Curriculum

Ph.D.

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Indian Institute of Technology Jodhpur

Ph.D. (Chemistry)

Cat.	Course Number: Course Title	L-T-P	Credits		Cat.	Course Number: Course Title	L-T-P	Credits
I Semester					**II Semester**			
E	*Electives*				E	*Electives*		
	Total					*Total*		
III Semester					**IV Semester**			
H	**CY799 Ph.D. Thesis**				H	**CY799 Ph.D. Thesis**		
	Total					*Total*		
V Semester					**VI Semester**			
H	**CY799 Ph.D. Thesis**				H	**CY799 Ph.D. Thesis**		
	Total					*Total*		
VII Semester					**VIII Semester**			
H	**CY799 Ph.D. Thesis**				H	**CY799 Ph.D. Thesis**		
	Total					*Total*		

Electives

Semester I				Semester II			
CY751	Quantum Computing	3-0-0	3	CY753	Analytical Techniques and Spectroscopy	3-0-0	3
CY752	Principles of Nuclear Magnetic Resonance	3-0-0	3	CY754	*Statistical Mechanics and Molecular Simulations*	3-0-0	3
CY755	Advance catalysis			CY761	Art in Organic Synthesis	3-0-0	3
CY756	Group Theory and Molecular Spectroscopy	3-0-0	3	CY762	Quantum Chemistry	3-0-0	3
CY757	Chemical Binding	3-0-0	3	CY763	Catalysis for Energy	3-0-0	3
CY758	Stochastic Problems in BioPhysics	3-0-0	3	CY764	Chemical Reaction Dynamics	3-0-0	3
CY759	Advance Material Design	3-0-0	3	CY765	Molecular Dynamics Simulations	3-0-0	3
CY760	Polymer Dynamics	3-0-0	3	CY766	Stereochemistry of Organic Compounds	3-0-0	3
				CY767	Water Chemistry	3-0-0	3
				CY769	Sustainable Catalytic Design	3-0-0	3

S.No.	***Category***	***Category Title***	**Students with**	***Total Courses***	***Total Credits***
1	E	*ELECTIVES*	Master's Degree	4	12
			Bachelor's Degree	10	30
2	H	Thesis	-	-	-

Course Title	***Quantum Computing***	Course No.	**CY751**			
Focus Group	Chemistry	Structure	3	0	0	3
Offered for	PhD	Status	Core		*Elective* √	
Pre-requisite	Consent of Teacher	To take effect from				

Objectives

To impart mathematical framework of Quantum Computation to students familiar with basic concepts of quantum mechanics and quantum information

Learning Outcomes

To use the concepts taught in class to various aspects of quantum information, communication and cryptography

Contents

Mathematical Preliminaries: Quantum Mechanics, Matrix representations of quantum states and operators, Cauchy-Schwartz and Triangle Inequalities, Classical and Quantum Correlations
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
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
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
Quantum Error Correction: Bit flip and phase flip codes, Quantum Hamming Bound, Calderbank-Shor-Steane codes, Gottesman-Knil theorem, Fault-tolerant quantum computation

Reference Books:

1. Nielsen, M. A. and Chuang, I. L., *Quantum Computation and Quantum Information*, Cambridge University Press, 2000
2. Griffiths, D. J., *Introduction to Quantum Mechanics*, Pearson Prentice Hall, 2006
3. Bouwmeester, D., Ekert, A. and Zeilinger, A., *The Physics of Quantum Information*, Springer, 2000
4. Bellac, M. L., *A Short Introduction to Quantum Information and Quantum Computation*, Cambridge University Press, 2006
5. Vedral, V., *Introduction to Quantum Information Science,* Oxford University Press, 2006
6. Fano, U., Rev, Mod. Phys. **55**, 855 (1983)
7. Bennett, C. H., Brassard, G., Crepeau, C., Jozsa, R., Peres, A., and Wootters, W. K., *Phys. Rev. Lett.* **70,** 1895 (1993)
8. Horodecki, M., Horodecki, P., and Horodecki, R., *Phys. Lett. A* **223,** 1 (1996)

Course Title	***Principles of Nuclear Magnetic Resonance***	Course No.	**CY752**			
Focus Group	Chemistry	Structure	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite	*Consent of Teacher*	To take effect from	July 2014			

Objectives

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

Learning Outcomes

1. Basic understanding of the theoretical background of solution state NMR.
2. Application of NMR as a biophysical technique in chemistry, biology, material science, medicine.
3. Exposure to 500 MHz NMR spectrometer available in the institute.

