micelles and macromolecules. Self-assembly. Characterization of solid surface structure and composition using electron microscopy, XPS, Auger, Mossbauer and EELS.

Text books:
1. C. Kittel, *Introduction to Solid State Physics*, 6th Ed., Wiley, 1991.
2. A. R. West, *Solid State Chemistry and Its Applications*, Wiley, 1989.

References:
1. D. K. Chakrabarty, *Adsorption and catalysis by solids*, Wiley Eastern, 1990.
2. F. P. Kane and G. B. Larrabee (Eds.), *Characterisation of solid surfaces*, Plenum, 1978.
3. P. A. Cox, *Electronic Structure and Chemistry of Solids*, Oxford University Press, 1991.
4. G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, 2nd Ed., John Wiley, 1989.

Common Elective Courses

CH 603: Concepts for Molecular Machine 3-0-0-6

[Note: This is a new course]

Prerequisite: Fundamentals aspects of spectroscopy

Miniaturization of machines, Terminologies in molecular machine, Energetic and states of molecular machines. Operational aspects and design; Tweezers, Molecular rotors, brake, bevel gear, gyroscopes, Nano-car, Molecules walking, Thermodynamics of interlocked systems, Motions in rotaxanes and catenanes, Switching in rotaxanes, Knots, Molecular elevator, Photochemical switching, photosensitiser, Photochemically driven molecular shuttle, Light driven conformation adjustments, Light-powered molecular pedal, photosensitive liquid crystalline materials, Electrochemically driven machines, Rotations by redox couple; Bio-inspired concepts in molecular machines - Protein synthesis, ATP synthesis; Biological molecular machines for transport - Movement of Kinesins and Dyneins. DNA based tweezers, walker, molecular gear, DNA nano-machine, molecular assembler.

Text books:
1. Credi A, Silvi S, Venturi M, (eds) Molecular Machines and Motors: Recent Advances and Perspectives (2014) *Topics in Current Chem.* Volume 354, Springer, Heidelberg.
2. Baruah JB (2018) Concepts for Molecular machines, World Scientific, Singapore.

Reference:
1. Erbas-Cakmak S, Leigh DA, McTernan CT, Nussbaumer AL (2015) Artificial molecular machines. *Chem. Rev.* **115**: 10081-10206.

CH 614: Supramolecules: Concepts and Applications 3 0 0 6

[Note: The course structure remains as before. Only course number is changed. Old course number was CH 603]

Pre-requisites: Nil

Host design, preorganised hosts, complementarity, Cation, anion and neutral molecule binding hosts. Ionophores, receptors, recognitions, nano-dimensional hosts, supramolecular isomerism. Noncovalent synthesis, multicomponent cocrystals, synthons, halogen-bonds, pi-interactions, interplay of weak interactions. Clathrates, inorganic solid state clathrates, layered solids, channel structures. Intracavity complexes of neutral molecules, crystal engineering, graph set analysis, conformational polymorphs, co-ordination polymers, liquid crystals. Porous materials, surfactants. Supramolecular approach for chemistry-biology interface, neurotransmitters, optical sensing, switches, enzyme substrate binding, supramolecular catalysis, biominerlisation, hydrophobic confinement in bio-mimicking molecules, MOFs as metalloenzymes.

Texts:

1. J. W. Steedand J. L. Atwood, Supramolecular chemistry, Wiley, New York, 2000.
2. J. M. Lehn, Supramolecular Chemistry, VCH, New York, 1995.
3. H. J. Schneider and A. Yatsimirsky, Principles and methods in Supramolecular chemistry, Wiley, New York, 2000.

Reference:

1. J. L. Atwood, J. E. D. Davies, D. D. McNicol and F. Vogtle (Exe. Ed), Comprehensive Supramolecular Chemistry, Pergamon, New York.

CH 615: Applied Crystallography 3 0 0 6

[Note: The course structure remains as before. Only course number is changed. Old course number was CH 605]

Pre-requisites: Nil

Symmetry and Symmetry operations: 1D, 2D and 3D symmetry, Symmetry in Molecule, Symmetry in Crystal; Crystal: Crystal lattice, Unit cell, Crystal systems, Bravais lattice, Planes in Lattices and Miller Indices, Reciprocal lattice, Postulates of Crystallography (law of constancy of angles, law of rational indices); Crystallographic point groups and Space groups; Crystal growth, Crystal defects and Twining; X-rays: Origin, Production, Absorption, Filtering, Detectors, Selection of radiation, Fundamentals of Diffraction Theory: Diffraction by a 3D-lattice, Bragg's law; Structure determination by X-ray crystallographic method: Choosing a crystal, Shaping a crystal, Crystal mounting, Optical alignment, Data collection, Data reduction, Phase problem, Direct method, Heavy atom method, Absorption correction, Refinement of crystal structures, Completing the structure. Disorders in crystal structures and their applications.

Text Books:

1. G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, The Macmillan Company, New York.
2. *Crystal Design: Structure and function*, Ed. G. R. Desiraju, Wiley 2003.
3. Lesley Smart and Elaine Moore, *Solid State Chemistry: An Introduction*, Chapman & Hall 1985.

