Syllabi for CST B.Tech. Curriculum (2023-2024 Batches)

6th Semester (Even, Jan-May)

CH3020: Computational Chemistry (3-0-0-6)

Computer programming in FORTRAN; Locating roots of equations; Numerical differentiation and integration; Systems of linear equations; Eigen value and eigenvector problems; Ordinary and partial differential equations: Euler, Runge-Kutta and finite difference methods; Solution to initial and boundary value problems; Problems on chemical kinetics; Solution of Newton's equation of motion; Solution of time-dependent Schrodinger equation for simple potentials. Approaches to solve the time-independent Schrodinger's equation, Use of standard available softwares to perform simple quantum chemical calculations.

Text Books:

1. S. J. Chapman, Fortran 90/95 for Scientists and Engineers, 2nd Ed., McGraw-Hill, 2003.
2. S. C. Chapra and P. Canale, Numerical Methods for Engineers 4th Ed., Tata McGraw -Hill, 2002.
3. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 5th Ed., Oxford University Press, 2010.

References:

1. Numerical Recipes in FORTRAN/C by W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 2nd edition, 1996.
2. J. M. Thijssen, Computational Physics, 2nd Ed. Cambridge Uni., 2007.
3. F. Jensen, Introduction to Computational Chemistry, 3rd edition, Wiley, 2017

CH3021 Application of nanomaterials (3-0-0-6)

History of nanomaterials; Origin of size-dependent properties; Zero, One, and Two dimensional nanomaterials; Syntheses and Characterization of nanomaterials. Nanocatalysts; Nanocomposites; Smart materials; Self-healing materials; Magnetic nanomaterials; Hydrogels and Aerogels; Nanosensors; Nanofluidics; Nanochannel fabrication techniques; Effect of surface charge; Ionic current rectification; Streaming potential; Water Desalination; Reverse electrodialysis; Fuel cells; Water splitting. Nanotoxicology; Environmental, health and ethical concerns.

Text Books

1. Introduction to Nanotechnology, 1st Edition, Frank J. Owens, Wiley, 2010.
2. A Textbook of Nanoscience and Nanotechnology, T. Pradeep Tata McGraw-Hill Education, 2003
3. C. P. Poole (Jr.) and F. J. Owens, Introduction to Nanotechnology, Wiley Interscience, John Wiley and Sons, Hoboken, New Jersey, 2003.
4. G. A. Ozin and A. C. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC Publishing, Royal Society of Chemistry, U.K, 2005.

References

1. Chemistry of Nanomaterials, C.N.R. Rao, A. Muller and A.K. Cheetham, Wiley-VCH, Weinheim, 2004. Reprinted 2006.
2. Nanofluidics: Nanoscience and Nanotechnology, Editors: Joshua Edel, Andrew deMello, RSC Nanoscience & Nanotechnology), 2008

3. Nanofluidics and Microfluidics, 1st Edition, Shaurya Prakash Junghoon Yeom, Elsevier, 2014
4. Nanocrystals: Synthesis, Properties and Applications, C.N.R. Rao, P.J. Thomas, G.U. Kulkarni, Springer-Verlag, 2007, Chinese Edition 2012.

CH 3022 Polymer Chemistry (3-0-0-6)

Introductory concepts, definition, common system chemistry and classification of polymers, resins, rubber, plastics; Conformations and properties of various types of polymers; Characterization: molecular weight studies and molecular weight distribution; Mechanistic aspects: addition, ionic, emulsion, suspension, aqueous, coordination, condensation polymerization; Relevant aspects of physical properties of polymer systems, rheological properties; Unit operations: calendering, extrusion and molding; fabrication processes, degradation and stabilization of polymer systems; Polymer Industry: manufacturing of some industrially important polymers (like PVC, Polyethylene, synthetic rubber, and synthetic fiber) and their characterization; Polymer Processing, Polymer additives and Curatives; Recent development in the field of biodegradable polymers.

Text Books:

1. G.S. Misra, *Introduction to Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.
2. J. R. Fried, *Polymer Science and Technology,* Prentice Hall, Englewood Cliffs, 1995.

