TEACHING SCHEME AND COURSE CONTENTS

FOR

MASTER OF TECHNOLOGY

IN

CHEMICAL TECHNOLOGY



DEPARTMENT OF CHEMISTRY

NATIONAL INSTITUTE OF TECHNOLOGY HAMIRPUR (H.P.)

Programme Objective:

- To provide extensive teaching and training in industry-oriented chemical techniques including analytical instrumentation, modern chemical technologies and novel research materials/methods.
- To emphasize the importance of understanding the functioning mechanism of diverse characterization devices and their applicability in emergence of enhanced, selective detection technologies. Special focus will be given to the fields of chemical/engineering materials, electrochemical devices, advance polymer/composite platforms, spectroscopic tools and their applications.
- To provide students hand-on exposure on advanced instruments, cutting edge R&D and promote them for carrying out interdisciplinary works to address national/regional issues.
- To inculcate good communication skills, technical/scientific curiosity and knowledge among students via regular presentations, seminars, quizzes, and project discussions.

Duration of the Programme:

Two years (Four Semesters)

Intake:

Fifteen students (reservation as per GOI norms)

Eligibility for admission:

The applicant must have a Master Degree in Chemistry (with Physics and Mathematics at UG level) or Bachelor Degree in Chemical Engineering/Biotechnology/Material Science and Engineering with CGPI of 6.5 on a 10-point scale (or equivalent) or 60% marks in case of Open/OBC candidates in qualifying degree. Whereas in case of SC/ST candidates, a CGPI of 6.0 on a 10-Point scale (or equivalent) or 55% marks in qualifying degree will be applicable. The admission to M.Tech. programme will be as per institute norms.

M. TECH. PROGRAMME IN CHEMICAL TECHNOLOGY
DEPARTMENT OF CHEMISTRY

SEMESTER-I

Course No.	Subject	Teaching Schedule			Hours/Week	Credits
		L	T	P		
CH-600	Industrial Catalytic Processes	3	0	0	3	3
CH-601	Electroanalytical Chemistry	3	0	0	3	3
CH-602	Advanced Transport Phenomena (*from Chemical Engineering Department*)	3	0	0	3	3
	Programme Elective -I	3	0	0	3	3
	Programme Elective -II	3	0	0	3	3
CH-603	Electrochemical Techniques: Lab.	0	0	3	3	2
Total		**15**	**0**	**3**	**18**	**17**

SEMESTER-II

Course No.	Subject	Teaching Schedule			Hours/Week	Credits
		L	T	P		
CH-604	Industrial Chemical Technology	3	0	0	3	3
CH-605	Modern Spectroscopic Techniques and Instrumentation	3	0	0	3	3
CH-606	Chemical Reaction Engineering (*from Chemical Engineering Department*)	3	0	0	3	3
	Programme Elective -III	3	0	0	3	3
	Open Elective-I (from other Dept.)	3	0	0	3	3
CH-607	Material Synthesis and Characterization Lab.	0	0	3	3	2
Total		**15**	**0**	**3**	**18**	**17**

SEMESTER-III

Course No.	Subject	Teaching Schedule			Hours/week	Credit
		L	T	P		
CH-799	Self Study				3	2
CH-800	Seminar	0	0	3	3	2
CH-801	Dissertation (to be continued in IVth Sem)				24	12
Total					**30**	**16**

SEMESTER-IV

Course No.	Subject	Teaching Schedule			Hours/week	Credit
		L	T	P		
CH-801	Dissertation (continued from IIIrd Sem)				40	20
Total					**40**	**20**

Programme Elective Courses

Course No.	Course Title	L	T	P	C
CH-700	Advanced Polymer Technology	3	0	0	3
CH-701	Numerical & Computational Methods in Chemical Engineering (*from Chemical Engineering Department*)	3	0	0	3
CH-702	Advanced Nanostructured Materials	3	0	0	3
CH-703	Industrial Safety in Process Industries (*from Chemical Engineering Department*)	3	0	0	3
CH-704	Modern Materials Characterization Techniques	3	0	0	3
CH-705	Environmental Chemical Technology	3	0	0	3

Open Electives

(To be offered to the students from other Departments/Centres except Department of Chemistry)

(i) **CH-750** Composite Materials
(ii) **CH-751** Molecular Modelling

Course Syllabus

CH-600: Industrial Catalytic Processes (Program core-1)

(3-0-0, 3 hours, 3 credits)

- **Catalysis and its Industrial Applications:** Homogeneous & heterogeneous catalysis; Role of catalytic processes in modern chemical manufacturing— catalysis in syngas manufacture, catalysis in organic polymer chemistry; catalysis in petroleum industry; catalysis in environmental control.
- **Enzyme Catalysis:** Transition states and enzyme catalysis; Enzymes in chemical bio-transformations; Pre-steady state and steady state kinetics; Kinetics in industrial processes, Toxicological considerations and safety in handling enzymes; Enzyme immobilization and concept of protein and enzyme engineering, Applications of enzymes in industry and medicine, Enzyme inhibition.

