University of Dhaka

Department of Chemistry

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.

3. **Reactions in solutions:** Review of reactions in solutions: The Brönsted relation, linear free energy relations, ion-dipole and dipole-dipole reactions, theory of diffusion-controlled reactions, full microscopic and partial microscopic diffusion-controlled reactions, diffusion control in ionic reactions, substituent and correlation effects, Hammett equation and its applications.

4. **Kinetics of fast reactions:** Flow techniques: plug and stirred flow method, stopped flow and continuous flow methods, contact time. Relaxation methods: temperature jump and pressure jump. Flash photolysis: light sources for flash photolysis, detection techniques for flash photolysis experiments.

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 ($H + H_2$) and ($Br + H_2$). 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

1. K. J. Laidler, Chemical Kinetics, Pearsons Education Inc., 3rd edition 1987.
2. M. J. Pilling, P. W. Seakins, Reaction Kinetics, Oxford University Press, UK, 2nd edition 1996.
3. A. A. Frost, R. G. Pearson, Kinetics and Mechanism, John Wiley and Sons, New York, 2nd edition 1961.
4. I. Chorkendorff, J. W. Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, Wiley-VCH, 2nd edition 2007.
5. J. H. Fendler, E. J. Fendler, Catalysis in Micellar and Macromolecular Systems, Academic Press, 1975.
6. M. N. Khan, Micellar Catalysis, Surfactant Science Series, Volume 133, CRC Press, 2007.
7. S. M. Lindsay, Introduction of Nanoscience, Oxford University Press, UK, 2010.

PC 502 Advanced Surface Chemistry and Catalysis *(3 Credits)*

1. **Properties of solid surface**: Physical properties of solid surface: pore structure, pore volume distribution, void volume and solid density, surface area, determination of surface area. Electrical properties of solid surface: surface electron potential, surface space charge, surface free energy. Structures of metals and metallic oxides: surface structure and stepped planes. Surface modification: coatings, crack formation and propagation.

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.

3. **Surface reactions kinetics:** Elementary surface reaction, adsorption and sticking, determination of sticking coefficient, Lagergren pseudo-first order and pseudo-second order equation, intra-particle diffusion model, Elovich equation, Langmuir isotherms for associative, dissociative and competitive adsorption. Langmuir-Hinshelwood and Eley-Rideal mechanism kinetics, micro-kinetic modeling.

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 NH_3 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.

7. **Techniques for characterization of solid surfaces and adsorbed species:** Electron Emission Spectroscopy: Ultraviolet Photoelectron Spectroscopy (UPS), X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES) and Extended X-ray Absorption Fine Structure Spectroscopy (EXAFS), Electron Energy Loss Spectroscopy (EELS), Low Energy Electron Diffraction (LEED). Electron Microscopy: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Surface Enhance Raman Spectroscopy (SERS) and Reflectance Spectroscopy (RS).

