

Chemistry

CHEM F110 Chemistry Laboratory 0 2 1

This laboratory course consists of experiments based on fundamental principles and techniques of chemistry emphasizing on physical-chemical measurements, quantitative & qualitative analysis and preparations.

CHEM F111 General Chemistry 3 0 3

Principles of thermodynamics, phase and chemical equilibrium, electrochemistry, kinetics; Atomic structure, chemical bonding, solid state and structural chemistry, molecular spectroscopy; organic compounds, functional groups, structure and isomerism, stereochemistry, reactions and mechanisms, aromaticity, coordination chemistry, chemistry of representative elements.

CHEM F211 Physical Chemistry I 3 0 3

Kinetic - molecular theory of gases; perfect gas; pressure and temperature; Maxwell distribution; collisions, effusion, mean free path; Boltzmann distribution law and heat capacities; first law of thermodynamics; p-V work, internal energy, enthalpy; Joule-Thomson experiment; second law; heat engines, cycles; entropy; thermodynamic temperature scale; material equilibrium; Gibbs energy; chemical potential; phase equilibrium; reaction equilibrium; standard states, enthalpies; Temperature dependence of reaction heats; third law; estimation of thermodynamic properties; perfect gas reaction equilibrium; temperature dependence; one component phase equilibrium, Clapeyron equation; real gases, critical state, corresponding states; solutions, partial molar quantities, ideal and non-ideal solutions, activity coefficients, Debye-Huckel theory; standard state properties of solution components; Reaction equilibrium in non-ideal solutions, weak acids-buffers, coupled reactions; multi component phase equilibrium- colligative properties, two and three component systems, solubility; electrochemical systems- thermodynamics of electrochemical systems and galvanic cells, standard electrode potentials, concentration cells, liquid junction, ion selective electrodes, double layer, dipole moments and polarizations, applications in biology, concept of overvoltage.

CHEM F213 Physical Chemistry II 3 0 3

Origin of quantum theory - black body radiation, line spectra, photoelectric effect; wave particle duality; wave equation: normal modes, superposition; postulates of quantum mechanics, time dependence, Hermitian operators, commutator; Schrödinger equation - operators, observables, solution for particle in a box, normalization, variance, momentum; harmonic oscillator, vibrational spectroscopy; rigid rotor, angular momentum, rotational spectroscopy; Hydrogen atom - orbitals, effect of magnetic field; Variation method - variation theorem, secular determinants; Many electron atoms and molecules; Born Oppenheimer approximation, VB Theory, H₂ in VB, Coulomb, exchange, overlap integrals states of H₂; antisymmetric wavefunctions - two electron systems, Slater determinants, HF method; SCF method; term symbols and spectra - configuration, state, Hund's rules, atomic spectra, spin orbit interaction; basic MO theory, homonuclear diatomics - N₂, O₂, SCF-LCAO-MO, molecular term symbols; HMO theory - π electron approximation, conjugated, cyclic systems.

CHEM F214 Inorganic Chemistry I 3 0 3

Structure of molecules: VSEPR model; ionic crystal structure, structure of complex solids; concepts of inorganic chemistry: electronegativity, acid-base chemistry, chemistry of aqueous and non-aqueous solvents; descriptive chemistry of some elements: periodicity, chemistry of transition metals, halogens and noble gases; inorganic chains, rings, cages and clusters.

CHEM F223 Colloid and Surface Chemistry

3 0 3

Surface phenomena; intermolecular forces relevant to colloidal systems; forces in colloidal systems; experimental and theoretical studies of the structure, dynamics and phase transitions in micelles, membranes, monolayers, bilayers, vesicles and related systems; technical applications.

CHEM F241 Inorganic Chemistry II

3 0 3

Coordination Chemistry: Bonding - Valence Bond, Crystal Field, and Molecular Orbital theories; Complexes - nomenclature, isomerism, coordination numbers, structure, electronic spectra, magnetic properties, chelate effect; Reactions - nucleophilic substitution reactions, kinetics, mechanisms; descriptive chemistry of Lanthanides and Actinides; Organometallic Chemistry: structure and reaction of metal carbonyls, nitrosyls, dinitrogens, alkyls, carbenes, carbynes, carbides, alkenes, alkynes, and metallocenes; catalysis by organometallic compounds; stereochemically non-rigid molecules.

