

# CHEMICAL SCIENCES

*Programme Code:* CHEM04

*Programme Outcome:*

- Foundation in the fundamentals of core chemical sciences fields including those in Analytical, Inorganic, Nuclear and Physical Chemistry.
- Skill development in critical thinking and problem solving applied to scientific problems.
- Development of skills to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
- Development of skill set necessary for starting a research career in chemical sciences and allied areas
- Appreciate the central role of chemistry in DAE programmers and apply these to take up research in key issues such energy, health and medicine

## DETAILED COURSE STRUCTURE

| Sl. No.      | Course Code | Course name  | Credits   | Hours |
|--------------|-------------|--|-----------|-------|
| 1            | ***         | Theory course 1 *                                  | 4         | 60    |
| 2            | ***         | Theory course 2 *                                  | 4         | 60    |
| 3            | CHE700      | Research Methodology & Research Publication Ethics | 4         | 60    |
| 4            | CHE699      | Chemistry Research Project                         | 6         | 180   |
| <b>Total</b> |             |  | <b>18</b> |       |

| Sl. No | Course Code | Course name                                    | Credits | Hours |    |
|--------|-------------|--|---------|-------|----|
|        |             |  |         | L     | T  |
| 1      | CHE601      | Physical Methods in Chemistry II               | 4       | 45    | 15 |
| 2      | CHE602      | Chemical Rate Processes                        | 4       | 45    | 15 |
| 3      | CHE603      | Chemistry of Heterocycles and Natural Products | 4       | 45    | 15 |
| 4      | CHE604      | Coordination Chemistry                         | 4       | 45    | 15 |
| 5      | CHE605      | Chemical Binding                               | 4       | 45    | 15 |
| 6      | CHE606      | Physical Methods in Chemistry I                | 4       | 45    | 15 |
| 7      | CHE651      | Molecular Modelling                            | 4       | 45    | 15 |
| 8      | CHE652      | Solid State Chemistry                          | 4       | 45    | 15 |
| 9      | CHE653      | Classics in Molecules                          | 4       | 45    | 15 |
| 10     | CHE654      | Crystallography                                | 4       | 45    | 15 |
| 11     | CHE655      | Principles of Drug action                      | 4       | 45    | 15 |
| 12     | CHE656      | Advanced Bio-inorganic Chemistry               | 4       | 45    | 15 |
| 13     | CHE657      | Nuclear Magnetic Resonance                     | 4       | 45    | 15 |
| 14     | CHE658      | Advanced Functional Materials                  | 4       | 45    | 15 |
| 15     | CHE659      | Supramolecular Chemistry                       | 4       | 45    | 15 |
| 16     | CHE660      | Chemistry of Nanomaterials                     | 4       | 45    | 15 |
| 17     | CHE661      | Advanced Bio-organic Chemistry                 | 4       | 45    | 15 |
| 18     | CHE662      | Polymer Chemistry                              | 4       | 45    | 15 |
| 19     | CHE663      | Molecular Reaction Dynamics                    | 4       | 45    | 15 |
| 20     | CHE664      | Theory of Molecular Spectroscopy               | 4       | 45    | 15 |

|    |        |   |   |    |    |
|----|--------|---|---|----|----|
| 21 | CHE665 | Advanced Organic Chemistry                      | 4 | 45 | 15 |
| 22 | CHE666 | Catalysis: Reaction Mechanisms and Applications | 4 | 45 | 15 |
| 23 | CHE667 | Advanced Main group Chemistry                   | 4 | 45 | 15 |
| 24 | CHE668 | Advanced Fluorescence Spectroscopy              | 4 | 45 | 15 |
| 25 | CHE669 | Bio macromolecules                              | 4 | 45 | 15 |
| 26 | CHE670 | Advanced Heterocyclic Chemistry                 | 4 | 45 | 15 |
| 27 | CHE671 | Statistical Mechanics                           | 4 | 45 | 15 |

*\*The theory courses 1 and 2 are any two courses from the above list offered from the School of Chemical Sciences (SCS) or courses offered by other schools as recommended by the monitoring committee or standing academic committee to a student.*

**\*\*\* List of theory courses for SCS Ph.D. program**

## CORE COURSES COORDINATOR

| CORE COURSE  |                         |                         |
|--|-------------------------|-------------------------|
| Course name  | Coordinator Name        | Email ID                |
| Research Methodology & Research Publication Ethics | Prof. V. Krishnan       | krishv@niser.ac.in      |
| Physical Methods in Chemistry II                   | Prof. A. Srinivasan     | srini@niser.ac.in       |
| Chemical Rate Processes                            | Prof. Moloy Sarkar      | msarkar@niser.ac.in     |
| Chemistry of Heterocycles and Natural Products     | Prof. C. Gunanathan     | gunanathan@niser.ac.in  |
| Coordination Chemistry                             | Dr. Deepak Samanta      | dsamanta@niser.ac.in    |
| Chemical Binding                                   | Dr. Arindam Ghosh       | aringh@niser.ac.in      |
| Physical Methods in Chemistry I                    | Dr. Bishnu P. Biswal    | bp.biswal@niser.ac.in   |
| Molecular Modelling                                | Prof. U. Lourderaj      | u.lourderaj@niser.ac.in |
| Solid State Chemistry                              | Prof. J. N. Behera      | jnbehera@niser.ac.in    |
| Classics in Molecules                              | Dr. S. Peruncheralathan | peru@niser.ac.in        |
| Crystallography                                    | Prof. J. N. Behera      | jnbehera@niser.ac.in    |
| Principles of Drug action                          | Dr. S. Peruncheralathan | peru@niser.ac.in        |
| Advanced Bio-inorganic Chemistry                   | Dr. N. K. Sharma        | nagendra@niser.ac.in    |
| Nuclear Magnetic Resonance                         | Dr. Arindam Ghosh       | aringh@niser.ac.in      |
| Advanced Functional Materials                      | Prof. Sudip Barman      | sbarman@niser.ac.in     |
| Supramolecular Chemistry                           | Dr. C. S. Purohit       | purohit@niser.ac.in     |
| Chemistry of Nanomaterials                         | Prof. Sudip Barman      | sbarman@niser.ac.in     |
| Advanced Bio-organic Chemistry                     | Dr. N. K. Sharma        | nagendra@niser.ac.in    |
| Polymer Chemistry                                  | Prof. V. Krishnan       | krishv@niser.ac.in      |
| Molecular Reaction Dynamics                        | Prof. U. Lourderaj      | u.lourderaj@niser.ac.in |

|   |                           |                           |
|---|---------------------------|---------------------------|
| Theory of Molecular Spectroscopy                | Prof. U. Lourderaj        | u.lourderaj@niser.ac.in   |
| Advanced Organic Chemistry                      | Dr. Rajkumar Misra        | rajkumarmisra@niser.ac.in |
| Catalysis: Reaction Mechanisms and Applications | Prof. C. Gunanathan       | gunanathan@niser.ac.in    |
| Advanced Main group Chemistry                   | Prof. Sharanappa Nembenna | snebenna@niser.ac.in      |
| Advanced Fluorescence Spectroscopy              | Prof. Moloy Sarkar        | msarkar@niser.ac.in       |
| Bio macromolecules                              | Dr. C. S. Purohit         | purohit@niser.ac.in       |
| Advanced Heterocyclic Chemistry                 | Dr. N. K. Sharma          | nagendra@niser.ac.in      |
| Statistical Mechanics                           | Dr. B. L. Bhargava        | bhargava@niser.ac.in      |

