Curriculum for Master of Science (MSc) in Chemistry (Material Chemistry Specialization)

(Credits are subject to changes)

Semester	Course Code	Course Name	LTP	Credits	Course Instructor
Semester 1	JCL 202	Organic Chemistry	3-0-0	3	Prof. Sarit S. Agasti
	JCL 207	Physical Chemistry	3-0-0	3	Prof. Balasubramanian S
	JCL 223	Basics Mathematics	3-1-0	4	Dr. Abhishek Kumar
	JML 213	Inorganic Chemistry	3-1-0	4	Prof. Eswaramoorthy M.
	JCP 203	Laboratory I- Organic and Inorganic Chemistry Lab	0-1-3	4	Dr. Aruna Sathyamurthy
Semester 2	JCL 301	Reaction Mechanisms	3-1-0	4	Prof. Sridhar Rajaram
	JCL 305	Organic Spectroscopy	3-1-0	4	Prof. Bani Kanta Sarma
	JCL 307	Quantum Chemistry and Chemical Bonding	3-1-0	4	Prof. Ranjani Viswanatha
	JML 306	Advanced Inorganic Chemistry	3-1-0	4	Prof. Tapas Kumar Maji
	JCP 204	Laboratory II- Physical Chemistry Lab	0-1-3	4	Dr. Aruna Satyamurthy
	JCD 210	Research Project I	0-2-3	5	Prof. Bani Kanta Sarma
Semester 3	JCL 311	Molecular Structure and Spectroscopy	3-0-0	3	Prof. Kanishka Biswas
	JCL 206	Energy and Environment	3-0-0	3	Prof. Kanishka Biswas Prof. Premkumar Senguttuvan Prof. Tapas Kumar Maji Prof. Eswaramoorthy M
	JCL 315	Recent Trends in Inorganic and Nanomaterials	3-1-0	4	Dr. Pratap Vishnoi
	JCL 316	Solid State Chemistry	3-0-0	3	Prof. Premkumar Senguttuvan
	JCD 211	Research Project II	0-2-4	6	Prof. Bani Kanta Sarma
Semester 4	JCL 302	Polymer and Supramolecular Chemistry	3-1-0	4	Prof. Subi Jacob George
	JCQ 209	Seminar	1-0-0	1	Dr. Pratap Vishnoi
	JCD 212	Research Project III	0-2-8	10	Prof. Bani Kanta Sarma
	Elective Course			3	
			Total	**80**	

Curriculum for Master of Science (MSc) in Chemistry (Chemical Biology Specialization)

(Credits are subject to changes)

Semester	Course Code	Course Name	LTP	Credits	Course Instructor
Semester 1	JCL 202	Organic Chemistry	3-0-0	3	Prof. Sarit S. Agasti
	JCL 207	Physical Chemistry	3-0-0	3	Prof. Balasubramanian S
	JCL 223	Basics Mathematics	3-1-0	4	Dr. Abhishek Kumar
	JML 213	Inorganic Chemistry	3-1-0	4	Prof. Eswaramoorthy M.
	JCP 203	Laboratory I- Organic and Inorganic Chemistry Lab	0-1-3	4	Dr. Aruna Sathyamurthy
Semester 2	JCL 301	Reaction Mechanisms	3-1-0	4	Prof. Sridhar Rajaram
	JCL 305	Organic Spectroscopy	3-1-0	4	Prof. Bani Kanta Sarma
	JCL 307	Quantum Chemistry and Chemical Bonding	3-1-0	4	Prof. Ranjani Viswanatha
	JML 306	Advanced Inorganic Chemistry	3-1-0	4	Prof. Tapas Kumar Maji
	JCP 204	Laboratory II- Physical Chemistry Lab	0-1-3	4	Dr. Aruna Satyamurthy
	JCD 210	Research Project I	0-2-3	5	Prof. Bani Kanta Sarma
Semester 3	JCL 311	Molecular Structure and Spectroscopy	3-0-0	3	Prof. Kanishka Biswas
	JCL 304	Bioorganic and Medicinal Chemistry	3-1-0	4	Prof. Jayanta Haldar
	JCL 312	Chemical Biology	3-0-0	3	Prof. T. Govindaraju
	JCL 314	Biophysical Chemistry	3-0-0	3	Prof. K. N. Ganesh
	JCD 211	Research Project II	0-2-4	6	Prof. Bani Kanta Sarma
Semester 4	JCL 302	Polymer and Supramolecular Chemistry	3-1-0	4	Prof. Subi Jacob George
	JCQ 209	Seminar	1-0-0	1	Dr. Pratap Vishnoi
	JCD 212	Research Project III	0-2-8	10	Prof. Bani Kanta Sarma
	Elective Course			3	
			Total	**80**	

JCL 202 Organic Chemistry

Chemical bonding and Molecular structure, Electronic effects, Resonance, Aromaticity, Acids and Bases, Weak bonding.

Stereochemistry and conformational analysis: Stereoisomerism definitions, optical isomerism, Resolution of racemic mixture, Enantioselective synthesis, Effect of conformation on reaction.

Basic organic reaction and their mechanism, nucleophilic, electrophilic addition to double bond.