References:

1. R. E. Fornes and R. D. Gilbert, *Polymer and Fiber Science: Recent Advances*, VCH, New York, 1991.
2. L.H. Sperling, *Introduction to Physical Polymer Science*, John Wiley & Sons, New York, 1992.
3. S. R. Sandler and W. Koro, *Polymer Syntheses*, Academic Press, Boston, 1992.

CH3023L Chemical Technology Lab - III (0-0-6-6)

Experiments based on various physical properties such as viscosity, surface tension, optical rotation and refractive index, light absorption and emission (spectroscopy); Experiments based on chemical kinetics and thermodynamics: determination of order of simple reactions, energy of activation, equilibrium constants, determination of thermodynamic functions; Experiments based on EMF and conductance measurements: determination of electrode potentials, solubility product, pH equivalent conductance; Experiments based on micro-fluidics; Experiments based on surface and interfacial chemistry: surface tension, CMC measurements, HLB values, adsorption isotherms and determination of surface area; Experiments based on phase equilibria: Study of binary and ternary liquid systems; Experiments based on deposition of thin polymer film on substrates and its characterization; Experiments based on syntheses of nanoparticles and their characterizations.

Texts/References:

1. B. Viswanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books Private Ltd., 2005.
2. D. P. Shoemaker, C. W. Garland and J. W. Nibler, *Experiments in Physical Chemistry*, 5th Ed., McGraw- Hill International Editions, 1989.
3. J. M. Postma, J. L. Roberts (Jr.) and J. L. Hollenberg, *Chemistry in the Laboratory*, 6th Ed., W. H. Freeman and Company, 2004.
4. V. D. Athawale and Parul Mathur, *Experimental Physical Chemistry*, New Age International Publishers, 2001.
5. R. A. Day (Jr.) and A. L. Underwood, *Quantitative Analysis*, 6th Ed., Prentice-Hall of India Pvt. Ltd., 2006.
6. G. D. Christian, *Analytical Chemistry*, 6th Edition, John Wiley & Sons, Inc. ,2003.

7th Semester (Odd, July-November)

CH4120 Modern Chemical Technology (3-0-0-6)

Fine chemicals and their synthesis: bio-catalysis, enantioselective catalysis; catalysis in fine chemicals: mechanism of catalysis, homogeneous and heterogeneous catalysis; catalyst performance, phase transfer catalysis; Selectivity engineering, Process development, Energy and its biological resources; Bio-Fuels: Biofuel feedstocks: sugar, starch, lignocelluolosic, plant and animal fats feedstock; Market and product process of bioethanol; Raw materials to produce low cost bio-diesel; Harvesting energy from biochemical resources.

Text Books:

A. Cybulski, J. A. Moulijn, M. M. Sharma, and R. A. Sheldon, *Fine Chemicals Manufacturing and Engineering* , Elsevier Science, 2001.

2. C. M. Drapcho, N. P. Nhuan and T. H. Walker, *Biofuels Engineering and Process Technology,* McGraw Hill, 2008.

References:

1. P. Pollak, *Fine Chemicals: The industry and the Business,* John Wiley and Sons, 2007.
2. A. Nag, *Biofuels refining and performance,* McGraw Hill, 2008.
3. D. M. Mousdale, *Biofuels: Biotechnology, Chemistry and Sustainable Development* CRC Press, 2008
4. R. N. Shreve and J. A. Brink, *Chemical Process Industries*, 4th Ed., International Students Edition,1977.
5. G. F. Austin, *Shreve's Chemical Process Industries*, 5th Ed., McGraw Hill Pub., 1984.

CH4121P BTP-1 (0-0-12-12)

Department Electives

CH4122 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 Dinitrogen compounds; Alkyls, Carbenes, Carbynes, Hydrides, Metallocenes, Alkenes, Alkynes, and Allyl complexes; Metal arene complexes; Carbonylate anions, agostic interaction, Oxidative addition and reductive elimination, insertion and elimination reactions; Industrial organometallic catalysis: Homogeneous and heterogeneous catalysis; Organometallic reagents in drugs synthesis Fluxional molecules; Metal-Metal bonding and Metal clusters; Organometallic materials : synthesis and applications; Biological and environmental aspects of organometallic compounds.

Text Books:

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.

