UNIVERSITY OF PUNE
Department of Chemistry

M.Sc. Part II- Physical Chemistry Syllabus from July 2014

Course no.	Course name	Credits
Semester III	**Compulsory courses**	
CHP 340	Quantum Chemistry	4 Credits
CHP 341	Nuclear, radiation and photochemistry	4 Credits
CHP 342	Physicochemical Methods of analysis	4 Credits
	Optional courses (any one from following three)	
CHP 343	Topics in Theoretical Chemistry	4 Credits
CHP 344	Polymer Materials : Principles and Processing	4 Credits
CHP 345	Molecular Reaction Dynamics and Non-equilibrium thermodynamics	4 Credits
	Compulsory courses	
CHP 346	Practical I:	6 Credits
CHP 347	Practical : II	6 Credits

Semester IV	Compulsory courses	
CHP 440	Molecular Structure and Resonance Spectroscopy	4 Credits
CHP 441	Solid State Chemistry and Electrochemistry	4 Credits
CHP 442	Surface Chemistry and Catalysis	4 Credits
	Optional courses (any one from following three)	
CHP 443	Advanced Quantum Chemistry	4 Credits
CHP 444	Special Topics in Nuclear and Radiation Chemistry	4 Credits
CHP 445	Principles and applications of Nanoscience and Nanotechnology	4 Credits
	Compulsory course	
CHP 446	Project	6 credits

Semester III

Compulsory courses

CHP-340: Quantum Chemistry (4 Credits)

1. Recapitulation: Classical Mechanics, Lagrangian and Hamilton formulation, Postulates of Quantum mechanics, interpretation of wave function, operators, hermitian, linear, unitary, projection operators, eigenfunctions and eigenvalues, expectation values, Bohr correspondence principle, Theorems in quantum mechanics (12L)

2. Angular Momentum: Recapitulation, commutative relations, spherical harmonics, Ladder operators (12L)

3. Approximate methods: The variational theorem, excited states, Helium atom, Applications of variational method. (12L)

4. Perturbation theory, energy and wave-function corrections to wave-function applications, degenerate states, stark effect (12L)

Text Books:

1. Quantum Chemistry, *I. N. Levine*, Fifth Edition, Prentice Hall, New York(1998)
2. Quantum Chemistry, *D. A. McQuarrie*, Viva Books, New Delhi (2003)

CHP-341: Nuclear, Radiation and Photochemistry (4 Credits)

Nuclear and Radiation Chemistry

1. Nuclear reactions: Discovery of Nuclear reaction, Energetics of nuclear reactions, Q value of equation and threshold energy of reaction, Reaction cross section, Types of nuclear reaction (4L)

2. Nuclear Models: Liquid drop model, Assumption of LDM, Semi-emperical mass formulae, BE equation and properties of isobars, Merits and limitation of LDM
   Shell Model: Assumption of shell Model, Shell Model potential and spin orbit coupling, Periodicity in nuclear properties (4L)

3. Nuclear fission: Discovery, Classification and mechanism of fission reactions, Fission mass and charge distribution, Fission energy (4L)

4. Nuclear Reactors: Classification of reactors, The four factor formula, Reactor power, Basic features of nuclear reactor, Nuclear power and Breeder reactions. (4L)

5. Radiation detectors: Scintillators and their properties inorganic and organic, solid state semiconductor detectors-theory, surface barrier, Li drifted and intrinsic detectors (4L)

6. Radiolysis of aqueous solutions : Radiolysis of water,ferric sulphate,ceric sulphate, cupric sulphate solutions , Radiolysis Kinetics: Pulse Radiolysis and competition kinetics, non-homogeneous kinetics, flash photolysis (4L)

Photochemistry

1. Introductory concepts: Laws of photochemistry, Quantum nature and interaction of light with matter, theory of photoluminescence, Efficiency of photochemical processes; Quantum yield Primary and Overall quantum yield, general features of photochemical and photophysical processes (2L)

2. Mechanism of absorption and emission of radiation: Einstein's treatment, selection rules, Life times of excited electronic states of atoms and molecules Types of electronic transitions in organic molecules, photochemical deactivation pathways, Jablonski diagram, Fluorescence, Phosphorescence (4L)

3. Fluorescence emission, factors affecting fluorescence, viz. structure, solvent, pH, temperature etc. Triplet state and phosphorescence, heavy atom effect (4L)

4. Photophysical kinetics of uni and bimolecular processes, delayed fluorescence mechanisms, kinetics of collisional quenching, Stern-Volmer equation, quenching by added substances charge transfer mechanism, energy transfer mechanism (4L)

5. Photolysis, Laser-general principles, types of lasers: two, three and four level lasers, solid state Ruby and Nd/YAG laser, self phase modulation, single photon counting, experimental techniques, flash photolysis: conventional microsecond flash photolysis, Nanosecond laser flash photolysis, Actinometry, Time Correlated Single Photon Counting (TCSPC) an introduction (6L)