Books recommended

1. A. W. Adamson & A. P. Gast, Physical Chemistry of Surfaces, Wiley, New York, 6th edition 1997.
2. P. W. Atkins & J. W. Paula, Atkin's Physical Chemistry, Oxford University Press, 9th edition 2010.
3. E. M. McCash, Surface Chemistry, Oxford University Press, 1st edition 2001.
4. R. P. H. Gasser, An Introduction to Chemisorption and Catalysis by Metals, Clarendon Press, 1st edition 1987.
5. I. Chorkendoff & J. W. Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, Wiley-VCH, 2nd edition 2007.
6. G. A. Somorjai, Introduction to Surface Chemistry and Catalysis, Wiley, New York, 1st edition 1995.
7. K. W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, Wiley, New York, 3rd edition 2012.
8. M. Milosevic, Internal Reflection and ATR Spectroscopy, Wiley, 1st edition 2012.
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.
2. **Light sources in photochemistry:** Solar energy and solar simulation, filament lamp, discharge lamp. Lasers: basic principle of laser action, various types of lasers, characteristics of laser radiation, continuous and pulsed laser. Determination of light intensity: actinometry.
3. **Photophysical and photochemical processes:** Excited species and their fates: Jablonski diagram, non-radiative and radiative processes, fluorescence, factors contributing to fluorescence, delayed fluorescence, P-type and E-type delayed fluorescences, phosphorescence. Kinetics of photophysical processes: unimolecular and bimolecular processes, photochemical quenching. Stern-Volmer equation, excimers, exciplexes. Intermolecular electronic energy transfers: radiative mechanism, long range dipole-dipole energy transfer, short range electron exchange energy transfer (photosensitization). Kinetics of some photochemical reactions: photochemical processes in atmosphere, photochemical formation and degradation of ozone, photochemistry of troposphere, photochemistry of metal complexes, ligand exchange, redox processes, photolysis of anthracene in an inert solvent, photochemistry of alkenes, photochemistry of carbonyl compounds. Chemiluminescence and bioluminescence.
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 (H_2O_2/UV), ozone/ultraviolet light (O_3/UV), hydrogen peroxide/ozone (H_2O_2/O_3),

hydrogen peroxide/ultraviolet light/ozone (H_2O_2/O_3/UV), TiO_2 or ZnO/UV and TiO_2 or ZnO/UV + H_2O_2 processes.

6. **Photodegradation:** Degradation of dyes and other organic substances in aqueous system, roles of mediators, hydrogen peroxide and ozone, influence of light on TOC and BOD of the dye house effluents in the presence of photocatalysts and other agents, kinetics of photodegradation of dyes in aqueous solution.

7. **Techniques in photochemistry:** Fluorescence spectroscopy, phosphorescence spectroscopy. Flash photolysis techniques in photochemistry: pico- and femto-second photolysis, flash photolysis studies of bimolecular electron transfer and other photochemical reactions. Time resolved IR spectroscopy. Detection of short-lived species: matrix isolation. Laser induced breakdown spectroscopy (LIBS).

Books Recommended

1. J.G. Culvert & I. N. Atkins, Photochemistry, John Wiley & Sons.
2. B. Wardle, Principles and Applications of Photochemistry, John Wiley & Sons, 2009.
3. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Principles of Molecular Photochemistry: An Introduction, Univ. Sci. Books, USA, 2009.
4. R. P. Wayne, Principles and Applications of Photochemistry, Oxford University Press, 1988.
5. K. K. Rohatgi-Mukharjee, Fundamentals of Photochemistry, revised edition, Wiley Eastern Ltd., Calcutta, 2007.
6. J. H. O' Donnel & D. F. Sangster, Principles of Radiation Chemistry, Hodder & Stoughton Educational, 1970.
7. Selected articles from recent journals.

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

1. **Electrified interface and electrodics:** Formation of electrified interfaces. Electrical double layer and different models. Butler-Volmer equation and its modifications and applications. Thermodynamic treatment of the equilibrium state for charge transfer at the metal/solution interface. Mass transport and electrode processes: Faradaic and non-Faradaic processes, Nernst-Planck equation, Nernstian and non-Nernstian behaviour, Fick's first and second law and their application in mass transport, kinetic and transport controlled processes.

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

3. **Step techniques**: Basic principles, potential excitation signals and response signals of chronoamperometry, chronocoulometry and chronopotentiometry (single and double potential steps). Use of Cottrell and Sand equations and applications. Evaluation of heterogeneous kinetic parameters and adsorption of species on the electrode surface.

4. **Pulse and stripping techniques:** Pulse techniques: tast, 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).

5. **Hydrodynamic voltammetry:** Useful parameters (comparison of diffusion layer thickness: dynamic and static conditions, relation of hydrodynamic condition with Reynolds, Schmidt, Peclet and Sherwood numbers). Practical considerations: potentiostat and electrodes in hydrodynamic system, RDE and RRDE. Reversible and irreversible kinetics in hydrodynamic condition, use of Levich, Koutecky-Levich equations and Tafel plot and applications. Evaluation of kinetic control and diffusion control processes. Applications of hydrodynamic voltammetry.

