#### **AcSIR-CSIR Chemical Sciences Course Work Syllabus**

#### 100 level courses

(Minimum Credit requirement: 02)

CHE-NEIST-1-3901 (Core)

Research Methodology: 1-0-0-1

Good laboratory practices, Safety in the laboratory, First Aid in the laboratory, Maintenance of laboratory records, Scientific literature management, Communication skills (scientific writing and presentation), Intellectual property management & planning, Ethics in Science, Computer applications and tools, Statistical methods & Data analysis

CHE-NEIST-1-3902 (Core)

**Analytical Tools and Instrumentation: 1-0-0-1** 

Thermal methods (TG, DTG, DTA, TMA, DSC), X-ray methods (XRD, XRF, SAXS), NMR (1H, 13C) and other Spectroscopic methods (EPR, IR, UV, Fluorescence), Chromatographic methods (TLC, GC, LC), Mass spectroscopy, Electron Microscopy (SEM, TEM), Electron Probe Micro Analysis (EDS, WDS), Quantitative Analysis (AAS, ICP, CHN)

CHE-NEIST-1-3903 (Elective)

Basic Chemistry for Interdisciplinary sciences: 1-0-0-1

Basics of inorganic, organic, physical and biochemistry, Nomenclature (IUPAC), molarity, molality and normality, types of bonding, Ionic, covalent and non-bonding interactions, Acids and bases, Atomic structure, periodic table and periodic properties, stoichiometry, chemical reactions and kinetics, solvent effects, functional groups in organic compounds, general named reactions and reaction mechanisms, carbohydrates, lipids, proteins, nucleotides, enzymes, photosynthesis.

#### CHE-NEIST-1-3904 (Elective)

Introduction to Nanoscience and Nanotechnology: 1-0-0-1

General considerations, Introduction, definitions, consequences of size reduction, Properties: structural, thermodynamic, optical, electrical and magnetic properties, Methods of synthesis, Surface modifications, factors governing the stability and assembly, Characterization of nanomaterials, Applications of Nanomaterials

CHE-NEIST-1-3905 (Elective)

Introduction to Chemical Biology: 1-0-0-1

Chemical biology/synthetic biology, Structure, function and chemistry of biological macromolecules including amino acids, proteins, nucleic acids and carbohydrates, Chemical kinetics and thermodynamics in biology, Chemical reactions and chemical diversity in Biology The Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Drugs from Nature, Drug interaction

#### 200 level courses

(Minimum Credit requirement: 06)

[\*Note: ANY ONE AS CORE OF 3901/ 3902/ 3903]

CHE-NEIST-2-3901\* (Core)(ANY ONE)
Advanced Physical Chemistry: 2-0-0-2

Thermodynamics and chemical kinetics, Quantum Mechanics, Atomic structure and spectroscopy, Chemical bonding in diatomics, Chemical applications of group theory, Colloids and Surface science, surfactants, Interface and Interfacial properties, Electrochemistry.

### CHE-NEIST-2-3902\* (Core)(ANY ONE) Advanced Inorganic Chemistry: 2-0-0-2

Structure & Bonding in Inorganic Compounds, Chemistry of Coordination Compounds, Symmetry in Chemistry & Group Theory, Main group chemistry, Organometallic chemistry, Electronic Spectra of Transition Metal Compounds, Magneto Chemistry, Metal Cluster Compounds, Inorganic Reaction Mechanism, Electron Transfer Reactions in Metal Complexes, Bioinorganic Chemistry (Metalloenzymes, Metal complexes as oxygen carriers, Photosynthesis), Metal Complexes in Medicinal Chemistry, Catalysis by Inorganic Complexes.

#### CHE-NEIST-2-3903\* (Core)(ANY ONE) Advanced Organic Chemistry: 2-0-0-2

Stereochemistry, reaction mechanism, C-C and C-X bond formations, Retrosynthetic analysis, photochemistry, pericyclic reactions, reactive intermediates, Methods of asymmetric synthesis and their application in total synthesis, oxidation-reduction reactions, organocatalysis, metathesis reactions.

