Course Contents offered by Chemistry Department for PhDs

Index

Electives

Title	**Catalysis for Energy**	Number	CY6xx
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	MSc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:
1. To give a overview about defining a roadmap for the role of catalysis in energy production
2. Relate catalysis with fuel cells, hydrogen production and storage, methane storage and industrial catalysis

Learning Outcomes

The students are expected to have the ability to:
1. Understand role and the possibilities of catalysis in the production of new energy carriers and in the utilization of different energy sources.
2. to go beyond conventional application identifying new developments that may lead to breakthroughs in the production of alternative energy.

Contents

Catalysis: Introduction to heterogeneous catalysis, including models of surface reactivity, surface equilibria, kinetics of surface reactions, electronic and geometrical effects in heterogeneous catalysis.(Lectures 14)
Catalytic reactions and application: Trends in reactivity, catalyst structure and composition, electro-catalysis and photo-catalysis.(Lectures 12)
Selected applications and challenges in energy transformations: fuel cells, hydrogen production, OER and HER reactions, CO_2 oxidation, methane and hydrogen storage and industrial catalysis. (Lecture 14)

Textbooks

1. Hanefeld, U, Lefferts, L. (2018) Catalysis: An Integrated Textbook for Students, 1st Edition, Wiley

Reference Books:

1. Okada, Tatsuhiro, Kaneko, Masao, (2009), *Molecular Catalysts for Energy Conversion* Springer.
2. Guczi, László, Erdôhelyi, András, *Catalysis for Alternative Energy Generation*, Springer.
3. Pierluigi Barbaro, Claudio Bianchini, *Catalysis for Sustainable Energy Production,* Wiley

Self Learning Material

1. Xile Hu, Angamuthu, R and Bera, J. K., Catalysis for Energy Storage, GIAN Course material, Indian Institute of Technology Kanpur, https://www.youtube.com/watch?v=LvTfsIAI-VE

Title	**Nanomaterials and Nanodevices**	Number	CY653
Department	Chemistry	L-T-P [C]	2-0-1 [3]
Offered for	MSc/PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:
1. Underlying scientific basis for the behavior of nanomaterials
2. Methods of synthesis, fabrication and characterization of nanomaterials
3. Scope of nanomaterials and potential translation as products

Learning Outcomes

The students are expected to have the ability to:
1. Able to describe the basic science behind the properties of materials at the nanometer scale
2. Learn principles behind advanced experimental techniques for studying nanomaterials
3. Systematically solve scientific problems related specifically to Nano technological materials

Contents

Concepts, Definitions and Examples: Nanoscale processes, nanosystems, nanostructures, important nanomaterials such as clusters, nanocrystals, nanotubes and nanowires. (2 Lectures)
Size-dependent properties: Quantum confinement, Bandgap, Surface effects in nanosystems. Optical, mechanical, electronic and magnetic properties along with surface reactivity.(6 Lectures)
Synthesis of nanomaterials: Top-down and bottom-up, soft versus hard methods, chemical and physical methods, hybrid methods for synthesis of nanomaterials.(6 Lectures)
Experimental methods for study of nanomaterials: Electron microscopes (SEM and TEM), scanning probe microscope (AFM and STM), X- ray photoelectron spectroscopy, BET surface area, electroanalytical techniques and miscellaneous methods (6 Lectures)
Nanolithography for Nanodevices: Concepts and methods; fabrication of devices, clean room practices, optical, electron, ion- beam lithography, soft lithography, micromolding, nanoimprint lithography. (6 Lectures)
Applications: Translating nanomaterials and nanodevices as commercial products.(4 lectures)

Laboratory Experiments

Synthesis of metal nanoparticles, Particle size analysis by UV Visible spectroscopy, synthesis of semiconducting ZnO nanoparticles, quantum dots, optical band gap analysis by emission spectrum, SEM imaging, AFM analysis, patterning by Photo/Soft Lithography,graphene synthesis and surface property analysis

Text Books

1. Pradeep, T., (2012), *Textbook of Nanoscience and Nanotechnology*, Mc Graw Hill
2. C. N. R. Rao, P. J. Thomas and G. U. Kulkarni (2007)Nanocrystals: Synthesis, Properties and Applications,Springer.

Reference Books

1. Nalwa, H. S., (2004), *Encyclopedia of Nanoscience and Nanotechnology*, Edition American Scientific Publishers, Los Angeles
2. Rao, C.N.R. and Govindaraj, A., (2005), *Nanotubes and nanowires*, RSC Publishing
3. C. N. R. Rao, P. J. Thomas and G. U. Kulkarni (2007)Nanocrystals: Synthesis, Properties and Applications,Springer.

Preparatory Course Material

1. Subramaniam, A., Balani, K. *Nanostructures and Nanomaterials: Characterization and Properties*, NPTEL Course Material, Department of Materials Science & Engineering, Indian Institute of Technology, Kanpur, http://nptel.ac.in/courses/118104008/;

Title	**Compounds of p-block elements and Applications**	Number	CY6XX
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. To give better insights into the interesting class of compounds such as rings, clusters, polymers and low valent complexes of the main-group elements.
2. To learn about the synthesis, structure and properties of inorganic heterocyclic and homocyclic rings.
3. To discuss about structure, properties and reactivity of clusters and cages of main group elements.

Learning Outcomes

The students are expected to:

1. Appreciate the interesting class of compounds such as rings, clusters and polymers of main group metal compounds.
2. Gain deeper insights into the synthesis and reactivity of novel main group compounds.
3. Understand structure-property relationships and applications of inorganic, organometallic polymers and low valent compounds.

Contents

Inorganic Rings: Synthesis, structure and reactivity of compounds containing heterocyclic rings of elements such as Phosphorus, Boron, Silicon, Tin and Aluminum. Structure and reactivity of compounds containing homocyclic rings of germanium, boron, silicon, aluminum. Synthesis and properties of inorganic macrocycles. (10 Lectures)
Clusters: Clusters and Cages of Main Group Elements, Boron Hydrides and Carboranes. Homo and Heteropolyatomic Anions of the Post-Transition Elements. (8 Lectures)
Inorganic polymers: Synthesis, structure-property relationships and applications of Polysiloxanes, Polyphosphazenes, polysilanes and organometallic polymers. (10 Lectures)
Chemistry of Low valent compounds: Low valent compounds of main group elements, Recent advances in NHCs and their analogous group 13, 14 and 15 compounds. (6 Lectures)
Applications: Main group element containing rings, clusters and polymers as single source precursors for nanomaterials. Low valent compounds in small molecule activation. (9 Lectures)