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

1. J. O'M. Bockris & A. K. N. Reddy, Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science, Springer, 2nd Edition 2001.
2. C. M. A. Brett & A. M. O. Brett, Electrochemistry: Principles, Methods and Applications, Oxford University Press, 1993.
3. J. Wang, Electroanalytical Chemistry, John Wiley & Sons Inc., 3rd Edition 2006.
4. A. J. Bard & L. R. Faulkner, Electrochemical Methods, Principles and Applications, John Wiley & Sons Inc., 2nd edition 2001.
5. P. Kissinger & W. R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, CRS Press, 2nd edition 1996.

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.

2. **Bioenergetics:** Introduction, bioenergetics and thermodynamics. Bioenergetics systems, mechanism of collection and utilization of energy in biological systems, coupling mechanism, phosphorylation, oxidative chain and substrate level phosphorylation. Self regulation of energy production, Biochemist's standard state, ATP-the carrier of energy, glycolysis, anaerobic and aerobic glycolysis, Krebs cycle, Limitations of thermodynamics.

3. **Biological membrane:** Structure and functions of biological membrane, diffusion through membrane- simple diffusion, facilitated diffusion, active transport, Na^{+}-K^{+} pump, co-transport. Membrane equilibria: general comments on equilibria across a membrane, osmotic pressure and pH difference across a membrane, Donnan effect, Donnan equilibria involving protein bearing single and multiple charges.

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.

5. **Biological macromolecules:** Introduction, structure of proteins: primary, secondary, tertiary and quaternary structures, stability of protein conformation, factors responsible for stabilization, thermodynamic treatment of stability constant, protein binding, protein-ligand binding, binding equilibria, equilibrium dialysis, dynamic dialysis, hydrophobic interaction, denaturation of proteins, denaturating agents, mechanism of denaturation, protein binding and pharmacodynamics, complexation and drug action, metal complexation in biological systems, solubility of proteins: salting-in and salting-out effects.

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

1. R. Chang, Physical Chemistry for the Biosciences, University Science Books, California, 2005.
2. D. R. Ferrier, Biochemistry (Lippincott Illustrated Reviews Series), Lippincott Williams & Wilkins

3. M. F. Chaplin & C. Bucke, Enzyme Technology, Cambridge University Press, 1990.
4. A. P. F. Turner, I. Karube, G. S. Wil, Biosensors: Fundamentals and Applications, Oxford University Press, 1990.
5. C. R. Cantor & P. R. Schimmel, Biophysical Chemistry Part III: The Behaviour of Biological Macromolecules, W. H. Freeman and Company, New York, 1980.
6. R. K. Murphy, D. K. Granner, P. A. Mayes, V. W. Rodwell, Harper's Biochemistry, Appleton and Lange, 1996.
7. D. L. Nelson & M. M. Cox Lehninger, Principles of Biochemistry, W.H. Freeman and Company, New York.
8. Recent publications.

PC 506 Chemistry of the Atmospheric Environment (*3 credits*)

1. **Atmosphere**: Earth atmosphere: its origin, composition, particles, aerosols, clouds. Cyclic processes: nitrogen, oxygen, water, carbon dioxide, sulphur, trace metal cycles, carbon cycles, link between biosphere and atmosphere. Structure of atmosphere: troposphere, stratosphere, mesosphere and ionosphere.

2. **Atmospheric transport**: Solar radiation, radiative heating, temperature profile, inversion layer in the troposphere, atmospheric transport and turbulence, geostrophic flow, vertical transport, winds, effects of changes in atmospheric composition on climate.