6. Frontiers of photochemistry, Picosecond, Femtosecond flash photolysis, applications: Semiconductor Photochemistry, Solar energy conversion and storage, An Introduction to Supramolecular Photochemistry: Host-Guest supramolecular photochemistry and photosynthesis (4L)

Reference Books:

1. Essentials of Nuclear Chemistry, *H. J Arnikar*, Wiley Eastern Limited, 4th Edition.(1995)
2. Nuclear and Radiochemistry, *G. Friedlander, J. W. Kennedy and J. M. Miller*, John Wiley (1981)
3. Introduction to Radiation Chemistry, *J. W. T. Spinks and R. J. Woods*, John Wiley (1990)
4. Introduction to Nuclear Physics and Chemistry, *B. G. Harvey*, Prentice hall (1963).
5. Sourcebook on Atomic Energy-*S. Glasstone*, Van Nostrand Company (1967)

6. Radiochemistry and Nuclear methods of analysis-*W. D. Ehman and D. E. Vance*, John Wiley (1991)
7. Fundamentals of photochemistry by *K. K .Rohatgi-Mukherjee*, New Age International Publishers Revised Edition (Reprint 2003)
8. Chemistry and light by *Paul Suppan*, The Royal Society of Chemistry
9. Introduction to Instrumentation Analysis by *R. D. Braun* Pharmamed. Press

CHP-342: Physicochemical Methods of Analysis (4 Credits)

1. Neutron Activation Analysis : Principle, target, matrix, cross-section, fluxes, saturation activity, excitation function, Different steps involved in NAA, radiochemical and instrumental NAA, prompt radiation and pulse neutron activation analysis, applications , advantages and disadvantages (8L)

2. Radiometric titrations: Principle, Radiometric titrations based on precipitate formation, complex formation and neutralization reactions (4L)

3. Thermal methods of analysis: Different methods of thermal analysis, TGA: Principle, Factors affecting TGA curve, Instrumentation and applications, DTA, DTA curve and factors affecting it, instrumentation and applications, DSC: Principle, Instrumentation and applications and thermometric titrations– principle and different types (6L)

4. Inductively coupled plasma atomic emission spectroscopy: principle, various stages involved in the analysis, instrumentation, ICP torch, Different nebulizers, applications, advantages and disadvantages (6L)

5. X-ray methods: Generation and properties of X-rays, generation of X-rays, -spectra, X-ray absorption, Concept of absorption edge, application, X-ray absorptive apparatus, radiography and radiotherapy, applications, X rays fluorescence, fundamental principles, instrumentation, wavelength dispersive and energy dispersive, quantitative analysis, X-ray emission, fundamental principles, X ray diffraction, powder diffractometer, applications in material science, electron microprobe, further advanced techniques, Introduction to STEM, SEM (10L)

6. XPS (X-ray photoelectron spectroscopy): Theory, satellite peaks, chemical shift, apparatus, chemical analysis, using ESCA, AES-fundamental principles UPS (8L)

7. Mass spectrometry: Theory, instrumentation-basic components, ionization sources, analyzers, resolution, chemical analysis, advanced techniques-GC/MS, MS/MS introduction (6L)

Text Books:

1. Principles of activation analysis - *P. Kruger*, John Wiley (1971)
2. Nuclear analytical chemistry- *J. Tolgyessy and S. Verga*, Vol. 2, University park press (1972)

3. Instrumental methods of chemical analysis- *Chatwal and Anand*
4. Introduction to Instrumental Analysis- *R. D. Braun*, Pharmamed Press, Indian Reprint (2006)
5. Principles of Instrumental Analysis, 5th edition- *D. A. Skoog, F.J. Holler, T. A. Nieman,* Philadelphia Saunders College Publishing (1988)

Optional courses (any one from following three)

CHP-343: Topics in Theoretical Chemistry (4 Credits)

(Reasonable mathematical background and knowledge of quantum chemistry principles and chemical bonding is a prerequisite for this optional course. ANY THREE of the FOLLOWING TOPICS will be offered.