CHEM F242 Chemical Experimentation I

0 3 3

This course is based on laboratory experiments in the field of organic chemistry. Qualitative organic analysis including preliminary examination, detection of functional groups, preparation and recrystallization of derivatives, separation and identification of the two component mixtures using chemical and physical methods; quantitative analysis such as determination of the percentage/ number of hydroxyl groups in organic compounds by acetylation method, estimation of amines/ phenols using bromate-bromide solution/ acetylation method, determination of iodine and saponification values of an oil sample; single step synthesis such as benzaldehyde to cinnamic acid; multistep synthesis such as phthalic anhydride - phthallimide - anthranilic acid; extraction of organic compounds from natural sources: isolation of caffeine from tea leaves, casein from milk, lactose from milk, lycopene from tomatoes, β - carotene from carrots etc.; demonstration on the use of software such as Chem Draw, Chem-Sketch or ISI-Draw.

CHEM F243 Organic Chemistry II

3 0 3

Introduction to stereoisomers; symmetry elements; configuration; chirality in molecules devoid of chiral centers (allenes, alkylidenecycloalkanes, spiranes, biphenyl); atropisomerism; stereochemistry of alkenes; conformation of acyclic molecules; conformations of cyclic molecules; reaction mechanisms; asymmetric synthesis; photochemistry and pericyclic reactions.

CHEM F244 Physical Chemistry III

3 0 3

Symmetry: symmetry operations, point groups, reducible and irreducible representations, character tables, SALC, degeneracy, vibrational modes IR-Raman activity identification; matrix evaluation of operators; stationary state perturbation theory; time dependent perturbation theory; virial and Hellmann-Feynman theorems; polyatomic molecules: SCF MO treatment, basis sets, population analysis, molecular electrostatic potentials, localized MOs; VB method; configuration interaction, Moller Plesset perturbation theory; semi empirical methods-all valence electron methods: CNDO, INDO, NDDO; Density Functional Theory: Hohenberg-Kohn theorems, Kohn-Sham self consistent field approach, exchange correlation functional; molecular mechanics.

CHEM F266 Study Project

3

These courses include projects which are oriented towards readings from published literature or books about new frontiers of development or analysis of available database. These courses are normally available to students in second or higher levels. These courses must coterminate with project reports.

CHEM F311 Organic Chemistry III 3 0 3

Applications of important reagents and reactions in organic synthesis and disconnection or synthon approach will be emphasized in this course. Basic principles of disconnection, order of events, chemoselectivity, regioselectivity etc. Common organic reagents, Organometallic reagents, Transition metal catalyzed reactions, introduction to retrosynthetic analysis using one group C-X and C-C disconnections, two group C-X and C-C disconnections, ring synthesis (saturated heterocycles), synthesis of heterocyclic compounds and complex molecules.

CHEM F312 Physical Chemistry IV 3 0 3

Weak forces; surface chemistry: interphase region, thermodynamics, surface films on liquids, adsorption of gases on solids, colloids, micelles, and reverse micellar structures; transport processes: kinetics, thermal conductivity, viscosity, diffusion, sedimentation; electrical conductivity in metals and in solutions; reaction kinetics, measurement of rates; integrated rate laws; rate laws and equilibrium constants for elementary reactions; reaction mechanisms; temperature dependence of rate constants; rate constants and equilibrium constants; rate law in non ideal systems; uni, bi and tri molecular reactions, chain reactions, free-radical polymerizations; fast reactions; reactions in solutions; heterogeneous and enzyme catalysis; introduction to statistical thermodynamics; theories of reaction rates; molecular reaction dynamics.

CHEM F313 Instrumental Methods of Analysis 3 1 4

Principles and practice of modern instrumental methods of chemical analysis. Emphasis on spectroscopic techniques such as UV-Visible, infrared, NMR (¹H, ¹³C and other elements, NOE, correlation spectroscopies), ESR, atomic absorption and emission, photoelectron, Mössbauer, and fluorescence. Other topics will include mass spectrometry, separation techniques, light scattering, electroanalytical methods, thermal analysis, and diffraction methods.

