Department Electives

CH 431: Quantum Molecular Dynamics (3-0-0-6)

The time-dependent Schrödinger's equation, Wavepackets, Correspondence between classical and quantum dynamics, The Wigner representation and the density operator, Correlation functions, Approximate solutions of the time-dependent Schrödinger's equation, Methods of quantum propagation of wave functions: Split operator method and the fast Fourier transform, The Born-Oppenheimer approximation and potential energy surfaces, Electronic absorption and Emission spectroscopy, Two-level system, Effect of strong fields, Variational formulation of control of chemical reactions, photodissociation, Reactive scattering problems.

Text Book

1. Introduction to quantum mechanics: A time-dependent perspective, D. J Tannor, 2007, Universty Science Books.

Reference

1. S. A. Rice, and M. Zhao, Optical Control of Molecular Dynamics 1st Edition, Wiley-Interscience, 2000

CH 427 Medicinal Chemistry (3-0-0-6)

Introduction to medicinal and pharmaceutical chemistry: Methods of classification of drugs based on structure and biological activity; Study of the chemistry and synthesis of the following classes of drugs: Anti-infective agents such as antiseptic and disinfectant, antibiotics (including stability and degradation products), antiparasitic, antiamoebic, antihelminitic, antimycobacterial, antifungal, anticancer, antiviral; Non-steroidal anti-inflammatory agents (NSAIDs); Drugs used in hypertensive, vasodilator, immunopharma-cology; Large scale synthesis: bench-scale experimentation, scale up, scale up from bench to pilot plant, commercial scale operation, example - Nevirapine.

Texts:

1. D. A. Williams and T. L. Lemke, *Foye's Principles of Medicinal Chemistry*, Lippincott Williams & Wilkins, Philadelphia, 2002.
2. D. Lednicer, *Strategies for Organic Drug Synthesis and Design*, John Wiley & Sons Inc., New York, 1998.

References:

1. D. J. Abraham (ed.), *Burger's Medicinal Chemistry and Drug Discovery, Vol. 1 - 6*, Wiley-Interscience, 2003.
2. D. Lednicer, *Organic Chemistry of Drug Synthesis, Vol. 1 - 6*, John Wiley & Sons Inc., New York, 1977.
3. S. Warren, *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons, 2002.

CH 428 Drug Design and Development (3-0-0-6)

Drug targets; Pharmacokinetics: ADME, administration and dosing; Drug testing: *in vivo*, *in vitro*; Drug discovery: natural lead, synthetic lead, combinatorial synthesis; Pharmacokinetics based drug design; Computer aided drug design: Principles of QSAR, 2D QSAR, 3D QSAR; Chemical development, Patenting, Process development; Toxicology, Pharmacology, Drug metabolism, Clinical trials, Commercialization: regulatory affairs, pipeline development, pharmaceutical market places, business opportunities.

Texts:

1. G. Thomas, *Fundamentals of Medicinal Chemistry,* John Wiley & Sons Ltd., 2006.
2. G. Patrick, *Instant Notes: Medicinal Chemistry,* Viva Books Pvt. Ltd., 2002.

References:

1. G. Patrick, *An Introduction to Medicinal Chemistry,* Oxford University Press, 2001.
2. T. Nogrady, *Medicinal Chemistry: A Biochemical Approach,* Oxford University Press, 2004.
3. S. Pidgeon, *Wiley handbook of Current and Emerging Drug Therapies, Vol. 4,* Wiley-Interscience, 2007.

CH 417 Organometallic Chemistry (3-0-0-6)

18-electron rule; Stabilisation of low oxidation state of metals; Metal carbonyls, nitrosyls, cabonyl hydrides, isolobal analogy, dioxygen and dinitrogencompoun ds; Metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes; Hydrides, Metallocenes, Metal arene complexes; Carbonylate anions, agostic interaction, Oxidative addition and reductive elimination, insertion and elimination reactions; Industrial organometallic catalysis: Homogeneous and heterogeneous catalysis; Organomeatllic reagents in drugs synthesis Fluxional molecules; Metal-Metal bonding and Metal clusters; Organometallic materials : synthesis and applications; Biological and environmental aspects of organometallic compounds.

Texts:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity;* 4th Ed., Harper Collins, 1993.
2. B. E. Douglas, D. H. McDaniel and J. J. Alexander, *Concepts and Models of Inorganic Chemistry*; 3rd Ed., John Wiley, 1993.

References:

1.C. Elschenbroich and A. Salzer, *Organometallics*; 2nd Ed., VCH, 1995.