Methods of deducing organic reaction mechanisms, Curtin-Hammett Principle, Organic Reaction Mechanism.

Fundamental reactions of functional groups including amines, carboxylic acids, ethers, alcohols, aldehydes, ketones, and aromatic compounds; functional group transformation: retrosynthetic approach.

Organic Transformations/molecular rearrangements/ isomerizations/ reactions involving additions, eliminations, and substitutions.

Reactive Intermediates: carbocations, carbanions, free radicals, carbenes, nitrenes, arynes, radical ions, diradicals.

Concerted reactions, thermal pericyclic reactions-Organic photochemistry, Forward and backward approach in organic synthesis.

Reference Books:

1. Smith, M. B.; March, J. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th ed. Wiley (2000)

2. Carey F. A.; Sundberg, R. J. Advanced Organic Chemistry, Part A. 5th ed. Harper & Row(1986)

3. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. Organic Chemistry. Oxford University Press, (2000)

4. Corey, E. J. Cheng, X. The Logic of Chemical Synthesis 1989

5. Warren, S. Organic Synthesis: The Disconnection Approach, 1982

JCL 207 Physical Chemistry

Thermodynamics: Specific heats, enthalpy, entropy, free energies, laws, standard energies.

Reaction Equilibria, equilibrium constant, Le Chatelier principle.

Phase equilibrium, phase rule, phase diagrams, Clausius-Clapeyron equation, phase transitions, Landau theory, equations of state.

Solution equilibrium: Nonideal solution, activity, fugacity, partial quantities, Gibbs-Duhem equation.

Intermolecular forces: Van der Waals, hydrogen bonding, electrostatic interaction.

Statistical mechanics of gases and liquids: Theory of ensembles, entropy, partition function, configuration integral, thermodynamic limit, relationship to thermodynamics, molecular partition function.

Electrolytes: Debye-Huckel theory, ion association.

Thermodynamics of electrochemical systems: Galvanic cell, Daniel cell, standard electrode potential, electrical double layer.

Quantum theory for He atom, H2+-ion, H2 molecules.

Reference Books:

1. Physical Chemistry by I.N. Levine

2. Physical Chemistry by Atkins

3. Modern Quantum Chemistry by Szabo and Ostlund

4. Statistical Mechanics by D.A. McQuarrie

5. Physical Chemistry by R.S. Berry, S.A. Rice and J. Ross

6. Quantum Chemistry by I.N. Levine

JCL 223 Basic Mathematics

Multivariable Calculus: Exact and inexact differentials, partial differentiation, Integrals

Vector Calculus: Gradient, Divergence, and curl and their physical significance, Vector products, Line integral, Green's theorem and Stoke's theorem.

Linear Algebra: Matrices, Eigen-value problems, Application of linear algebra tools

Differential Equations: Introduction and notation, Chain rule, Application of differential equations in quantum chemistry and chemical kinetics.

Function of complex variable: Analytical function, Contour integral, The residue theorem,

Evaluation of Definite integral

Introduction of special functions: Fourier series, Dirac Delta function, Fourier transformations,

Gaussian function, Error function, Application of mathematical functions in optical properties of materials

Numerical methods: Interpolation, root finding, curve fitting and error analysis.

Reference books:

1. Mathematical Methods for Physicists by Arfken, Weber and Harris

2. Mathematical Methods in the Physical Sciences by Mary L. Boas

JML 213 Inorganic Chemistry

Periodic properties of the elements and Introduction to Bonding: Arrangements of the elements in group in the periodic table and their general properties, chemistry of main group elements, periodic trends, acid-base behavior, inorganic thermodynamics, oxidation-reduction, symmetry and structure, ionic bond, covalent bond, metallic bond, crystal structures.

Coordination Chemistry: Bonding of transition metal complexes; Valence bond, Crystal Field and MO theory, and their limitations; d-orbital splitting in octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; Effect of CFT on Oh and Td symmetries, Jahn-Teller distortion, molecular orbital in coordination complexes (acceptor and donor), isomerism, magnetism and spectra, reaction mechanism in inorganic compounds/complex, stereochemistry, inner and outer sphere electron transfer mechanism. Electronic Spectra - UV-Vis, charge transfer, colors,

intensities and origin of spectra, term symbols, selection rules for electronic transitions, Orgel and Tanabe-Sugano diagram.

Supramolecular Chemistry: Introduction, noncovalent interactions, concepts of supramolecular synthons, supramolecules and host-guest chemistry, applications in molecular biology and material chemistry.

Bioinorganic Chemistry: Metalloporphyrin (hemoglobin, myoglobin, chlorophyll), metalloenzymes (electron transfer protein), Na/K ion pump, Iron-Sulfur protein, Vitamin B12, Nitrogen fixation. O2 binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocyanin& hemerythrin), their coordination geometry and electronic structure, co-operativity effect, Hill coefficient and Bohr Effect.

Biomineralization: Biomineral types of functions, general principles of biomineralization, chemical control of biomineralization, bio-inspired material chemistry.