CHEM F320 Introductory Computational Chemistry 0 4 2 Laboratory

In this course the major focus is on practical computation of electronic structure of atoms and molecules using open source and proprietary software; specific computational experiments will be in the areas of potential energy surfaces, geometry optimization, molecular geometry from symmetry and trigonometric relations without visualization software, molecular orbitals and bonding patterns, Hartree-Fock calculations, correlation energy and size-consistency, DFT based calculations, computing excited states using CIS, EOM-CCSD jobs for computing energies of excited, ionized and electron-attached states; methods to estimate activation energy, solvent effects etc.; molecular dynamics simulation, molecular mechanics will also be explored; the actual experiments may vary and can have more specific learning outcomes so as to enhance the course with the latest developments in electronic structure theories of chemistry.

CHEM F323 Biophysical Chemistry 3 0 3

The principles governing the molecular shapes, structures, structural transitions and dynamics in some important classes of biomolecules and biomolecular aggregates will be discussed. The topics will include: structure, conformational analysis, conformational transitions and equilibria in proteins and nucleic acids; protein folding; lipids - monolayers, bilayers and micelles; lipid-protein interactions in membranes.

CHEM F324 Numerical Methods in Chemistry 3 3 4

Selected problems in chemistry from diverse areas such as chemical kinetics and dynamics, quantum mechanics, electronic structure of molecules, spectroscopy, molecular mechanics and conformational analysis, thermodynamics, and structure and properties of condensed phases will be discussed. The problems chosen will illustrate the application of various mathematical and numerical methods such as those used in the solution of systems of algebraic equations, differential equations, and minimization of multidimensional functions, Fourier transform and Monte Carlo methods.

CHEM F325 Polymer Chemistry 3 0 3

Types of polymers; structures of polymers; molecular weight and molecular weight distributions; kinetics and mechanisms of major classes of polymerization reactions such as step growth, radical, ionic, heterogeneous, and copolymerization methods; polymer solutions- solubility, lattice model and the Flory- Huggins theory, solution viscosity; bulk properties- thermal and mechanical properties such as the melting and glass transitions, rubber elasticity, and viscous flow; polymerization reactions used in industry.

CHEM F326 Solid State Chemistry 3 0 3

X-ray diffraction; point groups, space groups and crystal structure; descriptive crystal chemistry; factors which influence crystal structure; crystal defects and non-stoichiometry; solid solutions; interpretation of the phase diagrams; phase transitions; ionic conductivity and solid electrolytes; electronic properties and band theory; magnetic properties; optical properties; analysis of single crystal XRD data; preparation of solid state materials and the chemistry of device fabrication.

CHEM F327 Electrochemistry: Fundamentals and Applications 3 0 3

Electrode Processes: Overpotential, Faradaic and non-Faradaic processes, the ideal polarized electrode, capacitance and charge of an electrode, electrical double layer; primary and secondary cells, variables in electrochemical cells, factors affecting electrode reaction, cell resistance; Mass transfer: steady-state mass transfer, semiempirical treatment of the transient response, coupled reversible and irreversible reactions, reference electrodes; Kinetics of electrode reactions: Arrhenius equation and potential energy surfaces, equilibrium conditions, Tafel Plots; rate determining electron transfer, Nernstian, quasi-reversible, and irreversible multistep processes; Marcus Theory; mass transfer by migration and diffusion; basic potential step methods; Ultramicroelectrodes (UME) potential sweep methods; polarography and pulse voltammetry; controlled current techniques; impedance; bulk and flow electrolysis; electrochemical instrumentation; scanning probe techniques, STM, AFM, Scanning Electrochemical Microscopy, approach curves, imaging surface topography and reactivity, potentiometric tips, applications.

CHEM F328 Supramolecular Chemistry 3 0 3

Non-covalent interactions and their role in "supermolecules" and organized polymolecular systems; concepts of molecular recognition, information and complementarity; molecular receptors: design principles, binding and recognition of neutral molecules and anionic substrates, coreceptor molecules and multiple recognition, linear recognition of molecular lengths by ditopic coreceptors, heterotopic coreceptors, amphiphilic receptors, large molecular cages; supramolecular dynamics; supramolecular catalysis: reactive macrocyclic cation and anion receptor molecules, cyclophane type receptor, metallocatalysis, catalysis of synthetic reactions, biomolecular and abiotic catalysis, heterogeneous catalysis; transport processes and carrier design: cation and anion carriers, electron, proton and light coupled