2. A. Yamamoto, *Organotransition Metal Chemistry: Fundamental Concepts and Applications*; John Wiley, 1986.

3. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals*; 2nd Ed., John Wiley, 1993.

4. F. A. Cotton and G. W. Wilkinson, *Advanced Inorganic Chemistry*; 5th Ed., John-Wiley & Sons, 1988.

CH 418 Biological Chemistry of Metal Ions (3-0-0-6)

Essential and trace metals; Role of alkali and alkaline earth metal ions, Na^+-K^+ Pump, ionophores and crown ethers; Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein; Electron Transfer: Cytochromes, Fe-S proteins and Copper proteins; Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin; Oxygen activation: Cytochrome P450, Cytochrome c oxidase; Others: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogenase, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center; Hazardous coordination complexes; Coordination complexes as medicines.

Texts:

1. S. J. Lippard and J. M. Berg, *Principle of Bioinorganic Chemistry*, University Science Books, 1994.

2. J. J. R. F. da Silva and R. J. P. Williams, *The biological chemistry of the elements: the inorganic chemistry of life;* 2nd Ed., Oxford University Press, New Delhi, 2006.

References:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity;* 4th Ed., Harper Collins, 1993.

2. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*; 3rd Ed., Oxford University Press, New Delhi, 2004.

CH 419 Consumer Chemistry (3-0-0-6)

Chemistry in the laundry: Soaps, domestic laundry detergents, other household cleaning agents, chemistry of washings.

Chemistry in the kitchen: Butter, margarine and other fats, oils and waxes, body fat, fish oils, chocolate, cholesterol, prostaglandins, antioxidants, chemistry of cooking.

Chemistry in the boudoir: Chemistry of cosmetics, lipsticks, toothpaste, deodorants, sunglasses, baby care products.

Chemistry in the garden: Pesitcides and alternatives, fertilizers, insect repellents, swimming pool chemistry.

Chemistry in the medicine cabinet: Medicinal chemistry of drugs, drugs action, tranquillisers, anaesthetic drugs.

Chemistry in the dining room: Food additives, alchoholic products, caffeine, nutrition, digestion, allegies.

Text Book:

Consumer Chemistry, Sarah Bent Ransom, John Chiocca and Robert Van Reen, 2005

CH 426 Green Chemistry and Technology (3-0-0-6)

Principles and Concepts of Green Chemistry: Sustainable development, atom economy, reducing toxicity; Waste: production, problems and prevention, sources of waste, cost of waste, waste minimization technique, waste treatment and recycling; Alternate solvents: safer solvents, green solvents, water as solvents, solvent free conditions, ionic liquids, super critical solvents, fluorous biphase solvents; Alternative Energy Source: Energy efficient design, photochemical reactions, microwave assisted reactions, sonochemistry and electrochemistry; Process and Operations: Industrial preparation, reaction, reactor design, inherently safer design (ISD), process intensification (PI), in process monitoring, micromixers, unit operations; Reaction with separation operations, process integration; Industrial Case Studies: Greening of acetic acid manufacture, EPDM rubbers, Vitamin C, Leather manufacture (tanning, fatliquoring), green dyeing, polyethylene, ecofriendly pesticides, sugar and distillery industry, paper and pulp industry, pharmaceutical industry; An integrated approach to green chemical industry.

Texts:

1. M. Lancaster, *Green Chemistry: An Introductory Text*, Royal Society of Chemistry, 2002.

2.M. Doble and A. K. Kruthiventi, *Green Chemistry and Engineering*, Academic Press, Amsterdam, 2007.

References:

1. P. T. Anastas and J.C. Warner, *Green Chemistry, Theory and Practice*, Oxford, 2000.

2. V. K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, Ane Books India, New Delhi, 2006.

3. M. M. Srivastava and R. Sanghi, *Chemistry for Green Environment*, Narosa, New Delhi, 2005.

4. R.E. Sanders, *Chemical Process Safety: Learning from Case Histories*, Butterworth Heinemann, Boston, 1999.

5. P. Tundo, A. Perosa, and F. Zecchini (eds.), *Methods and Reagents for Green Chemistry*: *An Introduction*, Wiley, 2007.