# CHE-NEIST-2-3904 (Elective) Advanced Analytical Chemistry: 2-0-0-2

Analytical instrumentation, signal and noise, Overview of optical methods of analysis: Components of optical instruments, atomic and molecular spectrometry based on scattering. absorption. emission and Electroanalytical techniques (basic electrochemistry, voltammetry, potentiometry), Analytical separations introduction to chromatographic methods, GC, LC, Mass spectrometry. electromigration techniques, hyphenated techniques, detectors, Analytical tools for petroleum refining.

### CHE-NEIST-2-3905 (Elective) Advanced Organometallic Chemistry: 2-0-0-2

Fundamentals, The 18 Valence Electron Rule; Structure and bonding of organometallic complexes using molecular orbital theory.σ-Donor Ligands:

Transition-Metal-Alkyl and -Aryl compounds;  $\sigma$ -Donor/ $\pi$  -Acceptor Ligands: Transition-Metal-Alkenyl, -Aryl and -Alkynyl Complexes, Transition-Metal-Carbenes (Fischer and Schrock Carbenes); Metal Carbonyl; Structure, properties and principal reaction types of the above complexes;  $\sigma$ ,  $\pi$  -Donor/ $\pi$  -Acceptor Ligands: Olefin Complexes; Alkyne, Allyl and Enyl Complexes, Complexes of the cyclic CnHn,Fundamental Mechanism of Organometallic Transformations: Oxidative addition, Migratory Insertion,  $\beta$ -hydride elimination and reductive elimination; Interaction of C-C and C-H  $\sigma$ -bonds with Transition Metals.

#### CHE-NEIST-2-3906 (Elective)

**Advanced Coordination Chemistry: 2-0-0-2** 

Naming of coordination compounds, classification of ligands, chelate and macrocyclic effect, Theories dealing with the formation of Coordination Compounds, Spectrochemical Series; Splitting of d-orbitals, Jahn–Teller Effect; Stability constants of Transition metal complexes and their determination by Job's Method. Spin–Orbit Coupling, Electronic states and term symbols, Selection rules (Laporte and spin selection rule), Interpretation of electronic spectra of Transition metal complexes, Orgel and Tanabe Sugano diagrams. Charge Transfer spectra, Magnetic Properties of Transition elements, Chemistry of Inner Transition Elements.

#### CHE-NEIST-2-3907 (Elective)

**Advanced Polymer Chemistry: 2-0-0-2** 

Techniques of polymerization, polymer characterization techniques, Stereochemistry of Polymers, polymer nano-architectures, random and block copolymers, Liquid Crystalline Polymers, Conducting Polymers, Non-linear Polymers, Polymer Blends and Composites, polymer rheology, inorganic, bio and supramolecular polymers.

### CHE-NEIST-2-3908 (Elective)

**Advanced Electrochemistry: 2-0-0-2** 

Basic electrochemistry concepts, Reference electrodes, Electrochemical Thermodynamics, Kinetics of electron transfer, the Taft equation, Diffusion, Double Layers, electrode Kinetics, the Gibbs adsorption isotherm, the Lippmann equation, infinitely dilute solutions and thermal balance, Electro capillary phenomena, Faradaic vs. capacitive currents, transport properties, potential theory, Electrochemical Techniques, Voltammetry, Reversible and irreversible reactions, Mass transport by convection, rotating electrodes, Equivalent circuits, A.C. voltammetry, Electrolysis methods, Adsorption, Thin layer cells, Electrochemistry of polymers and inorganic solids, Spectroelectrochemistry, Applications.

#### CHE-NEIST-2-3909 (Elective)

Advances in Bioinorganic chemistry: 2-0-0-2

Metal ions in biology, structure and function of metallo-proteins and enzymes, Communication role for metals in biology. Heme and non-heme systems with one-, two- or multi-metal, photosynthesis and photosystem II; O2-binding, reduction to O2-, O22-, and O2-species their utilization in hydroxylation and epoxidation; nitrogen fixation, water-oxidation reactions. Synthetic models, Correlation with structure and

function of the natural enzymes, design and synthesis, mechanisms. Metal based drugs, Porphyrins, Corrins, hydroporphyrins.

