

**INDIAN INSTITUTE OF TECHNOLOGY ROORKEE****NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry**Subject Code:** CYC-501      **Course Title:** Quantum Chemistry, Symmetry and Group Theory**L-T-P:** 3-1-0**Credits:** 4**Subject Area:** PCC

**Course Outlines:** Mathematical formulations, postulates, different quantum mechanical models, orbitals, multi-electron systems, term symbols, approximation methods, valence bond and molecular orbital theories, Hückel-molecular orbital approach, mathematical treatments of hybridized orbitals, semi-empirical and ab initio methods. Concept of groups, symmetry operations and matrix representations, molecular point groups, reducible and irreducible representations, great orthogonality theorem, Applications of group theory: linear combination of molecular orbitals, infrared and Raman activity, electronic transitions.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-509

**Course Title:** Coordination Chemistry

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Application of group theory for construction of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes; calculation of d orbital energies in the complexes; interpretation of electronic spectra of coordination complexes using Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral complexes, ligand field parameters; effect of triplet state stability in phosphorescent complexes; origin of magnetism other than unpaired electron spin, molecular magnetism - diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects, orbital angular moment, spin crossover phenomenon, spin admixed states, single molecular magnets.

**INDIAN INSTITUTE OF TECHNOLOGY ROORKEE****NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry**Subject Code:** CYC-502**Course Title:** Advanced Organometallic Chemistry**L-T-P:** 3-0-0**Credits:** 3**Subject Area:** PCC

**Course Outlines:** 18 electron rule and its application, bonding models for  $\pi$ -acceptor ligands, physical evidences and consequences of  $\pi$ -bonding. Main group organometallics. Mechanism of ligand substitution, oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands,  $\beta$ -hydrogen elimination,  $\alpha$ -abstraction or  $\alpha$ -elimination and  $\gamma$ - and  $\delta$ -remote C-H functionalization. Metal carbenes and carbynes, their reactions,  $\pi$ -metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cycloheptatrienyls and cyclooctatetraenes; reactions and bonding in ferrocene; fluxionality in organometallic compounds, Applications of organometallics and clusters in catalysis: Alkene metathesis, Cativa and Monsanto processes, carbonylation/ decarbonylation reactions, Wacker process, cyclooligomerisation of acetylene, Fischer-Tropsch processes, polymer-bound catalysts.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-503

**Course Title:** Thermodynamics, Interfaces and Solids

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Classical thermodynamics, phase equilibria, chemical potential, fugacity, mixing, excess functions; Statistical thermodynamics, microstates, ensembles, partition functions, thermodynamic properties, different statistics; Thermodynamics of surfaces and interfaces, adsorption, adsorption isotherms, macromolecules, electrical phenomenon; Thermodynamics of ionic systems, electrochemical systems, ionic interaction, electrolytes, living systems, polymers; Solids, classification, diffraction, bonding, electronic structure, properties.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-504

**Course Title:** Kinetics and Photochemistry

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Theoretical calculation of energy of activation using potential energy surfaces; Kinetics of unimolecular reactions, chain reactions and branched reactions, Solvent effect, kinetic isotope effect and salt effect on kinetics, fast reaction kinetics; Electron transfer reactions – homogenous and heterogenous systems, theories of electron transfer, Marcus-inverted region; Photochemistry – quantum efficiencies and kinetics of photochemical and photophysical processes, Franck-Condon principle and applications, Quenching of fluorescence, energy transfer processes, radiation chemistry.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-505

**Course Title:** Advanced Analytical Methods

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Advanced analytical techniques, concepts in atomic, nuclear, thermal, electro-analytical, chromatography, mass spectrometry, microanalysis techniques, hyphenated techniques; Data handling, and statistical data treatment.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-506

**Course Title:** Organic Reaction Mechanisms

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Single bond forming reactions involving nucleophilic additions to carbonyls and their theoretical models and enolates. Metal catalyzed C-C bond forming reactions. Carbon-carbon double bond forming reactions involving phosphorus, nitrogen and sulfur reagents, eliminations, reductions and important name reactions. Examples and theories of electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-507

**Course Title:** Structure and Reactivity of Organic Molecules

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Basic concepts of physical organic chemistry, structure and shape of organic molecules, conformational analysis of cyclic systems, physical properties and their reactivity, structure and bonding in organic compounds, ring strain, and stability; Methods for elucidating mechanism for various organic transformations; Catalysis, transition state *vs* ground state.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-510