Textbook

1. Chivers, T. and Manners, I., (2009), Inorganic Rings and Polymers of the p-Block Elements, 1st Edition, Royal Society of Chemistry

References

1. R. D. Archer, (2001), Inorganic and Organometallic Polymers, Wiley
2. H. R. Allcock, (2003), Chemistry and Applications of Polyphosphazenes, Wiley
3. V. Chandrasekhar, (2005), Inorganic and Organometallic Polymers, Springer-Verlag
4. M. Driess, (2004), Molecular Clusters of the Main Group Elements, Wiley-VCH
5. P. Atkins, (2008), Inorganic Chemistry, Indian Edition, 4th Ed, Oxford University Press

Preparatory Course Material

1. Balakrishna, M. S., *Chemistry of Main Group Elements*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/117101105/

Title	**Advanced Materials Design**	Number	CY7xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Provide a comprehensive overview of synthesis and characterization of bulk materials, nanoparticles, nanocomposites and hierarchical materials with nanoscale features.
2. cover the fundamental scientific principles controlling assembly of nanostructured
3. materials; synthesis, characterization tools; new properties at the nanoscale, and
4. existing and emerging applications of nanomaterials

Learning Outcomes

The students are expected to:

1. Understand a variety of different methods for synthesizing materials.
2. Evaluate the synthesis methods against each other and be able to make assessments as to what form the final products will be.
3. Should be able to assess appropriate methods for the synthesis of stable nanomaterials

Contents

Introduction to Materials Chemistry: Structure, property and their relationship with materials performance (3 Lectures)

Semiconducting Materials Chemistry: Semiconductor Devices, Phase Change Materials in Memory Technology, Thermoelectric, Superconductors, Topological Insulators, Emerging materials in the device industry such as graphene and 2D materials.(8 Lectures)

Optical/Opto-electronic Materials: Light Emitting Diodes, Photosensors, Photovoltaics (6 Lectures)

Structural & Basic Applied Materials: Structural Materials, Amorphous Materials, Smart & Responsive Materials, Bio-inspired materials (8 Lectures)

Thermal Materials Application: Thermochromics (2 Lectures)

Energy Materials: Batteries and Supercapacitors, Fuel Cells,Hydrogen generation,Hydorgen storage, Carbon capture and sequestration (12 Lectures)

Student Seminars on Selected Topics from above

Textbooks

1. Fahlman, Bradley, (2011), Materials Chemistry, 3rd Edition, Springer
2. P. Yang (2003), The Chemistry of Nanostructured Materials, 1st Edition, World Scientific Publishing Company, Singapore

Reference Books

1. G. Cao, (2004), Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press: Hackensack, NJ
2. Goldstein, J.I. *et al.* (1992), *Scanning Electron Microscopy and X-Ray Microanalysis: A Textbook for Biologists*, Materials Scientists and Geologists, 2nd Edition, Springer, US.

Preparatory Course Material

1. Qureshi, M. *Chemistry of Materials*, NPTEL Course Material, Indian Institute of Technology Guwahati, http://nptel.ac.in/courses/104103019/2

Course Title	**Characterization Techniques in Inorganic Chemistry**	Course No.	CY 6xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc/PhD Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To provide introduction to various characterization methods that are applied to inorganic chemical systems.

Learning Outcomes

The students are expected to:

1. Appreciate different important characterization methods that are applied to inorganic chemical systems.
2. Analyze the chemical and physical characterization of molecular (solution and solid-state) inorganic chemical systems.

Contents

Fundamental aspects of characterisation methods in inorganic chemistry.

Molecular Symmetry: Point group analysis of simple inorganic compounds. Infrared and Raman spectroscopy of simple inorganic molecules; predicting number of active modes of vibrations, analysis of representative spectra of metal complexes with various functional groups. (6 Lectures)

Electronic spectroscopy: electronic absorption and emission spectroscopy (4 Lectures)

Multinuclear NMR: Use of 1H and 13C NMR to study fluxionality and dynamics in inorganic and organometallic chemical systems; NMR spectral analyses of B, Al, Si, F, and P containing compounds. Inorganic and Organometallic compounds of some other NMR active nuclei will also be discussed. (11 Lectures)

EPR: Elementary aspects of Electron paramagnetic resonance (EPR) spectroscopy of inorganic compounds- g-values, hyperfine and super hyperfine coupling constants; selected applications in inorganic chemistry. (5 Lectures)

Mass spectrometry: basic principles, ionization techniques, isotope abundance, molecular ion; illustrative examples from supramolecules, inorganic/coordination and organometallic compounds. (5 Lectures)

X-ray and Photoelectron Spectroscopy: *Electron microscopy and energy dispersive analysis of X-rays (5 Lectures)*

Cyclic voltammetry: Introduction to cyclic voltammetry and discussion on cyclic voltammogram of some representative examples. (5 Lectures)

Text Books

1. R. S. Drago, Physical Methods for Chemists, 2nd Edition, Saunders, 1992.

Reference Books

1. M. Weller, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014.
2. J. E. Huheey, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Pearson, 2006.
3. F. A. Cotton, Advanced Inorganic Chemistry, 6th Edition, Wiley, 2007.
4. A. Abragam and B. Bleaney, Electron Paramagnetic Resonance of Transition Ions, Oxford University Press, 1970. (Reprint Edition 2013)

Preparatory Course Material

1. Alagarsamy P, *Characterization of Materials* NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Guwahati,https://nptel.ac.in/courses/115103030/

Course Title	**Advance Catalysis**	Course No.	CY6XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	MSc/PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. Provide knowledge of key aspects of organometallic chemistry including the different binding modes of organic ligands, variation in oxidation states and electron counts.
2. Provide an understanding of the fundamental types of organometallic reaction, such as insertion, oxidative-addition

Learning Outcomes

The students are expected to:

1. understand some fundamental organometallic transformations that underpin the catalytic formation of carbon-containing species.
2. understand basic knowledge, skills and experience useful to those students progressing into the chemical industry and research in the area of catalysis

Course Contents

*Fundamentals of Catalysis :*Definition, reaction coordinate diagram, homogeneous catalysis, mechanism, catalytic cycle, fundamental organometallic processes, ligand substitution, oxidative addition, migratory insertion, transmetallation, reductive elimination, transition metals versus homogeneous catalysts, turnover limiting step, features of a catalytic process, Effective Atomic Number Rule (18-electron-rule). (8 Lectures)

Stereochemistry and Selectivity: Concepts and Definitions, Isomers, constitution, configuration enantiomers and diastereomers, conformation, stereochemical terms-a primer, optical activity, methods for determination of enantiomeric excess-chiral stationary phase (CSP) GC and CSP-HPLC and NMR. (8 Lectures)

