Courses for MS in Physical Chemistry

Students wishing to study for the MS degree in Physical Chemistry must take six of the following theory courses. Each course carries three credits. The courses PC 503 and PC 507 must be taken by all the students. There will be an in-course assessment of 30 marks (comprising two one hour incourse examinations of 25 marks and 5 marks for attendance) and a three hours final examination of 70 marks. Besides, the students must submit a thesis equivalent to 10 credits and appear at two viva-voce examinations, of which one is for the courses (2 credits) and another is for the defense of the thesis (2 credits).

1. **PC 501** Advanced Chemical Kinetics
2. **PC 502** Advanced Surface Chemistry and Catalysis
3. **PC 503** Advanced Photochemistry
4. **PC 504** Advanced Electrochemistry and Electroanalytical Techniques
5. **PC 505** Biophysical Chemistry
6. **PC 506** Chemistry of the Atmospheric Environment
7. **PC 507** Molecular Symmetry and Advanced Spectroscopy
8. **PC 508** Supramolecular and Nano-Chemistry
9. **PC 509** Chemistry of Materials
10. **PC 510** Advanced Concepts of Liquids
11. **PC 511** Advanced Polymer Chemistry
12. **PC 512** Computational Chemistry
PC 501 Advanced Chemical Kinetics (3 Credits)

1. **Composite reactions**: Composite reactions: concept of steady state approximation and steady-state treatment, rate equations for composite reactions: decomposition of ozone, hydrocarbon oxidation and combustion of hydrocarbons, oscillatory reaction, Belousov-Zhabotinski (B-Z) reaction, a schematic representation of the B-Z reaction, chemistry of B-Z reaction, stationary flames, thermal explosion, isothermal explosion, branching chain explosion, hydrogen oxygen reaction, explosion limits.

2. **Theories of reaction rates**: Review of theories: collision theory and conventional transition state theory (CTST), thermodynamic treatment of the TST, statistical treatment of TST, contour diagram, potential energy surface, some applications of the CTST, reactions between atoms and molecules, reaction between H and HBr. Unimolecular reactions: RRK and RRKM, Slater theorem.


5. **Micellar catalysis**: General features of micellar catalysis, aqueous micelles as models for enzymatic interactions, micellar catalysis, general mechanisms of micellar catalysis: kinetic models.

6. **Kinetics of chemical reactions in nanosystems**: Stochastic approach, diffusion controlled reaction in nanosystems. Reactions inside the sphere mean reaction time approximation, reactions on the surfaces of the nanospheres.

7. **Reaction dynamics**: Molecular dynamical calculations for the reactions (H + H₂) and (Br + H₂). Potential energy surfaces: attractive, repulsive, and intermediate type surfaces for exothermic reactions, selective enhancement of reactions, disposal of excess energy, gradual and sudden surface, influence of rotational energy. Molecular beams, state to state kinetics.

**Books recommended**

PC 502 Advanced Surface Chemistry and Catalysis (3 Credits)


2. **Adsorption energetics**: Physisorption and chemisorptions: isotherms, isobars, enthalpy and entropy changes. Trends in surface reactivity: one dimensional model of energetics of physisorption and chemisorption. Work function, work function change due to adsorption, spontaneous self-organization.


4. **Mechanism of surface reactions**: General considerations in the determination of surface reaction mechanism: adsorption sites, orientation of adsorbate, adsorbate induced reconstruction, lateral interactions in surface reactions, intermediates in surface reactions, transition state theory of surface reactions, reaction pathway of catalyzed and noncatalyzed reaction, Tempkin equation, surface diffusion of adsorbed species, geometry of adsorbate and adsorbent after chemisorption, mechanism of chemisorption process on solid surface. Desorption, activation energy of desorption, temperature programmed desorption studies.

5. **Catalysis**: General description of catalyst, catalyst preparation, metallic catalyst, supported metal catalyst, non-metallic catalyst, metal oxide, mixed metal oxide, zeolite and bio-catalysts. Modification of catalyst, catalyst deactivation, turnover number, specificity and selectivity in catalysis, catalytic activity, the volcano curve, catalytic oxidation of CO and NH₃ on metal and metal oxide surfaces, hydrocarbon conversion, reforming catalysts.

6. **Solid catalysts in environmental and industrial processes**: Automotive exhaust catalysis, three way catalyst, catalytic reactions in three-way catalyst, selective catalytic reduction. Hydrogenation of vegetable oils, ammonia and nitric acid production, synthesis gas conversion, sulphuric acid production, catalytic cracking, synthetic gasoline production.