Organometallic Chemistry: Valence electron count (16/18 electron rules); structure and bonding in mono and polynuclear metal carbonyls; substituted metal carbonyls and related compounds; synthesis and reactivity of metal carbonyls; vibrational spectra of metal carbonyls; dinitrogen and dioxygen as ligands in organometallic compounds. Reactions of organometallic complexes: Substitution, oxidative addition, reductive elimination, insertion and deinsertion; Catalysis- Hydrogenation, Hydroformylation, Monsanto process, Wacker process, alkene polymerization, Ziegler-Natta polymerization; Metal carbonyls and other transition metal complexes with pi acid ligands.

Reference Books:

1. Inorganic Chemistry: Principles of Structure and Reactivity (Fourth Edition) James E. Huheey, Ellen A. Keiter, R. L. Keiter, (Addison-Wesley Publishing Company)

2. Concepts and Models of Inorganic Chemistry (Third Edition) Bodie Douglas, Darl McDaniel, John Alexander

3. Inorganic Chemistry (Third Edition) D.F. Shriver and P. W. Atkins

4. Advance Inorganic Chemistry F. A. Cotton, G. Wilkinson, (6th or 7th Edition) Wiley, New York.

5. Concise Inorganic Chemistry J. D. Lee, Fifth Edn., Blackwell Science.

JCP 203 Laboratory I- Organic and Inorganic Chemistry Lab

Organic Chemistry Lab

 Synthesis of anthracene maleic anhydride adduct through the Diels Alder reaction by chemical method

 Synthesis of aspirin

 Extraction of caffeine from tea leaves

 Acetylation of ferrocene and its purification by column chromatography

Inorganic Chemistry Lab

 Synthesis and characterization of porous silica materials and to also study the change in the npore size distribution by altering the temperature of hydrothermal treatment.

 Hydrothermal synthesis of ZnS microspheres.

 Synthesis of MoS2 nanoparticles on reduced graphene oxide (RGO) sheets suspended in solution which serves as an advanced catalyst for Hydrogen Evolution Reaction (HER)

 Preparation of the following inorganic complexes:

 Bis (acetyl acetonato) copper (II)

 Tris (acetyl acetonato) iron (III)

 Tris (acetyl acetonato) manganese (III)

 Synthesis and characterization of Mn-Anderson Polyoxometallate complex with ligand TRIS (TBA)3 [(MnMo6O18 {(OCH2)3 CNH2}2]

JCL 301 Reaction Mechanisms

1. Introduction to Reaction Mechanisms

• Curved arrow formalism with examples from current literature.

• Chemical kinetics: Orders, approximations, case-study of Baylis-Hillman reaction Baldwin's Rules, Burgi-Dunitz trajectory, and Felkin-Ahn model.

2. Retrosynthetic Analysis

• Retrosynthetic transforms, role of symmetry, recognizing patterns: Wender's taxol synthesis.

3. Enzymatic Reactions

• Thermodynamic model of catalysis, non-covalent interactions, proximity effects, acidbase catalysis, small molecule mimics of bifunctional catalysis.

• Mechanism of proteases.

• Redox enzymes and their mechanisms.

4. Mechanism of Oxidation Reactions

• Chromium-based oxidants, DMSO-based oxidations, MnO_2 oxidation, oxidation to acids

• C-H oxidations: SeO_2 oxidations, oxaziridines, enolate oxidations.

• Hypervalent iodine oxidations: Periodinane, PIFA and SET

5. Introduction to Organometallic mechanisms

• Basic reaction mechanisms

• Mechanism of Schwartz reaction, Zeigler-Natta polymerization, Brookhart and Grubbs polymerization, hydroamination, enzyme-cyclization, hydrogenations, allylic substitution, and cross-coupling reactions.

6. Peptides and lactams

• Mechanistic ideas for coupling and prevention of racemization, mechanistic rationale for protecting groups, native chemical ligation, solid phase peptide synthesis

• Stereoselective synthesis of β-lactams, stereochemical models

7. Aldol reactions

• Diastereoselective aldol reactions, stereochemical models for selective enolization, soft enolization, Evans aldol, Crimmins aldol, anti-aldol reactions, aldol reactions of α- chiral aldehydes

• Enzymatic aldol reactions

• Organocatalytic aldol reactions

Reference Books:

1. Writing Organic Reaction Mechanisms by A. Miller and P. H. Solomon

2. Logic of Chemical Synthesis by E. J. Corey and X. M. Cheng

3. Introduction to Enzyme and Co-enzyme chemistry by Tim Bugg

4. The Organometallic Chemistry of Transition Metals by Robert H. Crabtree

5. Current literature

305 Organic Spectroscopy

• Electromagnetic spectrum, various spectroscopic methods, and information they provide. Factors that affect the spectral line width and intensity of lines, concept of selection rule.

• Basic principle of UV-Vis spectroscopy, concept of chromophore, orbitals involved UV-Vis spectroscopy, effect of conjugation on HOMO-LUMO gap, Beer's and Lambert's law, Solvent effect in UV-Vis Spectroscopy, Woodward rules, Isosbestic point and its importance, Applications of UV-Vis spectroscopy with examples.