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 green house gases, sources and individual contribution of green house gases, CO_2 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 PM_{10}, $PM_{2.5}$, Soot Carbon, SO_x, NO_x and VOCs, field sensors for CO, SO_x, NO_x, O_3 and hydrocarbons analysis.

7. **Environmental regulation for air quality management**: Air quality standards. International legislative initiatives of global warming: Different protocols, Kyoto protocol. Legislative measures of O_3 depletion, HCFCs and their ODP. International legislative initiatives: Montreal protocol.

Books recommended

1. M. Z. Jacobson, Atmospheric pollution: History, Science and Regulation, Cambridge University Press, 2002.
2. T. Godish, Air quality, Lewis publishers (A CRC press company), New York, 4th edition 2004.
3. J. Wright, Environmental Chemistry, Routledge (CRC press), London, 2003.
4. P. V. Hobbs, Introduction to Atmospheric Chemistry, Cambridge University Press, 2000.
5. D. J. Jacob, Introduction to Atmospheric Chemistry, Princeton University Press, 1999.
6. A. K. Dey, Environmental Chemistry, New Age International Publishers, 6th edition 2006.
7. J. H. Seinfeld, S. N. Pandis, Atmospheric Chemistry and Physics from Air Pollution to Climate Change, Wiley-Interscience, 2nd edition 2006.
8. R. D. Griffin, Principles of Air Quality Management, CRC Press, 2nd edition 2006.
9. M. W. Sigrst (Edited), Air Monitoring by Spectroscopic Technique, John Wiley, 1st edition 1994.
10. S. Manahan, Environmental Chemistry, Lewis Publisher, 6th edition 2000.

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.

4. **Electronic spectra of molecules**: Electronic angular momentum of molecules, spectroscopic term symbols for atoms and molecules, photoelectron spectroscopy: principle, light sources for UV and X-ray. P.E. spectrophotometer and its instrumentation, position, multiplicity and fine structure of bands in P.E. spectrum, UV-photoelectron spectra of simple atoms and molecules, X-ray photoelectron spectra of gases and solids.

5. **Mössbauer spectroscopy**: Nuclear properties and nuclear gamma resonance, Mössbauer isotopes, Doppler effect, M**ö**ssbauer 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 $I = ½$ and $I > ½$. Zeeman anisotropy, hyperfine anisotropy. Rules of interpretation of esr spectra, esr spectrometer and scope of esr technique.

Books recommended

1. F. A. Cotton, Chemical Application of Group Theory, Wiley, New York, 3rd edition 2003.
2. C. N. Banwell & E. M. McCash, Fundamental of Molecular Spectroscopy, Tata McGraw-Hill, UK, 4th edition 1995.
3. J. M. Brown, Molecular Spectroscopy, Oxford University Press; 1st edition 1998.
4. J. A. Weil, J. R. Bolton, J. E. Wertz, Electron Paramagnetic Resonance, John Wiley & Sons Inc. 1994.
5. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons Ltd, 4th edition 2004.
6. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 3rd edition 2001.
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 nanochemistry.

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.

7. **Nanostructured materials and emerging applications:** Core-shell nanoparticles. Fullerenes: properties, aromaticity, solubility, endohedral and exohedral fullerenes. Carbon nanotubes (CNT): single and multi-walled nanotube, electronic structure and properties. Micro and mesoporous materials: ordered mesoporous structures, zeolites. Nanocomposites, nanowires, quantum dots. Nanostructure for electronics, photonic applications of nanoparticles, biomimetic chemistry, superparamagnetic nanoparticles, nanostructured thermal devices.

Books recommended

1. F. Vögtle, Supramolecular Chemistry, John Wiley and Sons, 1993.
2. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, Wiley, 2nd edition 2009.
3. J. W. Steed, D. R. Turner, K. J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley and Sons, 2007.
4. S. M. Lindsay, Introduction to Nanoscience, Oxford University Press, UK, 2009.
5. G. Cao, Nanostructures and Nanomaterials: Synthesis, Properties & Applications, Imperial College Press, UK, 2nd edition 2004.
6. A. Hirsch, M. Brettreich, F.Wudl, Fullerenes: Chemistry and Reactions, John Wiley & Sons, 2004.