Books recommended

9. Selected articles from recent journals.

PC 503 Advanced Photochemistry (3 credits)

1. **General consideration:** Pathways of dark reactions and photochemical reactions, photochemistry and radiation chemistry, dosimeters, current trends in photochemistry.


4. **Photoactive materials and their applications:** Semiconducting metal oxides and their photochemistry, types of photoelectrochemical solar cells, solar energy conversion by photovoltaic cells, dye sensitized photovoltaic cells, semiconductor sensitized water splitting, semiconductor mediated photocatalysis, organic solar cells, storage of solar energy, mechanism of energy conversion, energy conversion efficiency.

5. **Advanced oxidation processes (AOP’s) in water treatment:** Types of AOP’s, the hydrogen peroxide/ultraviolet light (H₂O₂/UV), ozone/ultraviolet light (O₃/UV), hydrogen peroxide/ozone (H₂O₂/O₃),
hydrogen peroxide/ultraviolet light/ozone (H₂O₂/O₃/UV), TiO₂ or ZnO/UV and TiO₂ or ZnO/UV + H₂O₂ processes.


**Books Recommended**

7. Selected articles from recent journals.

**PC 504 Advanced Electrochemistry and Electroanalytical Techniques (3 Credits)**


2. **Sweep voltammetry**: Linear and cyclic voltammetry: principles, switching potential and potential excitation signal, generation of cyclic voltammogram from concentration-distance profiles. Diagnosis of reversiblre, quasi-reversiblre and irreversible charge transfer and coupled chemical kinetics from cyclic voltammetry. Cyclic voltammetry at microelectrodes. Applications of linear and cyclic voltammetry.

4. **Pulse and stripping techniques:** Pulse techniques: fast, normal & differential pulse and square wave voltammetry (principle, comparative potential excitation signals and response signals), pulse width, diminution factor. Application and relative advantages of different pulse techniques. Some special pulse techniques: reverse pulse, differential normal pulse and double differential pulse voltammetry. Stripping techniques: different types of stripping techniques (anodic, cathodic, potentiometric, adsorptive and abrasive) and their comparative pre-concentration and determination step, use of pre-concentration techniques at trace and ultra trace level analysis, use of pre-concentration step for mercury film electrode in metal-ligand complex study (de Ford and Hume method).


6. **Impedance techniques:** Impedance, detection and measurements of impedance, equivalent circuit of an electrochemical cell, the Faradaic impedance and the total impedance of a simple electrode process, impedance plots for complex plane. Admittance and its use. Hydrodynamic electrodes and impedance. Transforms and impedance, application of impedance for characterization of corrosion and capacitors.

7. **Electrochemical quartz crystal microbalance, spectro-electrochemistry and scanning electrochemical microscopy:** Principles, electrochemical set-up and applications, electro-chemiluminescence, optical probing of electrode-solution interfaces. Approach curves for scanning electrochemical microscopy, imaging surface topography, applications in homogeneous reaction kinetics and others.

**Books Recommended**

PC 505 Biophysical Chemistry (3 Credits)

1. **Enzyme kinetics**: Introduction to enzyme, characteristics, mechanisms, kinetic equations, enzyme-substrate interactions, multisubstrate systems, enzyme inhibition, effect of pH on enzyme kinetics. Cooperative binding, quantitative analysis of cooperative binding by Hill plot, oxygen binding of myoglobin and hemoglobin, factors influencing the oxygen binding, Bohr effect. Allosteric interactions, features and properties of allosteric enzymes, Monod-Wyman-Changeux (MWC) model, experimental tests of the MWC model, alternative models for allosteric proteins; a sequential model, a more general scheme.


4. **Models for artificial membrane and cell**: Introduction, common lipids and their phase behavior, interactions of amino acid and protein with lipids. Models of biological membrane and cell; Langmuir monolayers, bilayers, vesicles or liposomes: structure and preparation of these models, conventional liposome formulations, targeted drug delivery using liposomes.


6. **Biophysical processes**: Dissociation of amino acids, isoelectric point, titration of proteins, buffer in biological systems, structure and function of DNA and RNA, molecular recognition.

7. **Biosensors**: Introduction, basic design, types of biosensors: calorimetric, potentiometric, amperometric, optical, acoustic biosensors. Immunosensors. Micro-organism based sensor: glucose sensor, alcohol sensor, formic acid sensor, methane sensor, BOD sensor, ammonia sensor, urea sensor, DNA sensors and their applications.