*Consequences of diastereoisomerism: (*i) resolution of enantiomers via formation of diastereomeric salts, (ii) resolution via chromatography (GC and HPLC), (iii) identification of absolute stereochemistry, (iv) determination of enantiomeric ratio (er), or enantiomeric excess (ee), NMR shift reagents, (iv) diastereoselective synthesis, (v) kinetic resolution, examples and (vi) enantioselective synthesis, examples. (7 Lectures)

Hammond Postulate: Kinetic and Thermodynamic Control. Kinetic and thermodynamic control, use of energy diagrams, examples: DBr addition to 1,3-butadiene, enolate formation from 2-methylcyclohexanone, Hammond postulate, examples: Markovnikov regioselectivity of HX addition to monosubstituted alkenes, Orientation in electrophilic aromatic substitution reactions (7 Lectures)

Asymmetric Catalysis Using Organometallic Reagents: Hammond Postulate and Curtin Hammett Concepts, Methods and Origin of Selectivity. CurtinHammett principle,reactivity ofconformations pyrolytic elimination, Felkin-Anh model for predicting acyclic stereoselection, [Rh(L*)]+ X− , L* =chiral ligand)]-catalyzed asymmetric hydrogenation of dehydroamino-acids for the synthesis of enantiopure alpha-amino-acids Diastereomeric intermediates and origin of selectivity, Pd(0)-catalyzed allylation of stabilized carbon nucleophiles and Rh Catalyzed hydrogenation two classical examples with different reaction profiles (10 Lectures)

Text Books

F A Cotton, G. Wilkinson, C A Murillo and M Bochmann, *Advanced Inorganic Chemistry*, 6th ed, 1999, WileyInterscience

C Elschenbroich and A Salzer, *Organometallics*, VCH Publishers, 1st ed 1989, 2nd ed 1993.

R H Crabtree, *The Organometallic Chemistry of the Transition Metals*, Wiley, 1998

C Masters, Homogeneous Transition-metal Catalysis - A Gentle Art, Chapman and Hall, 1981

Course Title	**Water Chemistry**	Course No.	CY6XX
Department	Chemistry	L-T-P [C]	2–0–1 [3]
Offered for	BTech/MTech/MSc/PhD(CY) Program	Type	Elective
Pre-requisite	*Consent of Teacher*		

Objectives

The instructor will:

1. Provide the objective of this course is to provide a fundamental and advance understanding of the chemical and biochemical processes that are involved in water treatment for drinking purposes and treatment of industrial and domestic wastewaters for water reuse and discharge to the environment
2. Provide knowledge of the key chemical processes relevant to research in water chemistry

Learning Outcomes

The students are expected to:

1. Perform quantitative and qualitative interpretations for water quality analysis
2. Apply concepts of chemical equilibrium to solve water related practical problems

Course Contents

Polar nature of water: Acids and bases, Buffering capacity of water (3 Lectures)
Equilibrium constant expressions: aqueous system including concentration, activities, activity coefficients and pH of equilibrium. (4 Lectures)
Chemical reaction equation: Arrenhius and Bronsted-Lowry acids and bases (4 Lectures)
Ionization constant reactions and expressions: Self-Ionization of water, Solubility-product expressions (4 Lectures)
Measurments: pH, Filtration, Alkalinity and aqueous titrations (3 Lectures)
Cycling of water and residence time (3 Lectures)
Water availability, usage, quality: water treatment methods (5 Lectures)
Analytical methods for water quality analysis (6 lectures)

Laboratory Experiments

Measuring color in water, removing turbidity, acidity determination, alkalinity determination, chloride in water, hardness test for water, dissolved oxyzen by winkler's method

Reference Books

Sawyer, C., McCarty, P., & Parkin G*, Chemistry for Environmental and Engineering Science*. 5th Edition. Toronto: McGraw-Hill, 2003
Mark M. Benjamin, 2015, Water Chemistry, Waveland Press, Second Edition, ISBN 1-4786-2308-X

Text Books

Werner Stumm, James J. Morgan*, Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, 3rd Edition*, Wiley
Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussell, *Principles of Water Treatment*, George Tchobanoglous, Wiley

Preparatory Course Material

1. NPTEL Lectures: https://nptel.ac.in/courses/122106030/

Title	**Frontiers in Organometallic Catalysis**	Number	MT6XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. and Ph.D	Type	Elective
Prerequisite	Consent of teacher		

Objectives

1. To impart advanced knowledge on frontiers of organometallic chemistry.
2. To teach practical applications of organometallic compounds in homogeneous catalysis particularly relevant to industrial applications.

Learning Outcomes

1. The learners are expected to gain knowledge of independent thinking in designing, characterizing and fine tuning of organometallic complexes suitable for potential catalytic transformations.
2. Learners will be able to delineate mechanistic proposal of catalytic reactions based on available experimental data.
3. Learners will have the update on current trends and challenges of organometallic chemistry towards molecular activation and organic transformations focusing on sustainable development.

Contents

Introduction: Basics of organometallics, 18 e- rule, sigma and pi donor/acceptor ligands (5 lectures)

Synthetic, characterization and reactivity strategies of Transition Metal hydrides bearing carbonyl, nitrosyl, carbene, phosphine, olefins, and so on as ancillary ligands. Inert bonds (C-H, C-C, O-H, N-H) and small molecules (H_2, CO, CO_2) activation mediated by organometallic complexes. (12 lectures)

Definition and concepts of catalysis: Important terminologies in catalysis Hydrogenation, dehydrogenation, dehydrogenative coupling reactions, hydrosilylation, hydroformylation, hydroamination, hydrocyanation, hydrozirconation, carbonylation, Wacker oxidation, Fischer Tropsch synthesis, water gas shift reaction, Olefin polymerisatization, olefin metathesis, Mechanistic pathway interpretation: Kinetic studies, Deuterium Kinetic Isotope effect, Rate limiting step, Resting state, Scrambling experiments. (13 lectures)

Approaches towards Sustainability using organometallic complexes: Pincer catalysts design, Utilization of CO_2 and other feed stocks; Sustainable Energy: H_2 economy, Methanol economy, Liquid organic hydrogen carrier. (6 lectures)

Frustrated Lewis pair Chemistry: Hydroboration, carboboration, small molecule activation, catalysis. (5 lectures)

Textbooks

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, Wiley, 1998
2. Gupta, B. D.; Elias, A. J. Basic Organometallic Chemistry: Concepts, Syntheses and Applications Paperback, Universities Press; 2nd Edition (May 30, 2013).