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,

structural composites: laminar composites, sandwich panels, materials of importance- nanocomposites in tennis balls, biomaterials and advanced ceramics.

Books recommended

1. W. D. Callister, Materials Science and Engineering: An Introduction, Wiley, 9th Edition 2013.
2. D. R. Askeland, P. Phulé, The Science and Engineering of Materials, PWS Publishing Company, 4th edition 2002.
3. W. F. Smith, Foundations of Materials Science and Engineering, McGraw-Hill, New York, 3rd edition 2004.
4. P. W. Atkins, J. D. Paula, Physical Chemistry, W. H. Freeman; 9th edition 2010.

PC 510 Advanced Concepts of Liquids (*3 Credits*)

1. **Theories and concepts of liquid state:** Cluster theory, optimized cluster theory: Lennard-Jones fluid, X-rays and solid like state theory of liquids, distribution of molecules in liquids, Monte-Carlo method of molecular distribution in liquid: radial distribution functions. Models of liquid: microscopic, Cybotactic, kinetic molecular, random close-packed, hard sphere, lattice and defect solid state model. Liquid as a modified solid/gas.
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.
3. **Viscous flow of liquids**: Maxwell's theory of gas viscosity, difference between the mechanism of gas and liquid viscosity: Lord Rayleigh and Chapman and Enskog contributions. Viscous flow of liquids: Navier-Stokes equation, Newtonian and non-Newtonian liquids, flow as a rate process, Eyring equation, Hole theory and application of absolute reaction rate theory in viscosity. Thermodynamic activation parameters for viscous flow of liquids, correlation between enthalpy of vaporization and enthalpy of activation for viscous flow, viscosity of mixtures, types of fluids on the basis of viscous flow of liquids.
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.

6. **Ionic liquids**: Definition, structure of ionic liquids: cations and anions in ionic liquid, types of ionic liquids, properties of ionic liquids, ionicity of ionic liquids, scopes of ionic liquids: designer solvents, green credentials.

7. **Experimental techniques**: Viscosity: Falling ball viscometer and Ladenburg correction, Cannon-Finske viscometer, Ostwald viscometer. Surface tension: Wilhelmy plate, du Noüy ring, maximum bubble pressure and growing drop, capillary rise and drop volume, pendent drop and sessile drop, spinning drop and micropipette methods. Dipole moment: derivation from relative permittivity, refractive index, heterodyne-beat method.

Books Recommended:

1. J. O. Hirschfelder, C. F. Curtiss, R. B. Bird. Molecular Theory of Gases and Liquids, John Wiley & Sons, Inc., New York, 1954.
2. A. W. Adamson and A. P. Gast, Physical Chemistry of Surface, Wiley Inter-Science, New York, 1997.
3. A. Bondi, Physical Properties of Molecular Crystals Liquids and Glasses, John Wiley & Sons, New York, 1968.
4. The Structure and Properties of Solution, Discussion of Faraday Society, Chemical Society, London, **43**, 1967.
5. M. Freemantle, An Introduction to Ionic Liquids, RSC Publishing, 2010.
6. F. Vögtle, Supramolecular Chemistry, John Wiley & Sons, Inc., New York, 1991.

PC 511 Advanced Polymer Chemistry (*3 Credits*)

1. **Kinetics of polymerization**: Free radical polymerization: Initiators, kinetics and mechanism, kinetic chain length, chain transfer agents, reversible addition fragmentation termination (RAFT). Step reaction polymerization: kinetics, Carother's equation, stoichiometric imbalance, reactivity and molecular size, dendritic polymers, ring-opening polymerization. Ionic and coordination polymerization: cationic and anionic polymerization, living polymers, Ziegler-Natta catalyst.