**Books Recommended**

2. D. R. Ferrier, Biochemistry (Lippincott Illustrated Reviews Series), Lippincott Williams & Wilkins
8. Recent publications.

PC 506 Chemistry of the Atmospheric Environment (3 credits)


3. **Air pollution and chemical processes in the troposphere**: Criteria and non-criteria pollutants, classification of air pollutants: primary and secondary pollutants, regional and global air pollution, regional air pollution: particulate, smog, acid rain, toxic effects of various pollutants. Generation of reactive species: singlet and triplet oxygen atoms, hydroxyl radicals, nitrate radicals, the day-time chemistry, formation of ozone and organic nitrates, the night-time chemistry, wet and dry deposition of pollutants.

4. **Greenhouse effect in the troposphere and its impact on climate changes**: Various greenhouse gases, sources and individual contribution of green house gases, CO₂ and methane concentration in the atmosphere, global warming and its impact on living system, GHG trading and clean technology.

5. **Stratospheric ozone depletion**: Ozone layer and stratospheric ozone, Chapman mechanism for the formation of ozone layer, catalytic processes, ozone depletion, role of CFCs, ozone depletion potential (ODP) of CFCs, UV spectrum of oxygen and ozone, ozone measurement in the stratosphere: earth stations and satellite stations, antarctic ozone hole, its detection and its formation, impact of stratospheric ozone depletion.

6. **Monitoring of atmospheric pollutants**: Air sampling techniques; spectrophotometric, chemicals and gas chromatographic techniques for analysis of PM₁₀, PM₂.₅, Soot Carbon, SOₓ, NOₓ and VOCs, field sensors for CO, SOₓ, NOₓ, O₃ and hydrocarbons analysis.

Books recommended


PC 507 Molecular Symmetry and Advanced Spectroscopy (3 Credits)

1. **Molecular symmetry and symmetry groups**: Symmetry elements and symmetry operations, products of symmetry operations, the symmetry classification of molecules into point groups, classes of symmetry operations, Marci matrix representation of symmetry operation, some immediate consequences of symmetry.

2. **Group theory and its application**: Definition and properties of a group. Group multiplication tables, representations of groups, properties of materials and vectors, reducible and irreducible representations, great orthogonality theorem, character tables and their uses, symmetry species of point groups, distribution of fundamentals among the symmetry species, vanishing integral and orbital overlap: vanishing integrals and selection rules for infrared and Raman activities.

3. **Advanced treatment of Raman spectroscopy**: Polarization of Raman scattered light, quantum mechanical interpretation of Raman effect, molecular polarizability, classical theory of Raman effect, pure rotational Raman spectra of linear and symmetric top molecules, Raman activity of vibrations, change in size, shape or direction of polarizability ellipsoid of simple molecules, rule of mutual exclusion, vibrational Raman spectra and rotational fine structure, Raman investigation of phase transitions, resonance Raman scattering, structure determination using IR and Raman spectroscopy, surface enhanced Raman scattering, non-linear Raman phenomenon, stimulated Raman scattering, multi-photon spectroscopy.


5. **Mössbauer spectroscopy**: Nuclear properties and nuclear gamma resonance, Mössbauer isotopes, Doppler effect, Mössbauer theory, isomer shift, quadrupole interactions, and magnetic splitting in Mössbauer spectrum,
effect of electronegativity in isomer shift, application of isomer shift and quadruple splitting measurements in tin and iron complexes, detection of cis-, trans-isomers from quadruple splitting value and estimation of covalent character of complex compounds from isomer shift value.

6. **Nuclear magnetic resonance spectroscopy:** General theory of high resolution of nmr, pulse and Fourier transformation methods, experimental techniques, double resonance methods, relation between structure and chemical shifts, spin-spin coupling (general, vicinal and long range), investigation of molecular fluxional properties using nmr technique, $^{13}$C nmr spectra, comparison with $^1$H nmr, hyperfine splitting, proton decoupling, interpretation of $^{13}$C nmr spectra. Introduction to 2D nmr: COSY and NOESY techniques, ENDOR technique in nmr.