Reference Books

1. Collman J. P.; Finke R. G.; Norton J. R. *Principles & Applications of Organo-transition Metal Chemistry*, University Science Books
2. Bhaduri S.; Mukesh, D. Homogeneous Catalysis: Mechanisms and Industrial Applications

Preparatory Course Material

1. Maiti, D. *Organometallic Chemistry*, NPTEL Course Material, Indian Institute of Technology Bombay, https://www.youtube.com/watch?v=ITfwjQemwMg&list=PLj_Alq7xw30l8iUgacWidP_83A0rZqlBR&index=1

Title	**Numerical Methods and Group Theory**	Number	CY515
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. Basic mathematics and numerical techniques required for Chemistry students
2. Knowledge on error analysis to be used for laboratory courses
3. Provide the fundamentals of group theory to understand structure, chemical bonding and spectroscopy

Learning Outcomes

The students are expected to:

1. Ability to analyze data and perform error analysis on the data
2. Ability to understand and appreciate the mathematical and group theoretical concepts behind chemical theories

Contents

Mathematical Concepts: Vectors and Vector spaces, Operators, Orthogonal and Unitary matrices, Diagonalization, Matrix eigenvalue problems, Systems of linear algebraic equations, Determinants, Ordinary and partial differential equations, Fourier and Laplace transformation (15 lectures)

Numerical Methods: Errors in Data, Absolute and relative errors, Distribution of Errors, Central Limit Theorem, Linear regression and correlation, Interpolation, Roots of Equations, Algorithms for Matrix (15 Lectures)

Group Theory: Symmetry elements and Point Groups, Group postulates and definitions, Group multiplication tables, Subgroups and cosets, Symmetry classes and conjugates, Reducible and irreducible representations, Representations and character tables, Group theory and quantum mechanics, Group theory and chemical bonding, Applications of group theory to structures and spectroscopy, Group theory and crystal symmetry (12 Lectures)

Text Books

1. Kreyszig, E., (2011) *Advanced Engineering Mathematics*, 9th Ed., Wiley
2. Cotton, F. A., (2008) *Chemical Applications of Group Theory*, 3rd Ed., Wiley India

Reference Books:

1. Louis, L., (1991) *A Practical Guide to Data Analysis for Physical Science students*, Cambridge University Press
2. Louis, L., (2005) *Mathematics for Science Students*, Cambridge University Press
3. Arfken, W. and Harris, P. (2012) *Mathematical Methods for Physicists*, 7th Ed., Elsevier
4. Bishop, D. M., (1993), *Group Theory and Chemistry,* 2nd Ed., Dover Publications, New York

Preparatory Course Material:

1. Iyengar, S. R. K., *Numerical Methods and Computation,* NPTEL course material, Department of Mathematics, IIT Delhi
https://www.youtube.com/watch?v=88ys5ZIolSg&list=PL6E313980EF23CA6E
2. Chandra, M., Chemical Applications of Symmetry and Group Theory, NPTEL course material, Department of Chemistry, IIT Kanpur
https://www.youtube.com/watch?v=Av9f25sqLG0&list=PLj_Alq7xw30knZPTpa9whzqiSn_RZHGWP

Title	**Chemical Binding**	Number	CY524
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./Ph.D (Chemistry)	Type	Elective
Pre-requisite	CY 514 (Quantum Chemistry and Spectroscopy)		

Objectives

The Instructor will:

1. Provide high level understanding of a chemical bond using quantum mechanics.
2. Describe knowledge of modern techniques in quantum chemistry.

Learning Outcomes

The students are expected to:

1. Use modern quantum chemistry techniques to solve fundamental problems related to basic chemistry.
2. Understand a chemical bond.

Contents

Electronic structure: Variation theory, perturbation theory, electron spin, He atom, Pauli exclusion principle, Slater determinant (13 lectures)

Electronic structure of diatomic molecules: Born Oppenheimer approximation, Atomic units, H_2^+ ion, H_2 molecule, VB theory, MO theory, Semi-empirical methods (13 lectures)

Wave function based theory: Hartree-Fock theory, Electron correlation, Self-consistent field wave function, Moller-Plesset theory, Coupled cluster formulation (12 lectures)

Density functional theory (DFT): Principles of density functional theory, commercial functionals and applications (4 lectures)

Textbook

1. Levine, I. N., (2000) *Quantum Chemistry*, Pearson education.
2. Lowe, J. P., (1995) *Elementary Quantum Chemistry*, Academic Press.

Reference Books

1. Szabo, A. and Ostlund, N. S., (1996) *Modern Quantum Chemistry*, Dover.

Preparatory Course Material

K. Mangala Sunder, Introduction to Chemistry & Quantum Chemical Methods, NPTEL course material, Department of Chemistry, IIT Madras, http://nptel.iitm.ac.in

Title	**Principles of Nuclear Magnetic Resonance**	Number	CY6XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite	CY211		

Objectives

The Instructor will:

1. Introduction to Nuclear Magnetic Resonance (NMR) Spectroscopy with an emphasis on the basic principle along with instrumentation and application.
2. Enable students to understand the design of NMR experiments and analyze NMR spectrum to extract information of interest.
3. Introduce to NMR experiments by giving hands on experience on the instrument available in the institute.

Learning Outcomes

The students are expected to:

1. Understand the theoretical background of solution state NMR.
2. Apply NMR experimental methods as an analytical tool in chemistry, biology, material science, medicine for structure and dynamic studies of molecules.
3. Understand instrumentation of NMR spectrometer available in the institute.

Contents

Introduction to NMR: Spin density operator, concept of density matrix, Liouville-Von-Neuman equation, the nuclear spin Hamiltonian- gyromagnetic ratio –energy level Diagrams-Zeeman Splitting. (12 lectures)

Introduction to NMR parameters: Chemical shifts and couplings, longitudinal and transverse relaxation process – Redfield relaxation theory – paramagnetic relaxation, correlation times and relaxation times. (10 lectures)

Introduction to 1D Fourier Transform spectroscopy: Bloch equation in the rotating frame – pulse sequence design – 1D 1H and 13C NMR for structure elucidation – measurement of relaxation rates, Nuclear Overhauser effect, effect of chemical exchange. (10 lectures)

Introduction to 2D NMR, correlation spectroscopy: common pulse sequences –homo and hetero nuclear correlation spectroscopy –examples of COSY, TOCSY and NOESY – Application –chemical structure –biological processes – molecular dynamics etc.
aboratory demonstration of standard NMR experiments. (10 lectures)

Textbook

1. Farrar, T.C. and Becker, E.D., (1971), *Pulse and Fourier Transform NMR*, 1st Edition, Academic Press
2. Gunther, H., (1995), *NMR Spectroscopy*, 2nd Edition, Wiley
3. Derome, A. E., (1987), *Modern NMR Techniques for Chemistry Research*, 1st Edition, Pergamon Press