2. **Polymerization processes**: Introduction, homogeneous systems: bulk and solution polymerization. Heterogeneous systems: suspension, emulsion, interfacial polymerization and solution polycondensation.

3. **Functional polymers**: Conducting polymer, polymer electrolyte, liquid crystalline polymer, polymer composite, polymer blends and alloys, polymer gels: hydrogels, self-oscillating gel, click polymer, self–healing polymer, inorganic polymer.

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

5. **Polymer processing**: Plastic technology: molding: compression, transfer, injection, reaction injection. Extrusion: co-extrusion, film extrusion, pultrusion. Fiber technology: textile terms, textile and fabric properties,

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

1. F. W. Billmeyer, Jr, Textbook of Polymer Science, John Wiley and Sons, 3rd edition 2002.
2. M. P. Stevens, Polymer Chemistry, Oxford University Press, 3rd edition 1998.
3. R. O. Ebewele, Polymer Science and Technology, CRC Press, Boca Raton, New York, 1st edition 2000.
4. P. Ghosh, Polymer Science and Technology, McGraw Hill, 3rd edition 2011.
5. P. C. Hiemenz, T. P. Lodge, Polymer Chemistry, CRC Press, 2nd edition 2007.
6. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International Limited, Publishers, 1st edition 1996.
7. F. M. Gray, Solid Polymer Electrolytes, Wiley-VCH, 1991.
8. R. D. Rogers, C. S. Brazel, Ionic Liquids in Polymer Systems: Solvents, Additives, and Novel Applications, ACS, Washington DC, 2005.

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.

3. **Molecular mechanics (MM):** Basic principles, force-field, force-field energy, force-field parameterization: parameter reduction in force-fields, force-fields for metal coordination compounds, universal force-fields; differences in force-fields, validation of force-fields, calculations using force-field, performance of MM.

4. ***ab initio*** **theory:** Hartree-Fock theory: Hartree-Fock equations, Fock operator. Self-consistence field (SCF) approach. Linear combination of atomic orbitals, Roothaan-Hall equations. Basis sets: Slater and Gaussian functions, contractions, polarization and diffuse functions, classification of basis sets, even and well-tempered basis set, basis set superposition errors. Restricted and unrestricted Hartree-Fock theory. Electron correlation, Møller–Plesset approach to electron correlation. Applications: geometry, energy, frequency, IR, UV and NMR spectra, ionization energy and electron affinity.

5. **Semiempirical methods:** Origin of semiempirical methods, π-methods: simple Huckel method and Pariser-Parr-Pople method. Neglect of differential overlap methods: CNDO, INDO, MNDO, AM1, PM3. Applications of semiempirical methods.

6. **Density functional theory (DFT):** Electron density distribution, functionals, Hohenberg–Kohn Theorems, Kohn-Sham (KS) energy, KS orbitals, KS equations. Various levels of Kohn-Sham DFT/Jacob's ladder: Local density approximation (LDA), local spin density approximation (LSDA), generalized gradient approximations (GGA), meta generalized gradient approximations (MGGA), hybrid generalized gradient approximations (HGGA), hybrid-MGGA (HMGGA), fully nonlocal theory. Applications: Geometry, energy, frequency and IR spectrum, dipole moment, ionization energy, electron affinity, electronegativity, hardness, softness, Fukui function.

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

1. Errol G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer Dordrecht Heidelberg London New York, 2nd edition 2011.
2. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2nd edition 2007.
3. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, 2nd edition 2004.
4. W. J. Hehre, L. Raelem P. R. Schleyer and J. A Pople, AB Initio Molecular Orbital Theory, John Wiley & Sons, 1st edition 1986.
5. E. Clementi, Modern Techniques in Computational Chemistry, ESCOM, 2nd edition 1990.
6. Ira N. Levine, Quantum Chemistry, Prentice Hall, 7th edition 2013.