1. Molecular Mechanics: Force fields in molecular mechanics, applications (Ref. 1 and 5) (16L)

2. Molecular dynamics: Simulations, Principles underlying MD methods, Classical and Quantum molecular dynamics, Applications (Ref. 2 and 3) (16L)

3. Case studies in Applied MO Theory: Structure, energetics, charge distributions and spectral data, interpretations in some simple systems, understanding reactivity, visualization of molecular properties (Ref. 4). (16L)

4. Quantitative Structure-Activity Relationships: Electronic and steric effects on organic reactions, topological indices, Hydrophobic parameter, Octanol-water, Partition coefficients, QSAR of Nonspecific Toxicity, QSAR of Proteins and Enzymes, QSAR in metabolism, Carcinogenesis and antitumor drugs, CNS agents, Microbial QSAR, Design of Bioactive Compounds (Ref. 1) (16L)

Text books:

1. Molecular Modelling, *A. Leach*, Longman, London (1996)
2. Introduction to Computational Chemistry, *F. Jensen*, John Wiley, New York (1999)
3. Computational Chemistry (Theories and Models), *D. Cra*mer, John Wiley, New York (2002)
4. J. B. Foresman and A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc. (1996)
5. Approximate Molecular Orbital Theory, *J. A. Pople and D. L. Beveridge*, McGraw Hill, New York (1971)

CHP-344: Polymer Chemistry: Principles and Processing (4 Credits)

1. Brief history of macromolecular sciences: Basic concepts of polymer science, classification of polymers, Chemical Bonding in polymers, stereochemistry of polymers (4L)
2. Kinetics of polymerization: Addition and condensation polymerization with specific examples

Copolymerization: Classification of copolymers, Kinetics and mechanism of copolymerization and determination of its composition (6L)

3. Thermodynamics of polymer solutions, The Flory-Huggins Theory, Flory Krigbaum and modified Flory-Huggins Theory (3L)
4. Structure and Properties: Crystalline melting point, The glass transition temperature (Tg), States of aggregation, states of phase, Factors influencing Tg. Determination of Tg by dilatometry, calorimetry. Heat distortion temperature. Properties involving large deformations, melt viscosity, tensile strength, stress, strain, crazing, shear banding, solubility and related properties, electrical and related properties. (6L)
5. Molecular weight of polymer: Number average and weight average molecular weight and degree of polymerization,
   Measurement of molecular weight of polymers: End group analysis, Colligative property measurement, Light scattering, Solution viscosity and molecular size and GPC. (5L)
6. Characterization of polymers: Chemical analysis of polymers, IR and Raman spectroscopy, X-ray diffraction analysis, Thermal analysis TG-DSC, Thermomechanical analysis (4L)
7. Commonly used polymers: Polyethylenes, Polyacrylates, Nitrile polymers, Polyamides, Polyesters, Polycarbonates, Polytetrafluoroethylene, Polyurethanes etc, Structure, preparation and applications (5L)
8. Special Polymers: Conducting polymers, mechanism of conduction, properties and applications. Biodegradable polymers, Polymer Blends and alloys, polymer gels, rubber and elastomers (6L)
9. Polymer Processing:- (5L)
   i) Plastic Technology:- Molding, Extrusion and casting, calendaring
   ii) Fibre technology: Melt, dry and wet spinning,
   iii) Elastomer Technology: Vulcanization, chemistry of vulcanization,
   iv) Reinforcement, Types of fillers
10. Polymer Degradation, Stability and Environmental Issues: Types of degradation, Thermal degradation, Mechanical degradation, Photodegradation. Recycling and biodegradation (4L)

References:

1) Polymer Science and Technology by Joel R. Fried Third edition, 2002.
2) Polymer Science, V.R.Gowarikar ,N.V.Vishwanathan and JaydevSreedhar Reprint edition, 2002.
3) Text book of Polymer Science, Fred W. Billmeyer Jr. Third edition, 2000.
4) Principles of Polymerization, George Odian, Third edition 2002.
5) Handbook on Conducting Polymers – T.A.Skotheim, Ed Marcel Dekker Inc, New York, 1 and2, 1986.

CHP-345: Molecular Reaction Dynamics and Nonequilibrium Thermodynamics
(4 Credits)

1. **Molecular Reaction Dynamics**
   Recapitulation- collision theory, transition state theory, molecular-dynamical calculations, chemiluminescence, potential energy surfaces, molecular beams,

state-to-state kinetics, spectroscopy of transition species, ultra fast laser techniques, electron transfer processes (24L)

2. **Non-equilibrium Thermodynamics**
   Entropy of irreversible processes, Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow, Entropy production in open systems; rate of entropy production, generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; electro-kinetic phenomena; TPD and thermo-mechanical effects; stationary non-equilibrium states, states of minimum entropy production; non-linear thermodynamics of irreversible processes, applications (24L)

Text book:

1. Non-Equilibrium Thermodynamics – Principles and Applications, *C. Kalidas and M. V. Sanganarayana*, Macmillan, India (2002)
2. Introduction to Thermodynamics of Irreversible Processes, *I. Prigogine*, 3rd Ed, Interscience, New York (1968)
3. Non Equilibrium Thermodynamics in Biophysics, *Katchalsky, A. & Curren, P. F.*, Harvard University Press, Cambridge (1965)

Compulsory courses

CHP-346: Physical Chemistry Practical-I (6 credits)

Computer programming and applications in computational chemistry (3 credits)

Part A: Computer programming

Hardware and software, binary and decimal numbers, constants and variables, assignment statement, flow chart and their use, IF and GO TO statements, Do loops. Input, output and format statements, Subroutines, function subprograms, Algorithms, Introduction to BASIC/Fortran/C programming languages

Part B: The students are expected to write and execute at least six of the following computer programs in BASIC/Fortran/C, Linear regression.