Books and References:

1. Enzyme catalysis in organic synthesis, third Edition Editor(s): Karlheinz Drauz, Harald Gröger, Oliver May, Wiley-VCH Verlag GmbH & Co, 2012
2. Homogeneous transition metal catalysis – Christopher Masters
3. Petrochemical Economics, by Duncan Seddon, Catalytic Science Series, Volume 8.
4. Environmental Catalysis, Edited by: F J J G Janssen and R A van Santen, Catalytic Science Series, Volume 1.
5. Concepts of Syngas Manufacture by Jens Rostrup-Nielsen and Lars J Christiansen**.**

CH-601: Electroanalytical Chemistry (Program core-2)

(3-0-0, 3 hours, 3 credits)

Principles of electro-chemical methods, electrochemical reactions, types of electrochemical cells. Application of EMF and conductometric measurements in determining (i) free energy, enthalpy, entropy and kinetic parameters of reactions, (ii) equilibrium constants, and (iii) solubility limits of different salts. Commonly used electrode types and their functioning. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Detailed qualitative discussion of potentiometric/conductometric titrations (acid-base, redox, precipitation), Kinetics of electrode reactions, polarography, electroanalytical voltammetry as applied to analysis and the chemistry of heterogeneous electron transfers. Working of fuel cells and batteries. Electrochemically-driven scanning probe techniques. Applied Electrochemistry: electrocatalysis, prevention of corrosion and ultra-sensitive biosensing of molecules.

Books and References:

1. Bard, A. J.; Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., John Wiley and Sons, New York, 2002.
2. Koryta, J.; Dvorak, J.; Kavan, L. *Priniciples of Electrochemistry*, John Wiley and Sons; New York, 1993.
3. Bockris, J. O. M.; Reddy, A. K. N. *Modern Electrochemistry 1: Ionics*, 2nd Ed., Springer, 1998.
4. Bockris, J. O. M.; Reddy, A. K. N.; Gamboa-Aldeco, M. E. *Modern Electrochemistry 2A: Fundamental of Electrodics*, 2nd Ed., Springer, 2001.
5. Bockris, J. O. M.; Reddy, A. K. N. *Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science*, 2nd Ed., Springer, 2001.

CH-602: Advanced Transport Phenomena (Program core-3)

(3-0-0, 3 hours, 3 credits)

Summary of Vector and Tensor Notation: Vector operations from a geometrical view point, Vector operation from an analytical view point, the vector differential operations, second order tensors, vector and tensor components in curvilinear coordinates, differential operations in curvilinear coordinates.

Momentum Transport: Viscosity and the mechanism of momentum transport, Newton's law of viscosity, non- Newtonian fluids, pressure and temperature dependence of viscosity, theory of viscosity of gases at low density, theory of viscosity of liquids.

Velocity Distributions in Laminar Flow: Shell momentum balances: boundary conditions, flow of a falling film, flow through a circular tube, flow through an annulus, adjacent flow of two immiscible fluids.

The Equations of Change for Isothermal Systems: Equation of continuity, the equation of motion, the equation of mechanical energy.

Thermal Conductivity and the Mechanism of Energy Transport: Fourier's Law of heat conduction, temperature and pressure dependence of thermal conductivity in gases and liquids, theory of thermal conductivity of gases at low density, theory of thermal conductivity of liquids, thermal conductivity of solids.

Temperature Distributions in solids and in Laminar Flow: Shell energy balances; boundary conditions, heat conduction with an electrical heat source, heat conduction with a chemical heat source, heat conduction through composite walls: Addition of resistance, Forced Convection, Free Convection.

The Equations of change for Non isothermal systems: The equations of energy, the energy equation in curvilinear coordinates, the equations of motion for forced and free convection in non-

isothermal flow, summary of the equations of change, use of equation of change to set up steady – state heat transfer problems.