• Basics of Fluorescence spectroscopy, Jablonski diagram, Phosphorescence,

applications of FL with examples.

• Basic principle of CD spectroscopy and its applications, Examples of CD spectra of DNA and various protein secondary structures, differentiating polyproline I and polyproline II helices by CD spectroscopy, DNA and protein (e. g. collagen) melting studies by CD.

• Basics of mass spectrometry, introduction to EI, ESI and MALDI mass spectroscopic methods, concept of molecular ion peak, isotopic pattern, Nitrogen rule, fragmentation pattern, McLafferty rearrangement, fragmentation of peptides by MALDI MS.

• Basics of IR spectroscopy, concept degrees of freedom, determining the number of and bending modes in a molecule, various types of vibrational modes, combination bands, overtones and Fermi resonance, hot bands, various functional group analysis by IR, fingerprint region, effect of conjugation, ring strain and hydrogen bonding on IR bands.

• Basic principle of NMR spectroscopy, resonance condition in NMR, NMR active nuclei, 1H NMR, chemical shift, splitting and integration in 1H NMR, basic idea of 13C and 19F NMR. Study of keto-enol tautomerism, intramolecular hydrogen bonding, H/D exchange using NMR spectroscopy. Variable Temperature (V/T) NMR studies.

Determining molecular formula from elemental analysis, calculating double bond equivalents (DBE) and structure determination of organic molecules using combination of various spectroscopic methods. Introduction to 2D methods such as NOESY, 1H-1H COSY, HMBC, HMQC and TOCSY and their analysis for structure determination of complex organic molecules.

Reference Books:

1. Organic Spectroscopy by William Kemp

2. Spectroscopic Identification of Organic Compounds by Silverstein

JCL 307 Quantum Chemistry and Chemical Bonding

Basics: Energy quantization, wave particle duality, observation and probability, wave functions, Operators, Observables; Quantization Principles; Schrodinger Equations; The Uncertainty Principle; Exactly Solvable Problems: Free Particle, Particle in a box, Harmonic Oscillator, Hydrogen Atom; Time independent Perturbation theory and

Variational theory; Hatree Fock: A bird's eye view, spin orbit, slater determinants, unitary transformation

Study of electronic structure of metals and semiconductors from a quantum mechanical perspective, principle of scanning tunneling microscopy, Density of states in a particle in a box, Vibrational energy levels in an atom/ molecule.

Atomic and Molecular Structures: Pauli principle, classification of atomic spectra,

Atomic Orbitals, Atomic Transitions and Spin; Molecular Orbital Theory: H2-Molecule, Hydrogen Molecule from atomic orbitals – Bonding and non-bonding orbitals,

Hybridization; Electronic Configuration, term symbols, Exploiting Symmetry; Molecular Orbitals of homo and hetero diatomic molecules, poly atomic molecules; Results of HF – Orbital model of atom, nature of Chemical bond, Localization of Molecular orbitals, Molecular Geometry and VSEPR model, Shapes of polyatomic molecules, Conjugation and Resonance; Molecules to Solids: Band Structure, Solid state quantum Chemistry – An Overview.

Reference books:

1. Quantum Chemistry, I. N. Levine, 5th Edition, Allyn and Bacon

2. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A.

Szabo and N. S. Ostlund, Courier Dover Publications.

3. Orbitals in Chemistry: A Modern Guide for Students, Victor Gil, Cambridge

University Press.

4. Quantum Chemistry and Spectroscopy, T. Engel and P. Reid, Pearson Education

Inc.

5. Introductory Nanoscience; Physical and Chemical Concepts, M. Kuno, Garland

Science.

JML 306 Advanced Inorganic Chemistry

Bioinorganic Chemistry: Metalloporphyrin (hemoglobin, myoglobin, chlorophyll), metalloenzymes (electron transfer protein), Na/K ion pump, Iron-Sulfur protein, VitaminB12, Nitrogen fixation.

Organometallic Chemistry: Synthesis and characterization of different types of organometallic compounds, catalytic reactions (hydrogenation, hydroformylation, Ziegler- Natta polymerization etc.)

Metal carbonyls and other transition metal complexes with pi-acid ligands.

Supramolecular Chemistry: Introduction, Noncovalent interactions, Concepts of supramolecular synthons, Supramolecules and supermolecules, Host guest chemistry, applications in molecular biology and materials chemistry, catenation and interpenetration compounds, Metallo-supramolecular aggregation, and gels.

Materials: Zeolites (Silicates, aluminosilicates) and its various applications, Inorganic- organic hybrid materials; metal-organic frameworks and its applications.

Magnetism of the Coordination Compounds: Origin of magnetic properties; Ground Term and Microstates; Russell Saunders Term and Hole equivalency Theorem, Curie equation, Van Vleck equation; Magneto-structural correlations of some compounds.

Reference Books:

1. James E. Huheey, Ellen A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity (Fourth Edition).

2. D. F. Shriver and P. W. Atkins, Inorganic Chemistry (Third Edition).

3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry.