Course Content

1. Introduction to Nuclear Magnetic Resonance (NMR) – Spin density operator, concept of density matrix, Liouville-Von-Neuman equation, the nuclear spin Hamiltonian- Gyromagnetic ratio – energy level diagrams –Zeeman splitting
2. Introduction to NMR parameters - chemical shift and coupling, longitudinal and transverse relaxation processes – Redfield relaxation theory - paramagnetic relaxation – correlation times and relaxation times.
3. 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
4. Introduction to 2D NMR, correlation spectroscopy – common pulse sequences – homonuclear and hetero nuclear correlation spectroscopy – examples of COSY, TOCSY, NOESY – Application – chemical structure – biological processes - molecular dynamics *etc*.
5. Laboratory demonstration of standard NMR experiments - Experimental data analysis

Reference Books

1. Farrar, T.C., and Becker, E.D., *Pulse and Fourier Transform NMR*, Academic Press, New York, 1971
2. Gunther, H., *NMR Spectroscopy*, Wiley, 2nd Ed., 1995
3. Ernst, R. R., Bodenhausen, G., Wokaun, A., *Principles of Nuclear Magnetic Resonance in One and Two Dimension*, Clarendon Press, Oxford, 1987
4. Braun, S., Kalinowski, H., Berger, S., *150 and more NMR experiments: A practical course*, Wiley- VCH

Course Title	***Analytical Techniques and Spectroscopy***	Course No.	**CY753**				
Focus Group	Biologically Inspired System Science	Structure (LTPC)	3	0	0	3	
Offered for	PhD students	Status				*Elective*	
Pre-requisite	*Consent of Teacher*	To take effect from	December 2013				

Objectives

1. Introduction to a few spectroscopic methods used as analytical techniques in various fields of science and engineering
2. Introduction to theoretical background of these methods along with their instrumentation and application
3. Enable students to use such methods whenever needed by giving hands on experience with available instruments in the institute

Learning Outcomes

1. Basic understanding of the theoretical background of various spectroscopic techniques
2. Application of spectroscopic methods as analytical tool in chemistry, biology, material science, medicine
3. Exposure to various spectrometers available in the institute

Course Content

1. *Introduction to Spectroscopy:* properties of electromagnetic radiation – interaction of radiation with matter – classical picture – uncertainty and question of time scale – intensity of spectral line and line shape – Sensitivity and resolution of spectral line – Fourier Transformation
2. *UV-VIS and Fluorescence Spectroscopy:* Basic principle, Chromophores – Laws of photochemistry, Beer-Lambert law, electronic energy levels, Solvent relaxation, Jablonski diagram, Frank-Condon principle, Excited state life time, excited state kinetics, solvent effect, quantum yield expression and Stern-Volmer equation, excimer and exciplex, kinetics of luminescence quenching, photo induced energy transfer, FRET. Instrumentation and application – Laboratory demonstration of standard UV-VIS and Fluorescence experiments
3. *Infrared and Raman Spectroscopy:* Basic principle; Organic functional group identification through IR spectroscopy, IR and Raman activity, Raman shift, Instrumentation and application - Laboratory demonstration of standard FTIR experiments
4. *NMR Spectroscopy*: Basic principle, spin-1/2 nuclei and energy level diagram, Zeeman splitting, introduction to NMR parameters - chemical shift and spin-spin coupling, introduction to AB, AX, AMX spin system, 1D 1H and 13C NMR for structure elucidation, longitudinal and transverse relaxation processes, measurement of relaxation rates, NOE, 2D NMR, correlation spectroscopy -Instrumentation and application - Laboratory demonstration of standard NMR experiments
5. *Mass Spectrometry:* basic principle, ionization technique, molecular ion, fragmentation processes. Instrumentation and application

Reference Books

1. Farrar, T.C., and Becker, E.D., *Pulse and Fourier Transform NMR*, Academic Press, New York, 1971
2. Silverstein, R. M., Bassler, G. C., and Morril, T. C., *Spectroscopic Identification of Organic Compounds*, Wiley, 1991
3. Gunther, H., *NMR Spectroscopy*, Wiley, 2^{nd} Ed., 1995
4. Banwell, C. N., *Fundamentals of Molecular Spectroscopy*, Tata Mcgrow Hill
5. Bernath, P. F., *Spectra of Atoms and Molecules*, Oxford University Press, 2^{nd} Ed., 2005
6. Lakowicz, J. R., *Principles of Fluorescence Spectroscopy*, Springer, New York, 2006