# SYLLABUS FOR CORE COURSES

## CHE700: Research Methodology and Research Publication Ethics

Coordinators: Prof. V. Krishnan  
krishv@niser.ac.in

### Course Details:

- **Introduction:**  
Knowledge, Theory, Paradigms, Perspectives, What is “scientific method”? Underlying assumptions of science and scientific explanation
- **Making sense of Theories**  
Understanding theoretical frameworks, Critical thinking, theory building and testing
- **Literature Review**  
Identifying sources and conducting bibliographic searches. Identifying possible research problems, developing research questions, progressing from area of interest to research topic Ways of reading a text Identifying gaps in literatures Writing literature review- formats Making arguments and spotting fallacies, Analyzing research questions.
- **Research Design (Dept./School specific inputs)**  
Various facets of theoretical, analytical, experimental and evidence based research
- **Data Analysis and data interpretation**  
Tools and techniques of data analysis/interpretation, use of applicable packages
- **Good Research Practices (General and Dept/School specific inputs)**
  - Conduct of research (execution, documentation, checks and honest reporting)
  - Scientific norms and conventions in collaborative research, authorships, ownership and intellectual property
  - Dissemination (choice of forums, mediums, conferences and publications)
  - Responsibilities, Governance and Conflict of Interests
  - Safety Issues (context specific inputs as applicable) – Environmental and Radiation/LASER safety protocols, Occupational, health, radiation, chemical, fire and environmental safety at work place
  - Ethical values – Scientific integrity, truthfulness and accountability, recognizing uncertainty and sources of error. Research misconduct, fabrication of data and plagiarism. Bio-safety and ethics, Human and Animal ethics]
- **Report Writing**
  - Methods of writing/publishing scientific work – overview. Components of a good scientific report – the writing lexicon. Improving writing skills through critical summary writing. Various formats followed by research journals.

▪ **Presentation**

- The diverse formats of ‘science presentation’. Effective presentation of research Publicizing and outreach

**Course Outcomes:**

- To learn good research practices and ethics.
- To learn report writing and presentation.

**References:**

1. Patwardhan B., Desai A., Chourasia A, Nag S., Bhatnagar R. 2020. Guidance Document: Good Academic Research Practices. New Delhi: University Grants Commission.
2. Cook, Claire Kehrwald. (1986) Line by Line: How to Edit Your Own Writing. Mifflin Company, Houghton
3. Mertens, D. M., & Ginsberg, P. E. (2009). The handbook of social research ethics, Thousand Oaks, CA, SAGE Publications, Inc., doi: 10.4135/9781483348971
4. Research Methodology (The Aims, Practices and Ethics of Science) by Peter Pruzan
5. P. Corbetta, Social Research - Theory, Methods and Techniques, 2003, London: Sage
6. Writing Scientific Research Articles: Strategy and Steps by Margaret Cargill, Patrick O'Connor
7. Effective Science Communication, A practical guide to surviving as a scientist by Sam Illingworth and Grant Allen
8. Beins, B.C. (2004). Research methods: A tool for life. Boston: Allyn& Bacon

**CHE601: Physical Methods in Chemistry II (60 Hours)****Coordinators: Prof. A. Srinivasan  
srini@niser.ac.in****Course Details:**

- **Nuclear Magnetic Resonance Spectroscopy**  
Basic principles, Chemical shifts, Spin-spin interactions; Application of  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy including NOE, COSY, NOESY, and other 2D techniques in the structure determination of bioorganic compounds; Application in conformational analysis. Multinuclear ( $^{31}\text{P}$ ,  $^{19}\text{F}$ ,  $^{29}\text{Si}$ ) NMR of various inorganic and organo-metallic compounds. Instrumental aspects; NMR of paramagnetic sample: Contact shifts and pseudo contact shifts, Shift reagents; Pulsed NMR: Modern multiple-pulsed experiments including 2D NMR.
- **Electron Spin Resonance Spectroscopy (ESR)**  
A brief review of theory; Analysis of ESR spectra of systems in liquid phase; Radicals containing single set; Multiple sets of protons; Triplet ground states: Transition metal ions; Fe, Cu, Mo, Cr, Mn,  $\text{VO}_2^+$  containing systems: g values; Symmetry; The practical interpretation of ESR spectra in solid state and solution states; Multiple electron systems; Triplet ground state, Zero-field splitting, Kramers degeneracy, Spectral line-shapes when  $D \ll h\nu$ ,  $D \sim h\nu$  and  $D \gg h\nu$ . EPR of photoexcited triplet states.
- **Double resonance Techniques (ENDOR)**  
ENDOR in liquid solution, ENDOR in powders and non-oriented solids; ENDOR spectra of free-radicals coupled to multiple sets of nuclei with spin; ENDOR of paramagnetic metals and complexes; Biological Applications: Substrate free radical; Flavins and metal free flavin proteins; Photosynthesis; Heme proteins; Iron-Sulfur proteins; Spin labels.
- **Mossbauer Spectroscopy**  
Basic physical concepts; Spectral line shape; Isomer shift; Quadrupole splitting, Magnetic hyperfine interaction; Interpretation of Mossbauer parameters of  $^{57}\text{Fe}$ ,  $^{99}\text{Ru}$ ,  $^{101}\text{Ru}$ ,  $^{195}\text{Pt}$ ,  $^{193}\text{Ir}$ , and  $^{110}\text{Sn}$ ; Some special applications: Solid state reactions; Thermal decomposition, Ligand exchange, Electron transfer, Isomerism, Surface studies and biological applications.

**Course Outcomes:**

- To learn instrument techniques such as NMR and EPR.
- To interpret the data obtained from these techniques.
- To understand various aspects involved in NMR, EPR, ENDOR and Mossbauer.
- To find out the radical nature of the materials.

**References:**

1. NMR Spectroscopy: Basic principles, Concepts and Applications in Chemistry, H. Gunther, 2nd Edn. John Wiley & Sons, 1995.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York, 5th Edn., 1991.
3. Basic  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectroscopy, M. Balci, Elsevier Science, 2005.
4. Electron paramagnetic Resonance: Elementary Theory and practical applications, J. A. Weil, J. R. Bolton and J. E. Wertz, Wiley Interscience, New York, 1994.
5. Physical Methods in Chemistry, R. S. Drago, 2nd Edn., Saunders, 1992.

6. Mossbauer Spectroscopy: An Introduction for Inorganic Chemists and Geochemists, Mcgraw Hill, UK, 1973.
7. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman & Hall, 1971.
8. Electron Spin Resonance: Elementary Theory and Practical Applications, J. E. Wertz and J. R. Bolton, Mcgraw Hill, 1984.

