. Definition: Electrode potential, Std. potential and Formal potential; Physical significance of electrode potential.
6. Factors affecting the electrode potential: (i) effect of concentration, (ii) effect of pH e.g. formation of insoluble hydroxide and (iii) effect of precipitation and complexation.
7. Application of electrode potential; Periodic trend of the reduction potential; Pourbaix diagram.

8. Electroanalytical techniques: Potentiometry, Coulometry, Voltammetry and Amperometry.
9. How to measure electrode potential?; 3 electrode system: working electrode, reference electrode and counter electrode; comparison between three and two electrode system; Linear sweep voltammetry, Cyclic voltammetry (CV), Differential pulse voltammetry (DPV) etc.
10. Bulk electrolysis.

Prerequisites: Chemical principals and Chemical equilibrium.

CHY321: **Molecular chirality and Isomerism**

Structural and Stereoisomerism chemistry, conformational analysis & optical activity. Enantiomer, Diastereomer and mesomers. R and S configuration and their importance in biological system.

Prerequisites: Chemical Principles, Structure & Bonding, Organic Reactions and Mechanisms.

CHY323: **Organometallic Chemistry** [+ Lab] (4 credits) Monsoon

The course will discuss various organometallic compounds involving Pd, Pt, Cr, Mo, Mn, their various complexes with several organic ligands and their application in the synthesis of heterocycles and natural products. The course will also cover all the name reactions involving organometallics. Since the advent of Pd as a suitable metal for C-C bond formation along with Ru-in Grubbs Metathesis the present pharmaceutical industry relies heavily on organometallics. Nearly 40% of the reactions in the lab involve organometallics. The intricacies of the reactions, the subtlety of the condition in the reactions involving organometallic compounds requires utmost understand of the mechanism of the reactions. Hence this course will provide an indepth understanding of organometallic reactions and their applications.

Prerequisites: Chemical Principles, Structure & Bonding, Organic Reactions and Mechanisms, Coordination Chemistry.

CHY332: **Informatics & Medicinal Chemistry** (4 credits: 3 Lectures + 2-hour Computer Lab)

This course and the associated computer lab deal with Bioinformatics and Cheminformatics, applied to the search for new drugs with specific physiological effects (*in silico* Drug Discovery). Students will learn the general principles of structure-activity relationship modeling, docking & scoring, homology modeling, statistical learning methods and advanced data analysis. They will gain familiarity with software for structure-based and ligand-based drug discovery. Some coding and scripting will be required. At the end of the course, students will be expected to present a completed piece of software of significant utility and/or an analysis of experimental data from the published literature. Students will be encouraged to seek avenues for publication of their most significant results.

1. Introduction:
   - Drug Discovery in the Information-rich age
   - Introduction to Pattern recognition and Machine Learning
   - Supervised and unsupervised learning paradigms and examples
   - Applications potential of Machine learning in Chem- & Bioinformatics
   - Introduction to Classification and Regression methods

2. Representation of Chemical Structure and Similarity:

- Sequence Descriptors
- Text mining
- Representations of 2D Molecular Structures: SMILES
- Chemical File Formats, 3D Structure
- Descriptors and Molecular Fingerprints
- Topological Indices
- Substructural Descriptors
- Physicochemical Descriptors
- Descriptors from Biological Assays
- Representation and characterization of 3D Molecular Structures
- Pharmacophores
- Molecular Interaction Field Based Models
- Local Molecular Surface Property Descriptors
- Quantum Chemical Descriptors
- Shape Descriptors
- Protein Shape Comparisons, Motif Models
- Molecular Similarity Measures
- Cluster and Diversity analysis
- Network graphs
- Self-Organized Maps
- Semantic technologies and Linked Data

3. Mapping Structure to Response: Predictive Modeling:
   - Linear Free Energy Relationships
   - Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) Modeling
   - Ligand-Based and Structure-Based Virtual High Throughput Screening
   - 3D Methods - Pharmacophore Modeling and alignment
   - ADMET Models
   - Activity Cliffs
   - Structure Based Methods, docking and scoring
   - Model Domain of Applicability