1. Quadratic equation.
2. Simultaneous pH titration.
3. Michaelis Menten based enzyme kinetics.
4. Analysis of amino acid sequencing.
5. Analysis of DNA sequences,Complementary sequences, repeat frequencies etc
6. Handling of atomic coordinates files and distance statistics in large molecules.
7. Determination of number of covalent and weak bonds in a given co-ordinate data for protein molecule.

These programs are only indicative. The instructor may choose other programs to illustrate the use of computers in Chemistry.

Part C: Student are expected to use following packages for computational chemistry

1. Standard *ab initio* and molecular mechanics packages of Computational Chemistry for molecular geometry optimization, energy calculation, molecular physical property evaluation viz. Dipole moment, Atomic charges, Electron density, Molecular electrostatic potential. These properties are only indicative.

The instructor may choose other properties to illustrate the applications of computers in Chemistry.

2. Visualization of molecular properties

Examination of the Part A will be taken in the form of written test whereas practical examination will be conducted for Parts B and C.

Text Books:

1. Computers and Common Sense *R. Hunt and Shelley*, Prentice Hall, New Delhi (1998)
2. Computer Programming in Fortran-90 V. *Rajaraman*, Prentice Hall, New Delhi (1990)
3. Computer and Chemistry: introduction to programming and numerical methods *T. R. Dickson*, Freeman (1968)
4. Computer programs for chemistry *D. F. Detar* W. A. Benjamin Inc, New York Vol. 1-3 (1968-69)

Wet experiments **(3 credits)**

1. Construct the ternary phase diagram for microemulsion of Tx-100/water/cyclohexane.
2. To determine the critical miceller concentration (CMC) of sodium dodecylsulphate (SDS) using conductivity method.
3. Determination of surface tension of water in presence of surfactant and hence surface excess by capillary rise method/Du-Nouy Ring tensiometer..
4. Determination of diffusion co-efficient and hydrodynamic radius of $K_3Fe(CN)_6$ by cyclic voltammetry (CV).
5. Determination of the dipole moment of polar molecule in a nonpolar solvent by the measurement of refractive index and capacitance.
6. Surface tension and parachor of liquids by stalagmometer and differential capillary methods
7. Determination of activity coefficient of electrolyte/nonelectrolyte by cryoscopy.
8. To study the formation of complex ions by cryoscopy.

CHP-347: Physical Chemistry Practical-II **(6 credits)**

1. To determine the ionisation constant (pK_a) of an indicator spectrophotometrically.
2. To investigate reaction between H_2O_2 and KI.
3. Determination of order of reaction by iodine clock method.
4. Thermodynamic parameters of an electrochemical cell, temperature dependence of EMF.
5. To determine the dose rate of C0-60 source by Fricke dosimetry.
6. Use of thiocynate dosimeter for determining the radiation dose.
7. Determination of Rate constant (Oxidation/reduction of Substituted benzene) by Pulse Radiolysis technique.
8. Determination of half life of radioisotopes in a given mixture
9. Determination of Manganese content of steel sample by neutron activation analysis technique.

10. Study the characteristics of G. M. Counter and effect of distance on absorbed dose.
11. Determination of dead time of a G. M. Counter.
12. Study of counting errors
13. Absorption coefficient of lead for a given gamma source.
14. Determination of gamma energy of a given source using scintillation counter coupled with single channel analyser.
15. Determination of Manganese content of steel sample by neutron activation analysis technique.
16. Determination of molar magnetic susceptibility by Guoy Technique.
17. Determination of magnetic susceptibility and no. of unpaired electrons by Faraday technique.
18. Determination of isobestic point of a given dye molecule by spectrophotometric method.
19. Determination of Molecular weight of a given polymer by turbidimetry.
20. Determination of Molecular weight of a given polymer by end group analysis
21. Kinetics of condensation polymerization by dilatometry.
22. Determination of equilibrium constant for the reaction, $KI + I_2 \rightarrow KI_3$.
23. To determine critical composition and critical temperature for given naphthalene bi-phenyl binary phase system.
24. Determination of composition and stability constant of a complex formed between iron (III) and sulphosalicylic acid by Job's continuous variation method and verification by slope ratio and mole ratio method.
25. Investigation of the solubility of a three component system and hence draw a tie line on a binodal curve.
26. Study of kinetics of photolysis of uranyl oxalate.