Reference Books

1. Ernst, R. R., Bodenhausen, G. and Wokaun, A., (1987), *Principles of Nuclear Magnetic Resonance in One and Two Dimension*, 2nd Edition, Clarendon Press
2. Claridge, T. D. W., (1999), High Resolution NMR Techniques in Organic Chemistry, 1st Edition, Elsevier

Preparatory Course Material

1. Atreya, H. S., *Principles and Applications of NMR Spectroscopy,* NPTEL Course Material, NMR Research Center, Indian Institute of Science, Bangalore, https://onlinecourses.nptel.ac.in/noc18_ge07

Title	**Quantum Information**	Number	CY652
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Elective
Prerequisite	MA111		

Objectives

The Instructor will:

1. Provide fundamentals of quantum information and computation
2. Impart the knowledge of modeling efficiencies of a protocol in real experimental conditions

Learning Outcomes

The students are expected to:

1. Use the concepts taught in class to various aspects of quantum information, communication and cryptography
2. Understand and appreciate the technological evolution at theoretical and experimental front in QIC

Contents

Basics of quantum information: Review of linear algebra and basic laws of quantum mechanics, concept of bits and qubits, quantum gates, quantum parallelism, quantum algorithms, density operators and its applications (10 Lectures)
Quantum entanglement and nonlocality: Classical and quantum correlations, separability criterion, separable and entangled states, measures of two-qubit and multiqubit entanglement, Bell-type inequalities, discord (12 Lectures)
Quantum Noise: Classical and Markov Processes, Quantum Operations, Examples of Quantum Noise and Quantum Operations, Applications of Quantum Operations, Limitations of the Quantum Operations Formalism (6 Lectures)
Applications: Cryptography, quantum teleportation, dense coding, entanglement swapping, secret sharing, quantum games (10 Lectures))
Effects of noise on quantum information and computation (4 Lectures)

Textbooks

1. Nielsen, M. A. and Chuang, I. L., (2000) *Quantum Computation and Quantum Information*, 10th edition, Cambridge University Press.
2. Vedral, V., (2006) *Introduction to Quantum Information Science,* 1st edition, Oxford University Press

Reference Books

1. Griffiths, D. J., (2006) *Introduction to Quantum Mechanics*, 2nd edition, Pearson Prentice Hall.
2. Bouwmeester, D., Ekert, A. and Zeilinger, A., (2000) *The Physics of Quantum Information*, 2nd edition, Springer.
3. Bellac, M. L., (2006) *A Short Introduction to Quantum Information and Quantum Computation*, 1st edition, Cambridge University Press.

Preparatory Course Material

1. Goswami, D., *Quantum Computing*, *Mathematics for Chemistry,* NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Kanpur https://onlinecourses.nptel.ac.in/noc18_cy07/preview

Title	**Molecular Dynamics Simulations**	Number	CY665
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Provide high level understanding of the connection between dynamics of molecules and their macroscopic properties
2. Describe knowledge of modern techniques in molecular simulations using high speed computers

Learning Outcomes

The students are expected to:

1. Use modern simulation techniques to solve fundamental problems related to interdisciplinary areas of Physics, Chemistry and Biology
2. Find explanations for phenomena related to soft condensed matter

Contents

Basics of Molecular Dynamics: Theoretical foundation of classical statistical mechanics, Boltzmann's relation, harmonic oscillator and harmonic baths, introduction to molecular dynamics, Algorithms for equations of motions (10 lectures),
(few lectures overlap with "Computational Material Science" offered by Physics department)
Various ensembles: Purpose of ensembles in simulations, canonical ensembles, isobaric ensembles, grand canonical ensembles, applications of ensembles, thermostat, Barostat (10 lectures)
Advance Techniques: Free energy perturbation theory, Thermodynamic Integration, Jarzynski's equality, Umbrella Sampling (10 lectures)
Applications: How to set up Membrane system, protein and small biological molecules (10 lectures)

Textbooks

1. D. Frenkel and B. Smith, (2002), *Understanding Molecular Dynamics Simulations*, 1st Edition, Academic Press
2. Mark Tuckermann, (2010), *Statistical Mechanics and Molecular Simulations*, 1st Edition, Oxford University

Self Learning Material

1. M. P. Allen and T. J. Tildesley., (1993), *Computer Simulations of liquids*, 1st Edition, Oxford Science Publications

Preparatory Course Material

1. Banerjee, T. *Molecular simulations*, NPTEL Course Material, Department of Chemical Engineering, Indian Institute of Technology Guwahati, http://nptel.ac.in/courses/103103036/
2. Tembe, B.L., *Computational Chemistry and Classical Molecular Dynamics*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, https://onlinecourses.nptel.ac.in/noc18_cy13

Course Title	**Solid State NMR Methods for Materials**	Number	CY7XX
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	MSc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. Introduction to essential techniques of solid state NMR
2. Introduction to various spin interactions important in solid state e.g., chemical shift anisotropy, dipolar coupling etc.
3. To enable students to analyze NMR spectrum to extract information on solid state structure and dynamics.

Learning Outcomes

The students are expected to:

1. Have basic understanding of the theoretical background of solid state NMR.
2. Application of solid state NMR in the field of materials relevant in medicine, renewable energy, polymers etc.
3. Understanding of various solid state methods that can be applied to characterize materials of interest.

Contents

Introduction to various nuclear spins other than 1H relevant for solid state materials: quadrupolar nuclei, concept of chemical shift anisotropy (CSA), scalar coupling, dipolar coupling and quadrupolar interactions, relation between shielding tensor and electronic structure, powder averaging. (8 lectures)
Introduction to nuclear spin Hamiltonian relevant in solid state: cross polarization, isotropic mixing Hamiltonian, solid state echo sequence, Homo and heteronuclear decoupling, concept of spin diffusion and polarization transfer, concept of Nuclear Quadrupole Resonance (NQR) (10 lectures)
Introduction to NMR techniques: powder line shape, determination of anisotropy, Magic Angle Spinning (MAS), generation of spinning sideband patterns, sideband modulation, molecular structure and dynamics determination by probing ssb manifolds, Techniques for measuring CSA and orientation of shielding tensor, measurement of homo and heteronuclear dipolar coupling, correlation experiments. (10 lectures)
Introduction to molecular dynamics: powder line shape analysis-relaxation time studies-2D rotor synchronization and Exchange Spectroscopy (EXSY). (10 lectures)
Application of solid state NMR: in polymers, nanomaterials, drugs, narcotics, explosives etc., recent advances in 1D solid state methods for dynamics, application of NQR. (4 lectures)

Text Books

1. Duer, J. M., (2005), *Introduction to Solid State NMR*, Wiley.

Reference Books

1. Ernst, R. R., Bodenhausen, G., Wokaun, A., (1987), *Principles of Nuclear Magnetic Resonance in One and Two Dimension*, Clarendon Press, Oxford.
2. Bakhmutov, V. I., (2011), *Solid-State NMR in Materials Science- Principles and Applications*, CRC Press.