4. Data Mining and Statistical Methods:
   - Linear and Non-Linear Models
   - Feature selection
   - Principal Component analysis (*1 lecture*)
   - Partial Least-Squares Regression
   - kNN, Classification trees and Random forests
   - Introduction to Neural Nets
   - Support vector machines classification and regression (*3 classes*)
   - Data preprocessing and performance measures in Classification & Regression (*1 lecture*)
   - Introduction to evolutionary computing (*1 lecture*)
   - Data Fusion
   - Model Validation
   - Best Practices in Predictive Cheminformatics

5. Medicinal Chemistry:
    - Sources of Bioactive compounds and their sources
    - High-throughput screens of compound collections
    - Combinatorial chemistry in drug discovery
    - Peptidometics in drug design
    - Macrocycles and their advantages
    - mAB vs small molecules in drug discovery

Prerequisites: Organic Reactions and Mechanisms, Chemical Binding, Biochemistry, Statistics, Computer Science, Macromolecules.

CHY342: **Chemistry of Solids and Surfaces** [+ Lab] (4 credits) Spring

This course deals with solid state chemistry and surface chemistry. The use of techniques such as X-ray crystallography, surface plasmon resonance and microscopy to elucidate the structures of crystals and surfaces, and the details of bonding, will also be discussed.

Prerequisites: Chemical Principles, Structure & Bonding, Nature of Materials.

CHY344: **Topics in Nanotechnology** (3 credits) Spring

The next few years will see dramatic advances in atomic-scale technology. Molecular machines, nanocircuits, and the like will transform all aspects of modern life - medicine, energy, computing, electronics and defense are all areas that will be radically reshaped by nanotechnology. These technologies all involve the manipulation of structures at the atomic level - what used to be the stuff of fantasy is now reality. The economics impact of these developments has been estimated to be in the trillions of dollars. But, as with all new technologies, ethical and legal challenges will arise in their implementation and further development. This course will examine the science of nanotechnology and place it in the larger social context of how this technology may be, and already is, applied. Underlying physical science principles will be covered in lecture sessions and students will read articles from current news sources and the scientific literature. There will be presentations on scientific literature on topics of student interests, to examine the science and applications of a well-defined aspect of nanotechnology of their choosing. Lecture material will focus on the principles behind modern materials such as semi-conductors (organic, inorganic) and novel nanostructures.

COURSE CONTENT:

- Introduction
- Bulk Vs. Nano
- Quantum confinement effect
- Surface area to volume ratio
- Effect on Properties: Material (electrical, magnetic, mechanical etc.) and structural properties
- Carbon nano-architectures: Fullerene, SWNT, MWNT, Graphite etc., Classification of structure
- Q-Dots

- Bonding parameters
- Methods of preparation
- Nanomaterial's synthesis: Top down and Bottom up approach, Physical and chemical methods Applications (Nano-machines, solar cells, coatings, MEMS, nano-medicine, sensors, miscellaneous)
- Characterization Techniques and Instruments: Microscopy SEM, TEM, AFM, X-Ray diffraction, UV-vis, Photoluminescence, Raman, FTIR, ESR, XPS, BET, DLS, Zeta potential

Prerequisites: Chemical Principles or Applied Chemistry.

CHY351: **Macromolecules** (3 credits) Monsoon

In this course we will learn about cellular macromolecules namely nucleic acids, proteins, carbohydrates and lipids. The chemistry and biochemistry associated with these macromolecules will be discussed. The goal is to learn about this important natural molecules, not only from a structural but from a chemical point of view as well. We will talk about the chemistry associated with these molecules, their importance and how we can interfere with it. Classes will be through a combination of group discussions, reading assignments, projects, presentations and lectures. Students are expected to do library research, write papers, and present discussion in class. Review articles and papers used in this course will be provided.