transport processes, transfer via transmembrane channels; supramolecular assemblies: heterogeneous molecular recognition, supramolecular solids, molecular recognition at surfaces, molecular and supramolecular morphogenesis; supramolecular photochemistry: photonic devices, light conversion and energy transfer devices, photosensitive molecular receptors, photoinduced electron transfer and reactions, non-linear optical properties; supramolecular electrochemistry: electronic devices, molecular wires, polarized molecular wires, switchable molecular wires, molecular magnetic devices; ionic devices, tubular mesophases, ion-responsive monolayers, molecular protonics, ion and molecular sensors, switching devices and signals, photoswitching and electroswitching devices, switching of ionic and molecular processes, mechanical switching processes; self-assembly: inorganic architectures, organic structures by hydrogen bonding; helical metal complexes, supramolecular arrays of metal ions – racks, ladders and grids, molecular recognition directed self-assembly of organized phases; supramolecular polymers; ordered solid-state structures; supramolecular synthesis, assistance, replication; supramolecular chirality; supramolecular materials.

CHEM F329 Analytical Chemistry 3 1 4

Data handling; sample preparation; unit operations; volumetric and gravimetric analysis; chromatography; solvent and solid phase extraction; absorption and emission techniques; potentiometry, voltammetry; trace metal separation and estimation in biological and environmental samples with emphasis on green chemistry, sensors; laboratory training in some of these techniques.

CHEM F330 Photophysical Chemistry 3 1 4

Absorption of the electromagnetic radiation; photophysical processes such as fluorescence, phosphorescence, non-radiative transitions, and delayed luminescence, excimer and exciplex formation; triplet state: radiative and non-radiative transitions; energy transfer, fluorescence resonance energy transfer (FRET), quenching of fluorescence; fluorescence decay; protein and DNA fluorescence; time-resolved emission spectra (TRES); time-dependent anisotropy decays; application of photophysics for the characterization of biological and bio-mimicking systems. In addition to the theory, through simple experiments, laboratory training will be imparted.

CHEM F333 Chemistry of Materials 3 0 3

Solid state structure : unit cells, metallic crystal structures, polymorphism and allotropy, crystallographic direction and planes, closed packed crystal structures, polycrystalline materials, anisotropy; meso and micro porous materials: zeolites, composites, synthesis, characterization (XRD, SEM, TEM, AFM, FTIR, NMR, TGA, and DTA) and applications; ceramics and glass materials: crystalline and non-crystalline nature, glass-ceramics, processing; polymers: synthesis, structure, properties, inorganic polymers; mechanical properties: stress and strain, elastic and tensile properties, hardness, phase transformations, microstructure, alteration of mechanical properties; magnetic properties: atomic magnetism in solids, the exchange interaction, classification of magnetic materials, diamagnetism, pauli paramagnetism, ferromagnetism, antiferromagnetism, ferrimagnetism, superparamagnetism, ferromagnetic domains, hysteresis loop, hard and soft ferrites, applications; electrical properties: conductivity, band theory, types of semiconductors, time dependence of conductivity, mobility of charge carriers, metal-metal junction, metal-semiconductor junction, n-type and p-type semiconductors; optical properties: refraction, reflection, absorption, transmission, luminescence, photoconductivity, opacity and translucency in insulators, optical fibers; thermal properties: heat capacity, thermal expansion, conductivity, thermal stresses; corrosion: electrochemistry of corrosion of metals, different forms, environmental effects, prevention.

CHEM F334 Magnetic Resonance

3 0 3

Classical treatment of motion of isolated spins; quantum mechanical description of spin in static and alternating magnetic fields; Bloch equations; spin echoes; transient and steady state responses; absorption and dispersion; magnetic dipolar broadening; formal theory of chemical shifts; Knight shift; second order spin effects; spin-lattice relaxation; spin temperature; density matrix; Bloch-Wangsness-Redfield theory; adiabatic and sudden changes; saturation; spin locking; double resonance; Overhauser effect; ENDOR; pulsed magnetic resonance: Carr-Purcell sequence, phase alternation, spin-flip narrowing, real pulses; electric quadrupole effects; spin-spin coupling; 2D correlation spectroscopies: COSY, DQF, INADEQUATE experiments; CIDNP; electron paramagnetic resonance (EPR); nuclear quadrupolar resonance; muon spin resonance; magnetic resonance imaging.