References:

1. W. Massa, *Crystal Structure Determination*, Springer Verlag, Berlin, 2000.
2. W. Clegg, *Crystal Structure Analysis: Principles and Practice*, Oxford University Press, 2001.
3. *Organic solid-state Chemistry*, Ed. G. R. Desiraju, Elsevier, 1987.
4. J. J. Rousseau, *Basic Crystallography*, John Wiley & Sons, New York, 1998.
5. Jenny P. Glusker, Mitchell Lewis and Miriam Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH, New York, 1994.
6. B. D. Cullity and S. R. Stock, *Elements of X - ray diffraction*, Prentice Hall, New Jersey, 2001.

CH 625: Advances in Biological Macromolecules 3-0-0-6
[Note: This is a new course.]

Pre-requisites: Nil

Advances in proteins, solid phase peptide synthesis, synthesis of peptide antibiotics, post-translational modification; advances in carbohydrates, oligosaccharides; lipids - fatty acids, bilayer, lipidation of proteins and peptides, farnesylation of the ras protein; biological membranes, transport across membranes, model membrane, insertion of lapidated peptides into model membrane and their biophysical properties, concepts of fluorescence and fluorescence markers, synthesis of vesicles containing fluorescence quencher and lipidated peptides; advances in nucleic acids–DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, nucleic acids as molecular probes, peptide nucleic acids (PNAs) - synthesis, doubly labeled PNAs as probes for the detection of point mutations; use of small molecules to link a protein target to a cellular phenotype and as probes for biological processes.

Text Books:

1. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd., 2008.
2. C.M. Dobson, J.A. Gerrard and A.J. Pratt,*Foundations of Chemical biology*, Oxford Univ. Press. 2002.
3. J. M. Berg, J. L. Tymoczko and L. Stryer. *Biochemistry,* W. H. Freeman and Company, New York.
4. Lehninger, Nelson and Cox, *Principles of Biochemistry*, CBS Publishers, 1993.

References:

1. S.L. Schreiber, T. Kapoor and G. W. Wiley *Chemical Biology: from small molecules to systems biology and drug design,* Vol.-1, VCH Verlag GmbH & Co. 2007.
2. B. Larijani, C. A. Rosser and R. Woscholski *Chemical Biology: Application and Techniques*, John Wiley & Sons Ltd. England, 2006.
3. H. Waldmann and P. Janning. Wiley *Chemical Biology: A practical course,* VCH Verlag GmbH & Co. 2004.
4. C.M. Dobson, J.A. Gerrard and A.J. Pratt., *Foundations of Chemical biology*, Oxford University Press, 2002.
5. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd., 2008.
6. L. Stryer, J.M. Berg and J. L. Tymoczko, *Biochemistry*, 5th Ed. (Hardcover) 2002.
7. J. S. Davies, *Amino acids, peptides and proteins* Vol. 35, Royal Society of Chemistry, UK, 2006.
8. J.S. Fruton, *Proteins, Enzymes, Genes: the Interplay of Chemistry and Biology,* (xii 1 783 pages).Yale University Press, 1999.

CH 631: Advanced Quantum Chemistry 3 0 0 6

[Note: The course structure remains as before. Only course number is changed. Old course number was CH 637]

Pre-requisites: Prior knowledge of Quantum Chemistry

Introduction: Vector interpretation of wavefunction, Hermitian operator, approximate solutions to the Schroedinger equation: the variation method (time independent and time dependent), time independent perturbation theory (non– degenerate and degenerate), time dependent perturbation theory; electron spin and many - electron systems: the antisymmetry principle, spin angular momenta and their operators, the orbital approximation (Slater determinant, Pauli exclusion principle), two electron wavefunctions; the Hartree-Fock self-consistent field method: the generation of optimized orbitals, Koopman's theorem (the physical significance of orbital energies), the electron correlation energy, density matrix analysis of the Hartree-Fock approximation, natural orbitals, the matrix solution of the Hartree-Fock equations (Roothaan's equations); introduction to molecular structure: the Born-Oppenheimer approximation, solution of the nuclear equation, molecular Hartree- Fock calculations, electronic structure of linear molecule: the MO-LCAO approximation, the hydrogen molecular ion, the hydrogen molecule, molecular configuration–interaction calculations.

Text Books:

1. F. L. Pilar, *Elementary Quantum Chemistry,* 2nd Ed., Dover Publications, 1990.
2. I. N. Levine, *Quantum Chemistry*, 7th Ed., Pearson Education India, 2016
3. Szaboa and Ostlund, Modern Quantum Chemistry, Dover Publications, Inc. NY, 1989.

References:

1. D. A. McQuarrie, *Quantum Chemistry*, Oxford Univ. Press, 1983.
2. P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 4th Ed., Oxford Univ. Press, 2005.

CH 639: Principles and Applications of Molecular Fluorescence 3 0 0 6

[Note: The course structure remains same as before in all respect.]

Pre-requisites: Nil

Absorption and emission of light, radiative and non-radiative transitions, fluorescence and phosphorescence emission, delayed fluorescence, laws of photochemistry, principles of steady-state and time resolved fluorometric techniques, time-domain and frequency-domain lifetime measurements, lifetimes and quantum yield, effects of solvents, temperature and molecular structure on fluorescence spectra, mechanisms of quenching, photoinduced electron and proton transfer, resonance energy transfer, fluorescence polarization, extrinsic causes of fluorescence depolarization, additivity law, free and hindered rotation, effect of rotational diffusion on fluorescence anisotropies: the Perrin equation, molecular probes and sensors, optical clinical chemistry and spectral observables and mechanisms of sensing.