Diffusivity and the Mechanism of Mass Transport: Definition of concentrations, velocities and mass fluxes, fick's law of diffusion, theory of ordinary diffusion in gases at low density, theory of ordinary diffusion in liquids.

Concentration Distributions in Solid and in Laminar Flow: Shell mass balances: boundary conditions, diffusion through a stagnant gas film, diffusion with heterogeneous chemical reaction, diffusion with homogeneous chemical reaction, diffusion into a falling liquid film, forced – convection mass transfer, Analogies between Heat, mass and momentum transfers.

Books and References:

1. Bird R. B., Stewart W. E. and Light fort R. N.,"Transport Phenomena", John Wiley and Sons (2002).
2. Welty J. R. , Wilson R. E. and Wicks C. E. , "Fundamentals of Momentum", Heat and Mass Transfer",4th ed, John Wiley and Sons (2001).
3. John C. Slattery, "Momentum, Energy and Mass transfer in continua", McGraw Hill, Co. (1972).

CH-603: Electrochemical Techniques: Lab.

(3-0-0, 3 hours, 2 credits)

Use of Conductometry /Potentiometry in understanding precipitation reactions, inorganic complex formations, determination of kinetic parameters of chemical reactions, and micelle formation in soap solutions. Electrochemical estimation of dissociation constant of amino acids. Practical verification of electrochemical Tafel equation. Determination of amount of metal ions in samples using polarography.

Books and References:

1. Shoemaker, D. P.; Garland, C. W.; Nibler, J. W. *Experiments in Physical Chemistry*, McGraw-Hill, New York, 1996.
2. Das, R. C.; Behera, B. *Experimental Physical Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., 1993.
3. Khosla, B. D.; Garg, V. C.; Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co., New Delhi, 2008.

CH-604: Industrial Chemical Technology (Program core-4)

(3-0-0, 3 hours, 3 credits)

Dyes: Structure and properties, Natural colours/dyes for textile applications, Natural food colours and their health aspects, Biomedical applications of dyes: Photodynamic therapy, Dyes in

bioanalysis and medical diagnostics, DNA sequencing, Cancer detection, activity with diazonium salts, Dyes as therapeutic agents.

Sugar Technology: Introduction to sugar industry, Specification of raw sugar, Refining quality of raw sugar – evaluation, calculation of raw value, By-products and co-products of sugar industry

Chemistry of Food Preservatives: Objectives and techniques of food preservation; Structure, properties and use of foods preservative: chemical preservative, biopreservative including antibiotics.

Petrochemicals – Structure, Properties and Applications: Types of crude oil, Properties of Petroleum oil products: Definition and significance of various properties like API gravity, Aniline point, Diesel index, Cloud point, Pour point, Flash point, Fire point, Smoke point, Octane number, Cetane number, Softening point; Manufacturing process of Chemicals from methane: synthesis of methanol, Acetic acid, Vinyl Acetate, Poly Vinyl Acetate, Specific requirements for automotive lubricants, oxidation deterioration and degradation of lubricants, additives and additive mechanism, synthetic lubricants.

Books and References:

1. Functional Dyes, S H Kim, Elsevier BV 2006

2. Industrial Dyes-Chemistry, Properties, Applications by Klaus Hunger WILEY-VCH Verlag, 2003

3. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi

4. Natural Food Colorants by Gabriel J. Lauro and F. Jack Francis (eds), Marcel Dekker Inc.

5. Manufacture and Refining of Raw Cane Sugar – V E Baikow

6. Industrial Utilisation of Sugarcane & Its Co-products - P J Manohar Rao

7. Technology of Food Preservation by Desrosier

8. Modern Petroleum Refining Processes, B. K. Bhaskara Rao

9. Lubrication – A practical guide to lubricant selection by A.R.Lansdown — Pergamon press – 1982.

CH-605: Modern Spectroscopic Techniques and Instrumentation (Program core-5)

(3-0-0, 3 hours, 3 credits)

UV-Visible spectroscopy; Vibrational Spectroscopies (Raman, FTIR, SFG); NMR as characterization tool: instrumentation, recent advances and analytical applications; Mass spectrometry and its applications; Atomic absorption and emission spectrometry; Fluorescence and phosphorescence based methods; Chromatographic methods of separation; Gas chromatography and HPLC.