1. Introduction
2. Nucleic Acid (DNA and RNA)
    a. Background
    b. Function and importance
    c. Structure
    d. Biosynthesis/replication
    e. Chemical synthesis
    f. Sequencing
        i. Maxam Gilbert
        ii. Sanger dideoxy
        iii. Bisulfite sequencing
        iv. Mass spectrometry
        v. NGS
    g. DNA chemistry
        i. DNA damage
            1. Spontaneous depurination
            2. deamination
        ii. Alkylation
        iii. Oxidative DNA damage
        iv. DNA-DNA crosslinks
        v. DNA-Protein crosslinks
        vi. DNA methylation and demethylation
    h. Mutagenesis
    i. Repair
    j. Epigenetics
    k. RNA editing
    l. Ribozymes

    m. Diseases and carcinogenesis
3. Proteins
    a. What are proteins
    b. Functions
    c. Amino acids
    d. Structure (primary, secondary, tertiary, quaternary)
    e. Sequencing
        i. Chemical and proteomics
    f. Peptide synthesis
    g. Enzymatic reactions
    h. Diseases
4. Lipids
    a. Functions and importance
    b. Fatty acids
    c. Phospholipids
    d. Steroids
    e. Diseases
5. Carbohydrates
    a. Introduction
    b. Function and importance in chemistry and biology
    c. Glycoconjugates
    d. Structural features
    e. Biosynthesis
    f. Chemical synthesis
    g. Industrial preparation

Prerequisites: CHY221, CHY112, Biochemistry.

CHY 352: **Polymers** (3 credits) Spring [REAL]

The chemistry of polymers, their synthesis and characterization will form the subject matter of this advanced course, which will follow a case-study approach. Students will be expected to apply their knowledge to a real-world problem of their choice.

Prerequisites: Chemical Principles, Nature of Materials, Macromolecules.

CHY411: **Applications of group theory in chemistry** (2 credits)

The objective of this course is to familiarize the students about how the symmetry properties of molecules influence their physical properties. Apart from learning the basic principles of group theory, the students will learn to evaluate the properties of molecules using these principles.

Symmetry operations and symmetry elements, Concepts and properties of a group, group multiplication Tables, Similarity transformation, Class, Determination of symmetry point group of molecules, Matrix representation of groups, reducible and irreducible representations, Great orthogonality theorem, Character tables, Direct Product and Spectroscopic selection rule, Molecular Vibrations, Normal coordinates, Symmetry of normal mode vibrations, Symmetry Adapted Linear Combination, Infrared and

Raman active vibrations, Molecular orbitals, LCAO MO approach, HMO method, Hybrid orbitals, Free ion configuration, terms and states, splitting of levels and terms in a chemical environment, correlation diagrams, spectral and magnetic properties of the transition metal complexes.

Pre-requisites: Linear Algebra, Chemical Binding, Molecular Spectroscopy, Coordination Chemistry.

CHY412: **Dynamics of Chemical Reactions** (4 credits)

The principles of chemical kinetics, as well as equilibrium and non-equilibrium statistical mechanics will be covered in this advanced course. The associated computer lab will introduce the student to classical and *ab initio* quantum molecular dynamics and Monte Carlo simulations of liquids and proteins. The techniques learned in this course will applied to substantive research projects that the students will design, execute, and present. Students will be encouraged to seek avenues for publication of their most significant results

Prerequisites: Chemical Equilibrium, Chemical Binding, Macromolecules.

CHY413: **Topics in the Philosophy of Chemistry** (3 credits)

Chemical concepts such as atoms, molecular structure, electron density, equilibrium, reaction path, etc. will be discussed from a historical and philosophical context. There will be numerous short papers on topics of student interest, as well as a more comprehensive project in which students will examine the historical and/or philosophical aspects of a chemical concept of their choosing.

Prerequisites: Chemical Principles, Structure and Bonding.

CHY415: **Theoretical Chemistry Seminar** (3 credits)

This advanced course will cover special topics in quantum chemistry and statistical mechanics. Students will examine in-depth selected articles from the current scientific literature, and develop a viable research proposal in the chosen area.