Open Electives

CH 429 Petroleum and Petrochemicals (3-0-0-6)

Origin, formation and composition of petroleum, petroleum processing: fractionation, blending of gasoline, gasoline treatment, kerosene treatment, treatment of lubes, petroleum wax and purification; Thermal and catalytic processes: thermal cracking, catalytic cracking, catalytic reforming, naphtha cracking, coking, hydrogen processes, alkylation, isomerization processes; polymer gasoline, asphalt, upgradation of heavy crudes; Specialty products: industrial gases, liquid paraffin, petroleum jelly; Sources of petrochemicals; Synthesis of methanol, formaldehyde, acetylene, synthetic gas, ethanol, ethylene, ethylene glycol, vinyl acetate, acrylic acid and acrylates, acrylonitrile, acetone, acetic acid, chloroprene, vinyl chloride, vinyl acetate, acrylonitrile, propylene, butadiene, butanes, isobutene, adipic acid, adiponitrile, benzene, toluene, xylene, phenol, styrene, phthalic acid, phthalic anhydride and their applications in chemical industry.

Texts:

1. B. K. B. Rao, *Modern Petroleum Refining Processes*, 4th Ed., Oxford & IBH Publishing Co. Pvt Ltd., New Delhi, 2002.
2. P. Wiseman, *Petrochemicals*, John Wiley & Sons, 1986.

References:

1. R. A. Meyers, *Handbook of Petroleum Refining Processes*, 3rd Ed., McGraw-Hill, 2004.
2. S. Raseev, *Thermal and Catalytic Processes in Petroleum Refining*, Marcel Dekker, Inc., 2003.

CH 437 Chemical Approaches to Nanoscale Science and Technology (3-0-0-6)

Properties of materials with nanoscale dimensions; Zero, one, two and threedimensional materials; Inorganic Nanomaterials: Metallic nanocrystals with special emphasis on coinage metals, semiconductor nanocrystals, quantum dots, magnetic materials, syntheses, characterizations and properties; Carbonnantubes; Organic and biological nanostructures; Measurements: Optical spectroscopy and microscopy, scanning probe microscopy, scanning electron microscopy, transmission electron microscopy and X-ray diffraction; Applications: Catalysts, sensors, actuators, display systems, molecular devices and nanobiotechology.

Texts:

1. C. P. Poole (Jr.) and F. J. Owens, *Introduction to Nanotechnology*, Wiley Interscience, John Wiley and Sons, Hoboken, New Jersey, 2003.
2. G. A. Ozin and A. C. Arsenault, *Nanochemistry: A Chemical Approach to Nanomaterials*, RSC Publishing, Royal Society of Chemistry, U.K, 2005.

References:

1. L. M. Liz-Marsan and P. V. Kamat, *Nanoscale Materials*, Kluwer Academic Publishers, Boston, USA, 2003.
2. D. A. Bonnel, Scanning *Probe Microscopy and Spectroscopy: Theory, Techniques and Application*s. 2nd Ed.. New York, Wiley-VCH, 2001.
3. S. Amelinckx, *Electron Microscopy: Principles and Fundamentals*, Weinheim, VCH, 1997.
4. B. Valeur, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH Verlag, GmbH, Weinheim (Federal Republic of Germany), 2002.

5. D. Astruc, *Nanoparticles and Catalysis*, Wiley-VCH, Wiley-VCH Verlag GmbH and Co. KGaA, Weinheim, 2008.

CH 438 Application of Statistical Mechanics to Chemistry (3-0-0-6)

Introduction and reviews of classical mechanics, quantum mechanics and thermodynamics; Microstates, macrostates, canonical, grand canonical and microcanonical ensemble; Boltzmann distribution for distinguishable particles; The emergence of temperature from conditions for equilibrium; postulate for entropy; Partition function for a single particle; Thermodynamic potentials and variables in terms of partition function, energy degeneracy and partition functions, many (weakly interacting) particle partition function, derivation of thermodynamics of a simple harmonic oscillator, distinguishable and indistinguishable particles, counting states of a gas of indistinguishable particles, density of states, partition function of an ideal gas, derivation of the equation state of an ideal gas;the Gibbs paradox and indistinguishibility;Application of the theory of statistical mechanics to the chemical problems related to rotational specific heat of gases; Maxwell-Boltzmann distribution of velocities; Quantum statistics (Bose-Einstein and Femi-Dirac) for indistinguishable particles; Photon gas; Density of states for photons; Black body radiation; Debye frequency and specific heat of phonons, heat capacity of a Fermi gas, the classical limit from the quantum mechanical expression for paritition function, distribution functions in classical monatomic liquids, direct correlation function, density expansions of the various distribution functions.

Texts:

1. D. A. McQuarrie, *Statistical Mechanics*, University Science Books, 2000.
2. R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 1996.

Reference:

1. K. Huang, *Statistical Mechanics*, John Wiley Asia, 2000.