Books and References:

1. Fundamentals for Molecular Spectroscopy by Colin Banwell and Elaine Mccash

2. Organic Spectroscopy by W. Kemp

3. Spectrometric Identification of Organic Compounds by R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce

4. Organic Spectroscopy: Principles & Applications by Jag Mohan

5. Principles of Instrumental Analysis (6^{th} Edition) by Douglas A. Skoog, F. James Holler, Stanley R. Crouch

6. Biophysical Chemistry, Part 2: Techniques for the Study of Biological Structure and Function, by Charles R. Cantor and Paul R. Schimmel

7. Organic Spectroscopy by K. S. Mukherjee and B Mukhopadhyay

CH-606: Chemical Reaction Engineering (Program core-6)

(3-0-0, 3 hours, 3 credits)

Introduction: Kinetics of homogeneous chemical and biochemical reactions, single and multiple reactions, order & molecularity, rate constant, elementary and non elementary reactions, temperature dependent term of rate equation, Constant volume batch reactor, integral method of analysis of data, series and parallel reactions, reversible reactions, Variable volume batch reactor, Differential methods of analysis, Temperature and reactions rate; Types of Microorganisms: Structure and function of microbial cells; Fundamental of microbial growth; batch and continuous culture; Isolation and purification Enzymes from cells; Assay of Enzymes; Metabolism and bio-energetics.

Reactors: Fixed Bed Catalytic Reactor, Single and multi bed adiabatic reactors, Multi tubular fixed bed reactor. Kinetic Regimes for Mass Transfer and Reaction, Film Conversion parameter, Clues to the kinetic Regime from solubility data, Clues to the Kinetic Regime from equipment, Applications to design, Reactor Design and Analysis for soluble enzyme systems**.**

Bio Reactors — Effect of Transport Processes: Introduction to Bioreactor design: Continuously Stirred aerated tank bioreactors. Mixing power correlation; Determination of volumetric mass transfer rate of oxygen from air bubbles and effect of mechanical mixing and aeration on oxygen transfer rate, heat transfer and power consumption; Multiphase bioreactors and their applications; Downstream processing and product recovery in bioprocesses.

Rate Equations for Fluid solid catalytic reactions: Rates of Adsorption, Surface reaction, Desorption, Rate limiting step, Power Law, Langmuir Hinshelwood rate, Eley Rideal mechanism, Packed bed reactor and fluidized bed reactor, Numerical Problems.

Intra Pellet Mass Transfer: Gaseous diffusion in single cylindrical pore, Different modes of diffusion: Bulk diffusion, Knudsen diffusion and surface diffusion, Diffusion in Liquids, Diffusion in Porous Catalyst, Concepts of effective thermal conductivity and effective diffusivity, Effectiveness factors.

Books and References:

1. Biochemical Engineering Fundamentals, J. E. Bailey and D. F. Oilis. 2nd Edn., McGraw Hill, New York, 1986.

2. Biotechnology, Trevan, Boffey, Goulding and Stanbury, Tata McGraw Hill Publishing Co., New Delhi, 1987.

3. Bio Process Engineering: Basic concepts M. L. Shulerand and F. Kaigi, Ist Edn., Prentice Hall, Englewood Cliffs, New Jersey 07632, 1992.

CH-607: Material Synthesis and Characterization Lab.

(3-0-0, 3 hours, 2 credits)

Single and double stage preparation of organic/inorganic/polymeric materials; purification using column chromatography, thin layer chromatography, Flash chromatography, GC, HPLC, Identification and Characterization of the same using UV, FTIR, NMR (1D, 2D, 3D), Raman, X-ray diffraction and mass spectroscopic techniques.

Books and References:

1. Vogel's Textbook of Practical Organic Chemistry, 5th Edition, by A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith

2. Advanced Practical Organic Chemistry by N.K. Vishnoi

3. Organic Spectroscopy by W. Kemp

4. Spectrometric Identification of Organic Compounds by R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce.

Program Electives

CH-700: Advanced Polymer Technology

(3-0-0, 3 hours, 3 credits)

Introduction: Molecular weight distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationships, Methods of determination of molecular weight, distribution, size and shape of macromolecules, Mark-Houwink relationship, Thermodynamics of polymer solutions, Rubber elasticity concepts, thermodynamic equation of state.

Polymerization Techniques- bulk, solution, emulsion-description of the process, progress of polymerization, rate of polymerization, degree of polymerization, suspension, living radical polymerization technique, Mechanical properties of polymers and methods of determination, selected commercial polymers and applications.