## CHE602: Chemical Rate Processes (60 Hours)

Coordinators: Prof. Moloy Sarkar  
msarkar@niser.ac.in

### Course Details:

- **Kinetic Measurements**

General features of fast reactions; Study of fast reactions by flow techniques, Relaxation methods (T-Jump, P-Jump, ultrasonic, pulse radiolysis, NMR); Flash photolysis; Salt and solvent effects on reactions in solutions.

- **Chain Reactions**

Features of chain reactions; Thermal and photochemical reactions (hydrogen–bromine reaction, decomposition of aldehydes and ketones).

- **Kinetics of oscillatory reactions**

Introduction to oscillatory reactions; Belousov- Zhabotinsky and Field-Koros-Noyes models.

- **Rate Theory**

Concept of potential energy surfaces, Transition state theory including its statistical mechanical treatment, Phenomenological theories of unimolecular reactions (Lindemann, Hinshelwood), Statistical mechanical theories of unimolecular reactions (RRKM).

- **Chemical Dynamics**

Collision theory and Reaction Dynamics, Reaction Cross section and rate constant, Brief idea of Molecular Beam Scattering, Dynamics in condensed phase.

- **Femtochemistry**

Concepts and perspectives; Applications to studies of dynamics and control of chemical reactions. [6]

### Course Outcomes:

- Students can learn varieties of chemical reactions and the time scale of those reactions.
- Describes different spectroscopy and analytical techniques to study chemical kinetics.
- Introduces enzyme kinetics.
- It is a useful course for chemistry and biology students to learn about chemical and biological reactions

### Reference:

1. Basic Chemical Kinetics, H. Eyring, S. H. Lin and S. M. Lin, John Wiley & Sons, New York, 1980.
2. The World of Physical Chemistry, K. J. Laidler, Oxford University press, 1993.

## **CHE603: Chemistry of Heterocycles and Natural Products (45L+15T)**

**Coordinators: Prof. C. Gunanathan**  
**gunanathan@niser.ac.in**

### ***Course Details:***

- **Chemistry of Heterocycles**

Introduction and application of Heterocycles; Nomenclature of aromatic and non-aromatic Heterocycles; Synthesis and reactivity of 5&6-membered aromatic Heterocycles with One or Two hetero atoms.

- **Chemistry of Natural Products**

Introduction and application of Carbohydrates; Steroids, Terpenoids, Fatty Lipids, Prostaglandins and alkaloids; Total synthesis of selected natural products.

### ***Course Outcomes:***

- Understanding nomenclature, structure and reactivity of aromatic and non-aromatic heterocycles
- Understanding the classification, structure and synthesis of biomolecules
- Understanding the design and application of various organic reactions for the synthesis of natural products.

### **References:**

1. J. A. Joule, K. Mills, "Heterocyclic Chemistry" 5th Edn., Blackwell, 2010.
2. T. Eicher, S. Hauptmann, "The Chemistry of Heterocycles" 2nd Edn., Wiley-VCH, 2003.
3. R. J. Simmonds, "Chemistry of Biomolecules: An Introduction" RSC, 1992.
4. I. L. Finar, "Organic Chemistry" Vol. II, ELBS, 1990.
5. S. V. Bhat, B.A. Nagasampagi, M. Sivakumar, "Chemistry of Natural Products" Springer, 2005.
6. E. J. Corey, X.-M. Cheng, "The Logic of Chemical Synthesis" Wiley-Interscience, 1995.
7. T. Hudlicky, J. W. Reed, "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley-VCH, 2007.

## CHE604: Coordination Chemistry (45L+15T)

Coordinators: Dr. Deepak Samanta  
dsamanta@niser.ac.in

### Course Details:

#### ▪ Theories of bonding

CFT including Jahn–Teller Effects of ligand field, Spectrochemical series, Enthalpies of hydration, Spinel structures. Shortcomings of CFT. MO theory of coordination complexes. Electronic Spectra of complexes including Orgel diagrams and Tanabe Sugano diagrams.

#### ▪ Magnetism

Introduction to Magnetism. Origin of diamagnetism. Paramagnetism: Van Vleck formula and its approximated forms, Curie law. Magnetic susceptibility, Orbital quenching and spin-only moment; Magnetic exchange interactions in coordination compounds: Ferrimagnetism and Antiferromagnetism; Bulk magnetic properties and ferromagnetism; Molecule-based magnetic materials: Organic magnets and single molecule magnets.

#### ▪ Mechanisms of reactions of transition metal complexes

Substitution (Kinetic effects: labile vs inert) and electron-transfer reactions (Outer-sphere, Self-exchange; Inner-sphere).

#### ▪ Bioinorganic Chemistry

Basic principles (why specific metal ions are present in certain proteins/enzymes): Heme proteins, types, structure and function (including mechanism of function): Hemoglobin, myoglobin, Cytochrome C, Cytochrome p450, Catalases, peroxidases. non-Heme proteins: Hemerythrin, Ribonucleotide reductase, Methanol monooxygenase (a) Iron-Sulfur proteins: Rubredoxin, Ferredoxin; (b) DNA / RNA: Ribozymes.

### Course Outcomes:

- Importance of Crystal Field Theory and Molecular Orbital Theory with various inorganic complexes.
- Learn the concept of magnetism and also to know about single molecular magnet
- Understanding the inner and outer sphere reaction mechanisms.
- Role of metal ions in bioinorganic chemistry
- Understand the basic concepts of supramolecular chemistry

### References:

1. Advanced inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M. Bochmann, Wiley Interscience, 2001.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 1999.
3. Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, 1995.
4. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
5. Bioinorganic Chemistry; Inorganic Elements in the Chemistry of Life. Kaim, B. Schwederski Wiley, 1994.

6. Biological Inorganic Chemistry: Structure and Reactivity Harry B. Gray, E. I. Stiefel, J. S. Valentine, I. Bertini University Science Book; 2006.
7. Reaction Mechanism of Inorganic and Organometallic Systems, R. B. Jordan, 2nd Edn., Oxford University press, 1991.
8. Bioinorganic Chemistry, A. K. Das, Allied Books, Kolkata, 2004.
9. Molecular Symmetry and Group Theory: A programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.
10. Mechanism of Inorganic Reactions, F. Basolo and R. G. Pearson, 2nd Edn. Wiley, 1967.
11. Inorganic Reaction Mechanisms, M. L. Tobe and J. Burgess, 1st Edn., Wesley Longmans Ltd. 1999.
12. Inorganic Chemistry- Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. Medhi, Pearson Education, 2007.

## CHE605: Chemical Binding (45L+15T)

Coordinators: Dr. Arindam Ghosh  
aringh@niser.ac.in

### Course Details:

#### ▪ Introduction

Review of basic principles of quantum mechanics, Atomic structure, Variation and perturbation methods.