Text Books:

1. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002.
2. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Ed. 2006.

References:

1. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 1: Techniques, Plenum Press, 1991.
2. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 4: , Probe Design and Chemical Sensing, Kluwer Academic Press, 1994.
3. B. Valuer and J. C. Brochon, New Trends in Fluorescence Spectroscopy: Applications to Chemical and Life Sciences, Springer, 2001.

DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

Departmental Elective Courses for M. Sc./PhD/Common In Chemistry

M. Sc. Elective Courses
(Syllabus as part of newly revised M. Sc. Course structure)

CH 611 Advanced Organometallic Chemistry 3 0 0 6
CH 612 Inorganic Clusters 3 0 0 6
CH 613 Applied Inorganic Chemistry 3 0 0 6
CH 621 Modern Reagents in Organic Synthesis 3 0 0 6
CH 622 Methods in Organic Synthesis 3 0 0 6
CH 623 Supramolecular Chemistry 3 0 0 6
CH 624 Fundamentals of Chemical Biology 3 0 0 6
CH 632 Solid State and Interfacial Chemistry 3 0 0 6

[All the syllabi are placed under the newly revised M.Sc. curriculum with a Note at the bottom. A summary sheet also is provided]

Common Elective Courses

CH 603 Concepts for Molecular Machine 3 0 0 6
CH 614: Supramolecules: Concepts and Applications 3 0 0 6
CH 615: Applied Crystallography 3 0 0 6
CH 625 Advances in Biological Macromolecules 3-0-0-6
CH 631: Advanced Quantum Chemistry 3 0 0 6
CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6

[All the syllabi are placed under the newly revised M.Sc. curriculum with a Note at the bottom. A summary sheet also is provided]

Ph. D. Elective Courses

CH 601 Physical Methods in Chemistry 3 – 0 – 0 6
CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6
CH 617 Organometallics 3 – 0 – 0 6
CH 618 Bioinorganic Chemistry 3 – 0 – 0 6
CH 633 Chemical Applications of Group Theory 3 – 0 – 0 6
CH 634 Time Dependent Quantum Mechanics 3 – 0 – 0 6
CH 635 Basic Statistical Mechanics 3 – 0 – 0 6
CH 636 A Fundamental Approach to Physical Chemistry 3 – 0 – 0 6
CH 637 Computational Methods in Chemistry 2-0-2 6
CH 626 Art in Organic Synthesis 3 – 0 – 0 6
CH 627 New Reagents for Organic Synthesis 3 – 0 – 0 6
CH 628 Chemistry of Biological Macromolecules 3 – 0 – 0 6
CH 629 Advances in Bioorganic Chemistry 3 – 0 – 0 6

[All the syllabi are placed below which are total Ph.D. electives with a Note at the bottom. A summary sheet also is provided]

CH 601 Physical Methods in Chemistry 3 – 0 – 0 6
[Note: The course structure/course no. remains the same as before.]

Prerequisite: Nil

Nuclear magnetic resonance spectroscopy: General principles, sensitivity of the method, CW and FT-NMR, instrumentation. Application in chemical analysis (with special reference to 1H – NMR): Chemical shift, spin-spin splitting, area of peak, shift reagents, off-resonance decoupling, nuclear Overhauser effect, selective population inversion, inter nuclear double resonance (INDOR). Two dimensional and three dimensional NMR spectroscopies, solid state and gas phase NMR spectra, polarization transfer techniques. Infrared spectroscopy: Principles, factors influencing vibrational frequencies, preparation of samples, the range of IR radiation, selection rules. Instrumentation: Representation of spectra, dispersive and Fourier- transform IR– spectroscopies. Application of IR spectroscopy to inorganic and organic compounds. Raman Spectroscopy: Principles, normal, resonance and laser Raman spectroscopies. Structure determination by symmetry selection rules (normal coordinate analysis). Application of Raman spectroscopy to structural chemistry. Electronic spectroscopy: General principles, electronic absorption by molecules, absorption peaks and molar absorptivity, absorption and intensity shifts. Selection rules and their implications. Analytical applications: qualitative and quantitative analyses. Electronic spectra of inorganic and organic compounds. Mass spectrometry: Principles, advantages and limitations of mass spectrometry; instrumentation, methods of ionization, metastable ions. Theory of mass spectrometry, structure elucidation of inorganic and organic compounds. Mossbauer spectroscopy: The Mossbauer effect, the Mossbauer nuclei, chemical isomer shift, quadrupole splitting, magnetic hyperfine interaction. Elucidation of electronic structure of ^{57}Fe, ^{119}Sn etc. compounds using Mossbauer data; Mossbauer of biological systems. Chromatography: General principles, different types of chromatographic techniques, characteristics of working components and analytes. Normal phase and reverse phase chromatography. Efficiency and resolution: Theoritical plate concept, van Deemter equation. Gas Chromatography: types of GC, basic components of GC, optimization of the method, GC-MS, Applications. High performance Liquid Chromatography: Different types of HPLC, basic components of HPLC, optimization of methods, applications. Electrochromatography: Principles and applications. Thermal Analysis: General principles of thermal analysis. Thermogravimetric Analysis (TGA): Principles, instrumentation, study of thermogram, applications, limitations, DTG, Chemical Vapor Deposition (CVD), Metal Oxide Vapor Deposition (MOVD). Differential Thermal Analysis (DTA*):* Principles, instrumentation, study of thermogram, applications and limitations. Differential Scanning Calorimetry (DSC*):* Principles, instrumentation, study of thermogram, applications and limitations.