#### CHE-NEIST-2-3910 (Elective)

Advances in hydrocarbon chemistry: 2-0-0-2

Chemistry of crude oil, thermal cracking, visbreaking and coking processes, catalytic cracking, hydro cracking and hydrogen production processes, catalytic reforming process, Chemistry and industrial processes for alkylates, isomerisation processes, Petrochemicals, Basic Building blocks; C1-Chemistry; Petrochemicals from n-paraffins; Petrochemicals from olefins and aromatics; Refinery-Petrochemical Integration, Future Prospects

### CHE-NEIST-2-3911 (Elective) Advanced Catalysis: 2-0-0-2

Homogeneous and heterogeneous catalysis, adsorption, diffusion, kinetics, equilibrium andrate expressions; Chiral catalysis, Surface Science in Catalysis, Catalytic Materials; Supports; Active Components, Classes of reactions and types of reactors; Catalyst preparation methods; Characterization of catalysts; Catalysis in super critical media; Brief introduction of organo and electro-catalysis; Structure-activity-property-stability of catalysts, Catalysts in chemical industry, Catalysis in petroleum refining and petrochemicals; Catalysis in the utilization of renewable feed stocks and concepts of sustainable chemistry.

#### CHE-NEIST-2-3912 (Elective)

Advanced Surface Science: 2-0-0-2

Introduction to Surface Science - Surface phenomena - Adsorption, Desorption, Adsorption Models, Special properties of surfaces and interfaces, Electronic structure of surfaces, Surface modification and its applications, Nanoscale catalysis and applications, Surface spectroscopy and microscopy tools for nanocatalysis

#### CHE-NEIST-2-3913 (Elective)

**Advanced Materials Characterization Techniques: 2-0-0-2** 

Optical Microscopy, Electron microscopy: TEM, HRTEM, SEM, STEM, EDX, FIB, e-beam lithography, Scanning probe microscopy: AFM, STM, MFM, confocal, etc, Raman spectroscopy/microscopy, Thermal analysis techniques, Magnetic measurements, Electrical measurements, Spectroscopic ellipsometry.

#### CHE-NEIST-2-3914 (Elective)

Advances in Nanoscience and Nanotechnology: 2-0-0-2

Low-dimensional structures: Quantum wells, Quantum wires, and Quantum dots, Nano clusters & Nano crystals, fullerenes, carbon nano tubes and graphene, Nano Composites, synthesis and characterization techniques, Properties at Nano Scales and comparison with bulk materials, fabrication techniques, general applications, nanomaterials in biology.

#### CHE-NEIST-2-3915 (Elective)

Advances in Chemical Biology: 2-0-0-2

Amino Acids, Peptides & Proteins, Design of poly peptides, Peptide hormones and their pharmaceutical significance, Peptide mimetics as therapeutics, Chemistry of Carbohydrates, Nucleic acids, Structure & function of DNA and RNA, Nucleic acid mimetics & their therapeutic applications, Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Basic principles of medicinal chemistry, Drugs from Nature, Natural products based drug discovery, Kinetics and thermodynamics of biological process, Enzyme

Catalysis, consecutive, parallel and competitive reactions in biological systems, Thermodynamics, alosteric effect in biology, types of bonds, hydration and their specific contribution towards specific thermodynamic parameters, enthalpy or entropy, Scatchard analysis, hill plot analysis.

### CHE-NEIST-2-3916 (Elective) Sol-gel chemistry: 2-0-0-2

Introduction, Hydrolysis and condensation reactions, Solution chemistry and physics of intermediates, Role of the anion on the hydrolysis and condensation reactions, Kinetics of Hydrolysis and Condensation, Non-Hydrolytic Sol-Gel Processing, Gelation, Ageing, Drying, Densification, Characterization, Chemistry of Sol-Gel Silicates, Solution chemistry of transition metal alkoxide precursors, Sol-gel synthesis and characterization of important materials, structure-property relationships

# CHE-NEIST-2-3917 (Elective) Green chemistry: 1-0-0-1

Green chemistry concepts: Basic understanding, scope and interdisciplinary nature of green chemistry; Environmental factors; Carbon credit, Energy efficiency and atom economy, Catalysis and green chemistry, Alternate reaction media and reaction systems, ionic liquids, supercritical fluids, solventless chemistry.