Semester IV

Compulsory courses

CHP-440: Molecular Structure and Resonance Spectroscopy (4 Credits)

1. **Nuclear Magnetic Resonance (NMR)**

Nuclear spin and magnetic moment, effect of Boltzmann distribution, spin lattice relaxation, line widths, saturation, magnetization, Bloch equations, the rotating frame of reference, ringing (4L)

Instrumentation, signal to noise ratio and size of sample, intensity measurements, references, magnetic susceptibility measurements, sampling techniques (2L)

Chemical shifts theory of chemical shifts, effect of electron density, magnetic anisotropy and chemical shifts, ring currents, nuclei other than hydrogen, isotope effects (4L)

Spin-spin interactions, origin of spin-spin coupling, first order analysis. Correlations of coupling constants with other physical properties (3L)

Structure elucidation, AX system, selection rule, intensities, AB, ABC, A_2B, ABX AB' BB' and AA'XX' systems (3L)

Relaxation, nuclear magnetic dipole interactions, chemical shift anisotropy, measurement of relaxation times (2L)

Solvent effects and hydrogen bonding solvent effects on chemical shifts, coupling constants, relaxation and exchange rates, hydrogen bonding (2L)
Multidimensional NMR, NMR imaging (2L)

2. **Electron Spin Resonance Spectroscopy (ESR)**
   ESR Basic theory, hyperfine structure, ESR Spectrophotometer (source, sample cavity, magnet, sampling procedure), line width and anisotropy, dynamic processes, electron transfer, proton exchange, fluxional molecules, the triplet state, illustrations (10L)

Text Books:

1. High Resolution N.M.R, *E. D. Becker*, Academic Press (1969)
2. Physical Methods in Chemistry, *R. S. Drago*, Saunders College Publishing (1977)
3. An introduction to Electron Paramagnetic Resonance, *M. Bersohn & J. C. Baired, W. A. Benjamin*, Inc N.Y. (1966)
4. High resolution ESR Spectroscopy, *F. Gerson*, John Wiley & sons (1970)

3. **Electric and Magnetic Properties of Molecules**
   Refractive index and electric permittivity Polarization and Polarizability, Mossotti–Clausius Equation The molar refraction, polar compounds, the measurement of permittivity, Debye Equation, Dipole moment determination, molecular dipole moment, Onsager equation, Dielectric breakdown, piezoelectricity, ferroelectrics (8L)

   Diamagnetisation and paramagnetisation theories, susceptibility and molecular magnetic moments, Zeeman splitting, multielectron systems, Ferro, anti-ferromagnetism, magnetic resonance, applications (8L)

Text Books:

1. Some electrical and optical aspects of molecular behaviour *M. Davies*, Pergamon Press (1965)
2. Lecturers on the electrical properties of materials *L. Solymar and D. Walsh*, 4th Ed., Oxford Science Publication
3. Introduction to magnetochemistry. *A. Earnshaw*, Academic Press, London (1968)
4. Magnetic Susceptibility, *L. M. Mulay*, Interscience, New York (1973)
5. Elements of magnetochemistry, *R. L. Dutta, A. Syamal*, East West Press Pvt. Ltd., (1993)

CHP-441: Solid State Chemistry and Electrochemistry (4 Credits)

Solid State Chemistry

1. Crystal growth techniques: General principles, Crystal growth from melt: Different methods of crystal growth, mehods of heating,materials for containers, seed holders, crucibles, crystal cutting, purification of material. Crystal growth from solution: Flux growth method, slow evaporation method, temperature gradient method. Theory of crystal growth (6L)

2. Imperfections and related phenomenon: Defects in solids: point defects and line defects, diffusion in solids- mechanism, elastic and plastic deformations (6L)

3. Optical properties: Photoelectric emission, Metal-Metal junctions, Metal-semiconductor junctions, Junction rectification, Luminescence and color centers (6L)

4. Solid state reactions: Reactions of single solids : Thermal decomposition reactions and their kinetic characteristics, Gas-solid reactions and their kinetics, Solid-solid reactions: addition reactions and double decomposition reactions with and without electron transfer, photographic process (6L)

Text Books:

1. Introduction of Solids, *L. V. Azaroff* , Tata McGraw Hill
2. Principles of the solid state, *H. V. Keer*, Wiley Eastern (1993)
3. Selected topics in solid state physics Vol. 12, The growth of crystals from liquids – *J. C. Brice*, North Holland/American Elsevier (1973)
4. Defects and diffusion in solids, *S. Mrowec*, Elsevier Publ.(1960)
5. Treatise on solid state chemistry, ED- *N. B. Hannay*, Plenum press Vol –2 (1975)