Cyclic Voltammetry and Coulometry: Basic principles and applications to the study of electroactive species.

References:

1. R. M. Silverstein, G. Clayton Bassler and C. Morril, *Spectrometric Identification of Organic Compounds*, 5th Ed., John Wiley & Sons, 1991.
2. W. Kemp, *Organic spectroscopy*, 3rd Ed., ELBS, 1991.
3. R. S. Drago, *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing, 1992.
4. W. Kemp, *NMR in Chemistry: A Multinuclear Introduction*, Macmillan, 1986.
5. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Ed., Elsevier, 1986.
6. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A & B, John Wiley and Sons Inc., 5th Ed., 1997.
7. E. A. V. D. Ebsworth, D. W. H. Rankin and S. Cradock, *Structural Methods in Inorganic Chemistry*, 2nd Ed., Blackwell, 1991.

CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6

[Note: The course structure/course no. remains the same as before.]

Prerequisite: Nil

Overview of electronic devices, band theory, zone theory, conjugated systems, electronic excitation, chromophores, phosphorescence and fluorescence. Theories and application of one dimensional substances: Electron-phonon coupling, Peirerls transition, solitons and polarons, superconductivity, conducting polymers, solution switching, molecular cellular automata, biocomputing, switching molecules, Langmuir Blodgett layers, holographic storage, light emitting diodes; semiconductor devices, defect structures, p, n-type semiconductor, structure property relations in high Tc superconductors. Chemical vapour deposition: Epitaxial growth, crystalline and amorphous films, metal organic vapour deposition, micro and nano crystalline materials, ceramic materials. Electrochemistry of corrosion: thermodynamics of corrosion, electrode kinetics, corrosion mechanism of electronic material systems, corrosion and protection. Fuel cells: operational characteristic, power generation. Lithography: Principle, optical Lithography, deep-UV resists, multi layer systems, top surface imaging systems, plasma etching, dielectric and optical interconnects; biological application of photochemical switches, biosensors, immunoassay, neurotransmitters, fluorescence labels, supramolecular devices, supramolecular electrochemistry, supramolecular ionics, molecular magnets, ion response monolayers, molecular channels, photohysteresis, dual mode photoswitching, self assembly of supramolecular liquid crystalline polymers, supramolecular material and composites.

Texts books:

1. H. B. Pogge and Mercel Dekker (Ed), *Electronic Material Chemistry*, New York, 1996.
2. S. Roth, *One – dimensional metals: Physics and material science,* VCH, New York, 1995.
3. H. Morrission (Ed), *Biological application of photochemical Switches*, John Wiley, New York, 1993.

Reference:

1. J. M. Lehn, *Supramolecular Chemistry: Concept & perspective*, VCH, New York, 1995.
2. C. N. R. Rao and J. Gopalakrishnan, *New Direction in solid state Chemistry*, Cambridge University Press, 1997.
3. R. Arshahy (Ed.), *Desk reference of functional polymers: synthesis and application*; American Chemical Society, Washington, DC, 1996.
4. G. Burns, *High temperature superconductivity an introduction*, Academic press, New York, 1992.

CH 617 Organometallics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 610]

Prerequisite: Nil

Definition, classifications and bonding in organometallics, isolobal analogies, structural aspects of organometallics, preparative methods. Spectroscopic techniques in organometallics chemistry. Electronic and magnetic properties of organometallic compounds. Stoichiometric and catalytic reactions: Fundamental process in reactions of organotransition metal complexes. Application of transition metal complexes to catalysis. Organometallics directed towards organic synthesis. Bio-organometallics, organometallics in environmental chemistry. Metal clusters and models for heterogeneous catalysis. Application of organometallics in industry.

Text books:
1. Yamamoto, *Organotransition metal in Chemistry, Fundamental concept and applications*; John Wiley, 1986.
2. R. H. Crabtree, *The organometallic Chemistry of the transition metals*, John Wiley, 1994.