# CHE-NEIST-2-3918 (Elective) Coal chemistry: 2-0-0-2

Mining processes, mine safety, Sampling methods of coal and its importance, Coal classification systems, Physical characterization, proximate analysis, Ultimate analysis, Sulphur analysis, Ash fusion temperature, Low temperature Carbonization, Swell Index, Cracking Index, Thermogravimetric analysis etc, Size Reduction and Size Classification of Coal, Structure of coal, Organic functionality of coal, aromatic Index, Mineral matter content, Mineralogy of coal, Geological origin of coal, petrographic analysis, geochemical processes during mining of coals, Coal Utilization, Coal Conversion processes, Other useful products from coal, Environmental Issues, CO2 sequestration.

#### CHE-NEIST-2-3919 (Elective)

#### Alternative feedstock options for petrochemicals: 2-0-0-2

Global scenario of Petrochemicals, Renewable resources; categorization of resources; chemicals from edible renewable resource; Chemicals from non-edible renewable resources; Catalytic reactions (mineral acid, bases; enzymes, homogeneous and heterogeneous catalysts); alternate fuels; fuels derived from renewable resources; biodiesel, bioethanol, biobutanol; Hydrogen generation from renewable feed stocks, Conversion of glycerol; Naphtha as a conventional source, Need for sustainability in production of Petrochemicals, Alternate Options; from Refineries sources, Natural Gas/Methane as an Option and other Non Refinery Sources, CO2 utilization, Identification and Recommendations based on technoeconomic analysis for India.

### CHE-NEIST-2-3920 (Elective) Natural products: 2-0-0-2

Carbohydrates and polysaccharides, Structure and functions of important derivatives of monosaccharides, Classification and nomenclature and synthesis of some simple Alkaloids; Terpenoids and Steroids such as pinene; Camphor and Cadenine; α-vetinone; Hirsutene and Abietic acid (Terpenoids); Cholesterol; Testosterone and Andestrone (Steroids) etc. isolation and characterization, elucidation of structure-property relationships. Biosynthesis of steroids, terpenoids, fatty acids, alkaloids and polysaccharides, biosynthesis of natural products

### CHE-NEIST-2-3921 (Elective) lonic liquids: 1-0-0-1

Introduction to ionic liquids, ionic liquids vs. molecular solvents/ionic salts (solids), ionic liquids vs. eutectic mixtures, solvent polarities using different spectral techniques (parameters), physicochemical properties of ionic liquids, effect of functional groups on the properties of ionic liquids, surface active ionic liquids, aggregation behavior of ionic liquids, interaction of ionic liquids with different molecular solvents, interaction of ionic liquids with biopolymers, thermodynamics of the binary mixtures of ionic liquids, structure property relationship in ionic liquids.

# CHE-NEIST-2-3922 (Elective) Synthetic methods for organic chemists: 2-0-0-2

Formation of carbon-carbon bond employing various kinds of organometallic reagents, C-C double bonds through different reactions, oxidation, reduction through various kinds of reagents, functional group interconversion, by substitution including protection and deprotection, alkylation of enolates, and other carbon nucleophiles, reaction of carbon nucleophiles with carbonyl compounds, electrophilic addition to C-C multiple bonds, reactions of C-C multiple bonds, Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

#### CHE-NEIST-2-3923 (Elective)

Organic reaction mechanisms: 2-0-0-2

Basics, The concept of Aromaticity, How to write an organic reaction mechanism?, Popular name reactions, Reactive intermediates: Generation, stability, structures and reactivity of carbocation, carbaion, carbene, radicals, benzyne, nitrene, Types of mechanism: classification, limitations examples of aliphatic nucleophilic substitution aliphatic electrophilic substitution - aromatic nucleophilic substitution - aromatic electrophilic Substitution - types of radical reactions - molecular rearrangements oxidation and reduction; Electrophilic reactions-Friedel crafts reaction, Riemer Beckmann rearrangements; nucleophilic reactions-Tiemenn reaction. perkin reaction. benzoin condensation;free radical condensation. reactionhalogenation of alkane, addition of HBr on alkene in presence of peroxide; allylic halogenation - using N-Bromo Succinamide (NBS), thermal halogenation of alkene CH3 - CH = CH2