4. I. S. Butler, J. F. Harrod, Benjamin Cummings, Inorganic Chemistry: Principles and applications.

JCP 204 Laboratory II - Physical Chemistry lab

• Powder X-ray diffraction (XRD) study of NaCl, KCl and Cu

• TGA and DSC of $CuSO_4.5H_2O$

• Characterization of charge transfer spectra in $KMnO_4$ and $K_2Cr_2O_7$

• Band gap analysis of a solid semiconductor by diffuse reflectance spectroscopy

• Study of thermoelectric properties of a chalcogenide material

• Study of synthesis, characterizations, and optical properties of a thermochromic material

• Study of gas adsorption behavior of porous solids

• Charge transfer studies of benzene-iodine system

• Study of ferricyanide by cyclic voltammetry

• Study of intercalation cathodes through galvanostatic cycling

• Photocatalysis of organic dyes by TiO_2 nanoparticles

• Raman spectroscopy of graphene and carbon nanotubes

• UV and PL studies of various materials

• Study of magnetism of a ferromagnetic and antiferromagnetic compound

JCD 210, JCD 211 and JCD 212

Research Project I, Research Project II, and Research Project III

Research Projects I, II & III aim at providing a hands-on research experience to students wherein each student is assigned a laboratory to carry out research activities under the guidance of the Supervisor.

Research Project I entails the following:

1. The student is required to submit a short Progress Report on the research conducted at the end of each Research Project.

2. The student is required to present the work before a committee and the evaluation will be done based on the research work performed during the tenure.

3. As part of Research Project I (JCD 210), an additional Term Paper needs to be submitted on the completion of the project. The topic will be suggested by the Research Supervisor and the Term Paper has to be prepared as per the format provided which will be evaluated and graded by the Committee. Detailed format can be collected from the NCU office.

Term Paper (Part of JCD 210):

The Term Paper includes:

(A) Abstract

(B) Introduction

(C) Research Methodology

(D) Conclusion

(E) References

Research Project II entails the following:

1. The student is required to submit a short Progress Report on the research conducted

for Research Project II (JCD 211) at the end of the Research Project.

2. The student is required to present the work before the Committee and the evaluation

will be done based on the research work performed during the tenure.

Research Project III entails the following:

1. The student is required to submit a short Progress Report on the research conducted

for Research Project III (JCD 212) at the end of the Research Project.

2. The student is required to present the work before the Committee and the evaluation

will be done based on the research work performed during the tenure.

JCL 311 Molecular Structure and Spectroscopy

Introduction: Electromagnetic spectrum - Different type of molecular energies - Different type of spectroscopy - Probability of transition and selection rules (derivation from perturbation theory) - Einstein absorption coefficient - Absorption and emission spectra - spectral line width Symmetry and point group: Use in spectroscopy: Symmetry elements and operation - point group -point group of simple chemical compound - character tables and irreducible representation - use in vibrational spectroscopy and determination of hybridization.

Rotational Spectroscopy: Rigid rotor energy level - Selection rule - Intensity of spectral line – Effect of isotopic substitution - Application of spectrum to determine bond strength - Non rigid rotator -polyatomic molecules- Application of rotational spectroscopy.

Infrared and Raman spectroscopy: Part A. Energy of diatomic molecule - Simple harmonic oscillator - Anharmonic oscillator - Diatomic vibrating rotator - Energy level diagram – selection rules of vibration-rotation spectra- Breakdown of the Born-Oppenheimer approximation - Vibrations of polyatomic molecules - influence of rotation on the vibration of poly atomic molecule - Simple examples.

Part B. Classical and quantum theory of Raman effect - Pure rotational Raman spectra – Vibrational Raman spectra - Rule of mutual exclusion - overtone and combination vibration - rotational fine structure - simple structure determination from Raman and infrared spectra.

Electronic spectroscopy: Part A. Electronic structure of atom- Angular and spin moment – coupling of angular momentum - Russel-Saunders coupling - spectroscopic term symbols and selection rule - spectra of alkali metal and hydrogen atom - Franck-Condon principle - electronic-vibrational coupling - d-d transition - charge transfer transition- electronic spectra of molecules- π to π* transition in organic compound.

Part B. The fates of electronically excited states - Fluorescence & phosphorescence -Dissociation & pre-dissociation - Quantum yield - Quenching (Static & Dynamic) - Resonance energy transfer.

Laser spectroscopy: Laser action - Population inversion - Different type lasers - Application (Flash photolysis, Determination of fluorescence lifetime, Femtosecond spectroscopy) Principles of magnetic resonance

Reference Books:

1. Fundamentals of Molecular Spectroscopy by Banwell & McCash

2. Chemical Applications of Group Theory by F. A. Cotton

3. Principles of Fluorescence Spectroscopy by Lakowicz

4. Modern Spectroscopy by Hollas

JCL 304 Bioorganic & Medicinal Chemistry

Fatty acid, Essential Fatty Acids, Lipids classification, Energy-storage lipids (triacylglycerols), Chemical Reactions of Triacylglycerols, Triacylglycerols and diseases, Lipid absorption, Membrane lipids (phospholipids, sphingo glycolipids, and cholesterol), Cell Membrane, Apolipoproteins & Lipoproteins, transport of lipoproteins and diseases, Lipid-lowering drugs, Lipid aggregates (Liposome, Vesicle, micelle), Membrane dynamics, Prokaryotic cell membrane and envelope, Antimicrobial peptide targeting bacterial cell membrane, Transport Across Cell Membranes, drugs targeting transport mechanism and diseases, Emulsification lipids (bile acids) and diseases, Protective-coating lipids (biological waxes), Messenger lipids (steroid hormones and eicosanoids) and diseases-related drugs, Cationic synthetic lipids and use in gene delivery,

membrane (lipids) as drug target (Antifungal drug, Antimicrobial peptides), lipids (liposome) use

as drug delivery system; Carbohydrates, Classification of Carbohydrates, nomenclature of Carbohydrates, Reaction of Monosaccharide, Glucose testing and diabetes and drugs, Disaccharide (Maltose, Cellobiose, Lactose, and Sucrose), Lactose Intolerance, Galactosemia, Artificial Sweeteners, oligosaccharide, polysaccharide (Starch, glycogen, cellulose, chitin, hyaluronic acid and heparin), Glycogen, Glycogenesis, Glycogenolysis, Carbohydrate Digestion, Carbohydrate metabolism, Warburg effect, Targeting Glucose metabolism for Cancer therapy, Glycolipids and Glycoprotein, Cell Recognition, viral entry into host cells (Influenza virus, Herpes Simplex Virus), Bacterial Cell wall, Sugar based drugs and their mechanism (anti-flu, glycopeptides antibiotics, aminoglycosides, anti-cancer drugs like doxorubicin). Nucleic Acids, Primary and Secondary Structure of DNA, Replication of DNA, Transcription: RNA Synthesis, Genetic Code, Translation:

Protein Synthesis, Recombinant DNA and Genetic Engineering, Polymerase Chain Reaction (PCR), Nucleic Acids as drug targets specially for cancer and infectious diseases, DNA-DNA crosslinker, Alkylating agents, DNA intercalator, Topoisomerase inhibitors, Chain cutters, Chain terminators (Acyclovir), Telomere and Telomerase inhibitors, Antisense Therapy, RNA Interference (micro-RNA or Si-RNA therapy)

Reference Books:

1. Biochemistry by D. Voet and J. G. Voet

2. Biochemistry by A. L. Lehninger

3. Medicinal Chemistry T. L. Lemke, D. A. Williams, V. F. Roche and S. W. Zito

4. An Introduction to Medicinal Chemistry by G. L. Patrick

JCL 312 Chemical Biology

Introduction to the structural aspects of biomolecules: Periodic table of life, General Introduction on structure and function of Proteins, nucleic acids, Carbohydrate, Lipids and their building blocks and derived systems and materials; Structural forces in biological macromolecules.

Chemical and biological synthesis: Introduction to synthesis in chemical biology; Biological synthesis of biomolecules- proteins; nucleic acids, oligosaccharides and lipids; Chemical synthesis of peptides, proteins; nucleic acids; oligosaccharides; Chemical synthesis of lipids. Manual to automated synthesis.

Protein engineering and in vitro evolution: General Introduction; Protein chemical ligation: Native Chemical ligation (NCL), Expressed protein ligation (EPL) and recent developments.

Molecular biology as a toolset for chemical biology: Key concepts in molecular biology, tools and techniques in molecular biology, Cloning and identification of genes in DNA, Integrating cloning and expression, Site-directed mutagenesis.

Molecular recognition and binding: Molecular recognition and binding in chemical biology, Theoretical models of binding, Analysing molecular recognition and binding, Biological molecular recognition studies.

Kinetics and catalysis: Catalysis in chemical biology, Steady state kinetic schemes, Pre-steady-state kinetics, Theories of biocatalysis.

Electron transfer Molecular selection and evolution: Chemical biology and the origins of life, Molecular breeding; natural selection acting on self-organisation, Directed evolution of protein function, Directed evolution of nucleic acids, Catalytic antibodies.

Molecular tools for imaging in chemical biology: Design and application of biological sensors.

Small molecular probes: chemical genetics: Chemical probes and tool compounds, diversity oriented synthesis (DOS), Biologically oriented organic synthesis (BIOS), Target discovery and validation: drug discovery, high throughput screening, Small molecule arrays, DNA arrays, protein arrays

Chemical Biology in animal models: Genetic loss of function vs chemical perturbation, In vivo visualization of biological activities, Crossing the blood-brain barrier to engage targets in the brain,

Chemical probes applied in tissues and living organisms.

Special topics: Activity based protein profiling and chemoproteomics; peptide-mimic-peptoid in drug discovery; Posttranslational modifications; Bioconjugation (Bio-orthogonal conjugation chemistries, Labeling tools and methods etc.; Bioinformatics resources to aid chemical biology.