Preparatory Course Material

1. Atreya, H. S., *Principles and Application of NMR spectroscopy*, NMR Research Center, IISC Bangalore, https://onlinecourses.nptel.ac.in/noc18_ge07/preview
2. Molugu, T. R., Lee, S., Brown, M. F., Concepts and Methods of Solid State NMR Spectroscopy Applied to Biomembranes, 2017, Chem. Rev., 117, 12087-12132
3. Dybowski, C., Bai, S., Solid State NMR Spectroscopy, 2008, Anal. Chem., 80, 4295-4300.

Title	**Quantum Computing**	Number	CY751
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	Ph.D. (CY) Program	Type	Elective
Prerequisite	MA111/CY514/PH513		

Objectives

The Instructor will:

1. Impart mathematical framework of Quantum Computation to students familiar with basic concepts of quantum mechanics and quantum information
2. Discuss advanced topics and State-of-the-Art research in quantum information and computation (QIC)

Learning Outcomes

The students are expected to:

1. Use the concepts taught in class to various aspects of quantum information, communication and cryptography
2. Understand and appreciate the technological evolution at theoretical and experimental front in QIC

Contents

Mathematical Preliminaries: Quantum Mechanics, Matrix representations of quantum states and operators, Cauchy-Schwartz and Triangle Inequalities, Classical and Quantum Correlations (6 Lectures)

Notions of Quantum Information: Classical and Quantum state Registers, Pure and Mixed states, Reduction and Purification of states, Quantum Channels, Completely Positive and trace Preserving Maps (6 Lectures)

Entropy: Quantitative bounds on Shannon and relative Entropy, Von-Neumann and quantum relative entropy, Klein's inequality, Concavity and subadditivity of von Neumann entropy, Strong subadditivity of von Neumann entropy, Accessible Information, Holevo information (8 Lectures)

Entanglement and Nonlocality: Separability Criteria, Classical, Separable and Entangled states, Local Operations and Classical Communications, Distillable entanglement and entanglement cost, Bound entanglement, Bell's Inequality and Nonlocality, Nonlocality in multiqubit Systems, Entanglement Measures (12 Lectures)

Quantum Error Correction: Bit flip and phase flip codes, Quantum Hamming Bound, Calderbank-Shor-Steane codes, Gottesman-Knil theorem, Fault-tolerant quantum computation, quantum algorithms and cryptography (10 Lectures)

Textbooks

1. Nielsen, M. A. and Chuang, I. L., *Quantum Computation and Quantum Information*, Cambridge University Press, 2000
2. Vedral, V., *Introduction to Quantum Information Science,* Oxford University Press, 2006

Reference Books

1. Griffiths, D. J., *Introduction to Quantum Mechanics*, Pearson Prentice Hall, 2006
2. Bouwmeester, D., Ekert, A. and Zeilinger, A., *The Physics of Quantum Information*, Springer, 2000
3. Bellac, M. L., *A Short Introduction to Quantum Information and Quantum Computation*, Cambridge University Press, 2006

Preparatory Course Material

1.Goswami, D., *Quantum Computing*, *Mathematics for Chemistry,* NPTEL Course Material,

Department of Chemistry, Indian Institute of Technology Kanpur https://onlinecourses.nptel.ac.in/noc18_cy07/preview

Title	**Group Theory and Molecular Spectroscopy**	Number	CY6xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	MSc./Ph.D. (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Provide basic and advanced group theoretical concepts and their applications in bonding, spectroscopy, and solid state chemistry.

Learning Outcomes

The students are expected to:

1. Analyze and understand the concept of point group and symmetry associated with molecular frameworks
2. Apply the knowledge of group theory to understand bonding, and structure in chemical species.

Contents

Introduction: The nature of the problem, symmetry operations, elements and operators, groups and group theory- general definitions, defining, deriving and recognizing point groups, subgroups and cosets, classes, group multiplication table (10 Lectures)

Theory of group representations: The great orthogonality theorem, character of a representation, reducible and irreducible representations, construction of character tables and physical interpretation, application of representation theory in quantum mechanics, direct-product groups (10 Lectures)

Applications to Chemical Bonding and spectroscopy: Molecular orbitals, applications to valence bond theory and molecular orbital theory, bonding in homonuclear diatomic molecules of transition metal, molecular orbitals in complex compounds, Huckel molecular orbital theory, application of group theory to UV-Visible, IR and Raman spectroscopy (14 Lectures)

Group theory and crystal symmetry: Crystal systems and classes, translational and space groups, symmorphic and nonsymmorphic space groups, applications of space group, factor group (8 Lectures)

Textbooks

1. Cotton, F. A., (1990) Chemical Applications of Group Theory, 3rd edition Wiley-Interscience
2. Vincent, A., (2013) *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications*, 2nd Edition Wiley

Reference Books

1. Engel, T. and Reid, P., (2012), *Quantum Chemistry and Spectroscopy*, 3rd Edition, Pearson

Preparatory Course Material

1.Chandra, M., *Chemical Applications of Symmetry and Group theory*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Kanpur, https://onlinecourses.nptel.ac.in/noc18_ch02/preview

Title	**Modern Electronic Structure Theory**	Number	CY6XX
Department	Chemistry	L-T-P [C]	3–0–3 [4]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite	CY 514 (Quantum Chemistry and Spectroscopy)		

Objectives
The Instructor will:
1. Provide knowledge of modern electronic structure theories and basic computational chemistry techniques and tools to carry out electronic structure calculations and interpret experimental spectra

Learning Outcomes
The students are expected to:
1. Carry out electronic structure calculations and interpret experimental spectra
2. Write simple computer programs to carry out calculations

Contents
Review of basics: Linear algebra, numerical techniques, postulates of quantum mechanics, Born-Oppenheimer approximation, concept of potential energy surface, variational and perturbation approaches (14 lectures)
Electronic structure theories: Hartree-Fock (HF) and post-HF theories, Moller-Plesset theory, density functional theory, coupled cluster theory, electron correlation, configuration interaction, excited states, time dependent density functional theory (14 lectures)
Techniques: Energy minimization, vibrational frequency analysis, symmetry analysis, zero point energy calculation, intrinsic reaction coordinate, distinguishing stationary points, atomic charges, Mulliken analysis (14 lectures)