CH 618 Bioinorganic Chemistry 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 611]

Prerequisite: Nil

Role of metal ions in Biology: Physiological effects of presence or absence of metal ions in biology. Role of ions in respiration, metabolism, photosynthesis and gene regulation in brief. Hard-Soft Acid-Base Concept, chelate effect, pKa values of coordinated ligand, redox potential, Nernst equation, some kinetic aspects such as ligand exchange rate, substitution reactions and electron transfer reactions. Brief description of peptide bond, primary, secondary and tertiary structure and hydrogen bonding. Various spectroscopic methods used in bioinorganic chemistry: Infrared, electronic spectra (specially d-d transitions), EPR (emphasis on first row transtion metal ions and their spectra), brief description of CD/MCD and multinuclear NMR. Brief descrieption and capability of newer methods like EXAFS, XANES, ENDOR. Classifications of metalloproteins and enzymes based on function with example: Metalloproteins; Dioxygen transport (Hemoglobin, Hemocyanin), electron transfer (blue cuprotiens, cytochromes, iron-sulphur protein), structural roles (zinc finger), uptake and storage proteins (ferritines). Metalloenzymes: Hydrolytic enzymes (zinc enzymes), redox enzymes (Binuclear redox enzymes, SODs photosystem II), oxygen-atom-transfer reactions (methane monooxygenase, catechol dioxygenase). Metalloproteins or enzymes either newly discovered or of current research interest not covered above should be included. Discussion about different approach employed in solving the problems in bioinorganic chemistry: Use of coordination complexes as model. Models for various enzymes will be discussed along with the above mentioned enzymes/proteins. Brief descriptions of other approaches like use of mutant enzymes. Topics of current interest: Thrust areas of research in bioinorganic chemistry such as role of nitric oxide and other topics will be discussed and student will participate writing a short report on one such topic and discuss in class.

Text book:
1. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, California. (Other journal articles and books will be referenced during the course.)

CH 633 Chemical Applications of Group Theory 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 632]

Prerequisite: Nil

Definitions and Theorems of Group Theory: Properties of Group and examples, subgroups, slasses. Molecular Symmetry and the Symmetry Groups: Symmetry elements and operations: symmetry planes and reflections, the inversion Center, proper axes and proper rotation, and improper axes and improper rotations, products of symmetry operations, equivalent symmetry elements and equivalent atoms, General relations among symmetry elements and operations, Symmetry elements and optical isomerism, symmetry point groups, symmetries with multiple high- order axes, classes of symmetry operations, a systematic procedure for symmetry classification of molecules. Representations of Groups: Comments on matrices and vectors, representation of groups, the "Great Orthogonality Theorem" and its consequences, character tables, representation for cyclic groups. Group Theory and Quantum Mechanics: Wave function as bases for irreducible representations, the direct product, detection of non–zero integrals. Symmetry Adapted Linear Combinations: Derivation of Projection Operators. Use of projection operators to construct SALCs. Molecular Orbital Theory and its Application in Organic Chemistry: General remarks, Symmetry factoring of secular equations, Carbocyclic system. More general cases of LCAO-MO π bonding, naphthalene. Electronic excitations of naphthalene: Selection rules and configuration interaction, three center bonding. Symmetry based selection rules for cyclization reactions. Molecular Orbital Theory for inorganic and organometallic compounds: Transformation properties of atomic arbitals. Molecular orbitals for σ bonding in AB_n molecules: The Tetrahedral AB_4 cases. Molecular orbitals for π bonding in AB_n molecules.

Texts book:

1. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Ed., John Wiley & Sons, 1990.

Reference:

1. F. L. Pilar, *Elementary Quantum Chemistry*, 2nd Ed., Dover Publications, INC, 1990.

CH 634 Time Dependent Quantum Mechanics 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 638]

Prerequisite: M.Sc. Chemistry or Physics.

Introduction; mathematical review; evolution operator: The Schrodinger, Heisenberg and interaction pictures; perturbation theory: Fermi's Golden Rule; numerical methods for wave packet representation and propagation: The Fourier grid, discrete variable representation, finite difference, split operator, Chebychev, Lanczos and the t,t' method; wave packet dynamics in harmonic oscillator; wavefunction auto-correlation: electronic wavefunction calculation, molecular spectra; two level system: Rabi oscillations; quantum tunneling: resonances; laser matter interaction: dipole approximation and the center of mass transformation, Gauge transformation, multiphoton interactions, above threshold ionization and dissociation, high harmonic generation; control of molecular dynamics; laser cooling and trapping.

Texts books:

1. M. H. Mittleman, *Introduction to the Theory of Laser-Atom Interactions*, 2nd Ed., Plenum US, 1993
2. G. C. Schatz, and M. A. Ratner, *Quantum Mechanics in Chemistry*, Dover Publications, 2002.
3. S. A. Rice, and M. Zhao, *Optical Control of Molecular Dynamics* 1st Ed., Wiley-Interscience, 2000.

References:

1. N.B. Delone, and V.P. Krainov, *Multiphoton Processes in Atoms, Springer Series on Atoms and Plasmas*, Vol 13, Springer, 1994.
2. A. Szabo, and N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications, 1996.
3. H. J. Metcalf, and P. van der Straten, *Laser Cooling and Trapping* 1st Ed., Springer, 2001.

CH 635 Basic Statistical Mechanics 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 643]

Pre-requisites: Nil

Introduction of Statistical Mechanics: Macroscopic states, microscopic states, maximum-entropy principle, determination of the number of microstates, and statistical origin of thermodynamics, Entropy of mixing and the Gibbs correction, Ensemble Theory: Phase space, Liouville's theorem, theory of microcanonical ensemble, Canonical Ensemble Theory: Theory of distribution function for canonical ensemble, statistical quantities in canonical ensemble, ideal gases in canonical ensemble theory, energy fluctuation, equipartition theorem, molecular partition function, translational, rotational, vibrational, electronic and nuclear partition function, concepts of negative temperature, Grand Canonical Ensemble: Distribution function of grand canonical ensemble, statistical quantities in the theory of grand canonical ensemble, Quantum ideal gases: Fermi-Dirac and Bose-Einstein statistics.