7. **Electron spin resonance spectroscopy:** Quantization of angular momentum, relation between magnetic moment and angular momentum, characteristics of spin system, $g$ factor, characteristics of dipolar interaction, electronic and nuclear Zeeman interaction, spin Hamiltonian including isotropic hyperfine interaction. Isotropic hyperfine splitting effect in esr spectra: single set of equivalent protons, multiple set of equivalent protons, other nuclei with $I = \frac{1}{2}$ and $I > \frac{1}{2}$. Zeeman anisotropy, hyperfine anisotropy. Rules of interpretation of esr spectra, esr spectrometer and scope of esr technique.

**Books recommended**

7. Recently published papers on the above topics in different journals.

**PC 508 Supramolecular and Nano-Chemistry (3 Credits)**

1. **Supramolecular chemistry:** Conceptual foundations of supramolecular chemistry, supramolecular, bioorganic, bioinorganic and biomimetic chemistry, from molecular materials to supramolecular structures, selectivity, supramolecular interactions, supramolecular design.

2. **Supramolecular systems:** Solution host-guest chemistry: guests in solution, macrocyclic vs. acylic hosts, cation binding, anion binding, neutral-molecule binding, self-assembly: rotaxanes, catenanes and knots, solid state supramolecular chemistry: clathrates, clathrate hydrates, crystal engineering.

3. **Organized systems:** Surfactants, micelles, vesicles, reverse micelles, microemulsions: preorganization of surface-active compounds. Interfaces and liquid assemblies. Order in liquids, interfacial ordering, surfactants,
micelles, vesicles and other ordered aggregates, surface self-assembled monolayers, supramolecular liquid crystals, ionic liquids, liquid clathrates.

4. **Chemistry of nanoparticles:** About size scales, history, Feynman scorecard, Schrodinger’s cat-quantum mechanics in small systems, fluctuations and “Darwininian nanoscience”, quantum effects and fluctuations in nanostructures, microscopy and manipulation tools in nanotechnology.

5. **Methods for the synthesis of nanomaterials:** Synthesis of nanoparticles through homogeneous and heterogeneous nucleation: fundamentals, subsequent growth of nuclei. *Bottom-up approach:* Common aspects of all assembly methods, synthesis inside micelles or microemulsions, laser vaporization technique, chemical bath deposition method, chemical vapor deposition technique, organic synthesis, electrodeposition, spin coating. *Top-down approach:* Photolithography, electron beam lithography, micromechanical structures, thin film technologies, molecular beam epitaxy, focused ion beam milling, laser ablation technique.

6. **Quantum size effect, bulk behavior and properties of nanomaterials:** Electrons in nanostructures and quantum effect, electrons passing through tiny structures: the Landauer resistance, charging nanostructures: Coulomb blockade, resonant tunneling. Optical and luminescent characteristics, surface plasmon resonance, mechanical properties, redox properties of nanoparticles. Dependence of thermodynamic parameters of nanocrystals on their size. Bulk behavior of nanomaterials.


**Books recommended**

PC 509 Chemistry of Materials (3 Credits)

1. **Materials:** Materials science and engineering, classification of materials, materials of the future, smart and intelligent materials, nanotechnology, modern materials’ needs.

2. **Mechanical properties of materials:** Concept of stress and strain, elastic deformation, stress-strain behavior, anelasticity, elastic properties of materials, tensile properties, plastic deformation, tensile properties, true stress and strain, elastic recovery after plastic deformation, compressive, shear, and torsional deformations, hardness. Variability of material properties, design/safety factors, dislocation, characteristics of dislocations, slip, slip systems, generalized creep behavior, stress and temperature effect, viscoelastic deformation.

3. **Thermal and electrical properties of materials:** Heat capacity, thermal expansion, materials of importance-Invar and other low expansion alloys, thermal conductivity and thermal stresses, electrical conduction in ionic ceramics and in polymers, dielectric behavior, capacitance, field vectors and polarization, types of polarization, frequency dependence of the dielectric constant, dielectric strength, dielectric materials, ferro-electricity, piezoelectricity, conducting polymers, polymer electrolytes; interaction between polymer and salts, polymer in salt and salt in polymer electrolytes.

4. **Magnetic materials:** Basic concepts, diamagnetism and paramagnetism, ferromagnetism, anti-ferromagnetism and ferri-magnetism. Influence of temperature on magnetic behavior, domains and hysteresis, magnetic anisotropy, soft and hard magnetic materials, magnetic storage, superconductivity, superconducting quantum interference device.