### CHE-NEIST-2-3924 (Elective)

Physical organic chemistry: 2-0-0-2

Hammett concepts-Quantitative structure activity relationships, linear free energy relationships, Molecular mechanics, Semi-empirical and ab initio molecular theory, Pericyclic Reactions; Substituent Effects; Frontier Molecular Orbitals, HOMO-LUMO Interactions, Aromaticity, Odd and Even Alternant Hydrocarbons, Pericyclic Reactions The Woodward-Hoffman Rules. Free Energy Changes, Transition State Theory, The Eyring Equation, The Mechanistic Significance of Kinetic versus Thermodynamic Control of Organic Reactions, The Hammond Postulate, The Curtin-Hammett Principle; Kinetic Isotope Effects, The Reactivity-Selectivity Principle, Substituent Effects, Absorption of Light by Organic Molecules, Jablonsky Diagrams, Morse Potential Energy Curves, Common Photochemical Reactions. Photocycloadditions.

### CHE-NEIST-2-3925 (Elective) Composite materials: 2-0-0-2

Concept of Composite materials, Various types of composites, Classification based on Matrix Material: Organic Matrix composites, Polymer matrix composites (PMC), Carbon matrix Composites or Carbon-Carbon Composites. Metal matrix composites (MMC), Ceramic matrix composites (CMC); Classification based on reinforcements: Fiber Reinforced Composites, Fiber Reinforced Polymer (FRP) Composites, Laminar Composites, Particulate Composites, Reinforcements/Fibers, Types of fibres, Multiphase fibers, Whiskers and Flakes, Mechanical properties of fibres, Processing of Advanced composites, Metal Matrix Composites: Casting - Solid State diffusion technique, Cladding - Hot isostatic pressing; Ceramic Matrix Composites: Liquid Metal Infiltration - Liquid phase sintering; Carbon - Carbon composites: Knitting, Braiding, Weaving; Polymer matrix composites: Preparation of Moulding compounds and prepregs - hand lay up method - Autoclave method - Filament winding method Compression moulding – Reaction injection moulding, Processing characteristics of nanocomposites, hybrid composites, functionally graded composites, smart and functional composites

### CHE-NEIST-2-3926 (Elective) Carbon allotropes: 1-0-0-1

Synthesis, characterization, structure, properties and applications of: Diamond, Graphite, Amorphous carbon, Charcoals, Fullerene and related compounds, Carbon nanotubes, Graphene.

#### CHE-NEIST-2-3927 (Elective)

Organic spectroscopy applications: 2-0-0-2

Mass spectroscopy, IR spectroscopy, Proton magnetic resonance spectroscopy, Structural assignment by employing NMR techniques, Carbon-13 NMR spectroscopy, Introduction COSY, HSQC, HMBC, NOESY, ROESY, Structural elucidation using 2D-NMR methods

#### CHE-NEIST-2-3928 (Elective)

Surface characterization techniques: 2-0-0-2

XPS, LEED, XAS, SEM, AFM, TEM, NSOM, SPR, SERS, static and dynamic contact angle measurements, Ellipsometry.

#### CHE-NEIST-2-3929 (Elective)

Oil Field Materials and Operations: 2-0-0-2

Oil well drilling, Clay based and oil based drilling fluids, clay structure and chemistry, Drilling Chemicals, Oil well cementing, formation of damage, Oil well simulation, Water injection, polymer flooding, Water shut off, EOR Chemicals, Fracturing Chemicals and Materials, Environmental aspects related to oil filed.

### CHE-NEIST-2-3930 (Elective)

**Ecology and Environmental Chemistry: 2-0-0-2** 

Meaning of ecology and environment, impact of mining on ecology, ecosystem reconstruction, environmental compartments, naturally occurring and anthrpogenic green house gases, global warming potential (GWP), Aerosols, Poly-aromatic Hydrocarbon, chemistry of organic pollutants, pollution from coal power generation, noise pollution, rehabilitation problem and health hazards from mining, impact of mining on air quality, production of solid waste from coal mining (including fly ash, bottom ash and fuel gas), environmental effect due to coal mining, reclamation, deterioration of water quality from acid mine drainage, rare earth elements in ground water, radioactive an heavy metal contamination, disturbance of hydrologic regime due to mining, biological damage due to environmental degradation, ecological compensation.