Prerequisites: Chemical Binding.

CHY421: **Organic Synthesis** [+ Lab] (4 credits) Spring [REAL]

Students will gain expertise in the techniques of organic synthesis. A major project will be the development of a research proposal based on the student's own question. Background from the literature will motivate the proposal and initial experiments will be proposed.

Prerequisites: Chemical Principles, Structure & Bonding, Organic Reactions & Mechanisms.

CHY442: **Chemistry and Ceramics** (3 credits)

What is clay? Why do glazes make such wonderful colors? Why does the water content of clay play such an important role in making pots? What do charges and ions and silicon have to do with ceramics? Making pottery is an art as old as civilization itself. The ancients who perhaps accidentally heated clay and discovered that heat gave the material different properties were among the first chemists. After thousands of years the basic procedure is still the same with some influences by modern technology. In this course we will learn basic ideas of chemistry and the more advanced ideas of transition metal chemistry to investigate the process of throwing and glazing pottery. Students will read papers and handouts, write a term paper exploring a chemistry problem in depth, and experiment with the ceramic form.

Prerequisites: Chemical Principles, Structure and Bonding.

CHY451: **Introduction to Bioorganic Chemistry**

Basic structure of nucleic acids, proteins, lipids and carbohydrates; biological functions and biosynthesis of precursors.

CHY453: **Forensic Chemistry**

Chemistry for Forensic Scientists, Skills for Forensic Scientists Crime Scene Science, Aspects of Forensic Science, Application of Forensic Science Forensic Science Dissertation, Advances in Forensic Chemistry, Forensic Toxicology.

Semester Plan for B.Sc. (Research) Chemistry degree

Semester	Course	Course Title	L:T:P	Chem. Minor	Prerequisites	Chem. Credits
1	CHY111	Chemical Principles	3:1:1	●	None	5
	PHY101/ PHY103	Introduction to/ Fundamentals of Physics-I	3:1:1			
	MAT101	Calculus I	3:1:0			
	MAT110	Programming	2:0:1		None	
2	CHY112	Structure and Bonding	3:1:1	●	CHY111	5
	PHY102/ 104	Introduction to Fundamentals of Physics-II	3:1:1			
	MAT102	Calculus II	3:1:0			
	MAT260	Linear Algebra	3:1:0			
3	CHY211	Chemical Equilibrium	3:1:1	●	CHY111, CHY112	11
	CHY213	Chemical Analysis lab	1:0:1	●	CHY111, CHY112	
	CHY221	Organic Reactions & Mechanisms	3:0:1	●	CHY111, CHY112	
	BIO201	Cell biology and Genetics	2:0:1		BIO113	
4	CHY242	Coordination Chemistry	3:0:1		CHY111, CHY112	10
	CHY244/ CHY 344	The Nature of Materials/Topics in Nanotechnology	3:0:0		CHY111, CHY112, CHY221	
	CHY252/ BIO 204	Biochemistry	2:0:1		CHY111, CHY112, CHY221	
	MAT284	Probability & Statistics	3:1:0			
	PHY202	Introduction to Quantum Mechanics	3:1:0		PHY101, PHY102	
5	CHY311	Chemical Binding	3:0:1		CHY111, CHY112, PHYS202,MAT260	15
	CHY313	Molecular Spectroscopy	3:0:1		CHY213, CHY311	
	CHY332	Informatics & Medicinal Chemistry	3:0:1		CHY221, CHY252, MAT284, MAT210	
	CHY351	Macromolecules	3:0:0		CHY244, CHY252	
6	CHY316	Electrochemistry	3:0:1		CHY111, CHY211	14
	CHY342	Chemistry of Solids and Surfaces	3:0:1		CHY244, CHY311	
	CHY499	Senior Project	0:0:6			
		Major Electives		●		
7		Major Electives		●		6
	CHY499	Senior Project	0:0:6			
8	CHY499	Senior Project	0:0:6			6
		Total Credits		**29**		**72**