CH4123 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 products), antiparasitic, antiamoebic, antihelminitic, antimycobacterial, degradation 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.

Text Books:

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.

CH4124 Machine Learning in Chemistry (3-0-0-6)

Introduction to encode molecules in a Format Readable and Processable by Computers: Cheminformatics learning, smiles representation, RDKIT, molecular to vector representation; Introduction to regression and classification style statistical analysis: types of regression and classification, data visualizations, simple chemical properties selection, feature identification, descriptor findings; Data-driven modeling: data and standardization, training set vs testing set, model validations, evaluating the model accuracy, simple chemical properties selection, feature identification, descriptor findings; Introduction to Deep Learning, Generative AI, Graph neural network; Property prediction models: example code for libraries (Pandas, Numpy, Matplotlib etc.), example code for materials, catalysis, potential energy surface, and reaction prediction.

Text Books:

1. Hugh M Cartwright, Machine learning in Chemistry: The Impact of artificial Intelligence, 1st Edition, Royal Society of Chemistry.2020

2. Jahan B. Ghasemi, Machine Learning and Pattern Recognition Methods in Chemistry from Multivariate and Data Driven Modeling,1st Edition, Elsevier, 2022

References

1. Etienne Bernard, Introduction to Machine Learning, 1st Edition, Wolfram Media Inc, 2021
2. Mark Lutz, Learning Python: Powerful Object-Oriented Programming, 5th Edition, O'Reilly Media, Inc, 2013
3. Aurélien Géron, Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow, 2nd Edition, O'Reilly Media, Inc, 2019

CH4021 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 storage: Ferritin, Transferrin, Siderophores and metallothionein; ion transport and Electron Transfer: Cytochromes, Fe-S proteins and Copper proteins; Oxygen transport and storage: Hemoglobin, Myoglobin, Hemerythrin, Hemocyanin; Oxygen activation: Cytochrome P450, Cytochrome c oxidase; superoxide dismutase, Others: Catalase, Peroxidase, 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.

Text Books:

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 4022 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.

Text Books:

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.

CH4023 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 partition function, distribution functions in classical monatomic liquids, direct correlation function, density expansions of the various distribution functions.

Text Books:
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.

Open Electives

CH4125 Petroleum Chemistry (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.

Text Books:

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.

CH4020 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: Pesticides and alternatives, fertilizers, insect repellents, swimming pool chemistry. Chemistry in the medicine cabinet: Medicinal chemistry of drugs, drug action, tranquillisers, anaesthetic drugs. Chemistry in the dining room: Food additives, alcoholic products, caffeine, nutrition, digestion, and allergies.

Text Book:

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

CH5644 Applied Quantum Chemistry (2-0-2-6)

Prerequisites : Basics Quantum Chemistry and Programming

Review of Quantum Chemistry: Molecular Schrödinger equation, Born-Oppenheimer approximation, variational principle, many-electron wavefunctions, Hartree-Fock theory and electron correlation, semi empirical theory; Some early density-functional theories: Thomas-Fermi model, Slater approximation of Hartree-Fock theory; Modern density-functional theory (DFT): Introduction to functionals and functional calculus, Hohenberg-Kohn theorems, Kohn-Sham approach, meaning and utility of the Kohn-Sham orbitals and eigenvalues, Approximate exchange-correlation functions; Practical DFT: Introduction to basis sets – localized and periodic basis sets, all-electron versus pseudopotential approximations, self-consistent methods to solve the Kohn-Sham equations. Hellmann-Feynman theorem and computation of forces, computation of electronic and structural properties; Introduction to a DFT code and some simple examples and case studies

Text Books

1. W. Koch and M. Holthausen, *A Chemist's Guide to Density-functional Theory*, 2nd Edition, Wiley-VCH, 2001.
2. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry*, Dover Publications, 1996.
3. R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, 2004.
4. R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules*, Oxford Science Publications, 1995.

References

1. F. Jensen, *Introduction to Computational Chemistry*, 3rd Edition, Wiley, 2017.
2. J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopoulos, H. Reis, M. K. Shukla (Eds.), *Handbook of Computational Chemistry*, 2nd Edition, Springer, 2017.