Reference Books:

1. Nucleic Acids in Chemistry and Biology- Blackburn, G. M. and Gait, M.

2. Introduction to Protein Structure. Garland- Branden, C. & Tooze, J.

3. Essentials of Chemical Biology: Structure and Dynamics of Biological Macromolecules-A. D. Miller and J. Tanner.

4. The Organic Chemistry of Drug Design-Silverman, R. B.

5. Chemical Biology: From Small Molecules to System Biology and Drug Design - Stuart L. Schreiber and others.

6. Chemical Biology: Approaches to Drug Discovery and Development to Targeting Disease – Natanya Civjan

7. Posttranslational Modification of Proteins: Expanding Nature's Inventory - Christopher T. Walsh

8. Primary literature, reviews will be used/referred extensively

JCL 315 Recent Trends in Inorganic and Nanomaterials

Extended inorganic solids:

Different types of complex metal oxides; perovskites (ABO3), Ruddlesden–Popper, Dion- Jacobson, Aurivillius, Brownmillerite, hexagonal phases, Spinel and pyrochlore; synthesis, structure, band theory in solids, electronic properties, optical properties, transport properties, phonon properties; electrochemistry of transition metal oxides (LiCoO2, LiNiO2, LiMn2O4) andutility in energy storage.

Antiperovskites and their functional properties.

Metal pnictides; Skutterudites (CoSb3 etc.), Zn4Sb3.

Metal chalcogenides; CuFeS2 (chalcopyrite), AgCuTe, Bi2Se3 and other complex chalcogenides.

Intermetallics; Stoichiometric and non-stoichiometric, half Heusler, full Heusler compounds.

Natrium Superionic CONductor (NaSiCON; e.g. Na1-xZr2SixP3-xO12, 0 < x < 3) compounds and ion conductivity in NaSiCONs.

Topological insulator, topological crystal insulator, Dirac semimetal, Weyl semimetal.

Metal halides:

All-inorganic halide perovskites and hybrid halide perovskites, structural descriptors (tolerance factor and octahedral factor), layered metal halides (α-RuCl3), and their optical and topological quantum behavior. Chemical control over dimensionality (0D, 1D, 2D and 3D). Metal to metal charge transfer in mixed-valence metal halides and ligand to metal charge transfer in metal halides.

2D nanomaterials:

Introduction, structure, classification of 2D materials the compound and the elemental materials.

Rise of various post-graphene elemental 2D materials; borophene, silicene, phosphorene, arsenene, antimonene etc. Binary, ternary and quaternary 2D materials; metal dichalcogenides (MoS2, MoSe2), metal phospho-chalcogenides (Mn2P2S6, AgInP2S3), MXenes. Top-down approach for synthesis of 2D materials; liquid and electrochemical exfoliation Tuning properties of 2D materials by chemical functionalization, self-assembly and heterostructures. Electronic, transport properties, and lattice anharmonicity.

Desirable prerequisites: basic knowledge of crystallography, ligand field theory, geometric aspects of metal complexes.

References:

1. Perovskites Structure–Property Relationships - Richard J. D. Tilley

2. Perovskite Photovoltaics and Optoelectronics: From Fundamentals to Advanced Applications -Tsutomu Miyasaka

3. N. Kumar, et al., Chem. Rev., 2021, 121, 2780–2815

4. X. Li et al., Chem. Rev., 2021, 121, 2230–2291

JCL 206 Energy and Environment

Energy scenario in World and India (demand and consumption), Alternative (Renewable energies).

Fuel cells: Basic principle, history of fuel Cell, different types of fuels and sources, electrochemical cell, different components of fuel cell, cell potential, thermodynamics, and kinetics of fuel cell reactions; different types of fuel cells, various approaches in designing materials as electrodes, applications.

Batteries: History and principles of batteries, Primary and Secondary Batteries, Zn-carbon, alkaline Batteries, Pb-acid, Ni-MH and Li-, Na- and Mg-ion Batteries, Redox flow batteries.

Capacitors and Supercapacitors: history, working principle, different types of capacitors, applications.

CO2 reduction: Chemistry of CO2, advantages and disadvantages, greenhouse effect, sources of CO2, carbon recycling, global warming, photosynthesis, CO2 capture, CO2 sequestration, CO2 reduction using different pathways, chemicals and fuels from CO2, reaction mechanisms, carbon footprint, zero carbon policy, industrial development.

N2 reduction: Fundamentals and Applications

Solar cell: What is solar cell? Definition and history of solar cell, Difference between Module and Solar Cell, Photovoltaic effect, Basic physics of solar cell, Solar cell parameters, Solar radiation and AM 1.5, Working principle – light absorption and band alignment, Charge carriers Generation Rate, Diffusion and Drift current, Construction of Si/Perovskite solar cell, Sensitized Solar Cells.

Water splitting and photocatalysis; electronic structure of semiconductors, hetero-structures, charge separation, band gap evolution, Z-scheme, thermo-chemical water splitting, artificial photo synthesis.

Hydrogen generation and storage; chemical processes, hydrogen storage in porous materials.

Thermoelectrics: Electronic structure modulation, resonance state, band convergence, low thermal conductivity, point defect phonon scattering, nano-structuring, intrinsic factors- bonding asymmetry, soft chemical bonding, effect of lone pair and rattling.

Piezoelectronics: Ferroelectric, dielectrics, piezoforce microscopy.