Course Title	***Statistical Mechanics and Molecular Simulations***	Course No.	**CY754**			
Focus Group	Biologically Inspired System Science	Structure (LTPC)	3	0	0	3
Offered for	PhD students	Status				*Elective*
Pre-requisite	*Basic thermodynamics*	To take effect from	December 2013			

Objectives

1. To understand the complex soft matter systems that bridge 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

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

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

Reference Books

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

Course Title	***Advance Catalysis***	Course No.	**CY755**			
Focus Group	Chemistry	Structure	3	0	0	3
Offered for	PhD	Status			Elective	
Pre-requisite		To take effect from	July 2014			

Objective

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

Learning Outcomes

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

Course Content

*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).

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.

*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.

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 (Definition IMPORTANT!) examples: Markovnikov regioselectivity of HX addition to monosubstituted alkenes, Orientation in electrophilic aromatic substitution reactions

Asymmetric Catalysis Using Organometallic Reagents: Hammond Postulate and Curtin Hammett Concepts, Methods and Origin of Selectivity. CurtinHammett principle (Definition, IMPORTANT!) examples: reactivity of conformations 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

Reference Books

1. F A Cotton, G. Wilkinson, C A Murillo and M Bochmann, *Advanced Inorganic Chemistry*, 6th ed, 1999, Wiley-Interscience
2. C Elschenbroich and A Salzer, *Organometallics*, VCH Publishers, 1st ed 1989, 2nd ed 1993.
3. R H Crabtree, *The Organometallic Chemistry of the Transition Metals*, Wiley, 1998
4. C Masters, Homogeneous Transition-metal Catalysis - A Gentle Art, Chapman and Hall, 1981

Course Title	***Group Theory and Molecular Spectroscopy***	Course No.	**CY756**			
Focus Group	Chemistry	Structure	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite	*Consent of Teacher*	To take effect from	July 2014			

Objectives

To discuss various group theoretical concepts in connection with molecular spectroscopy

Learning Outcomes

Students will understand how chemical theories are used to solve chemical problems in biology, environmental science, and material science

Course Content

The complete nuclear permutation and permutation – inversion group, molecular symmetry groups, Double groups, point group symmetry, representation and character tables. The molecular Hamiltonain and its symmetry. Nuclear spin statistics. Examples of application of MS group to non-rigid molecules and molecular complexes.

General formalism for molecular Hamiltonians in curvilinear coordinates –Podolsky transformation, Echart-Sayvetz. Rotational – vibrational Hamiltonians with emphasis on coupling terms for semirigid diatomic and polyatomic molecules. The Wilson – Howard – Darling - Dennison and the Watson Hamiltonians. Contact transformation and the derivation of effective rotational Hamiltonians for vibrational degrees of freedom. Coriolis and centrifugal coupling. Advanced theory of line intensities for infrared and Raman Spectra. Symmetry of ro-vibronic wave function and introduction to vibrational – rotational spectra of non-rigid molecules and molecular complexes

Applications to chemical and biological systems

Reference Books

1. Engel, T. and Reid, P., *Quantum Chemistry and Spectroscopy*, Benjamin Cummings, 2005
2. McHale, J. L., *Molecular Spectroscopy*, Prentice Hall, 1998

Course Title	***Chemical Binding***	Course No.	**CY757**			
Focus Group	Chemistry	Structure	3	0	0	3
Offered for	PhD	Status	Core		*Elective* √	
Pre-requisite	*Consent of Teacher*	To take effect from	July 2014			

Objectives

1. High level understanding of a chemical bond using quantum mechanics.
2. Knowledge of modern techniques in quantum chemistry

Learning Outcomes

1. Ability to use modern quantum chemistry techniques to solve problems
2. Theoretical understanding of a chemical bond

Contents:

Electronic Structure: Many electron atoms, Variational principle, Born-Oppenheimer approximation, H_2^+ ion, homo and hetero nuclear diatomic molecules, Valence bond and Molecular orbital theories
Hartree-fock (HF) and Moller-Plesset (MP) Theory: HF theory of atoms and molecules, Self-consistent field wavefunction, configuration interaction wavefunction, Moller-Plesset perturbation theory and CI calculations
Density functional theory (DFT): Principles of DFT, Commercial Functionals
Semi Empirical Methods: Introduction to CNDO (Complete neglect of differential overlap), INDO (Intermediate neglect of differential overlap) and NDDO (Neglect of of diatomic differential overlap)

Reference Books:

1. I. N. Levine, Quantum Chemistry, 5th edition, Pearson education (2000)
2. J. P. Lowe, Elementary Quantum Chemistry, 2nd edition, Academic Press
3. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover (1996).