Laboratory Experiments
Electronic structure calculations; Geometry optimization; simple Fortran programming; finding intrinsic reaction coordinates; computing potential and free energy profiles

Textbook
1. Levine, I. N., (2016), *Quantum Chemistry,* 7th Edition, Pearson Education
2. McQuarrie, D. A., (2016), *Quantum Chemistry,* 2nd Edition, Viva Books
3. Szabo, A., (1996), *Modern Quantum Chemistry,* Dover Publications

Reference Books
1. Jensen, F., (2017), *Introduction to Computational Chemistry,* 3rd Edition, Wiley-Blackwell
2. Cramer, C. J., (2004), *Essentials of Computational Chemistry*, 2nd Edition, Wiley-Blackwell

Self Learning Course Material
1. Simons, J.: https://www.youtube.com/watch?v=Z5cq7JpsG8I

Title	**Chemical Reaction Dynamics**	Number	CY764
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite	CY 514 (Quantum Chemistry and Spectroscopy)		

Objectives

The Instructor will:

1. Provide introduction to reaction dynamics in the gas phase and many advanced concepts in scattering theory.
2. Compare experimental data with dynamics simulations.

Learning Outcomes

The students are expected to:

1. Interpret experimental data in terms of classical and quantum scattering theory
2. Design and perform advanced dynamics simulations.

Contents

Reactive collisions: Fundamentals, Potential energy surfaces, Crossed molecular beams, state-to-state cross sections, Classical and quantum scattering process (15 lectures)
Rate theories: Kinetic theory of gases, Transition state theory (TST), Rice-Ramsperger-Kassel-Marcus (RRKM) theory, Microcanonical and thermal rate constants
Gas phase dynamics: Photodissociation, energy transfer dynamics, intramolecular vibrational energy flow, mode selective chemistry with Lasers (20 lectures)
Condensed phase dynamics: Solvation, Diffusion, Kramer-Grote-Hynes model, Correlation functions (7 lectures)

Textbooks

1. R. D. Levine, (2009) *Molecular Reaction Dynamics,* Reprint Edition, Cambridge University Press, USA.

Reference Books

1. T. Baer and W. L. Hase, (1996), *Unimolecular Reaction Dynamics: Theory and Experiments,* Oxford University Press, USA
2. A. Nitzan, (2006), *Chemical Dynamics in Condensed Phases,* Oxford University Press, USA

Preparatory Course Material

1. Halder, M., *Reaction Dynamics*, NPTEL lectures, Department of Chemistry, Indian Institute of Technology, Kharagpur, http://nptel.ac.in/courses/104105041/31

Title	**Biophysical Techniques: Theory and Applications**	Number	CY5XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc/PhD Program, B.Tech	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Introduce basic knowledge of a few biophysical methods and their application in the interdisciplinary area of chemistry and biology.
2. To have a greater understanding of the underlying theory of these methods and their practical applications in the laboratories.

Learning Outcomes

The students are expected to:

1. Understand the underlying principle of different biophysical methods.
2. To be able to use important biophysical methods to decipher problems relevant to biology.
3. Better understand the structure-function activity of biomolecules.

Course Content

Spectroscopic methods: Concepts of spectral transition and analysis of spectrum, Application of UV-VIS spectroscopy in protein folding kinetics, Advance topics in fluorescence such as anisotropy, resonance energy transfer and real time fluorescence; principle of Circular dichroism, optical rotatory dispersion methods and applications, Principle of Surface Plasmon Resonance spectroscopy, SPR optical phenomenon, application of SPR in ligand-protein interaction. (15 lectures)

Magnetic Resonance based methods: Principles of NMR and EPR, Concept of relaxation and polarization transfer, application of 1D and 2D NMR methods in biomolecules, EPR transitions, identification of metal centers in biomolecules, spin labelling and motions of side chains. (15 lectures)

Calorimetric techniques: Principles and applications of Isothermal Titration Calorimetry, Differential Scanning Calorimetry, applications in biomolecules. (7 lectures)

Centrifugation Techniques: Concepts and fundamentals of centrifugation. Ultracentrifugation techniques in biology. (5 lectures)

Textbook

1. Cox, M.M, Nelson, D.L., Lehninger (2009) *Principles of Biochemistry*, 6th Edition, W.H. Freeman & Co,
2. Gunther, H., (1995), *NMR Spectroscopy*, 2nd Edition, Wiley
3. *Circular Dichroism – Principles and Application*, (2000) Edited by Brova, N., Nakanishi, K., Woody, R. W., 2nd Ed., Wiley.

Reference Books

1. Claridge, T. D. W., (1999), High Resolution NMR Techniques in Organic Chemistry, 1st Edition, Elsevier
2. Stryer, L., Berg, J.M., Tymoczko, J.L., (2012) *Biochemistry*, W.H.Freeman & Co Ltd
3. Lakowicz, J. R., (2006), *Principles of Fluorescence Spectroscopy*, 3rd Edition, Springer, New York
4. Biophysical approaches determining ligand binding to biomolecular targets (2011), Edited by Podjarny, A., Dejaegere, A., Keiffer, B., RSC Publishing

Preparatory Course Material

1. NPTEL lectures: https://onlinecourses.nptel.ac.in/noc19_cy07/preview
2. Sharma, K. A., Analytical Technologies in Biotechnology, Dept. of Biotechnology, IIT Roorkee, https://onlinecourses.nptel.ac.in/noc19_cy07/preview

Course Title	**Stochastic Problems in Biophysics**	Number	CY758
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To understand applications of fundamental probability methods to wide variety of problems related to biophysics.
2. To show the mathematical literature on this subject
3. To understand non-equilibrium statistical mechanics

Learning Outcomes

The students are expected to:

1. Ability to translate complex phenomena into simple models
2. Ability to derive mathematical models for problems related to biophysics

Course Content

1. *Introduction:* Historical examples, Joint and conditional Probabilities, Correlation functions and Cumulants, Gaussian and Poissonian Probability Distributions (14 lectures)
2. *Markov Processes*: Chapman-Kolmogorov Equation, Examples of Markov Processes (10 lectures)
3. *Brownian Motion:* Basic assumptions, Langevin Equation, Fokker-Planck Equation, Master Equations and Jump Processes, Linear Response Theory (18 lectures)

Text Books

1. Landau and Lifshitz, *Statistical Physics*, Elsevier, 2005
2. David Chandler, *Introduction to Modern Statistical Mechanics*, Oxford University Press, 1987