Polymer modifications and recent technological advances toward live cell encapsulation and delivery, Surface modification of natural fibers for reinforcement in polymeric composites, Biopolymers based stimuli-sensitive functionalized graft copolymers as controlled drug delivery systems.

Role of polymers for high-tech areas such as light emitting diode, OSR in satellite communication, photovoltaic etc., High temperature polymers such as polyimides, polyetherimides, PEEK, silicone etc., their preparations, properties & applications, Liquid Crystalline polymers- their synthesis, properties and applications, High energy absorbing polymer, Super absorbent polymers - their synthesis, properties and applications.

Books and References:

1. Surface modification of Biopolymers, V. K. Thakur and A.S. Singha (Ed.), John Wiley & Sons, 2015.

2. Introduction to Physical Polymer Science, L.H. Sperling, Wiley Interscience, New York,

1986.

3. Principles of Polymerization, G. Odian, Third edition, Wiley Interscience. New York, 1992.

4. Principles of Polymer Chemistry, P.J. Flory, Cornell University, Press Ithaca, 1953.

5. Textbook of polymer Science, F.W. Billmeyer, 3rd Edition, John Wiley, London, 1994.

6. Polymer Science, Gowariker et al, Wiley Eastern, New Delhi, 1990.

7. Polymer Science and Technology by J. R. Fried.

CH-701: Numerical & Computational Methods in Chemical Engineering

(3-0-0, 3 hours, 3 credits)

Treatment of engineering data-graphical representation, empirical equations, Interpolation; Newton's formula, Lagrange's interpolation formula, extrapolation, integration, graphical Integration, graphical construction of integral curves, numerical integration.

Interpretation of Engineering Data- significant figure, classification of measurements, propagation of errors, variation and distribution of random errors, properties of variance, confidence limits for small samples.

Ordinary Differential Equations – formulation, application of law of conservation of mass– mixing in flow process. Classification of ordinary differential equations and its applications to common chemical engineering problem.

Numerical Solutions of Ordinary Differential Equations – linear second–order equations with variable coefficients, numerical solution by Runge kutta method. its application to higher–order equations

Formulation of partial differential equations, finite difference, linear finite difference equations, non-linear difference equations, optimization, types of methods, its application relating to chemical

processes.

Books and References:

1. Applied Mathematics in Chemical Engineering, Mickley HS, Sherwood and Reed, TMH pub.
2. Mathematical Methods in Chemical Engineering, Jenson & Jeffrey's, McGraw Hill
3. Process Modeling, Simulation and Control for Chemical Engineering, Luyben WL, McGraw Hill

CH-702: Advanced Nanostructured Materials

(3-0-0, 3 hours, 3 credits)

Introduction; fundamentals of colloidal chemistry; Synthesis, preparation and fabrication: chemical routes, self assembly methods, biomimetic and electrochemical approaches; Size controls properties (optical, electronic and magnetic properties of materials) - Applications (carbon nanotubes and nanoporous zeolites; Quantum Dots, basic ideas of nanodevices).

Books and References:

1. Nanotechnology: Principles and Practices, by Sulabha K. Kulkarni

2. Nanostructures & nanomaterials: synthesis, properties & applications, by Guozhong Cao, Imperial College Press, London

3. Introduction to nanoscience and nanotechnology, by Gabor L. Hornyak,Harry F. Tibba et.al., CRC Press, New York

CH-703: Industrial Safety in Process Industries

(3-0-0, 3 hours, 3 credits)

Introduction: Industrial safely principles, Site selection and plant layout, Legal Aspects, Design for ventilation, Emergency response systems for hazardous goods basic rules and requirements which governs the chemical industries.

Hazards: Chemical hazards classification, Hazards due to fire, explosion and radiation, Reduction of process hazards by plant condition monitoring, Materials Safety Data sheets and National Fire protection agency's classifications.

Diseases: Dangerous occupational diseases, poisoning, dust effect, Biomedical and engineering response to health hazards.

Control of Hazards: Engineering control of plants instrumentation, Color codes for pipe lines, Safety aspects of reactive chemicals.

Operation and Process Hazards: Safety in operations and processes, Runaway reactions, unstable products.