Course Title	***Stochastic Problems in Biophysics***	Course No.	**CY758**				
Focus Group	Chemistry	Structure	3	0	0	3	
Offered for	PhD	Status			*Elective*		
Pre-requisite	*Basic Statistical Mechanics*	To take effect from	December 2013				

Objectives

1. To understand applications of fundamental probability methods to wide variety of problems related to biophysics
2. To show the connection between mathematical literature on this subject

Learning Outcomes

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

Course Content

1. *Probability and Stochastic Processes :* Historical examples, Joint and conditional Probabilities, Correlation functions and Cumulants, Gaussian and Poissonian Probability Distributions
2. *Markov Processes :* Chapman-Kolmogorov Equation, Examples of Markov Processes
3. *Brownian Motion:* Basic assumptions, Langevin Equation, Fokker-Planck Equation, Master Equations and Jump Processes

Reference Books

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

Course Title	***Advance Material Design***	Course No.	**CY759**				
Department	Chemistry	Structure	3	0	0	3	
Offered for	PhD	Status				*Elective*	
Pre-requisite	*Consent of Teacher*	To take effect from	July 2014				

Objectives

1. This course aims to provide a comprehensive overview of synthesis and characterization of bulk materials, nanoparticles, nanocomposites and hierarchical materials with nanoscale features.
2. Course modules will cover the fundamental scientific principles controlling assembly of nanostructured materials; synthesis, measurement and computational tools; new properties at the nanoscale, and existing and emerging applications of nanomaterials

Learning Outcomes

1. Understanding a variety of different methods for synthesizing materials
2. Be able to 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
4. Practical skills with several techniques for synthesis of inorganic materials

Course Content

1. Physics and Chemistry of Nanomaterials
2. Electronic Structure of Nanomaterials
3. Solution Chemistry of Nanomaterials
4. Adsorption in Nanoporous Materials
5. Nanoporous Catalytic Materials
6. Self-assembly and Colloidal Phenomena
7. Nanostructured Fuel Cells and Solar Cells
8. Scattering Theory and Diffraction
9. Electron Microscopy and Nuclear Magnetic Resonance.

Reference Books

1. Nanoparticulate Materials: Synthesis, Characterization, and Processing by Kathy Lu, Wiley
2. Inorganic Nanostructures: Properties and Characterization by Petra Reinke, Wiley
3. Hybrid Materials: Synthesis, Characterization, and Applications by Guido Kickelbick, John Wiley & Sons

Course Title	***Polymer Dynamics***	Course No.	**CY760**			
Focus Group	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite		To take effect from				

Objectives
1. To understand basic principles and theory of modern macromolecules
2. To understand the analogy to other branches of science at a more fundamental level

Learning Outcomes
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

Polymer chains with volume interactions and Melts : Models with volume interactions, ideal melts, chains in solvents

Dynamics: Rouse model, Zimm Model, Real polymer coil, Reptation model

Biopolymers: Properties, Primary structure, Secondary structure, Helix-coil transition

Reference Books

1. M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford Science Publications, 1990
2. Alexander Yu. Grosberg and Alexei R. Khokhlov, *Statistical Physics of Macromolecules*, AIP Press, 1994
3. Pierre-Gilles de Gennes, *Scaling Concepts in Polymer Physics*, Cornell University Press, 1979

Course Title	***Art in Organic Synthesis***	Course No.	**CY761**			
Focus Group	Chemistry	Structure	3	0	0	3
Offered for	PhD	Status	Elective			
Pre-requisite	*Consent of Teacher*	To take effect from				

Objectives

1. Knowledge of key aspects of retrosynthesis of complex organic molecules.
2. An understanding of the fundamental mechanistic aspect of chemical transformations.

Learning Outcomes

1. An understanding of some total synthesis.
2. The basic knowledge, skills and experience on wise strategy and plan to design a molecule.

Course Contents

Introduction to Strategies for the Synthesis of Complex Molecules: General principles of retrosynthetic analysis and general strategies for stereochemical control.