#### ▪ Electronic structure of diatomic molecules

Born–Oppenheimer approximation, H<sub>2</sub><sup>+</sup> ion, Molecular orbitals of ground state and excited states of H<sub>2</sub><sup>+</sup> (LCAO-MO), Homo and heteronuclear diatomic molecules, Electronic term symbols, Valence Bond Theory of diatomic molecules, Comparison of VB and MO theories. Term symbols for diatomic molecules.

#### ▪ Self-consistent Field methods

Hartree–Fock theory of atoms and molecules, Post-Hartree–Fock theories, Configuration interaction wave functions.

#### ▪ Electronic structure of polyatomic molecules

SCF-MO treatment of closed shell systems and applications to molecules (H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>); Potential energy surface and equilibrium geometry, Molecular vibrational frequencies. Brief introduction to density functional theory. ]

Virial theorem and chemical bonding. The Hellman–Feynman theorem.

Semi-empirical and molecular mechanics treatment of molecules, Huckel molecular orbital theory for conjugated organic molecules and its applications to Ethylene, Butadiene, Benzene; Delocalization energy and stability.

### Course Outcomes:

- Understand the quantum mechanics of molecules
- Construct molecular orbitals for polyatomic molecules
- Apply symmetry and molecular orbital theory to derive molecular terms
- Understand the theory Hartree-Fock (HF), DFT, and semi-empirical methods

### References:

1. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, Dover, 1996.
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press, 3rd Edn., 1997.
3. Quantum Chemistry, I. N. Levine, 5thEdn., Pearson Education, 2000.

## CHE606: Physical Methods in Chemistry I (45L+15T)

Coordinators: Dr. Bishnu P. Biswal  
bp.biswal@niser.ac.in

### Course Details:

- **General Introduction to Spectroscopy**

Electromagnetic radiation and its interaction with atoms and molecules. Holistic view of spectroscopy.

- **Ultraviolet Spectroscopy**

Electronic Transition; Definitions of related terms and designation of UV-absorption band; Studies of conjugated and extended conjugated systems; Woodward-Fieser rules; Analytical use of UV-spectroscopy.

- **Infrared and Raman Spectroscopy**

Molecular Vibrations, Instrumentation of IR and Raman spectroscopic techniques; Interpretation of Infrared and Raman spectra, Identification of functional groups, Hydrogen bonding, Complexity of IR spectra, Utility of IR spectroscopy in structural elucidation. Raman spectroscopy in material science; SERS. [

### Fluorescence Spectroscopy

Phenomena of fluorescence; Photochemical laws; General characteristics; Quantum yield and its measurements; Radiation less transitions; Spin states and their interconversion; Kasha's rule and solvent effect; Spin orbit coupling; Energy transfer processes; Donor acceptor complexes, Excimers and Exiplexes. Fluorescence quenching (static and dynamic); Stern Volmer analysis; Timescale of molecular processes in solution. Steady-state and time resolved fluorescence. Fluorescence anisotropy; Biochemical fluorophores; New fluorescence technologies: Multiphoton Excitation, Fluorescence correlation Spectroscopy, Single molecule detection.

- **Photoelectron Spectroscopy**

Experimental methods, Ionisation processes and Koopmans theorem; Photoelectron spectra and their interpretation and applications.

- **Mass Spectrometry**

Basic concepts; Instrumentation, Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules; Isotope effects.

### Course Outcomes:

- Understand the basics of absorption and fluorescence spectroscopy.
- Theoretical prediction of absorption maximum of some organic molecules.
- Identifying and distinguishing various type of electronic transition using solvent perturbation techniques.
- Understanding the concept of micro polarity and the importance of this parameter in spectroscopy
- Understanding some important photoprocesses such as electron transfer and energy transfer and their applications in energy related applications.
- Applications of fluorescence spectroscopy in detecting various analytes (Sensing applications)

**References:**

1. Modern Spectroscopy J. M. Hollas. Wiley, 2004.
2. Physical Methods in Chemistry, R. S. Drago, 2nd Edn., Saunders, 1992.
3. Essentials of Photochemistry, A. Gilbert and J. Baggot, Blackwell Scientific Publications, 1992.
4. Fundamentals of Photochemistry, K. K. Rohatgi Mukherjee, Wiley Eastern Ltd., 1978.
5. Molecular Fluorescence, Bernard Valeur, Wiley-VCH, 2002.
6. Principles of Molecular Photochemistry: An Introduction, P. Walsh, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
7. Principles of Fluorescence Spectroscopy. Joseph R. Lakowicz, 3rd Edn., Springer, 2006.
8. Interpretation of Mass Spectra, F. W. McLafferty, 1980.
9. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York, 5th Ed., 1991.

## CHE651: Molecular Modeling (45L+15T)

Coordinators: Prof. U. Lourderaj  
u.lourderaj@niser.ac.in

### Course Details:

- **Introduction**  
What is molecular modeling? Computable quantities.
- **Concept of Potential Energy Surface**  
Stationary points, Born–Oppenheimer approximation, Geometry optimization, Normal modes of vibration.
- **Molecular Mechanics**  
Basic principles, properties that can be calculated, Strengths and weaknesses.
- **Quantum Mechanics**  
Hartree–Fock–Self-Consistent-Field theory, Post-Hartree–Fock (Electron correlation) methods, Density functional theory, Semi-empirical methods.
- **Chemical Dynamics**  
Unimolecular and Bimolecular reactions, Reaction path and transition states, Classical trajectories, Direct dynamics, Quantum dynamics.
- **Simulations of Molecular Ensembles**  
Properties as ensemble and time averages, Molecular dynamics simulations, Monte Carlo simulations.
- **Modeling Lab**  
Hands-on experience for using different simulations methods and algorithms pertaining to the course.

### Course Outcomes:

- Construct potential energy surfaces and forcefields for molecules
- Perform HF, DFT, and semi-empirical calculations on molecules
- Perform chemical dynamics simulations for simple reactions
- Apply molecular dynamics and Monte-Carlo simulations on large sized molecules

### References:

1. C. J. Cramer, Essentials of Computational Chemistry, Wiley, 2004.
2. I. N. Levine, Quantum Chemistry, Prentice-Hall of India, 2006.
3. P. W. Atkins, Molecular Quantum Mechanics, Oxford, 2008.
4. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford, 1987.
5. R. Leach, Molecular Modelling, Prentice Hall, 2001.
6. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2007.

**CHE652: Solid State Chemistry (45L+15T)****Coordinators: Prof. J. N. Behera**  
**[jnbehera@niser.ac.in](mailto:jnbehera@niser.ac.in)****Course Details:****Crystal Chemistry**

A brief introduction to crystallography, Lattices, unit cells, symmetry, point groups, space groups. packing: CCp, HCp, voids, radius ratio rules. Bonding in crystals: ionic, covalent, metallic, van der Waals, hydrogen bonds. Description of crystal structures: metallic & non metallic structures, AB, AB<sub>2</sub>, AB<sub>3</sub> (ReO<sub>3</sub>), spinels, pyrochlores, perovskites, K<sub>2</sub>NiF<sub>4</sub> etc. Pauling's rules for ionic crystal structures and the concept of bond valence. Methods of crystallography: powder, single crystals, X-ray, neutron and electron diffraction.