**Course Title:** Inorganic Chemistry Laboratory

**L-T-P:** 0-0-6

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Semi-micro qualitative analysis with interfering radicals; combination of volumetric and gravimetric analysis; syntheses and characterization of transition metal complexes; estimation of metal content in the synthesized complexes; comparison of the electronic spectra of metal complexes, verification of the spectrochemical series; quantitative estimation of metal ion; estimation of stability constant from Job's plot and continuous ligand variation method; photochemical reaction of inorganic complexes; synthesis of chiral inorganic complexes and inorganic polymer; estimation of metal ion in ore; identification of linkage and geometrical isomerism; basic electrochemical studies.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYC-511

**Course Title:** Organic Chemistry Laboratory

**L-T-P:** 0-0-6

**Credits:** 3

**Subject Area:** PCC

**Course Outlines:** Thin-layer chromatography, oxidation of hydroquinone, reduction of camphor, Diels-Alder reaction, extraction of oils, aldol condensation, Wittig reaction, synthesis of chalcone, *meso*-stilbene dibromide, phenyl acetylene, *p*-nitroaniline and pyridinium dichromate, bromination of acetanilide, Fisher indole synthesis.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-501

**Course Title:** Chemistry of Main Group and Transition Metals

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Chemistry of alkali and alkaline earth metals, their complexation reactions with crown ethers, cryptands, and calixarenes, Syntheses and reactions of hydrides, oxides, halides of boron, carbon, silicon, pnictogens (P, N), chalcogens (S, Se and Te) and halogens, Non-covalent interaction of main group and transition metal complexes, Separation, isolation, electronic and magnetic properties of lanthanides and actinides, lanthanide shift reagents, Inorganic composition of cells, metallobiomolecules in oxygen and iron transport and storage, electron transfer proteins-active site structure and functions of ferredoxin, rubridoxin and cytochromes, metal in medicine and diagnosis, Catenation, one-dimensional conductors: (SN)<sub>x</sub> chains, borazines, boron nitride, cyclic and acyclic phosphazenes, phosphazene polymers, syntheses, and reactions of boranes, carboranes and metallacarboranes.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-518

**Course Title:** Structure, Bonding and Properties of Solids

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Symmetry in the crystalline state with an emphasis on the translational symmetry elements, crystallographic point groups, understanding of space group symmetry and their representations according to the International Tables of Crystallography. Understanding crystal chemistry of close packed structures, structure-composition relationship, descriptive crystal chemistry, non-stoichiometry, defects and order-disorder phenomena in crystalline structures. X-ray diffraction from crystal planes, Bragg's law and sphere of reflection, structure factor and systematic absences, indexing of powder X-ray diffraction patterns. Bonding in solids: Ionic, covalent and metallic, band theory and classification of metals, semiconductors and insulators, Properties of solids: optical, electrical, magnetic, dielectric, magnetoresistive and superconducting.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-520

**Course Title:** Inorganic Rings and Polymers

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Synthesis and applications of Inorganic heterocyclic rings based on P, N, Si, Sn, B, Al and S, Al-N rings and cages, Al-C rings and cages. Inorganic polymers based on homo and heterocatenated inorganic polymers, Anionic and cationic polymerization methods, Synthesis, structure, bonding, unique optical and electronic properties and applications of polyphosphazenes, polysilanes, polysiloxanes, polythiophenes, polythiazyls, synthesis, properties and applications of organometallic polymers.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-608

**Course Title:** Chemical Biology

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Introduction to chemical biology, biological structures and its chemical constituents, spectroscopic tools to rationalize chemical reactions in biosystems, design nonfluorescent and fluorogenic probes and optical biosensor molecules; solid phase peptide synthesis, bioorthogonal reactions, functional group specific ligation techniques, strategies for attachment of synthetic molecules to biomolecules, Staudinger ligation, native chemical ligation, click chemistry, site selective protein modification; Green fluorescence protein (GFP), fluorescein arsenical hairpin (FAsH), SNAPtag, CLIPtag, mutant  $\beta$ -lactamase (BL) tag, halotag, and their selective significant applications; synthetic membranes, vesicles–ion transport, unnatural amino acids and their incorporation, DNA chemistry and its uses, nucleic acid template chemistry, chemistry of morpholino and locked nucleic acid (LNA), siRNA.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-610

**Course Title:** Molecular Modelling and Simulations

**L-T-P:** 2-0-2

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Basis function–hydrogen-like, classification of basis sets, basis set super position error, energy minimization methods. Approximation methods, self-consistent field treatment of polyatomic molecules, closed shell systems –restricted Hartree Fock calculations, open shell systems, The Roothan–Hall equations, Koopman’s theorem, HF limit and electron correlation, introduction to post Hartree-Fock and density functional methods. Molecular mechanics, Montecarlo and molecular dynamics simulations, periodic boundary conditions, radial distribution function, calculation of thermodynamic properties.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-613