#### 300 level courses

(Minimum Credit requirement: 04)

CHE-NEIST-3-3901 (Elective)

Computer aided drug design: 2-0-0-2

Definition of a drug molecule and factor affecting their biological activity, definition of chemotherapeutic index, therapeutic index, design of a drug molecule and relationship of functional groups, discovery of new drugs: drug discovery without a lead, lead discovery, random screen, non-random screen, concept of absorption, distribution, metabolism, and excretion (ADME), drug receptors, physicochemical properties, mechanism of a drug action, stereochemistry and drug action, synthetic and natural drugs and their modifications to increase oral bioavailability, chirality and drug action, bioisosterism, drug receptor-interactions, topographical and stereochemical considerations, concept of drug resistance, drug synergism, enzyme inhibition and activation, molecular modeling and insilico drug design, concept of structure-activity relationship(SAR) and quantitative structure-activity relationship (QSAR), Lipinski rule of five, mechanism of action of some important drug molecules.

### CHE-NEIST-3-3902 (Elective) Carbohydrate chemistry: 2-0-0-2

Mono and disaccharides, polysaccharides, Bacterial polysaccharides, starch and cellulose, derivatives of cellulose, Protecting groups, Glycosylation reactions, Dynamics and interactions, carboxy methyl cellulose and gun cotton, structure, Conformational analyses, glycoconjugates, Immunology of carbohydrates.

### CHE-NEIST-3-3903 (Elective) Total Synthesis: 1-0-0-1

Synthesis of complex organic molecules – planning and execution; Concepts of Retrosynthetic Analysis and Total synthesis of Natural products; Retrosynthesis; Disconnection; Synthons; Linear and Convergent Synthesis; Photochemistry in total synthesis; MCRs in total synthesis; Breakthrough synthesis – past and present.

### CHE-NEIST-3-3904 (Elective) Asymmetric Synthesis: 1-0-0-1

Strategies for the preparation of optically pure compounds; Stereoselective, Enantioselective and Diastereoselective reactions; Stochiometric asymmetric synthesis-chiral auxiliaries. Evans Alsdol and modified versions; Catalytic asymmetric synthesis; Asymmetric Dihydroxylation; Asymmmetric Aminohydroxylation; Asymmetric Hydrogenation; Asymmetric allylation, propargylation, and alkylation; Chiral Organocatalysis; Cascade reactions by organocatalysis; Transition Metal based catalysis; Asymmetric amplification and autocatalysis

#### CHE-NEIST-3-3905 (Elective)

Chemistry and biology of Heterocycles: 2-0-0-2

Privileged heterocycles, Electronic properties, reactivity (electrophilicity and nucleophilicity), Synthetic methodologies, Biological properties of Natural products and drug candidates, Biosynthesis, Dimeric compounds and related stereochemistry

### CHE-NEIST-3-3906 (Elective) Fluoro organic chemistry: 2-0-0-2

Importance of fluorine in organic compounds, Strategies to introduce fluorine/ trifluoromethyl group into organic molecules, Preparation of fluorinated reagents, Preparation of fluorinated carbon materials and their uses, Known fluorinated drugs and their mode of action, Overview on CFCs, HCFCs, HFCs, their preparation and applications, Halon susbsitutes, Harmful effects of fluorine and inorganic fluorides

### CHE-NEIST-3-3907 (Elective)

Nutraceuticals: 2-0-0-2

Raw material preparation, and characterization, extraction of valuable biomolecules, characterization of these molecules with stability study, preparation and formulations for functional foods. Characterization and stability study of neutraceuticals, properties and stability packaging of neutraceuticals.

#### CHE-NEIST-3-3908 (Elective) Homogeneous Catalysis: 1-0-0-1

Organometallic Catalysis, Applications in organic synthesis: Olefin Isomerization, C-C Coupling reactions: Heck, Suzuki, Stille and Sonogashira reactions, Alkene and Alkyne Metathesis, C-Heteroatom coupling: Hydroamination, Olefin Oxidation, C-H activation, Oxidation reactions, hydrogenation of Alkenes, Industrial Applications.