**Defects in Solids**

Origin of defects in crystals; perfect and imperfect crystals; thermodynamics of defect formation; types of defects: point defects, line defects, plane defects; Schottky and Frenkel defects; thermodynamics of Schottky and Frenkel defect formation; crystal classifications; Madelung constant and lattice energy.

**Electronic Structure of Solids**

Atoms to molecules to crystals; Orbitals to bonds to bands; Electronic structure of crystalline solids, Elementary band theory: Metals, Insulators and Semi-conductors., Solid state ionics; Intrinsic and Extrinsic semiconductors. Transport property measurement techniques: Electrical resistivity, Thermopower, Hall effect Magnetism of d vs. f block metal compounds.

**Critical Phenomena**

Phase transitions (Order-disorder, Martensite-austenite, Spinodal decompositions); Liquid crystals; Structure–property relations (magnetic, electrical, superconductivity, optical and thermal); Powder synthesis by conventional and modern chemical methods; Reactivity of solids; Decomposition mechanisms; Powder processing (sintering and diffusion processes), Tailoring of solids, Special methods for single crystal growth and thin film depositions.

**Synthesis of Solids**

Chemistry behind synthesis; Intercalations; Synthesis/preparation of single crystals; Hydrothermal methods. Framework Solids; Zeolites, Aluminophosphates and related structures; Metal-organic framework compounds – their structures and properties.

**Superconductivity**

Superconductivity: General aspects of superconductivity; Effects of magnetic field; BCS Theory; Oxide Superconductors.

**Course Outcomes:**

- Describe the principles concerning solid state structures
- Describe specific crystal structures by applying basic crystallographic concepts
- Describe the experimental use of the diffraction phenomenon
- Use powder diffraction data for characterising cubic substances
- Analyse thermograms and phase diagrams in known systems

**References:**

1. Solid State Chemistry and Its Applications, A. R. West, John Wiley, 1987.
2. Solid State Chemistry, L. Smart and E. Moore, Chapman and Hall, 1992.
3. Principles of the Solid State, H. V. Keer, Wiley Eastern Ltd., 1994.
4. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan, Cambridge University Press, 2008.
5. The Electronic Structure and Chemistry of Solids, P. A. Cox, Oxford University Press, 2005.
6. Ionic crystal, Lattice defect and Non-stoichiometry, N. N. Greenwood, Chemical Pub. Co., New York, 1970.
7. An Introduction to Crystal Chemistry, R. C. Evans, Cambridge University Press, 1964.

## CHE653: Classics in Molecules (45L+15T)

Coordinators: Dr. S. Peruncheralathan  
peru@niser.ac.in

### Course Details:

- Introduction, Understanding structural diagrams of organic molecules, Protein and Three-dimensional protein Structure, Nucleic acids, Synthesis, Biosynthesis.
- Urea & acetic acid, glucose, aspirin, Camphor, Terpeneol, Tropinone, Haemin, Quinine, Morphine, Steroids & the pill, Strychnine, penicillin, Longifolene, prostaglandins & Leukotrienes, Vitamin B12, Erythronolide B & Erythromycin a, Monensin, Avermectin, Amphotericin B, Ginkgolide B
- Cyclosporin, FK506 & Rapamycin, Calicheamicin  $\gamma$ 1, Palytoxin, Taxol, Mevacor, Zaragozic acids & Cp Molecules, Brevetoxin B, Ecteinascidin 743, Epothilones, Resiniferatoxin, Vancomycin, Thiostrepton.
- Modern Drug Discovery and Developments, Designed Small Drug Molecules for Mental illness, Viral infections, gastrointestinal Disorders, Heart diseases and Sexual Dysfunction.
- DNA Technologies, Vaccines, antibodies, Diabetes, anemia, Rheumatoid arthritis, Breast Cancer, Biologics.

### Course Outcomes:

- To learn discovery of organic molecules and their impact on the world such as Urea, Glucose, & Penicillin
- To understand the basic organic chemistry for learning chemical biology
- To learn the small organic molecules that interaction with molecular targets
- To find the nature of drugs and their function in biological changes

### References:

1. K. C. Nicolaou and Tamsyn Montagnon, "Molecules that Changed the World", Wiley-VCH, 2008.
2. E. J. Corey, LászlóKürti and Barbara Czak' o, "Molecules and Medicine", Wiley-VCH, 2008.
3. J. Block and J. M. Beale "Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry", 11th Edn., Lippincott Williams & Wilkins, 2003.

## CHE654: Crystallography (45L+15T)

Coordinators: Prof. J. N. Behera  
jnbehera@niser.ac.in

### Course Details:

- Origin of X-rays, Filters, Monochromators, Sealed tube, Rotating anode synchrotron radiation, Safety considerations.
- Crystals and their properties- Concepts of symmetry, Direct and reciprocal lattice, Planes, Indices, Unit cell, Bragg's law in direct and reciprocal lattices, Primitive and non-primitive lattices, Point and space groups, Equivalent positions, Systematic absences and space group determination, Occupancy factors.
- Theory of structure factors, Argand diagram and its use, Lorentz and polarization corrections, Absorption corrections, Absolute scale of intensities; Unit cell determination, Data collection parameters, Data reduction, Phase problem and structure solution by Patterson and direct methods.
- Structure refinement techniques, Presentation and interpretation of structural data, Examination of CIF file and critical evaluation of a structure, Errors and pitfalls, Twinning and disorder, Renninger effect, Extinctions, Anomalous scattering and its use.

### Course Outcomes:

- Define concepts such as lattice, point and space groups
- Be familiar with Bragg's Law and explain its relation to crystal structure
- Identify and describe different diffraction methods
- Interpret and assign X-ray and electron diffraction patterns
- Use crystallographic data for a validated phase analysis

### References:

1. X-Ray Structure Determination: A Practical Guide, G. H. Stout and L. H. Jensen, Springer, 1992.
2. Fundamentals of Crystallography, C. Giacovazzo, Oxford University Press.
3. X-Ray Analysis and the Structure of Organic Molecules, Jack. D. Dunitz, Wiley, 1996.
4. Crystal Structure Determination, Werner Massa, Springer.
5. Structural Inorganic Chemistry, A. F. Wells, Clarendon Press, 1986

## CHE655: Principles of Drug Action (45L+15T)

Coordinators: Dr. S. Peruncheralathan  
peru@niser.ac.in

### Course Details:

#### ▪ Pharmacodynamic Phase in Drug Action

Introduction to pharmacodynamics, Biochemical basis of drug action, Drug absorption, distribution and bioavailability, Passive diffusion, Active transport mechanisms, Excretion and reabsorption of drugs.

#### ▪ Pharmacokinetic Phase in Drug Action

General classification of pharmacokinetic properties, Pharmacokinetic models, Intravascular administration, Extravascular administration, Estimation of pharmacokinetic parameters, The use of pharmacokinetics in drug design.