5. **Optical properties of materials:** Light interactions with solids, atomic and electronic interactions, optical properties of metals, optical properties of nonmetals, refraction, reflection, absorption, transmission, color, opacity, and translucency in insulators, applications of optical phenomena, luminescence, materials of importance- light emitting diodes (LED), photoconductivity, lasers, optical fibers in communications; components, step index, graded index optical fiber design.

6. **Phase diagrams and microstructure in materials:** Definitions and basic concepts, binary phase diagrams, binary isomorphous systems, interpretation of phase diagrams, development of microstructure in isomorphous alloys, mechanical properties of isomorphous alloys, binary eutectic systems, materials of importance- lead-free solders. Ceramic and ternary phase diagrams, Gibbs phase rule, development of microstructure in eutectic alloys, equilibrium diagrams having intermediate phases or compounds, eutectic and peritectic reactions, congruent phase transformation, iron-iron carbide phase diagram, development of microstructure in iron-carbon alloys; superalloys.

7. **Composite materials:** Particle-reinforced composites: large-particle composites, dispersion-strengthened composites, fiber-reinforced composites: influence of fiber length, influence of fiber orientation and concentration, the fiber phase, the matrix phase, polymer-matrix composites, metal-matrix composites, ceramic-matrix composites, carbon-carbon composites, processing of fiber-reinforced composites, hybrid composites,
Books recommended


PC 510 Advanced Concepts of Liquids (3 Credits)


2. Intermolecular forces in liquids: Nature of intermolecular forces, different types of forces and their mathematical expression and resulting effect: dipole-dipole forces, dipole-induced dipole interaction, instantaneous dipole-induced dipole interaction, repulsive interaction, total potential energy of a pair of liquid molecules, relative magnitude of different intermolecular forces in a molecule, hydrogen bonding, hydrogen bonding in water, structure of water: cluster to bulk.


4. Nature and thermodynamics of liquid surfaces: Surface thermodynamic quantities and the temperature dependence of surface free energy, the total surface energy, change of vapor pressure for a curved surface (Kelvin equation), effect of curvature pressure and other variables on surface tension, contact angle and adhesion, surface concentration (Gibbs equation), surface film, surface equation of state.

5. Liquid crystal (LC): Liquid crystallinity: classification and properties, structural features, mesomorphic state, isotropic liquid, mesophases and their properties, amphiphilic and non-amphiphilic mesogens. Conversion of different types of mesogens. Theory of LC: molecular order, order tensor, chemical structure and thermal stability, idealized structure of a calamitic LC. Theories of phase transition: molecular field and mean field
theories, Landau theory, Landau-de Gennes free energy, McMillan theory. LCD, LC thermometers, polymeric and ferroelectric LCs.


Books Recommended:


PC 511 Advanced Polymer Chemistry (3 Credits)


4. Polymer modification: Copolymerization, post-polymerization reactions: cross-linking, block and graft copolymer formation, surface modification.

spinning. Elastomer technology: elastomer properties, chemistry of vulcanization. Polymer additives and reinforcements: plasticizers, fillers and reinforcements.

6. **Characterization techniques of polymers**: UV, IR, Raman, $^1$H NMR and $^{13}$C NMR spectroscopy, mass spectrometry for polymer characterization, gel permeation chromatography (GPC), thermogravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC), dynamic mechanical analysis (DMA), thermo-mechanical analysis (TMA).

7. **Polymer in wastes and their environmental impact**: Polymer industry and environment, natural resources scenario, classified waste materials, municipal solid wastes, waste management, recovery and recycling of organic wastes, polymer reprocessing, polymer incineration. Integrated waste management for sustainable development.

**Books recommended**


**PC 512 Computational Chemistry (3 Credits)**

1. **Review on basic quantum chemistry**: Atomic units, exact solution of the Schrödinger equation, Dirac notation, one- and two-electron systems. Approximation methods: Born-Oppenheimer approximation, perturbation theory, perturbation treatment of ground state of helium atom, variation principle. Slater determinants.

2. **Fundamentals of computational chemistry**: Definition, tools and scope of computational chemistry. Potential energy surfaces: stationary points, global minima, relative minima, saddle point, hilltops; Hessian index, intrinsic reaction co-ordinate. Geometry optimization, normal-mode vibrations and zero point energy.


7. **Some aspects of computational chemistry**: Evaluation of calculated data of simple molecules, comparison of data of a model molecule calculated with MM, ab initio and semi-empirical methods. Importance of molecular modeling in drug discovery.

**Books recommended**