Texts:

1. D. A. McQuarrie, Statistical Mechanics, University Science Books, 2000.
2. R. K. Pathria and Paul D. Beale, Statistical Mechanics, Elsevier, 2011.

References:

1. K. Huang, Statistical Mechanics, Wiley, 2008.
2. Y. V. C. Rao, Postulational and Statistical Thermodynamics, Allied Publishers Pvt. Ltd., 1994.

CH 636 A Fundamental Approach to Physical Chemistry 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 630]

Pre-requisites: Nil

Quantum Chemistry: The concept, foundation, postulates and general principles. The Schrödinger wave equation. Application – particle in a box, the harmonic oscillator and the rigid rotor, the hydrogen atom, approximate methods, multielectron atoms, the chemical bond (diatomic to polyatomic). **Spectroscopy:** Basic principles of electronic, vibrational and rotational spectroscopies. Fundamentals of nuclear magnetic resonance (n.m.r.) and electron spin resonance (e.s.r.) spectroscopies. Mossbauer Spectroscopy, Solid state and surface spectroscopies. **Photochemistry:** Fundamentals of Photophysical and photochemical processes. Lasers in photochemistry. **Statistical Thermodynamics:** The Boltzmann Factor and partition functions. Thermodynamic quantities e.g., entropy, Helmholtz and Gibbs Free Energies. **Reaction Dynamics:** Molecular collisions, Scattering, Molecular Energy Transfer and Chemical Reactivity. **Solids and Surface Chemistry:** The unit cell, Symmetry, X-Ray Diffraction in solids. The nature of surfaces compared to the bulk, Physisorption and Chemisorption on surfaces. Reactions on surfaces.

Text Books:

1. Physical Chemistry: A Molecular Approach by Donald A McQuarrie and John D. Simon; Viva Books Private Limited, New Delhi, First South Asian Edition, 1998.

References:

1. Quantum Chemistry; Ira N. Levine, Fourth Edition; Prentice / Hall of India Pvt. Ltd., New Delhi – 1994 (or later).
2. Molecular Reaction Dynamics and Chemical Reactivity by Raphel D. Levine and Richard Bernstein; Oxford University Press; 1987 or later.

3. Dynamics of Molecules and Chemical Reactions by Robert E. Wyatt and John Z. H. Zhang, Marcel Dekker, Inc. New York 1996.
4. Fundamentals of Statistical and Thermal Physics by F. Reif, Mc. Graw Hill, 1985.
5. Molecular Vibrations by E. Bright Wilson, jr., J. C. Decius and Paul C. Cross Dover Publications, Inc., New York 1980.
6. Molecular Rotation Spectra by H. W. Kroto, Dover Publications Inc., New York, 1992.
7. Symmetry and Spectroscopy: An introduction to Vibrational and Electronic Spectroscopy, Daniel C. Harris and Michael D. Bertolucci, Dover Publications Inc., New York, 1978.
8. Fourier Transform N. M. R. spectroscopy by Derek Shaw; Studies in Physical and Theoretical Chemistry Vol. 30, Elsevier 1987.

CH 637 Computational Methods in Chemistry 2-0-2 6

[Note: Only course number is changed. Old course number was CH 634]

Prerequisites : Nil

Introduction to linux operating system. Introduction to Fortran; Development of small computer codes involving simple formulae in chemistry: such as van der Waals equation, pH titration, kinetics, radioactive decay; Basic numerical analysis: Roots of equations, Interpolation and polynomial approximation, Numerical solution of differential equations: ODE and PDE, numerical integration, solution of linear systems using Gaussian elimination; Use of standard available software to perform simple quantum chemical calculations.

Text Books :

1. S. J. Chapman, Fortran 90/95 for Scientists and Engineers, 2nd edition, McGraw-Hill, 2003.
2. W. E. Mayo and M. Cwiakala, Programming with FORTRAN 77, Schaum's Outline Series, McGraw Hill, 1995.
3. Numerical Recipes in FORTRAN/C by W. H. Press , S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 2nd edition, 1996.
4. S. C. Chapra and P. Canale, Numerical Methods for Engineers, 4th edition, Tata McGraw -Hill, 2002.
5. F. Jensen, Introduction to Computational Chemistry, 3rd edition, Wiley, 2017.

References :

1. V. Rajaraman, Computer Programming in in Fortran 90 and 95, PHI, 1997.
2. M. Metcalf and J. Reid, Fortran 90/95 Explained, Oxford : O.U.P, 1999.
3. C. Xavier, Fortran 77 and Numerical Methods, Wiley Eastern, 1994.
4. J. Leszczynski (editor), Handbook of Computational Chemistry, 2nd edition, Springer, 2017.