CHEM F335 Organic Chemistry and Drug Design 3 0 3

An introduction to organic chemistry principles and reactivities vital to drug design, drug development and drug action; the role of molecular size, shape, and charge, and in drug action; proteins and nucleic acids as drug targets; bioisosterism; ADME, QSAR and drug design; applied molecular modeling and combinatorial synthesis; Synthesis of some selected chemotherapeutic agents (e.g antifungal, antibacterial, antimalarial, anticancer etc.)

CHEM F336 Nanochemistry 3 1 4

Nano and nature, importance of nanoscience, chemistry behind nano; instruments for characterizing nanomaterials; diversity in nanosystems: chemical aspects of metallic, magnetic and semiconducting nanomaterials, carbon nanotubes and fullerenes, self-assembled monolayers, monolayer protected metal nanomaterials, core-shell nanomaterials; applications of nano materials in nanobiology, nanosensors and nanomedicine; hands on experience in laboratory.

CHEM F337 Green Chemistry and Catalysis 3 0 3

Definition and overview of the twelve principles of Green Chemistry, alternative starting materials; alternative synthesis and reagents; E factor and the concept of atom economy; the role of catalysis, alternate energy sources (microwave & ultrasound), catalysis by solid acids and bases, bio-catalysis, catalytic reduction, catalytic oxidation, catalytic C–C bond formation, cascade catalysis, enantioselective catalysis, alternative reaction media, renewable raw materials, industrial applications of catalysis.

CHEM F341 Chemical Experimentation II 0 4 4

This course is based on laboratory experiments in the fields of inorganic, physical and analytical chemistry. Quantitative separation and determination of pairs of metal ions using gravimetric and volumetric methods; Ion exchange chromatography; Separation & estimation of metal ions using ion exchangers and solvent extraction techniques; Determination of K_{eq} of M – L systems by colorimetry; Preparation, purification and structural studies (magnetic, electronic and IR) of inorganic complex compounds; Physical property measurements such as conductance, pH, viscosity, surface tension, refractive index, specific rotation etc. Experiments to illustrate the principles of thermodynamics, kinetics, chemical equilibrium, phase equilibrium, electrochemistry, adsorption, etc.

CHEM F342 Organic Chemistry IV 3 0 3

The fundamental structural characteristics, synthesis and reaction of various heterocyclic compounds, natural products and biomolecules will be emphasized in this course. Structure, nomenclature and common reactions of heterocyclic compounds; synthesis, properties and reactions of three-, four-, five-, and six membered ring systems; condensed five and six membered ring systems, introduction to natural products; terpenoids, steroids, lipids, alkaloids, amino acids, peptides, proteins and vitamins.

CHEM F343 Inorganic Chemistry III 3 0 3

Inorganic elements in biological systems: role of alkali and alkaline earth metal ions, iron, copper and molybdenum; metalloenzymes. Metals in medicine: metal deficiency and disease; toxicity of mercury, cadmium, lead, beryllium, selenium and arsenic; biological defence mechanisms and chelation therapy. Molecular magnetic materials: trinuclear and high nuclearity compounds; magnetic chain compounds; magnetic long-range ordering in molecular compounds; design of molecular magnets. Other emerging topics in inorganic chemistry.

CHEM F366 Lab Project 3**CHEM F367 Lab Project 3**

These courses include projects involving laboratory investigation or laboratory development in the students discipline or interdisciplinary areas. These courses are normally available to students in third or higher levels. These courses must coterminate with project reports.

CHEM F376 Design Project 3**CHEM F377 Design Project 3**

These courses are intended to impart training in design of product/ process or other artifact to the students in the discipline or interdisciplinary areas. These courses are normally available to students in third or higher levels. These courses must coterminate with project reports.

CHEM F412 Photochemistry and Laser Spectroscopy 3 0 3

Photochemical events : absorption, fluorescence and phosphorescence; Jablonski diagrams; physical properties of molecules after photoexcitation; photochemical tools and techniques: spectrophotometers, fluorescence decay time measurement and analysis, flash photolysis; fundamental properties of laser light; principles of laser operation ; description of some specific laser systems : Helium-Neon, Argon ion, CO₂, Nd-YAG and ultrafast Titanium : Sapphire lasers.