#### ▪ Novel Therapeutic agents

Synaptic Pharmacology: Cholinergic and adrenergic systems, CnS agents: Antipsychotics, Antidepressants, CVS Agents: Antihypertensives, Antineoplastic agents, Analgesic and anti-inflammatory agents, Drug toxicity.

#### ▪ Concepts in Drug Metabolism

Basic principles and factors affecting drug metabolism, Secondary pharmacological implications of metabolism, Phase i metabolic reactions, Phase ii metabolic reactions, Drug metabolism and drug design, Prodrugs, Metabolic pathways for common drugs.

#### ▪ Stability of Drugs and Medicines

Oxidation and stability of free-radicals, Prevention of oxidative deterioration, Autoxidation of fats and oils, Examples of drugs susceptible to aging and hydrolysis, Other mechanisms of degradation.

#### ▪ Drug Development

Clinical trials (phase-i to phase-iv), Formulation development, Quality control aspects (methods of assay).

### Course Outcomes:

- To learn pharmacokinetics and pharmacology
- To understand absorption, distribution, metabolism, and excretion of drugs
- To learn various stages of drug discovery process such as clinical trials
- To find the modern drug discovery and development processes including the identification of molecular targets, High throughput screening (HTS)

### References:

1. Thomas G. (2003) Fundamentals of Medicinal Chemistry, Wiley.
  2. Cairns D. (2008) Essentials of Pharmaceutical Chemistry (3rd Edn.), Pharmaceutical Press.
  3. Block J. and Beale J. M. (2003) Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry (11th Edn.), Lippincott Williams & Wilkins.
  4. Rang H. P., Dale M. M. et al. (2007) Rang & Dale's pharmacology (6th Edn.), Churchill Livingstone.
  5. Hardman J. G., Limbird L. E. et al. (2001) Goodman & Gilman's. The pharmacological Basis of Therapeutics, Mcgraw-Hill Professional.
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## CHE656: Advanced Bio-inorganic Chemistry (45L+15T)

Coordinators: Dr. N. K. Sharma  
nagendra@niser.ac.in

### Course Details:

- Principles of bioinorganic Chemistry (Justification of why a certain protein/enzyme contains a particular metal ion).
- **Heme Proteins**  
Types, function and mechanisms, Myoglobin, Hemoglobin, Cytochrome C, Cytochrome-P450, Peroxidases (Horseradish peroxidase, Chloroperoxidase), Catalase, Cytochrome C Oxidase, Synthetic porphyrins of biological relevance.
- **Iron–Sulfur Proteins**  
Types, function and mechanisms, Rubredoxin, Ferredoxins, Aconitase.
- **Non-Heme Proteins**  
Types, function and mechanisms, Mononuclear Systems (Catechol-1,2-Dioxygenases, Transferrin, Ferritin, Superoxide Dismutase, Isopenicillin N Synthase) Dinuclear Systems (Hemerythrin, Ribonucleotide Reductase, Methane Monooxygenase, Purple acid phosphatases).
- **Copper Proteins (Type i, ii, and iii)**  
Types, function and mechanisms, Blue Copper proteins; Hemocyanin, Tyrosinase, Catechol Oxidase; Superoxide Dismutase; ascorbate Oxidase, Laccase; galactose oxidase
- **Molybdenum Enzymes**  
Types, function and mechanisms, Oxo-Transfer Enzymes, Xanthine Oxidase, Nitrogenase.
- **Manganese**  
Photosynthesis (Photosystem I and Photosystem II); function and mechanisms.
- **Zinc Enzymes**  
Function and mechanisms, Hydrolytic Enzymes (Carbonic anhydrase; Carboxypeptidase A; Alkaline phosphatase).
- **DNA/RNA**  
Types, function and mechanisms, DNA nicking enzymes; DNA polymerase; Ribozymes.
- **Environmental & Medicinal Aspects**  
Acid-rain; Green-house Effect etc. Radiopharmaceuticals; Photodynamic Therapy; Anti-Tumor Drugs (cis-platin, Carboplatins; Bleomycins); Ion-pumps.

**Course Outcomes:**

- Apply the basic principles in inorganic and general chemistry to interdisciplinary topics in the field of bio-inorganic chemistry.
- Describe the main roles of metal ions in biological processes and identify the chemical properties that are required for particular functions.
- Describe the role of metal ions in enzymes involved in acid-base reactions.
- Describe the role of metal ions that are involved in electron-transfer reactions in biological systems.
- Describe how oxygen is transported in different species and identify the metal centers involved in this task.
- Describe the different metal-activation sites in enzymes that are involved in the activation of oxygen.
- Identify the main toxicological mechanisms of metals and the biological defenses against the toxic effects.
- List some medical applications of inorganic compounds.
- Oral and written communication using the specific language of bioinorganic chemistry.

**References:**

1. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
2. Bioinorganic Chemistry; Inorganic Elements in the Chemistry of Life; W. Kaim, B. Schwederski Wiley, 1994.
3. Biological Inorganic Chemistry: Structure and Reactivity; Harry B. Gray, Edward I. Stiefel, Joan Selverstone Valentine, Ivano Bertini, University Science Book; 2006.
4. Specific Review Articles to be collected from the Internet

## CHE657: Nuclear Magnetic Resonance (45L+15T)

Coordinators: Dr. Arindam Ghosh  
arinhg@niser.ac.in

### Course Details:

- **Classical NMR Spectroscopy**  
Nuclear magnetism, Bloch equations, Chemical shift, Linewidth, Scalar coupling.
- **Theoretical description of NMR spectroscopy**  
Expectation value of magnetic moment, Density matrix, Pulses and rotation operator, Chemical shift and coupling Hamiltonians, Concept of coherence, One pulse experiment.
- **Product Operator Formalism**  
Operator spaces, Basis operators, Free precession, Pulses, Single and multiple quantum coherences, Application of pOF to study spin echo and standard polarization transfer protocols like in EpT.
- **Practical Aspects of NMR Spectroscopy**  
Tuning, Matching, Shimming, Temperature calibration, Spectrum referencing, Sampling theorem, Quadrature detection, Fourier transformation, Zero filling, apodization, Phasing, Signal to noise ratio, Spin decoupling, Pulse field gradients, Water suppression, One dimensional experiment.
- **Two-dimensional NMR Experiments**  
Two-dimensional spectroscopy, Coherence transfer, COSY, double quantum filtered COSY, TOCSY, NOESY, HSQC, HMQC, Sensitivity enhanced HSQC.
- **Higher-dimensional NMR Experiment**  
Need for higher dimensional experiments, HNCA, HN(CO)CA, introduction to the new trend of fast multidimensional experiments: GFT, spatially spatial encoding.

### Course Outcomes:

- Theoretical understanding of the basic working principle of NMR spectroscopy.
- Building in-depth knowledge of the routinely performed experimental steps.
- Analysis of pulse sequence of few key one- and two-dimensional experiments to understand how certain spectra are generated.
- Understanding the theory behind common problems encountered during routine operation of an NMR spectrometer.