Electrochemistry

1. Introduction and over view of electrochemical processes: Origin of electrode potential, Electrochemical cell and reactions, Faradiac and nonfaradiac processes, Basic electrochemical thermodynamics, free energy and cell EMF, half reaction and reduction potentials, formal potentials, reference electrodes, measurements of potential differences, Electrochemical potentials, Fermi level and absolute potentials, liquid junction potential. (Ref.1, Ch. 1 and Ref. 2, Ch. 1 and 2) (4L)
2. Ion-ion interactions: Ideal solution, deviation from ideality, Activity and activity coefficient, Debye-Huckel Theory, limited and extended law (derivation expected) (Ref. 3, Ch. 3) (6L)
3. Kinetics of Electrode reactions (Electrodics): Essentials of electrode reactions, Butler Volmmer Model for electrode kinetics, One step,one electron process through potential energy diagram, standard rate constants and transfer coefficients, equilibrium condition and exchange current, current over potential equation, Tafel behavior. Mass transfer by migration and diffusion, Ficks Law (Ref. 1, Ch. 3 and 4) (5L)
4. Electrochemical devices: Batteries, Fuel cells, photoelectrochemical and dye sensitized solar cells and electrochemical super capacitors and ion-selective electrodes (Ref. 4: Ch. 10 and 13) (5L)
5. Corrosion: Mechanism, Potential – pH diagram, Measurement of corrosion rates, corrosion inhibition-anodic and cathodic protection, passivation (Ref.4: Ch. 12) (4L)

Text Books:

1. Electrochemical Methods, Second edition, *A. J. Bard and L. R. Faulkner*, John Wiley and Son (2001)
2. Electrode Potentials, *Richard G. Compton and Giles H.W. Sanders*, Oxford University Press, Walton Street, Oxford (1998)

3. Modern Electrochemistry Vol 1: 2nd Edition, *John O'M. Bockris, Amulya K. N. Reddy*, Plenum Press N.Y. (1998)
4. Modern Electrochemistry Vol 2B: *John O'M. Bockris, Amulya K. N. Reddy*, Plenum Press N.Y. (1998)

CHP-442: **Surface Chemistry and Catalysis** **(4 Credits)**

Surface Chemistry

1. Adsorption: Adsorption definition, Thermodynamics of adsorption, Langmuir adsorption isotherm, Langmuir constant and Gibbs energy of adsorption, Langmuir adsorption with lateral interaction, BET adsorption isotherm, adsorption on heterogeneous surface, The potential theory of Polanyi (4L)

2. Surface Forces: Van der Waals Forces macroscopic solids, Microscopic approach, macroscopic calculation-Lifshitz theory, Surface energy and Hamaker constant, Derjaguin approximation, DLVO theory and application (5L)

3. Thermodynamics of Interface: The Surface excess, Helmholtz/ Gibbs surface energy and definition of surface tension, interfacial enthalpy, Surface tension of pure liquids, Gibbs adsorption isotherm for two component system (derivation expected), Experimental aspects (5L)

4. Liquid Surface: Microscopic Picture of liquid Surface, Surface Tension, Equation of Young and Laplace (derivation and application), Curve surface, Kelvin Equation, Capillary Condensation, Nucleation Theory (4L)

5. Thin films on surfaces of liquids: Phases of monolayer films, Experimental techniques to study monolayer; optical methods, X-ray reflection and diffraction, the surface potential, surface elasticity and viscosity, Langmuir-Blodgett transfer, problems (3L)

6. Surfactant Micelles, emulsions: Surfactants, spherical micelles, cylinders and bilayers, critical micelle concentration, thermodynamics of micellization (equilibrium and phase separation model, derivations are expected), Structure of surfactants aggregates, biological membranes (3L)

Text Books:

1. Physics and Chemistry of Interface, Second edition, *Hans-Jurgen Butt, Karlheunz Graf, Micael Kappl*, Willey VCH (2006),ISBN-13 978-3-527-40629-6
2. Physical Chemistry of Surface, *A. W. Admson*, Fifth edition, Wiley Interscience Publiation (1990)
3. Surfactant Science and Technology, Second edition, Drew Myers, VCH Publishers (1992)
4. Principles of Colloids and Surface Chemistry, *P. C. Hiemenz Marcel and Dekker, N.*

Catalysis

Introduction, history and importance of catalysis, concept of activity, selectivity, poisoning, promotion, turnover number and deactivation, Types of catalysis, homogeneous catalysis: examples of homogeneous catalysis in gas phase, and in solution phase, acid-base catalysis, enzyme catalysis, effect of temperature and pH on enzyme catalysis, heterogeneous catalysis: heterogeneous catalysis with gaseous reactants, liquid reactants, and gaseous reactants, biocatalysis, autocatalysis, negative catalysis, characteristics of catalytic reactions, activation energy and catalysis, theories of catalysis : the intermediate compound formation theory, the adsorption theory (10L)

Mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, Langmuir-Hinshelwood model, Catalysis by semiconductors, Boundary Layer theory, Wolkenstein's theory, Catalyst characterization: surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FT-IR and thermal methods (8L)