CHEM F413 Electron Correlation in Atoms and Molecules 3 1 4

Matrix algebra, Matrix representation of operators; mean-field approach: the Hartree-Fock method- formulation, coulomb and exchange integrals, Fock-operator, second quantization, Slater rules, self-consistency, correlation energy; Brillouin's theorem, Koopmans' theorem; basis-sets, restricted Hartree-Fock, Roothaan-Hall equations; unrestricted Hartree-Fock method, spin-contamination; restricted open-shell Hartree-Fock method; Recovery of correlation energy time independent perturbation approach: Brillouin-Wigner and Rayleigh-Schrodinger perturbation theories; Møller Plesset and Epstein-Nesbeth partitioning of molecular Hamiltonian, many-body perturbation theory; Feynman diagrams, connected and disconnected terms, size-consistency; Recovery of correlation energy: configuration interaction and other non-perturbative approaches, variational and projection approaches for obtaining CI ansatz, truncated CI and size-consistency problem, Davidson correction, pair-coupled-pair theory, coupled-electron-pair method and coupled-cluster approach; Density functional theory, N-representability, V-representability, Kohn-Sham approach, natural orbitals, exchange-correlation functionals, Levy functional.

CHEM F414 Bio and Chemical Sensors 3 0 3

Biological and chemical recognition: reaction kinetics, signals and noise, sensitivity, specificity, selectivity; IUPAC definition of biosensors, their classification based on receptors and transducers; analytical characteristics of various types of bio and chemical sensors, performance criteria of biosensors; electro-

chemical, optical, thermal, piezoelectric transducer selections for immunosensors and enzyme sensors; surface functionalization of transducers, novel self assembly techniques, coupling of biomolecules on different surfaces and their characterization; thermal biosensors, enzyme thermistor; miniaturization of sensors and flow injection techniques; applications in analysis such as urea, penicillin, pesticides, cholesterol; optical biosensor mechanisms: fluorescence and chemiluminescence techniques; electrochemical biosensors: impedimetric and amperometric biosensors; electrochemical quartz crystal micro balance, applications in chemical and biological analysis; flow injection systems vs. static measurements, protein-protein interaction and quantification; principle of inhibition based biosensor for enzyme and immunoassay, pretreatment techniques in bio-analysis.

CHEM F415 Frontiers in Organic Synthesis 3 0 3

Traditional and classic organic synthesis; modern synthetic strategies; systematic approach in terms of progress in reaction methodologies in synthesizing complex natural molecules; metal-catalyzed C-C and C-X couplings; direct functionalization via C-H and C-C activation; development of organocatalysis: metal-free catalysis; direct functionalization of olefins including hydroamination, hydrogenation, hydrosilylation, hydroformylation and other C-C bond forming reactions; the potential of radical chemistry for C-C and C-X bond formation; metal-catalyzed carbocyclization: from Ru and Rh-mediated cycloadditions to Pt and Au chemistry; one-pot multi-steps reactions: avoiding time and resource-consuming isolation procedures; tracing the development from the first total synthesis to the state of the art for some complex molecules.

CHEM F422 Statistical Thermodynamics 3 0 3

Review of classical thermodynamics, principles of statistical thermodynamics, ensemble averages; Boltzmann distribution; partition functions and thermodynamic quantities; ideal gases and crystals; thermodynamic properties from spectroscopic and structural data; dense gases and the second virial coefficient; statistical mechanics of solutions; Bose-Einstein and Fermi-Dirac statistics.

CHEM F430 Atmospheric Chemistry 3 0 3

This course aims to describe the chemical and physical processes of atmosphere by different models. The specific topics will include, the measures of atmospheric compositions, atmospheric pressure, models to explain variation in concentration of chemical species in atmosphere, atmospheric transport, continuity equation to provide quantitative measures about the variation of concentration, geochemical cycles, the green-house effect, aerosols, atmospheric chemical kinetics, stratospheric ozone, oxidation in troposphere, ozone air pollution, and acid rain.