CH 626: Art in Organic Synthesis 3 – 0 – 0 6

[Note: Old Course is modified and course number is changed. Old course number was CH 620/625]

Pre-requisites: Nil

Retrosynthetic Analysis: Basic for retrosynthetic analysis, Transforms and retrons, Types of Transforms, Biomimitic Approach to Retrosynthesis, Chemical degradation as a tool for retrosynthesis, Chiron approach. Transform-Based Strategies: Transform-guided retrosynthetic search, Diels-Alder cycloaddition as a T-goal, Retrosynthetic analysis by computer under T-goal guidance, Enantioselective transforms as T-goals, Mechanistic transform application, T-goal search using tactical combination of transforms. Structure-Based and Topological Strategies: Structure-goal

(S-goal) strategies, Acyclic strategies disconnections, Ring-bond disconnections-isolated rings, Disconnection of fused-ring systems, Disconnection of bridged-ring systems. Stereochemical Strategies: Stereochemical simplification-transform stereoselectivity, Stereochemical complexity-clearable stereocenters, Stereochemical strategies-polycyclic systems, Stereochemical strategies-acyclic systems. Functional Group-Based and other Strategies: Functional Group interconversion, functional group-keyed skeletal disconnections, disconnection using tactical sets of Functional Groupkeyed transforms, Strategies use of Functional Group equivalents, Acyclic core group equivalents of cyclic Functional Groups, Functional Group-keyed removal of functional and stereocenters, Functional Group and appendages as keys for connective transforms. Use of Several Strategies: Multistrategic retrosynthetic Analysis of longifolene, parontherine, perhydrohistrionicotoxin, Gibberellic acid, Picrotoxinin.

Texts:

1. E. J. Corey and Xue-Min Cheng, *The logic of chemical synthesis,* John Wiley, 1989.
2. M. B. Smith, *Organic synthesis,* McGraw-Hill Inc, New York, 1994.
3. Stuart Warren and Paul Wyatt, *Organic Synthesis: The Disconnection Approach*, Wiley; 2nd edition, 2008.

CH 627: New Reagents For Organic Synthesis 3 – 0 – 0 6

[Note: Old Course is modified and course number is changed. Old course number was CH 621/627]

Pre-requisites: Nil

Lanthanides in Organic Synthesis: General properties of Lanthanides, use of Lanthanide metal compounds at different oxidation states in synthesis. Reagents from (i) Cerium (ii) Samarium (iii) Ytterbium etc. Organotransition metal reagents: Principles, reagents developed from Titanium, Chromium, Iron, Rhodium, Nickel, Palladium. Reagents containing Phosphorous, Sulphur, Silicon or Boron: Introduction, Phosphorous-containing reagents, Sulphur-containing reagents, Silicon-containing reagents,, Boron-containing reagents. Oxidising reagents: Use of reagent such as Pyridinium Chloro Chromate, Pyridinium Fluoro Chromate, Swern oxidation, DCC oxidation, Tetrapropyl ammonium peruthenate, other oxidizing agent. Reducing agents: Reductions involving (NaBH) 4, (LiAlH)4, (NaBH)3CN, DIBAL, Red –Al.

Texts:

1. R. O. C Norman and J. H. Coxon, *Principle of Organic Synthesis*, 1st Ed, ELBS, 1993.
2. T. Imamoto, *Lanthenides in Organic synthesis*, Academic Press, 1994.
3. W. Carrutuer, *Some Modern methods of Organic Synthesis*, Cambridge, 1990.
4. L. W. Paqueette (Ed), *Reagents for Organic synthesis*, John Wiley, 1995.

CH 628: Chemistry of Biological Macromolecules 3 – 0 – 0 6

[Note: Old Course is modified and course number is changed. Old course number was CH 623]

Pre-requisites: Nil

Definition and history of chemical biology; amino acids, peptides and proteins, bio- and chemical synthesis of proteins, solid phase peptide synthesis, native chemical ligation, strategies of combinatorial synthesis, combinatorial solid phase synthesis of peptide antibiotics, post-translational modification - glycosylation, carbohydrates, oligosaccharides; lipids - fatty acids, bilayer, lipidation of proteins and peptides, farnesylation of the ras protein; biological membranes, transport across membranes, model membrane, insertion of lapidated peptides into model membrane and their biophysical properties, concepts of fluorescence and fluorescence markers, synthesis of vesicles containing fluorescence quencher and lipidated peptides; nucleic acids – DNA double helices, DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, nucleic acids as molecular probes, peptide nucleic acids (PNAs) - synthesis, doubly labeled PNAs as probes for the detection of point mutations; use of small molecules to link a protein target to a cellular phenotype and as probes for biological processes.

Text Books:

1. C.M. Dobson, J.A. Gerrard and A.J. Pratt,*Foundations of Chemical biology*, Oxford Univ. Press. 2002.
2. J. M. Berg, J. L. Tymoczko and L. Stryer. *Biochemistry,* W. H. Freeman and Company, New York.
3. Lehninger, Nelson and Cox, *Principles of Biochemistry*, CBS Publishers, 1993.