### References:

1. Protein NMR Spectroscopy, 2nd Edn., John Cavanagh, W. J. Fairbrother, A. G. Palmer.
2. M. Rance and N. J. Skelton, Elsevier Academic Press, 2007.
3. Spin dynamics 2nd Edn., Malcolm H. Levitt, John Wiley and Sons Ltd., 2008.

## CHE658: Advanced Functional Materials (45L+15T)

Coordinators: Prof. Sudip Barman  
sbarman@niser.ac.in

### Course Details:

- **Introduction to Materials in Modern Technology**  
Materials as an enabling element of technological progress; Functions that materials perform; The properties - structure - processing connection.
- **Semiconductor Materials**  
Intrinsic semiconductors, Band Structure of Semi- conductors, Impurity Semiconductors, ii-v and ii-vi compounds, Hall effect, SC devices. Charge carrier dynamics in semiconductor nanomaterials.
- **Dielectric Materials**  
Dielectric constant and polarizability, Insulating materials, Ferroelectrics, piezoelectrics, Measurement of Dielectric properties, Applications.
- **Nanosized Magnetic Materials**  
Basic concepts of magnetism; Types of magnetic behavior, Magnetic domains, Soft and hard magnets, Classification of magnetic nanomaterials, Ferrofluids, Single-domain particles, Physical Properties of Magnetic nanostructures, Nano magnetism for biological applications.
- **Polymer Materials and Nano-composites**  
Classification of Polymers, Structure–Property Correlation, Molecular weights, Conduction in polymers, Natural composites, Incorporation of nanomaterials into polymer Media, Organic polymer nanocomposites, Metal and Ceramic composites, Clay nanocomposite Materials, Polymer–Clay nanocomposites, Polymer/graphite nanocomposites, Polymer Composites with Carbon nanotubes.
- **Amorphous and Crystalline Porous Materials**  
Crystalline vs. Amorphous Solids, Glass Formation, Structural models of amorphous materials, Properties of meta glasses, Evolution and Development of porous materials, Chemistry of microporous materials, Mesoporous materials, Semiconductor nanoparticles in Zeolites, Polymers and carbon materials in Zeolites. [10]

### Course Outcomes:

- Introduction to materials in modern technology
- Learn about semiconductor and dielectric materials.
- Exploring the role of magnetic materials in inter-disciplinary sciences
- Use of polymer materials and nano-composites in chemistry and day-today life.

### References:

1. Fundamentals of nanotechnology, Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta, CRC Press, Taylor & Francis Group, 2009.
  2. Optical Properties and Spectroscopy of Nanomaterials, Jin Z. Zhang, World Scientific Publishing Co. Pte. Ltd, 2008.
  3. Science of Engineering Materials and Carbon nanotubes, C. M. Srivastava, C. Srinivasan, New Age International Publishers.
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4. Optimization of Polymer Nanocomposite Properties, Edited by Vikas Mittal, WILEY-VCH VerlagsgmbH&Co. KGaA, Weinheim, 2009.
5. Polymer Nanocomposites Handbook; Rakesh K. Gupta, Elliot Kennel, Kwang-Jea Kim, CRC Press, Taylor & Francis Group, 2008.

**CHE659: Supramolecular Chemistry (45L+15T)****Coordinators: Dr. C. S. Purohit**  
purohit@niser.ac.in**Course Details:****▪ Introduction**

Understanding of Supramolecular Chemistry (Multidisciplinary nature, Complementarities in biology); Selectivity; Supramolecular interactions; Chelate and Macrocyclic Effects; Characterizing Supramolecular Systems; Structural, Kinetic and Thermodynamic.

**▪ Molecular Self-assembly**

Non-Covalent Interactions: Electrostatic, Hydrogen Bonding,  $\pi$ - $\pi$  Stacking, Dispersion and Induction Forces, Hydrophobic or Solvophobic Effects,  $\pi$ -Electron Donor Acceptor Systems, Catenanes and Rotaxanes, Transition Metal Directed assemblies; Molecular Macrocycles and Boxes: Locked and Unlocked Molecular Boxes, Ladders and grids, Cages; Hydrogen Bond Directed assemblies: Rosettes and Ribbons, peptide nanotubes; Self-Replicating Molecular Systems.

**▪ Synthesis of Macrocycles**

High Dilution Technique; Coordination Template Effects; Cation Binding and Demetallation; Porphyrins; Corrins; Crown Ethers; Cryptands; Spherands; Sepulchrates; Siderophores; Calixarenes.

**▪ Molecular Sensors of Ions and Molecules**

Anions, Cations and Neutral molecules receptor design principles: Recognition by electrostatic and hydrogen bonding, Lewis acidic Hosts interactions etc.; Introduction to fluorescence probing techniques and applications: Fluorescent molecular sensors of ions and Molecules, Logic gate etc.; Expanded porphyrins, Amide functionalized metallo compounds, Cyclophanes, Electrostatics and hydrophobicity, Hydrogen bond receptors, Chiral recognition; Hydrophobic effect: Recognition in water; Solvent effect; Cyclodextrins; Calixarenes; Metallo receptor for nucleic acid and bases; Boronic acid receptors for Sugars.

**Course Outcomes:**

- Learn various noncovalent interactions.
- Design the synthesis of novel macrocycles
- Understand the stabilization of anions, cations and neutral substrates.
- To evaluate the binding and stability constants

**References:**

1. D. J. Cram and J. M. Cram, Container Molecules and their Guest, Monographs in Supramolecular Chemistry, Ed. J. F. Stoddart, The Royal Society of Chemistry, Cambridge, 1994.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim, 1995.
3. Comprehensive Supramolecular Chemistry, Edn. J. L. Atwood, J. E. D. Davies, D. D. Macnicol, F. Vogtle, Volumes 2 and 3, Elsevier Science, Oxford, 1996.
4. Supramolecular Chemistry of Anions, Edn. A. Bianchi, K. Bowman-James, E. Garcia- Espana, John Wiley and Sons, New York, 1997.
5. Supramolecular Chemistry, P. D. Beer, P. A. Gale and D. K. Smith, Oxford University Press, 1999.
6. A Practical Guide to Supramolecular Chemistry, Peter J. Cragg, John Wiley & Sons Ltd, England, 2005.

## CHE660: Chemistry of Nanomaterials (45L+15T)

Coordinators: Prof. Sudip Barman  
sbarman@niser.ac.in

### Course Details:

#### ▪ Introduction

Nano and nature, Fascination and Motivation of nanoparticle research, Bottom-up and Top-down approaches.

#### ▪ Zero and One-Dimensional Nanostructures

Introduction, aqueous and non- aqueous sol-gel chemistry, Surfactant-assisted synthesis, Solvent-controlled nanoparticle assembly: Introduction, Oriented attachment and Mesocrystals, Superlattices, Core-Shell nanoparticles: introduction, Types of systems, Characterization, properties.

#### ▪ Carbon Nanomaterials

Fullerenes and their derivatives, Carbon nanotubes: Structure and properties, nano crystalline diamond.

#### ▪ Self-assembled Monolayers

Introduction, Monolayers on gold, Growth process, Phase transitions, Patterning monolayers, Mixed monolayers structure, Electrochemistry and applications of self-assembled monolayers of thiols.