Reference Books:

1. Electrochemical Supercapacitors: Fundamentals and Applications, B E Conway, (Kluwer,1999.

2. Understanding Batteries, R.M. Dell and D.A.J. Rand (RSC), 2003.

3. Fuel Cell Technology, Sammes Nigel, (Springer), 2006.

4. Renewable Energy, Godfrey Boyle, (Oxford University Press) 2004.

5. Fundamentals of Atmospheric Modeling, Mark Z. Jacobson (RSC Publications, Cambridge),2004.

6. Carbon Dioxide Sequestration and Related Technologies, Ying Wu, (Wiley) 2011.

JCL 316 Solid State Chemistry

Chemical bonding in solids; ionic, covalent, metallic, van der Waals and hydrogen bonded crystals;metallic, non-metallic, semi-metallic and inorganic compounds; porous solids; Organic crystals;quasicrystals; clathrates; non-crystalline or amorphous solids.

Preparative methods: Solid state reaction, Chimie douce/soft chemistry routes; hydro- and solvo-thermal single crystal growth (Melt Growth-Bridgeman, Czochralski, Kyropoulus); Molten salt synthesis;

Electrosynthesis; High pressure synthesis; Arc techniques; combustion synthesis; mechanochemical and sonochemical methods; chemical vapor deposition and atomic layer deposition.

Phase transition: Thermodynamics; critical phenomena; structural changes and mechanism of phase transitions; incommensurate phases; cooperative Jahn-Teller effect; spin-state transitions; Plastic and liquid crystalline states; plastic and liquid crystalline states; non-crystalline state and glass transitions.

Defects and non-stoichiometry: Point defects; Color centers; Dislocations; Extended defects; superstructures; Clusters and aggregates, Non-stoichiometric compounds, Crystallographic shear (CS); block structures;

Lattice dynamics; Diffusion mechanisms, Fick's law, Solid-state Ionics; Kirkendall effect.

Characterization: X-ray, electron and neutron diffraction; Electron microscopy; X-ray absorption spectroscopy; Nuclear magnetic resonance spectroscopy. Electron spectroscopy; scanning tunnelling microscopy.

Electrical properties: Band theory of solids; Metals, semiconductor and insulator; localized electron model; chemical bond approach; Hall effect; Two / Four probe methods and thermal conductivity and Optical band gap; thermoelectric effects; insulators – dielectric, ferroelectric, pyroelectric and piezoelectric properties, multiferroics. Superconductivity: Meissner effect; High Tc superconductors.

Case studies on various metal oxide/sulfide/telluride/nitride compounds.

Magnetic properties: Dia, para, ferro, ferri, and antiferro magnetic types; Magnetic materials and measurements; magnetoresistance.

Reactivity of solids: Solid-state reactions; Solid-solid, solid-liquid and solid-gas reactions. Reactions of organic solids. Heterogenous catalysis

Intergrowth structures and misfit compounds; Intermetallic compounds; Zintl Chemistry.

Reference Books:

1. A. R. West, Solid State Chemistry and Its Applications, 2nd Edition, Wiley 2022.

2. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry, 2nd Edition Cambridge University Press 1997.

3. C. N. Rao and K. Biswas, Essentials of Inorganic Materials Synthesis, Wiley 2015.

JCQ 209 Seminar

This one-credit course provides the opportunity for students to give scientific talks based on any research papers or research topic of their choice in front of a scientific audience. The students can choose the research papers or topics in consultation with their research supervisors and have to submit the abstracts (~ 300 words). The duration of the talk is about 30 minutes in the case of paper seminar (MSc) and 45 minutes in the case of topic seminar (Int PhD) including discussion. The presentations will be evaluated based on the quality of the presentation, chemical aspect, and discussions.

References:

1. Current Literature

JCL 302 Polymer and Supramolecular Chemistry

Part I. Fundamentals of Polymer chemistry and Polymeric materials

Fundamentals **-** Introduction, Molecular weight, Dispersity, stereochemistry,

characterization, Step growth and chain polymerization. Types of polymerization **-** Condensation polymerization, Addition polymerization (cationic, anionic, free radical), Ring opening polymerization, ROMP. Living Polymerization- GTP, ATRP. Copolymerization - random, alternating and block copolymers Functional Polymeric materials **-** Conducting polymers-liquid crystals/Liquid crystalline polymersdendrimers/ dendritic polymers-Hyper branched/star polymers- supramolecular polymers-Biodegradable polymers-block copolymer lithography.

Part II. Supramolecular Chemistry and Materials: Concepts and Basic Principles - Molecular Recognition, Pre-organization, Non-Covalent Interactions, Co-operativity, Multivalency, Analytical Methods in Supramolecular Chemistry

Reference Books:

1. George Odian, “Principles of Polymerization”

2. Jonathan W. Steed, Jerry L. Atwood, “Supramolecular Chemistry”

3. Hans-Jorg Schneider and Anatoly Yatsimirsky, “Principles and Methods in Supramolecular Chemistry”

4. Fred W. Billmeyer, “Textbook of Polymer Science”

5. Hans-Jorg Schneider and Anatoly Yatsimirsky, “Principles and Methods in Supramolecular Chemistry”

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