CHEM F431 Sustainable Chemistry using Renewables 3 0 3

Importance of the utilization of renewable resources as alternative feedstock for the chemicals and fuels industry; alternatives to current petro-based technology and processes such as biomass utilization; chemicals from renewables, bio-refinery concept, strategies for biomass utilization, Platform molecules, Degraded molecules, Biomass conversions by new catalytic/ synthetic routes, catalytic cascade reactions, one-pot multi-product synthesis; chemistry in lignocellulose conversions; bio-based oleochemicals; fine chemicals from renewables; thermochemical conversion to fuels and other chemicals; analytical in thermal biomass conversions, kinetics based on tunable diode laser measurements, CFD modeling; bio-ethanol : production, upgradation and valorization; glycerol as feedstock; fatty acid epoxidation; hydrogen and carbon-di-oxide, hydrogen as a feedstock, electro-catalysis, solar-photo catalysis, fuel cells, Carbon-di-oxide capture and valorization.

CHEM F491 Special Projects 3

This is an unstructured open-ended course where under the overall supervision of an instructor-in-charge, batches of students will be attached to different instructors. Each batch will work on a specific time-bound project which is of basic or peripheral concern of his discipline. Each student must submit a project report as a culmination of his endeavour and investigation. The instructor-in-charge will determine the choice of the project and also whether or not the project report is to be submitted jointly by a group or individually by a student. The course will aim to evaluate student's actual ability to use the fundamentals of knowledge and to meet new unknown situations as demonstrated by the students' interaction with the instructors and instructor-in-charge and aggregated in the project report. The instructor-in-charge may assign specific hours for formal brain-storming sessions.

CHEM G511 Nuclear and Radio Chemistry 5

Course description is to be developed.

CHEM G513 Advanced Nuclear and Radio-chemistry 5

Nuclear stability, binding energy, properties of nucleons; Nuclear models (Shell Model, Liquid drop model), Radioactive decay characteristics, decay kinetics, α , β and γ decay, nuclear reactions, types, radiative capture, reaction cross section, theory of fission; Nuclear reactors – classification, Reactor power, Breeder reactors, Nuclear reactors in India, Reprocessing of spent fuel, Nuclear waste management (HLW, LLW and ILW); Detection and measurement of activity, GM counters, Gamma counters, Liquid Scintillation counting; Application of radioactivity, Szilard Chalmers reaction, Isotope dilution analysis, Neutron activation analysis, Diagnostic and therapeutic applications of radionuclides, interaction of radiation with matter.

CHEM G521 Environmental Chemistry 5

Energy-flows and supplies, fossil fuels, nuclear energy, nuclear waste disposal, renewable energy, industrial ecology, green chemistry, ozone chemistry, effect of SO_x , NO_x as pollutants, reformulated gasoline, water pollution and treatment, organochlorine and organophosphate pesticides, eco-system effects, Toxic chemicals – Effect of dioxins, polychlorinated biphenyls (PCBs) and species of metals such as lead, mercury, cadmium etc.

CHEM G531 Recent Advances in Chemistry 5

The course is aimed at providing an overview of recent developments in selected areas of chemistry. Topics to be covered may be drawn from: modern theories of structure, bonding and reactivity, spectroscopy, chemical dynamics, phase transitions, surface phenomena, solid state materials, and synthetic and mechanistic organic and inorganic chemistry, or such other topics as may emerge in the development of the subject.

CHEM G541 Chemical Applications of Group Theory 5

Groups, subgroups and classes : definitions and theorems; molecular symmetry and symmetry groups; representation of groups; character tables; wave functions as bases for irreducible representations; direct product; symmetry adapted linear combinations; symmetry in molecular orbital theory; hybrid orbitals; molecular orbitals of metal sandwich compounds; ligand field theory; molecular vibrations; space groups.

CHEM G551 Advanced Organic Chemistry 5

Recent advances in aromatic electrophilic and nucleophilic substitution reactions and nucleophilic addition reactions; oxidation and reduction; enolates in organic synthesis; retro synthetic analysis; multiple step synthesis; protecting groups.

CHEM G552 Advanced Inorganic Chemistry 5

Advanced coordination chemistry, reactions, kinetics and mechanism; advanced organometallic chemistry, bonding models in inorganic chemistry, inorganic chains, rings, cages and clusters; group theory and its applications to crystal field theory, molecular orbital theory and spectroscopy (electronic and vibrational); inorganic chemistry in biological systems.