Carbanionic in syhthesis: Chemistry of "carbanionic" synthetic building blocks. Directed metalation for the generation of organolithium compounds, and discussion of alkenyl and alkynylmetal compounds. Synthetic Application of organometallic species.

Electrophilic Substitution Reactions: Reaction of Caranion with alkyl halides, sulfonates, and related electrophilic substitution reactions. Stereocontrolled alkylation.

Addition to C=O group: Stereocontrol elements in 1,2-additions to carbonyl compounds. Stereocontrolled reduction of ketones and 1,2-addition of organometallic compounds to carbonyl groups.

Addition of Allylmetal Compounds to unsaturated bond: Introduction to reactions of carbocation with carbon-carbon pi bonds including organosilanes and stannanes.

Functional Group Transformations: Including reduction, oxidation, and functional group interconversions by nucleophilic substitution, and protective group chemistry

Reference Books

1. Organic Chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren, Oxford University
2. Classics in Total Synthesis: Targets, Strategies, Methods by , K. C.; Nicolaou, E. J. Sorensen, (1996), Wiley
3. Organic Synthesis: The Disconnection Approach by Stuart Warren and Paul Wyatt. Wiley

Course Title	***Quantum Chemistry***	Course No.	**CY762**			
Department	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite	*Basics of Quantum Mechanics*	To take effect from	July 2014			

Objectives

To discuss various aspects of multi-electron systems and computational chemistry

Learning Outcomes

Students will be able to use and understand the theoretical concepts related to computational aspects of theoretical chemistry

Course Content

Born-Oppenheimer approximation, hydrogen molecule ion, hydrogen molecule: valence bond and molecular orbital methods: Detailed calculations for energies and overlaps.

Polyatomic molecules and hybridisation. Conjugated pi-systems and Huckel theory, frontier orbital theory, configuration interaction.

Hartree-Fock method, self-consistent field method and derivation of Hartree-Fock, Roothaan Equations.

Polyatomic basis sets, Gaussian, double-zeta and polarized basis sets, population analysis and dipole moments. The Thomas-Fermi model of the atom.

The metallic bond. Bloch theory, free electron and tight binding model. Effective crystal field Hamiltonian: Steven's equivalent operator method.

Electric and magnetic properties of molecules. Introduction to multipole expansion, dipole moments, static polarizability and hyperpolarizability, magnetic susceptibility, vector functions and vector potential: shielding constants, spin-spin coupling and hyperfine interactions.

Reference Books

1. Levine, I. N., *Quantum Chemistry*, 5th edition, Pearson education (2000)
2. Lowe, J. P., *Elementary Quantum Chemistry*, 2nd edition, Academic Press
3. Szabo, A.and Ostlund, N. S., *Modern Quantum Chemistry*, Dover (1996).

Course Title	***Catalysis for Energy***	Course No.	**CY763**				
Focus Group	Chemistry	Structure (LTPC)	3	0	0	3	
Offered for	PhD	Status			*Elective*		
Pre-requisite		To take effect from	July 2014				

Objectives

To give a overview about defining a roadmap for the role of catalysis in energy production. Consciousness about fuel cells, hydrogen production and storage, methane storage and industrial catalysis.

Learning Outcomes

Role and the possibilities of catalysis in the production of new energy carriers and in the utilization of different energy sources. Students will learn to go beyond conventional application identifying new developments that may lead to breakthroughs in the production of alternative energy.

Course Content

1. Catalysis: Introduction to heterogeneous catalysis, including models of surface reactivity, surface equilibria, kinetics of surface reactions, electronic and geometrical effects in heterogeneous catalysis.
2. Catalytic reactions and application: Trends in reactivity, catalyst structure and composition, electro-catalysis and photo-catalysis. Selected applications and challenges in energy transformations.

Reference Books:

1. Molecular Catalysts for Energy Conversion by Okada, Tatsuhiro, Kaneko, Masao, Springer.
2. Catalysis for Alternative Energy Generation by Guczi, László, Erdôhelyi, András Springer.

Catalysis for Sustainable Energy Production by Pierluigi Barbaro, Claudio Bianchini, Wiley

Course Title	***Chemical Reaction Dynamics***	Course No.	**CY764**			
Focus Group	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite	*Consent of Teacher*	To take effect from	July 2014			

Objectives

1. Atomic level understanding of chemical reactions in gas and condensed phase.

Learning Outcomes

1. Knowledge of various rate theories and ability to calculate rate constants.
2. Use of scattering theory to calculate state to state reaction cross sections.