References:

1. S.L. Schreiber, T. Kapoor and G. W. Wiley *Chemical Biology: from small molecules to systems biology and drug design,* Vol.-1, VCH Verlag GmbH & Co. 2007.
2. B. Larijani, C. A. Rosser and R. Woscholski *Chemical Biology: Application and Techniques*, John Wiley & Sons Ltd. England, 2006.
3. H. Waldmann and P. Janning. Wiley *Chemical Biology: A practical course,* VCH Verlag GmbH & Co. 2004.
4. C.M. Dobson, J.A. Gerrard and A.J. Pratt., *Foundations of Chemical biology*, Oxford University Press, 2002.
5. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd., 2008.

CH 629 Advances in Bio-Organic Chemistry 3-0-0-6

[Note: Old Course is modified and course number is changed. Old course number was CH 641]

Pre-requisites: Basic knowledge in Biological Macromolecules/Biochemistry

Introduction to bioorganic chemistry; biomimetic chemistry; chemical biology: proteomics, glycomics, protein's secondary structures; peptidomimetics; peptide based drugs; recent trend in expanding genetic code; enzymes catalysis; drug targets: types, enzyme as drug target, inhibiton and drug design, enzyme catalysed reactions; antibody: catalytic antibodies, hapten design, examples of antibody catalyzed reactions; biomimetic polyene cyclisation; squalene biosynthesis; drug DNA interaction; RNAzymes; genetic alphabets; DNA detection-single nucleotide polymorphism (SNPs); human genome project; hap map project; gene therapy; human variome project; 1000 genomes project; personalised medicine.

Text Books:

1. Lehninger Principles of Biochemistry, 5th Ed. by Nelson and Cox.
2. Hermann Dugas: Bioorganic Chemistry-A chemical Approach to Enzyme Action; 3rd Edition.
3. The organic chemistry of enzyme-catalyzed reactions, by Richard B. Silverman, Academic Press, San Diego, **2000**, 717 pp.

References:

1. Biochemistry, 5th Ed. (Hardcover) by Lubert Stryer, Jeremy M. Berg, and John L. Tymoczko.
2. *NPTEL-Web based Course, Bio-Organic Chemistry by* S. S. Bag. Website: http://www.nptel.iitm.ac.in/courses/104103018/.
3. Amino acids, peptides and proteins, by J. S. Davies, Royal Society of Chemistry, UK, Vol. 35, **2006**.
4. Proteins, Enzymes, Genes: the Interplay of Chemistry and Biology by J.S. Fruton, Yale University Press, **1999**. (xii 1 783 pages).

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

MINUTES OF THE 96th MEETING OF THE INSTITUTE POSTGRADUATE PROGRAMME COMMITTEE (IPPC) held on 11 APRIL 2019

[SUMMARY SHEET]

Departmental Elective Courses for M. Sc./PhD/Common In Chemistry

M. Sc. Elective Courses
(Syllabus as part of newly revised M. Sc. Course structure)

CH 611 Advanced Organometallic Chemistry 3 0 0 6
CH 612 Inorganic Clusters 3 0 0 6
CH 613 Applied Inorganic Chemistry 3 0 0 6
CH 621 Modern Reagents in Organic Synthesis 3 0 0 6
CH 622 Methods in Organic Synthesis 3 0 0 6
CH 623 Supramolecular Chemistry 3 0 0 6
CH 624 Fundamentals of Chemical Biology 3 0 0 6
CH 632 Solid State and Interfacial Chemistry 3 0 0 6

Common Elective Courses

CH 603 Concepts for Molecular Machine 3 0 0 6
[Note: This is a new course → Syllabus is given].

CH 614: Supramolecules: Concepts and Applications 3 0 0 6
[Note: Only course number is changed. Old course number was CH 603 → Syllabus is given]

CH 615: Applied Crystallography 3 0 0 6
[Note: Only course number is changed. Old course number was CH 605 → Syllabus is given]

CH 625 Advances in Biological Macromolecules 3-0-0-6
[Note: This is a new course → Syllabus is given]

CH 631: Advanced Quantum Chemistry 3 0 0 6
[Note: Only course number is changed. Old course number was CH 637 → Syllabus is given]

CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6
[Note: The course structure/course no. remains the same as before → Syllabus is given]

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

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Ph. D. Elective Courses

CH 601 Physical Methods in Chemistry 3 – 0 – 0 6
[Note: The course structure/course no. remains the same as before. → Syllabus is given]

CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6
[Note: The course structure/course no. remains the same as before. → Syllabus is given]

CH 617 Organometallics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 610→ Syllabus is given]

CH 618 Bioinorganic Chemistry 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 611→ Syllabus is given]

CH 633 Chemical Applications of Group Theory 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 632→ Syllabus is given]

CH 634 Time Dependent Quantum Mechanics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 638→ Syllabus is given]

CH 635 Basic Statistical Mechanics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 643→ Syllabus is given]

CH 636 A Fundamental Approach to Physical Chemistry 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 630→ Syllabus is given]

CH 637 Computational Methods in Chemistry 2-0-2 6
[Note: Only course number is changed. Old course number was CH 634→ Syllabus is given]

CH 626 Art in Organic Synthesis 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 620/625→ Syllabus is given]

CH 627 New Reagents for Organic Synthesis 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 621/627→ Syllabus is given]

CH 628 Chemistry of Biological Macromolecules 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 623→ Syllabus is given]

CH 629 Advances in Bioorganic Chemistry 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 641→ Syllabus is given]

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