**Course Title:** Frontiers in Inorganic Biochemistry

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Homeostatic mechanism of metal ions in cells; metal transport and assembly of metalloproteins; transcription factors, heme synthesis in protein assembly; biocatalysis and electron transfer; iron, molybdenum and tungsten in biology; non-heme iron proteins in cancer research, biocatalysis and industrial applications; metal ions and diseases; protein aggregation and Alzheimer's disease; radiochemistry; manganism; inorganic NO-donors; bioinformatics and postgenomic era; metalloprotein and metal binding motif; de novo protein design, DNA intercalation; biomineralization; structural biology of metalloproteins; gene expression and protein purification; heme protein–cytochrome c vs cytochrome b; protein labelling.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-614

**Course Title:** Asymmetric Synthesis

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Importance of chiral compounds, stereoisomeric discrimination, determination of optical purity by using GC, HPLC and NMR techniques. Absolute configuration determination by using NMR and X-ray crystallographic techniques. Also, enrich the knowledge in resolution, organocatalysis, transition metal catalysis and bio-catalysis, Applications of asymmetric synthesis in industrially relevant molecules, such as L-DOPA, (*S*)-metolachlor, carbapenem and menthol.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-615

**Course Title:** Crystal and Molecular Structure

**L-T-P:** 2-0-2

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Crystal morphology and crystal symmetry, screw axis and glide plane, space groups, systematic absence; X-ray source, Bragg equation, concept of reciprocal lattice, atomic scattering factor, structure factor equation and limiting conditions, intensity and intensity statistics, polarization and Lorentz correction, temperature factor and anisotropic effect, phase problem, small angle X-ray scattering/diffraction; Fourier techniques for electron density calculation in X-ray structure, electron density map, heavy atom method, Patterson function, direct method, normalized structure factor,  $\Sigma_2$  relationship, least square refinement, anomalous dispersion, twinning in crystal, neutron diffraction, neutron sources and detection of neutrons, scattering cross sections.

Introduction to handling of single crystal data and structure solution; generation of crystallographic information file (CIF) and checking of CIF.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-621

**Course Title:** Organic Structure Determination

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Structural determination of organic compounds, spectroscopic methods such as electronic spectroscopy, infrared and Raman spectroscopy, mass spectrometry and NMR spectroscopy, Structure elucidation of organic compounds using spectroscopic methods.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-629

**Course Title:** Advanced topics in Statistical mechanics, and Quantum chemistry

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Statistical mechanics of equilibrium systems and thermodynamics, irreversible thermodynamics, entropy production, statistical mechanics of non-equilibrium systems, Langevin equation, Brownian motion, Fokker-Planck equation; Advanced Quantum mechanics: addition of angular momentum, ladder operators, approximation methods, Hartree-Fock method, introduction to post Hartree-Fock methods, Density-functional theory.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-638

**Course Title:** Reactivity, Structure Determination, Devices and Electronic Structure of Solids

**L-T-P:** 2-0-2

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** General principles and kinetics of solid-state reactions, phase transitions in solids. Powder X-ray diffraction (XRD) pattern simulation and Rietveld refinement for structure determination using powder XRD data. Introduction to powder neutron diffraction (PND) and concepts of magnetic structures. Understanding the structure, components and functioning of electronic and magnetic devices, energy production and storage devices including Josephson junctions, magnetic tunnel junctions, spin-valves, fuel cells, photocatalytic and electrocatalytic cells, solar cells and Li-ion batteries.

**List of computer-based laboratory experiments:**

- (i) Indexing of powder X-ray diffraction (P-XRD) pattern
- (ii) Lattice parameter refinement and chemical doping analysis
- (iii) Simulation of P-XRD pattern and occupancy modelling in doped systems
- (iv) Whole pattern fitting- Le Bail method
- (v) Rietveld refinement of structure using P-XRD data
- (vi) Drawing and visualization of crystal structures and analysis of structural parameters

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-644

**Course Title:** High Energy Density Materials

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Classification, properties, design and evaluation of high energy density materials, Military and civilian applications of high energy density materials; chemical safety of energetic materials, Classification, characterization and properties of explosives, synthetic routes to polynitro compounds, Chemistry of pentazole, energetic tetrazines and azoles based energetic compounds, Heat-resistant explosives, insensitive explosives, melt-cast explosives; energetic metal-organic frameworks (EMOFs) and energetic co-crystals; laser ignition of energetic transition metal complexes; nitrogen-rich energetic polymers and plasticizers, Classifications of propellants, liquid, solid, hybrid and thixotropic propellants, Ingredients of gun and solid rocket propellants, types of pyrotechnic formulations; performance assessment of pyrotechnic formulations; recent trends in pyrotechnics.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-648    **Course Title:** Synthesis and Applications of Tetrapyrroles