Course Content

Rate theories: Kinetic theory of gases, Transition state theory, RRKM theory, Microcanonical and thermal rate constants, classical and quantum scattering process

Reactive collisions: Potential energy surfaces, crossed molecular beams, state-to-state cross sections

Gas phase dynamics: Photodissociation, energy transfer dynamics, intramolecular vibrational energy flow, mode selective chemistry with Lasers

Condensed phase dynamics: Solvation, Diffusion, Kramer-Grote-Hynes model, correlation functions

Reference Books

1. Levine, R. D., Molecular Reaction Dynamics, Reprint edition, Cambridge University Press (2009)
2. Baer, T. and Hase, W. L., Unimolecular Reaction Dynamics: Theory and Experiments, OUP USA (1996)
3. Nitzan, A., Chemical Dynamics in Condensed Phases, OUP Oxford (2006).

Course Title	***Molecular Dynamics Simulations***	Course No.	**CY765**			
Focus Group	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite	*Consent of Teacher*	To take effect from				

Objectives

1. To understand the complex soft matter systems that bridge the traditional disciplines of physics, chemistry and biology using high-speed computers
2. To explore the connections between theory of statistical mechanics and real world applications in studying Physical, chemical and biological phenomena

Learning Outcomes

1. Ability to apply the mathematical formalism associated with the theory in modelling problems related to soft condensed matter
2. Building computational foundation to model problems related to biophysics or biochemistry
3. Familiarity to current developments in soft condensed matter

Course Content

Introduction : Entropy and Temperature, Ergodicity, Idea of Molecular Dynamics Simulations, Algorithms for equation of motion, Liouville Formulation for time reversible algorithm, Lyapunov Instability

Molecular Dynamics in various ensembles: Andersen Thermostat, Nose-Hoover Thermostat, MD at constant Pressure

Free energy Calculations: Thermodynamic Integration, Chemical Potentials, Umbrella Sampling, Free energy for chain molecules

Advanced Techniques: Long range interactions, Monte Carlo, Tackling Time-scale problems, Dissipative particle dynamics

Applications: Applications for proteins, membranes and polymers

Reference Books

1. M. P. Allen and T J Tildesley, *Computer Simulations of Liquids*, Oxford Science Publications, 1993
2. D. Frenkel and B. Smit, *Understanding Molecular Dynamics Simulations*, Academic press, 2002
3. Mark E Tuckerman, *Statistical Mechanics and Molecular Simulations*, Oxford University, 2010
4. Andrew R Leach, *Molecular Modelling: Principles and applications*, Prentice Hall, 2010

Course Title	***Stereochemistry of Organic Compounds***	Course No.	**CY766**			
Focus Group	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	PhD	Status	Core		*Elective* √	
Pre-requisite		To take effect from	July 2014			

Objectives

1. To be able to represent organic stereochemical structures correctly (diastereoisomers and enantiomers).
2. To be able to design synthetic routes to compounds containing more than one stereochemical feature, and especially to design enantioselective syntheses.

Learning Outcomes

1. Student will able to understand stereochemical nomenclature, classification of objects with regard to symmetry, desymmetrizations, chiroptical properties of organic compounds, stereochemical discrimination, separation of stereoisomers, and principles for stereoselective synthesis
2. Student will learn about the key aspects of modern synthetic reactions, especially reactivity, bond formation, and the origin of stereoselectivity and to be able to provide reaction mechanisms.

Course Contents

Structure, Symmetry, configuration and Stereoisomers: Constitution, configuration, conformation, determination of structure, symmetry elements, point groups, desymmetrization energy barrier, enantiomers and diasteriomers.

Properties of Stereoisomers: Stereoisomer Discrimination: Stereoisomer discrimination, Nature of racemates, properties of racemates and their enantiomer components.

Separation of Stereoisomers: Resolution, Racemization: Crystallization, Chemical separation of enantiomers and diastereomers, Resolution, Kinetic resolution and racemization.

Prostereoisomerism, Prochirality: Homotopic and heterotopic ligands, hetrotopicity and NMR, prochirality and centers.

Conformation of Acyclic and cyclic Molecules: Conformation of Acyclic molecule, disteromer equilibria in acyclic system, Physical and spectral properties of diastereomers and conformers, Conformational aspects of various ring size compound, stereochemistry of fused and bridged compouds.