Hazard identification: Hazard survey, checklist, HAZOP, safety reviews

Risk Assessment: Probability theory, event tree, fault tree, QRA and LOPA, Dow's fire and explosion index, Mond index, Dow's Chemical release model

Case Histories: Accident Investigations: Bhopal gas tragedy, flixborough disaster, Pasadena accident, IOCL disaster

Books and References:

1. Safety and Accident Prevention in Chemical Operation, H. H. Fawcett and W. S. Wood, 2nd Edn., Interscience, 1982.
2. Loss Prevention and Safety Promotion in Chemical Process Industries, Vol. 1, Published by Institution of Chemical Engineers U.K., 1983.
3. Safety of Reactive Chemicals, T.Yoshida, Vol. l, Elsevier, 1987.
4. Industrial Safely Handbook, 2nd Edn., H. Willium, McGraw Hill, 1968

CH-704: Modern Materials Characterization Techniques

(3-0-0, 3 hours, 3 credits)

Mechanical Testing of materials; Thermal analysis techniques: TGA, DTA & DSC; Magneto-Optical Characterization of Magnetic Thin Films, Surfaces, and Interfaces at Small Length and Short Timescales; Basic concepts of diffraction techniques (powder and single crystal) for inorganic, organic and hybrid materials; Applications of electron microscopic techniques (scanning and transmission) for morphological and nanostructural features; Scanning Probe Microscopies (STM, AFM, SNOM), Photoelectron Spectroscopy: XPS and Auger.

Books and References:

1. Characterization of Materials, Elton N. Kaufmann (Ed.)

2. Materials Characterization: Introduction to Microscopic and Spectroscopic Methods by Yang Leng.

3. Characterization of Materials by P.K. Mitra

CH-705: Environmental Chemical Technology

(3-0-0, 3 hours, 3 credits)

- Water and waste water analysis: Determination of acidity/alkalinity, turbidity, hardness, residual chlorine, BOD, COD and other inorganic/organic contaminants.
- Chemical Toxicology: Dose-response relationships, toxicology of metal ions, pesticides, insecticides and food additives.
- Waste management and application of Green technology
- Industrial pollution and its control by application of biotechnology, Radioactive wastes and their proper disposal, Pollution from agrochemicals and its control.

- INTERNATIONAL STANDARD IS0 14040: Environmental management - Life cycle assessment - Principles and framework

Books and References:

1. Sawyer, C.N. and McCarty, P.L., and Parkin, G.F. *Chemistry for Environmental Engineers,* 4th Edn. McGraw Hill, New Delhi, 1994.

2. Environmental Chemistry with Green Chemistry by A.K. Das and M. Das

3. INTERNATIONAL STANDARD IS0 14040

Open Elective

CH-750: Composite Materials

(3-0-0, 3 hours, 3 credits)

Introduction to composite materials, comparison of different materials with composites- advantages and disadvantages, Principles of composite reinforcement, Effect of fibrous reinforcement on composite strength, Types of reinforcement such as natural, glasses, carbon/graphite, aramid fiber, high strength and high modulus fibers, Surface treatment and various forms of fibers.

Processing and production techniques like hand-layup, bag moulding, filament winding, pultrusion, Prepegs, their manufacture and characterization, Sheet moulding and dough moulding compounds and their processing, resin transfer mouldings.

Application of self reinforced composites, Concept of nanofillers and polymer nanocomposites, Surface modification of cellulose nanocrystals for nanocomposites, Surface modification ofnatural fiber composites and their potential applications.

Books and References:

1. Surface modification of Biopolymers, V. K. Thakur and A.S. Singha (Ed.), John Wiley & Sons, 2015.

2. Hand Book of Composites, by George Lubin.

3. Hand Book of Fibre glass and Advanced Plastic Composites, by G. Lubin

4. Nanocomposite Science and Technology by Pulickel M. Ajayan, Linda S. Schadler,

Paul V. Braun, September 2003 Wiley

CH-751: Molecular Modelling

(3-0-0, 3 hours, 3 credits)

Molecular Mechanics, Simulation of Molecular Ensembles, Foundation of molecular orbital theory, Semi-empirical implementations of molecular orbital theory, *Ab initio* implementations of Hartee-Fock molecular orbital theory, Density Functional Theory, Charge Distribution and Spectroscopic

properties, Thermodynamic properties, Hybrid quantal/classical models, Gaussian Techniques, Docking, 2D and 3D QSAR, Applications in pharmaceutical industry and designing of new varieties of polymers/pesticides/pigments/materials.

Books and References:

1. Essentials of Computational Chemistry: Theories and Models by Christopher J. Cramer.

2. Molecular Modelling: Principles and Applications, by Andrew Leach

3. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, by Errol G. Lewars.