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** The pigments of life and their biological importance, IUPAC nomenclature, various synthetic routes to porphyrins and their analogues, synthesis of porphrin dimers and oligomers, metal-organic and covalent-organic frameworks, spectral characterization, applications of porphyrinic materials in the diverse arena.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-703

**Course Title:** Advanced Materials Characterization Techniques

**L-T-P:** 3-1-0

**Credits:** 4

**Subject Area:** PEC

**Course Outlines:** X-ray diffraction – lattices, types of crystal systems, principle of X-ray diffraction, instrumentation, powder diffraction and interpretation of diffraction data; Microscopic techniques – electron microscopy, TEM and SEM working principles and instrumentation, electron diffraction, energy dispersive X-ray analysis and atomic force microscopy; Texture analysis – N<sub>2</sub> sorption, BET and Langmuir isotherms, characterization of porous materials; X-ray photoelectron spectroscopy – working principle and instrumentation, photoelectron intensities, binding energy and chemical shifts; Thermal and magnetic measurements, Optical and Raman spectroscopy.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-902

**Course Title:** Advanced Inorganic Chemistry

**L-T-P:** 3-0-0

**Credits:** 3      **Subject Area:** PEC

**Course Outlines:** Symmetry and associated group theory, spectroscopic term symbols for free ions and metal ions in complexes having different geometries, irreducible representations and their use in interpretation of IR and Raman transitions, advanced organometallic catalysis, water splitting reactions, mechanism, ammonia activation, oxygen atom transfer reactions, ligand design, catalyst design, multimetallic catalysis, latest trends in bioinorganic research, oxygen carrier, anticancer drugs based on platinum and their mode of activity, superoxide dismutases, active site structure, function and mechanism, dioxygen activation by iron and copper enzymes and biomimics.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-904

**Course Title:** Advanced Physical Chemistry

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Quantum mechanics postulates and models, approximation methods, H-like and many-electron systems, Hartree-Fock and post Hartree-Fock methods, Density functional theory, Statistical mechanics of equilibrium systems, thermodynamics and ensemble formalism, irreversible thermodynamics, non-equilibrium statistical mechanics, Time dependent perturbation theory, transition probabilities, Rotational and vibrational spectroscopy of diatomic and polyatomic molecules, Electronic spectroscopy, term symbols, Introduction to non-linear spectroscopy.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-905

**Course Title:** Spectroscopic Methods of Structural Elucidation

**L-T-P:** 3-1-0

**Credits:** 4

**Subject Area:** PEC

**Course Outlines:** Instrumentation, principles, and interpretation of spectral data for various spectroscopic techniques such as IR, Raman, NMR including heteronuclei, Electronic transitions in inorganic complexes, charge transfer transitions, Fluorescence and phosphorescence emissions of metal complexes, delayed fluorescence, fluorescence quantum yield, lifetime, stokes shift, solvatochromism, photochromism, photocatalysis and photodynamic therapy, solid state and paramagnetic NMR, GC, ESI-MS, HR-MS, MALDI-MS and EPR, Determination of isotopic abundance, isotopic distribution pattern, molecular ion, Combinational spectral techniques for the structural elucidation.

# INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYT-501      **Course Title:** Computational Approaches to Catalysis & Reaction Design

**L-T-P:** 2-0-2

**Credits:** 3

**Subject Area:** STAR

**Course Outlines:** Quantum chemistry: Hartree-Fock theory, basis sets, correlated ab initio methods, configuration interaction, MP2 theory, Coupled-cluster methods, multi-reference methods, density functional theory, semi-empirical methods, solids and periodic models. Geometry optimization: features of potential energy surfaces, geometry optimization methods, geometry optimization with quantum chemical methods, transition states and reaction paths. Rate constant and Equilibria, statistical thermodynamics and equilibrium, transition state theory, homogeneous and heterogeneous catalysis, computational-based examples to understand catalysts role in reactions, screening of catalytic reactions to find best catalyst.

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

**NAME OF DEPARTMENT/CENTRE/SCHOOL:** Department of Chemistry

**Subject Code:** CYL-633

**Course Title:** Nanoscale Materials: Properties and Applications

**L-T-P:** 3-0-0

**Credits:** 3

**Subject Area:** PEC

**Course Outlines:** Introduction to nanomaterials, carrier confinement, bonding, quantum size effect; Structure of nanomaterials, surface energy, nucleation and growth; Physicochemical characteristics of nanomaterials, textural, composition analysis, agglomeration, sintering, dispersibility, surface modification, nanofabrication; Synthesis of nanomaterials, reactivity, applications, destructive adsorption, biocides; Toxicology of nanomaterials, toxicity types, case studies.