#### CHE-NEIST-3-3909 (Elective)

Catalysis for organic synthesis: 1-0-0-1

A background on fine and specialty chemicals in chemical industry; Concept of atom economy; Homogeneous and heterogeneous catalytic reactions: hydrogenation, hydrogenolysis, dehydrogenation, selective oxidation, alkylation & acylation, isomerization and C-C bond forming reactions, Enzyme catalysis in organic synthesis; Reaction mechanisms

### CHE-NEIST-3-3910 (Elective) Functional Ceramics: 1-0-0-1

Advanced Electronic Ceramics, high temperature ceramic super conductors, Dielectric ceramics, microwave ceramics, low k materials, SOFC materials, solidionic conductors, phosphor materials, Impedance analysis, varistors, sensors, ceramic magnets, thermal shock resistance and super plastic ceramics.

### CHE-NEIST-3-3911 (Elective) Porous structures: 2-0-0-2

Definitions, Micro-Porous and Mesoporous Solids, Structural Chemistry of Zeolite Framework Types, MOFs, COFs, Synthesis, Structure Determination, Role of the Structure-directing Agents, The Chemistry of Microporous Framework Solids, Adsorption and Diffusion, Catalytic Applications, hydrogen storage, separation, CO2 sequestration, sensors.

### CHE-NEIST-3-3912 (Elective) Alternate energy materials: 2-0-0-2

Energy scenario, Non-renewable and renewable energy sources; description of renewable sources and their importance. Technologies for biomass energy conversion, Solar energy, Wind Turbines, Geothermal Technologies; Applications; Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.

### CHE-NEIST-3-3913 (Elective) Natural gas to liquid fuels: 2-0-0-2

Generation processes; SMR; POx; ATR; DMR and Tri reforming, Syngas conversion processes; FT Synthesis, LTFT, HTFT, Low Pressure versus high pressure FT, Syncrude up gradation by hydrocracking, methanol synthesis, chemistry of the processes; catalysts, development in reactors; tubular; multitubular; fixed bed; fluidized bed; FFB; CFB, SBCR, variables affecting SCBR, Commercial Processes; MTO; UOP/Hydro MTO; Exxon Mobil MTO; Lurgi MTP, DME Synthesis, status and prospects of DME production; Challenges for DME commercialization, commercialization activities of GTL plants, SSPD, SMDS, AGC- 21 and Gasel Processes

### CHE-NEIST-3-3914 (Elective) Block copolymers: 2-0-0-2

Chain and controlled block copolymerization, monomer reactivity ratios, Copolymer compositions, molecular architecture, blends, grafts, melts, self assembly and phase separation, phase diagram, range of applicability of copolymerization equation; types of copolymerization; Block copolymers with controlled molecular weight, Living Polymerization, block copolymer synthesis, characterization techniques, block copolymers for biomedical and industrial applications, Amphiphilic block copolymer micelles, Block copolymer thin films.

### CHE-NEIST-3-3915 (Elective) Conducting polymers: 1-0-0-1

Synthesis and characterization, electrical transport properties, theory of conductivity, doping, electrochromic properties, Classification and types of organic conductors, Structure and properties of conducting charge-transfer salts, Conducting polymers based on organometallic compounds, Applications of conducting polymers, EMI shielding, supercapacitors, sensors

#### CHE-NEIST-3-3916 (Elective)

Polymers and Colloidal Solutions: 2-0-0-2

Intermolecular forces and potentials, Overview of Statistical physics, DLVO theory, charged colloids, Poisson Boltzmann theory, Debye radius, Bjerrum length, electrophoresis, zeta potential, diffusion, Hydrodynamic interactions. Brief overview of Phase transitions in hard sphere colloids, Random walk, self avoiding random walk, flexible polymers, persistence length, Excluded volume interactions, Polymer solutions in the dilute limit/semi-dilute limit, Entropy of mixing, theta temperature, rubber elasticity, Polyelectrolytes, polymer at surfaces: Brushes, polymer dynamics.

### CHE-NEIST-3-3917 (Elective) Biodegradable polymers: 2-0-0-2

Polymers from biomass, microbial production, synthetic polymers, structure and properties, Biodegradation mechanism, measurement techniques, processing techniques, sterilization and storage, global standards, market potential, applications.