Photocatalysis**:** Photoprocesses at semiconductor surfaces: concepts and mechanism. Applications of semiconductor photocatalysts in the field of energy and environment, photocatalytic pollutant degradation, photocatalytic water splitting, solar cells, etc. (6L)

Text/Reference Books:

1. Physical Chemistry of Surfaces, *W. Adamson*, Wiley Intersciences, (5^{th} edition) (1990)
2. Heterogeneous Catalysis: Principles and Application, *G. C. Bond*, Oxford University Press (1987)
3. Hetergogeneous Catalysis, *D. K. Chakrabarty and B. Viswanathan*, Hardcover - Oct 2008 New Age International Publishers)
4. Catalytic Chemistry, *B. C. Gates*, John Wiley and Sons Inc. (1992)

<u>Optional courses (any one from following three)</u>

CHP-443: Advanced Quantum Chemistry (Optional course) (4 Credits)

(Sound mathematical background and a good knowledge of quantum chemistry principles and chemical bonding is a prerequisite for this optional course. Any THREE OF THE FOLLOWING TOPICS will be discussed.

1. Hartree Fock Theory: Slater determinants, Postulate of antisymmetry, Slater-Condon rules for matrix elements, Hartree-Fock equations, Koopman and Brillouin theorems, Roothaan formulation, basis sets, computational aspects, UHF method, Pople Nesbet equations (Ref. 1). (16L)

2. Semi-empirical Theories: Recapitulation of Huckel method, extended Huckel method, ZDO approximation, CNDO/INDO methods, Molecular Properties,

Computational aspects, MINDO, AM1, PM3 methods, comparison of these methods (Ref. 2 and 4). (16L)

3. Density Functional Theory: Introduction, Hohenberg Kohn Theorem, N and V-representablity, Levy Functional, Kohn Sham equations, Functional derivatives and local potentials, Thomas Fermi theory, The Kohn-Sham construction, Fractional occupation numbers, Janak's theorem, Slater transition state, Electronegativity, hardness (Ref. 2). (16L)

4. Configuration Interaction: Multi-configuration wave function, full CI matrix, doubly excites CI, illustrations, Natural orbitals, Introduction to MC-SCF methods. Truncated CI and size-consistency (Ref. 1) (16L)

Text Books:

1. Modern Quantum Chemistry, *A. Szabo and N.L. Ostlund*, Dover, New York (1996)
2. Approximate Molecular Orbital Theory, *J. A. Pople and D. L. Beveridge*, McGraw Hill, New York (1971)
3. Density Functional Theory of Atoms and Molecules, *R. G. Parr and W. Yang*, Oxford University Press, Oxford (1989)
4. Molecular Modeling, *A. Leach*, Longman, Landon (1996)

CHP-444: Special Topics in Nuclear and Radiation Chemistry (4 Credits)

1. Radiation hazards and safety: Natural and manmade sources of radiations, internal and external radiation hazards, safe handling methods, personal dosimetry, reactor safety, the effects of Three miles and Chernobyl accidents, radiation protecting materials (4L)

2. Biological effects of radiations: The interaction of radiations with biological cells,somatic and genetic effects, maximum permissible dose-ICRP recommendations, Biological effects of various doses (4L)

3. Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In-vivo diagnostic procedures : Positron Emission Tomography and Thyroiditis, In-vitro diagnostic testing: Radio Immuno Assay, Therapeutic use of radiations, Use of radiations for food preservation and sterilization (8L)

4. The origin of chemical elements: cosmology and cosmochemistry premordial nucleosynthesis, stellar nucleosynthesis Various burning processes (4L)

6. Radiation Waste Management: Generation of radioactive waste from various sources, Classification of radioactive waste as per AERB guidelines, Treatment of radioactive waste: Solid waste and liquid waste (4L)

7. Accelerators: Basic components, Cockroft-Walton accelerator, Van de Graaff accelerator, Linear accelerators, cyclotrons, synchrotrons (4L)

8. Ion beam analysis techniques: Particle induced X-ray emissions- projectile accelerator and target preparation, ionization and X-ray emission detection,analysis and applications. Rutherford back scattering – scattering reaction,surface analysis,depth profiling, chanelling effects and applications (4L)

9. Radiolysis of aqueous solutions : Radiolysis of water, Basic units, ferric sulphate,ceric sulphate, cupric sulphate solutions , effect of solute concentrations on the molecular yields from water, radical scavenging, LET, Effect of LET on molecular yields ,chain reactions (5L)

10. Radiolysis of organic systems : Alkanes, aromatic hydrocarbons, alcohols (3L)

11. Radiolysis kinetics : Emperical rate studies, pulse radiolysis, molecular kinetics, non-homogeneous kinetics (8L)

References:

1. Radiation Chemistry: Principles and Applications, *Farhataziz and M. A. J. Rodgers (Eds.)*, VCH Publishers, New York (1987).
2. Essentials of Nuclear Chemistry, *H. J Arnikar*, Wiley Eastern Limited, 4th Edition.(1995)
3. Nuclear and Radiochemistry, *G. Friedlander, J. W. Kennedy and J. M. Miller*, John Wiley (1981)
4. Radiochemistry and Nuclear methods of analysis-*W. D. Ehman and D. E. Vance*, John Wiley (1991)
5. Fundamental of Radiochemistry, D.D.Sood, A.V.R.Reddy, N.Ramamoorthy, IANCAS, Mumbai, 4th Edition

CHP-445: Principles and Applications of Nanoscience and Nanotechnology
(4 Credits)

1. Introduction to Nanotechnology: Introduction to the nanoworld, A new realm of matter that lies between chemistery and solid state physics, historical perspective of nanomaterials, classification of nanomaterials (2L)
2. Metals:Structure and bonding, Properties, Reduction of Size, Size dependent properties, Applications, Synthesis of metal nanoparticles and structures (4L)
3. Chemical and catalytic aspects of nanocrystals: Nanomaterials in catalysis, Recent progress-Metals (2L)
4. Self Assembly and Self Organization: The advantages of self assembly, Intermolecular interactions and Molecular recognition, Self assembly monolayers (SAMs) (2L)
5. Energy and Power: Energy needs for future mobile devices, Basics of Battery and Power source Technology, Energy harvesting-Nanotechnology in portable systems (5L)
6. Flat Panel displays: The emergence of flat panel displays, New technologies for flat panel displays, Displays as an Intuitive human interface (3L)

7. Memory technologies for the future: Flash memory, Future options of memory technologies and their comparisons (1L)
8. Seeing beyond the hype: What the internet teaches us about the development of nanotechnology (1L)
9. Size and shape effect on biomedical applications of nanomaterials: Role of size and shape of nanomaterials in biomedical applications, Nanoparticles selection based on size, shape and surface,Targeted drug delivery by nanoparticles,The role of blood vessel,The significance of size, shape and surface characteristics of nanoparticles in biomedical applications, Comparison between nanorods and nanospheres, Thermotherapy or hyperthermia of tumors, Biomedical applications of Quantum dots, Carbon nanotubes and Silver nanoparticles (4L)
10. The optical and electron microscopy, Elementary principles of phase contrast microscopy, Fundamental properties of different types of electron microscopy (3L)
11. SEM and TEM: Importance of use of electrons, Electron sources: Electron Gun, Characteristics of Electron beam, Measurement of gun characteristics Scattering and diffraction Elastic and inelastic scattering, Diffraction in TEM, Diffraction from crystals and small (3L)
12. Lasers, apertures and resolution: Electron lenses, Apertures and diaphragms, The resolution of electron lenses, Lens Defects: Aberration: Spherical and chromatic astigmatism (3L)
13. Pumps and Holders: The vacuum, Diffusion, Turbomolecular ion and cryogenic pumps, Leak detection, contamination, Hydrocarbon and water, plasma cleaner. Different types of holders (3L)
14. Specimen preparation: SEM and TEM (2L)
15. Imaging: Amplitude contrast, mass thickness contrast, z-contrast, Phase contrast images, Bright and Dark field surface imaging, Secondary electron and back scattered electron imaging, Detectors: Electron detection and displays, Semiconductor detectors, scintillator,- PMT, TV cameras, CCD detectors, Faraday cup, Everhart-Thornley detector, SE and BSE detectors (4L)
16. Analysis of Samples: Qualitative and quantitative analysis using SEM and TEM (2L)
17. Other Techniques: X-ray spectrometry, EELS, EDX, X-ray emission spectroscopy, AFM (4L)

References:

1. Nanoscale Materials in Chemistry, *Editor: Kenneth J. Klabunde,* Publisher: John Wiley & Sons
2. Introduction to Nanoscale Science and Technology, *Edited by: Massimiliano Di Ventra, StephaneEvoy and James R. Heflin, Jr.* Publisher: Springer
3. Nanotechnologies for Future Mobile Devices, *Edited by: TapaniRyhanen, Micco A. Uusitalo, Olli Ikkala and AstaKorkkainen.*, Publisher: Cambridge University Press.
4. Biomedical Engineering-Technical Applications in Medicine, *Edited by: Radovan Hudak, MarekPenhaker and JaroslavMajernik,* Publisher: InTech, Croatia.
5. Physical Principles of Electron Microscopy: An introduction to TEM, SEM and AFM, *Ray F. Egerton*, Springer.
6. Handbook of Instrumental Techniques for Analytical Chemistry, *Frank Settle* Pearson Education (Singapore).

7. Transmission Electron Microscopy: A text book for Material Science, *David B Williams and C. Barry Carter*, Springer.
8**.** High Resolution Electron Microscopy, *John C. H. Spence*, Oxford Science Publications

Compulsory course

CHP-446: Project **(6 Credits)**