Stereoselective Synthesis: Convergent Synthesis, Distereoselective synthesis, Enantioselective synthesis and double sterodifferentations.

Chiroptical Properties: Optical activity, Anisotropic Refraction, Circular dichroism, application of optical activity and vibration optical activity.

Reference Books

1. *Stereochemistry of Organic Compounds* by Ernest L. Eliel, Samuel H., Wiley
2. *Stereoselectivity in Organic Synthesis"* by G. Procter, Oxford University Press
3. *Organic Synthesis: Strategy and Control* by Warren and Wyatt, Wiley

Course Title	***Water Chemistry***	Course No.	**CY767**			
Focus Group	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	PhD	Status			*Elective*	
Pre-requisite		To take effect from	July 2014			

Objectives

1. The objective of this course is to provide a fundamental and advance understanding of the chemical and bio-chemical 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. This course will provide knowledge of the key chemical processes relevant to research in water chemistry

Learning Outcomes

1. Chemical processes in aquatic environments.
2. Chemistry of the atmosphere.
3. chemistry of soil processes
4. Summarize the water chemistry for a separate field Deliver a report with high demands on time keeping, transparency and structure

Course Contents

1. Polar nature of water
2. Cycling of water and residence time
3. Analytical method
4. Equilibrium constant expressions
5. Chemical reaction equation and
6. Arrenhius and Bronsted-Lowry acids and bases
7. Ionization constant reactions and expressions
8. Acids and bases, Buffering capacity of water
9. Measuring pH, Filtration, Alkalinity
10. Water quality and water treatment, Solubility-product expressions

Reference Books

1. *Chemistry for Environmental and Engineering Science*. By Sawyer C., McCarty, P., & Parkin G . 5th Edition. Toronto: McGraw-Hill, 2003
2. *Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, 3rd Edition* by Werner Stumm, James J. Morgan, Wiley
3. *Principles of Water Treatment* by Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussell, George Tchobanoglous, Wiley

Course Title	**Sustainable Catalytic Systems**	Course No.	**CY 769**			
Department	Chemistry	Structure (L-T-P:C)	3	0	0	3
Offered for	Ph.D. Students	Status	*Elective*			
Pre-requisite	Consent of Teacher					

Objective

To generate a thoughtfulness in students to correlate catalyst for real life problems

Learning Outcomes

1. Understanding the behavior of Catalyst and materials using fundamental knowledge of their nature
2. Describe, explain and apply the principles of catalysis and characterization to solve problems related to energy
3. Collaboratively plan, implement and evaluate a series of experiments using analytical techniques
4. Real life correlation of catalysis and events

Contents

1. *Natural Catalysis*: Fundamental of a catalysts, Enzymes as models for catalyst development, Biomimetic catalysis, Redox, Hydrolytic catalysis
2. *Supramolecular Catalysis*: Recognition, Calixarenes and related, Metal-containing macrocycles, Self-assembled nanoreaction systems
3. *Zeolites, Clay, MCM-41 and Metal-Organic Frameworks*: Nature, structure and properties; Applications
4. *Dendrimers*: Chemical nature, Types of dendrimers, preparation and characterization methods; Applications
5. *Nanocatalysis*: Nature and properties of nanoparticles, Methods of characterization; Applications

References

1. Atkins,P.W., Langford,C.H., (2008), *Inorganic Chemistry*, 3rd Edition, Oxford University Press, _____
2. Astruc,D., (Ed.), (2008), *Nanoparticles and Catalysis*, Wiley-VCH, Weinheim, Germany
3. Viswanathan,B., (Ed.), (2009), *Catalysis : Selected Applications*, Alpha Science International, Oxford, UK
4. Sheldon,R.A., Arends,I., and Hanefeld,U., (Eds.), (2007), *Green Chemistry and Catalysis*, Wiley-VCH, Weinheim, Germany
5. ____, (2003), *Catalysis from A to Z : a Concise Encyclopedia*, 2nd Edition, Wiley-VCH, Weinheim, Germany
6. van Leeuwen,P.W.N.M., (2004), *Homogeneous Catalysis : Understanding the Art*, Kluwer Academic, Dordrecht, The Netherlands
7. Ribas,X., (Ed.), (2013), *C–H and C–X Bond Functionalization: Transition Metal Mediation*, RSC Catalysis Series N°11, RSC Publishing, Cambridge, UK