# CHE-NEIST-3-3918 (Elective) Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2

Controlled or Living Radical Polymerization, TEMPO-mediated polymerization and atom Transfer radical Polymerization (ATRP), Kinetics of ATRP, Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide mediated polymerization (NMP), Ring opening Metathesis polymerization (ROMP), living ROP, Macromolecular architectures using controlled living polymerizations

#### CHE-NEIST-3-3919 (Elective)

X-Ray Diffraction and Structure of Solids: 2-0-0-2

Introduction to X-ray crystallography, Crystal growth, evaluation and mounting, Symmetry and space group determination, Background theory for data collection, Data collection using four-circle diffractometers, Area detectors, Crystal lattices, Structure factors, Crystal symmetry, Structure solutions, Structure refinement, An introduction to maximum entropy, Least squares fitting of parameters, Practical aspects of structure refinement, Crystallographic Database, Structure solution from Powder Diffraction Data

### CHE-NEIST-3-3920 (Elective) NMR spectroscopy: 2-0-0-2

Quantum Mechanics of NMR, Multinuclear NMR spectroscopy, Periodic table of NMR, Heteronuclear double resonance experiments, Magnetization transfer and signal enhancement, NMR of diamagnetic and paramagnetic compounds, Multidimensional NMR: 2D NMR, 1H-1H correlations, Heteronuclear Correlation Spectroscopy, 2D Exchange (EXSY), 2D NOESY, ROESY, DOSY Structure elucidation of small molecules, NMR of macromolecules, Multidimensional NMR Spectra, NMR Spectroscopy of Solids, 2D experiments in solids, semi rigid systems: HR MAS, Magnetic Resonance Imaging: In Vivo NMR, Imaging, MRI, functional MRI, NMR imaging of materials.

### CHE-NEIST-3-3921 (Elective) Natural products and drug discovery: 2-0-0-2

Natural products: Importance, lead, clinical trials in drug discovery research, Case studies of marketed natural product drugs, Synthetic Biology and Genetic engineering in the production of natural product, A brief overview of drug discovery approach, Cause of diseases, Target identification, Target validation, Modeling, Synthesis and SAR, Drug Delivery, Clinical Trials, Etiology, pathogenesis, prevention, drug targets and chemotherapy, drug resistance and remedies of tropical infectious diseases, Etiology and remedies of diseases developed through metabolic disorders.

### CHE-NEIST-3-3922 (Elective) Environmental Nanotechnology: 2-0-0-2

Application of nanotechnology to environmental issues, nano-geochemistry, nano-mineralogy, use of nano clusters as catalyst, fullerene, cleaning up organic chemicals polluting ground water using nanotechnology, cleaning up oil spills, cleaning Volatile Organic Compounds (VOCs) from air, potential environmental benefits, use of nano materials for radioactive waste clean- up in water, nano pollution, toxicological impacts of nano -materials, potential health hazard posed by exposure to nano materials.

# CHE-NEIST-3-3923 (Elective) Coal and Biomass Conversion Technologies: 2-0-0-2

Origin of coal and biomass, resources, classification and characteristics, application of remote sensing, thermo-chemical conversion, direct combustion, incineration, pyrolysis, gasification, liquefaction, economics of thermo-chemical conversion, biological conversion, biodegradation and biodegradability of substrate, biochemistry and process parameters of bio-methanation, chemical kinetics and mathematical modeling of bio-methanation process, economics of bio-methanation plant with their environmental and social impacts, bioconversion of substrates into alcohol: methanol and ethanol production, organic acids, solvents, amino acids, antibiotics, chemical conversion, hydrolysis & hydrogenation; solvent extraction of hydrocarbons, solvolysis of wood, bio-crude and biodiesel, chemicals from coal and biomass, power generation, utilization of gasifier for electricity generation, operation of spark ignition and compression ignition engine with wood gas, methanol, ethanol and biogas, coal/biomass integrated gasification/combined cycles systems, sustainable co-firing of biomass with coal, biomass productivity, energy plantation and power programme.

#### 400 level courses

PHY-NEIST-4-0001 (Core)

Project Proposal writing & Presentation: 0-0-4-2

PHY-NEIST-4-0002 (Core)

Review Article Writing & Presentation: 0-0-4-2

PHY-NEIST-4-0003 (Core)

CSIR-800 Societal Programme: 0-0-8-4