CHEM G553 Advanced Physical Chemistry 5

Equilibrium: The laws of Thermodynamics, applications to phase equilibrium, reaction equilibrium, and electrochemistry; Structure: Principles and techniques of quantum mechanics, applications to atomic and molecular structure and spectroscopy, statistical thermodynamics, molecular interactions, macromolecules, solid state; Dynamics: Molecular motion in gases and liquids, reaction rate laws, mechanisms and rate theories of complex reactions, molecular reaction dynamics, surface processes, electron transfer dynamics.

CHEM G554 Physical Methods in Chemistry 5

Advanced spectroscopic and non-spectroscopic techniques used in chemistry; Topics will include electronic absorption spectroscopy of organic and inorganic compounds, ORD, CD; vibrational rotational spectroscopy symmetry aspects; Dynamic and Fourier transform NMR, NOE, Multipulse methods, Two-Dimensional NMR; EPR; NQR; Mossbauer spectroscopy; Magnetism; Ionization Methods: Mass spectrometry, Ion Cyclotron Resonance; Photoelectron Spectroscopy; Microscopic techniques: TEM, STM, AFM; EXAFS, XANES; X-ray Crystallography.

CHEM G555 Chemistry of Life Processes 4

Synthesis and structures of biopolymers such as proteins and nucleic acids; nucleic acid replication, transcription and translation; lipids and biomembranes; transport across membranes; neurotransmission; enzyme and enzyme inhibitors; citric acid cycle, pentose phosphate pathway and nucleic acid metabolisms; photosynthesis; electron transport systems in respiration and oxidative phosphorylation.

CHEM G556 Catalysis 4

A comprehensive survey of the catalytic processes along with the fundamental aspects of the catalyst design and evaluation; several classes of heterogeneous industrial catalysts; their preparation, characterization and applications, recent developments in catalysis, application of nanomaterials in catalysis.

CHEM G557 Solid Phase Synthesis and Combinatorial Chemistry 4

A comprehensive understanding of solid phase synthesis and combinatorial chemistry, basic principles of solid phase organic synthesis; solid phase organic synthesis strategies; introduction to combinatorial chemistry; analytical techniques in combinatorial chemistry; applications of the combinatorial approach in chemistry, drug development and biotechnology.

CHEM G558 Electronic Structure Theory 5

Advanced methods in theoretical and computational chemistry based on Quantum Mechanics: Review of mathematical background, N-Dimension complex vector spaces, linear variational problem, many electron wave functions and operators, operators and matrix elements; Ab-initio methods: Hartree-Fock (H-F), Configuration Interaction (CI), Many Body Perturbation Theory (MBPT); Density Functional Theory: Thomas-Fermi model, Hohenberg-Kohn theorems, derivation of Kohn-Sham equations; Development and use of software for such models.

CHEM G559 Bioinorganic Chemistry 4

Fundamentals of inorganic biochemistry; essential and non-essential elements in bio-systems, metalloproteins and metalloenzymes; role of metal ions in oxygen carriers, synthetic oxygen carriers, bioinorganic chips and biosensors; fixation of dinitrogen, environmental bioinorganic chemistry; transport and storage of metal ions *in vivo*, metal complexes as probes of structure and reactivity with metal substitution; fundamentals of toxicity and detoxification, chelating agents and metal chelates as medicines, nuclear medicines.

CHEM G561 Heterocyclic Chemistry 5

The fundamental structural characteristics; synthesis and reactions of various heterocycles with nitrogen, oxygen and sulphur heteroatom in the ring; heterocycles such as pyrrole, thiophene, furan, imidazole, thiazole, oxazole, indole, benzofuran, pyridine and quinoline; advanced synthesis and reaction mechanism of heterocyclic compound.

CHEM G562 Solid State Chemistry 4

Basics of solid state chemistry, comprehensive survey of different synthesis techniques, properties and their structural-property relationship of solid materials; introduction to special nanomaterials, ceramics, polymers, biopolymers and nanocomposites; thermal and mechanical properties of nanomaterials; nanocomposites in hydrophobic applications; recent advances in material science and technology.

CHEM G563 Advanced Statistical Mechanics 5

Review of ensembles, fluctuations, Boltzmann statistics, quantum statistics, ideal gases and chemical equilibrium; imperfect gases; distribution function theories and perturbation theories of classical liquids; electrolyte solutions; kinetic theory of gases; continuum mechanics; Boltzmann equation; transport processes in gases and Brownian motion; introduction to time-correlation function formalism.