Self Learning Materials

1. C. W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry and Natural Sciences*, Springer-Verlag, 1983
2. Edited and Introduced by John Stachel, *Einstein's Miraculous Year*, Princeton University Press, 1998.
3. S. Chandrashekhar, Reviews of Modern Physics, vol 15, No 1, APS

Preparatory Course Material

Prof. V. Balakrishnan, IIT Madras: https://www.youtube.com/watch?v=qNmB1qNjZ0k

Course Title	**Polymer Dynamics**	Course No.	CY760
Department	Chemistry	L-T-P[C]	3-0-0 [3]
Offered for	PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

To understand basic principles and theory of modern macromolecules

To understand the analogy to other branches of science at a more fundamental level

Learning Outcomes

The students are expected to:

1. Ability to realize that polymers are essential ingredients in biological machinery
2. Ability to do advanced calculations more modestly

Course Content

Ideal Chain : Freely joint chain, Flexibility of a polymer chain, Gaussian Chain, Ideal chain as a random walk, Ideal polymer by an external force, Flory Calculation (12 lectures)

Polymer chains with volume interactions and Melts : Models with volume interactions, ideal melts, chains in solvents (10 lectures)

Dynamics: Rouse model, Zimm Model, Real polymer coil, Reptation model (10 lectures)

Biopolymers: Properties, Primary structure, Secondary structure, Helix-coil transition (10 lectures)

Text Books

1. M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford Science Publications, 1990.

Self Learning Materials

1. Alexander Yu. Grosberg and Alexei R. Khokhlov, *Statistical Physics of Macromolecules*, AIP Press, 1994
2. Pierre-Gilles de Gennes, *Scaling Concepts in Polymer Physics*, Cornell University Press, 1979

Online course material

1. George Phillies lectures a series of graduate classes, based on his book "Phenomenology of Polymer Solution Dynamics" Cambridge University Press, 2011.
2. https://www.youtube.com/watch?v=mVzrYKkeJzE

Course Title	**Statistical Mechanics and Molecular Simulations**	Course No.	CY758
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To understand the complex soft matter system that bridges the traditional disciplines of physics, chemistry and biology using modern theoretical methodology and high-speed computers**.**
2. To explore the connections between basic statistical mechanical theories and real world applications in studying physical, chemical and biological phenomena.

Learning Outcomes

The students are expected to:

1. Understanding basic principles of Statistical Mechanics and Molecular Dynamics Simulations.
2. Mathematical formalism associated with theory and techniques of molecular modelling.
3. Few real world applications to understand the connections between microscopic and macroscopic world.

Course Content

*Statistical basis of thermodynamics***:** Introduction to Statistical Methods, Micro and Macro states, Ensemble theory (micro-canonical, canonical, isobaric, grand-canonical), Mathematical techniques (5 lectures)
Classical Statistical Mechanics: Partition functions, Thermodynamic functions, Phase space and Liouville equation, Distribution functions, Kirkwood integrals (10 lectures).
(Module 3 of ``Statistical Physics" by Physics department) *Fluctuations:* Thermodynamic fluctuations, Spatial correlations in a fluid, Einstein-Smoluchowski theory of Brownian motion, Langevin theory,Fokker-Planck equation, Fluctuation-dissipation theory, Onsager relations (12 lectures)
Introduction to Molecular Modeling: Algorithms, Periodic boundary conditions, Interaction functions and force fields, Electrostatics, Molecular dynamics in various ensembles (10 lectures)
Applications: Brownian dynamics simulations, Biological applications for proteins and membranes (5 lectures)

Text Books

1. Mark E Tuckerman, *Statistical Mechanics and Molecular Simulations*, Oxford University, 2010
2. David Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987

Self Study Material

1. M. P. Allen and T J Tildesley, *Computer Simulations of Liquids*, Oxford Science Publications, 1993
2. D. A. Mcquarrie, *Statistical Mechanics*, University Science Books, 2000
3. D. Frenkel and B. Smit, *Understanding Molecular Dynamics Simulations*, Academic press, 2002
4. Andrew R Leach, *Molecular Modelling: Principles and applications*, Prentice Hall, 2010
5. R K Pathria, Paul D. Beale, *Statistical Mechanics*, Elsevier, 2011

Preparatory Course Material

1. https://ocw.mit.edu/courses/mechanical-engineering/2-57-nano-to-macro-transport-processes-spring-2012/

Course Title	**Advanced Electrochemistry and Applications**	Number	CY6xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc/PhD Program	Type	Elective
Pre-requisite			

Objectives

The instructor will

1. Provide an introductory but thorough background in electrochemistry.
2. Provide fundamentals of electrochemical systems, electroanalytical techniques and advanced applications.

Learning Outcomes

The students are expected to:

1. describe the difference between equilibrium properties and properties of electrochemical systems and apply electrochemical methods for required information.
2. explain the functioning of electrochemical devices as well as the commonly employed underlying electrochemical reactions

Contents

Introduction to Electrochemistry: Nernst equation, electrode kinetics, dynamic electrochemistry, the Butler-Volmer and Tafel equations. Overpotentials. Kinetically and mass transport controlled electrochemical processes. Mass transport by migration, convection and diffusion. Conductivity. (Lectures 7)
Electrochemical Methods: Potentiostatic and galvanostatic electrochemical methods including chronoamperometry, coulometry, cyclic voltammetry, chronopotentiometry, ac impedance spectroscopy, spectroelectrochemistry and hydrodynamic methods.(Lectures 8)
Solid state electrochemistry. Ion conducting and electronically conducting polymers; The electrochemical double layer. (5 Lectures)
Surface confined electrochemical processes: The fundamentals of corrosion. Homogeneous and heterogeneous electrocatalysis (HER and OER). Electrochemical processes coupled to chemical steps. Nanostructured and surface modified electrodes. (8 Lectures)
Application: Introduction to batteries, fuel cells and electrochemical solar cells. (7 Lectures)
Electrochemical processes of particular relevance to energy conversion.(5 Lectures)

Text Books

D. I. Antropov, Theoretical Electrochemistry, Mir Publishers, 1972.
J. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol.1 and 2, Plenum Press, 1998.
Industrial Electrochemistry, 2nd ed, Pletcher, Derek/Walsh, Frank C., London: Chapman and Hall, 1990
Electrochemistry for Chemists, 2nd ed, Sawyer, Donald T./Sobkowiak, Andrej/Roberts, Julian L., New York: John Wiley, 1995

Reference Books

1. Transient Techniques in Electrochemistry, Macdonald, Digby D., New York: Plenum Press, 1977
2. Laboratory Techniques in Electroanalytical Chemistry, (2nd edition) by Peter Kissinger and William Heineman (Marcell Dekker) 1996

Preparatory Course Material

1. https://nptel.ac.in/courses/104106105/