#### ▪ Nano and Micro-emulsion

Surface active agents, Micellization, Mechanism of emulsion, Characterization of Microemulsion.

#### ▪ Application of Nanomaterials

Solar energy conversion, Molecular and nano-electronics, Nanocatalysis, Biological applications and other applications.

### Course Outcomes:

- Key concepts of Bottom-up and Top down approaches
- Understanding the mechanism of formation of 0-D, 1-D, 2-D, 3-D nanostructured materials.
- Understanding the structure-property relationship of carbon nanomaterials and self-assembled monolayers.
- Application of nanomaterials for energy applications and biological applications

### References:

1. Nanoparticles: Synthesis, Stabilization, Passivation, and Functionalization, Edited by R. Nagarajan, T. Alan Hatton, ACS Symposium Series 996.
2. Metal Oxide Nanoparticles in Organic Solvents, Markus Niederberger and Nicola Pinna, Springer-Verlag London Limited, 2009.
3. Fundamental of Nanotechnology, Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta, CRC Press, Taylor & Francis Group, 2009.

4. Carbon Nanomaterials, Advanced Materials Series, Edited by YuryGogotsi, Taylor and Francis Group, LLC, 2006.
5. Carbon Nanotubes and Related Structures, Edited by Dirk M. Guldi and Nazario Martin, WILEY– VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.
6. Nano: The Essential, Understanding Nanoscience and Nanotechnology, T. Pradeep, Tata Mcgraw–Hill publishing Company Limited.
7. Applied Surfactants, Thrwat F. Tadros, WiLEY-VCH VerlaggmbH& Co. KGaA, Weinheim, 2006.

## CHE661: Advanced Bio-organic Chemistry (45L+15T)

Coordinators: Dr. N. K. Sharma  
nagendra@niser.ac.in

### Course Details:

#### ▪ Enzymology

Mechanistic studies of enzymatic reactions. Studies of enzyme kinetics for substrate/inhibitors (reversible/irreversible) and their future aspects in drug design. The role of cofactors and hormones in enzymatic reactions. Enzymes as Catalysts in organic chemistry reaction (group Transfer Reactions, Reduction and Oxidation; Monooxygenation; Dioxygenation Substitutions, Addition/Elimination; Carboxylations; Decarboxylation; isomerizations; aldol and Claisen Reactions; and Retro-reactions; Formylations, Hydroxy methylations, and Methylations; rearrangements.

#### ▪ Application of Enzyme Kinetics

Substrate Kinetics; Kinetics of Enzyme inhibition; Substrate inhibition; Non-productive Binding; Competing Substrates; Multi-substrate Systems; Allostereism and Cooperativity.

#### ▪ Biosynthesis of Secondary Metabolites

Polyketide Biosynthesis; Saccharide Biosynthesis; Shikimate pathway (pDF); Shikimate pathway Flavonoids; alkaloid Biosynthesis; Alkaloid Biosynthesis: Tyrosine Derivatives; Terpene Biosynthesis with example-Taxol, Vancomycin, Penicillin and other recent discovered natural products; Design and synthesis of modified secondary metabolites analogues; Isotope labeling (radioactive/non-radioactive) and their application in biosynthetic pathways.

#### ▪ Non-natural Bio-active Molecules

Synthesis and importance of these amino acids ( $\beta$ ,  $\gamma$  &  $\delta$ ), non-ribosomal peptides and nucleotides (PNA, LNA, TNA & other stable analogues).

#### ▪ Introduction of Vital Bio-macromolecule Secondary Structures

g-Quadruplex, i-motif, RNAi (mi-RNA & si-RNA) & Collagen and their application in therapeutics.

### Course Outcomes:

- Introduction of Biomacromolecules, and Enzymology
- Synthesis and application of DNA, RNA and related analogues
- Understanding of biosynthesis of natural products
- Understanding the role biomacromolecules in therapy

### References:

1. Organic Chemistry of Enzyme-Catalyzed Reactions, Revised Edition by Richard Silverman, Academic Press, 2002.
2. Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding ByalanFersht, Publisher: W. H. Freeman; 1998.
3. Evaluation of Enzyme Inhibitors in Drug Discovery: A Guide for Medicinal Chemists and Pharmacologists (Methods of Biochemical Analysis); by Robert A. Copeland, Publisher: Wiley- interscience; 2005.

4. Dewick, Paul M. Medicinal Natural Products: A Biosynthetic Approach. 2nd Edn.. New York, NY: John Wiley & Sons, 2001.
5. Structural Diversity of g-Quadruplex Scaffolds; Stephen Neidle and Shankar Balasubramanian, CRC Press, 2006.
6. Gene Silencing by RNA Interference: Technology and Application, by Muhammad Sohail (Editor), CRC Press, 2004.
7. Modified Nucleosides: in Biochemistry, Biotechnology and Medicine (ed P. Herdewijn), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany.
8. Natural products: The Secondary Metabolites, James R. Hanson, RSC, 2003.

## CHE662: Polymer Chemistry (45L+15T)

Coordinators: Prof. V. Krishnan  
krishv@niser.ac.in

### Course Details:

- Classification of polymers, Nomenclature of polymers, Synthesis of polymers using different methods, viz Chain polymerization, Step polymerization, Ring-opening polymerization etc. Polymerization techniques, viz bulk polymerization, Solution polymerization, Suspension polymerization, Emulsion polymerization etc. [10]
- Polymer characterization, molecular weight-number average, weight average; significance of molecular weight; Methods of characterizing molecular masses, GPC, Viscosity, Mass analysis, End-group analysis, Thermal properties - melting point, Glass transition temperature (T<sub>g</sub>), Factors influencing T<sub>g</sub>, relation between T<sub>g</sub> and molecular weight, Crystallinity in polymers - degree of crystallinity in polymers, Structural regularity and crystallinity. [14]
- Kinetics of polymerization, Free-radical, Cationic and Anionic polymerization and polycondensation. [5]
- Copolymerization, Free-radical and ionic copolymerization and Copolycondensation.
- Stereochemistry of polymerization, Types of stereoisomerism in polymers, Properties of stereoregular polymers, Different methods for the synthesis of stereoregular polymers; Less traditional approaches: aTRp, RaFT, ROMp, Surface functionalization of polymers.
- Biodegradable polymers: Synthesis and challenges.

### Course Outcomes:

- Different types of polymers
- Concepts of polymers
- Applications of polymers
- Challenges involved in making bio-degradable polymers

### References:

1. Odian, G. Principles of Polymerization. 4th Edn. Hoboken, NJ: Wiley-interscience, 2004.
2. Allcock, H. R., Lampe, F. W. in Contemporary Polymer Chemistry; Prentice-Hall: Englewood Cliffs, NJ, 1990.
3. Billmeyer Jr. F. W. Textbook of Polymer Science Wiley-interscience.

## CHE663: Molecular Reaction Dynamics (45L+15T)

Coordinators: Prof. U. Lourderaj  
u.lourderaj@niser.ac.in

### Course Details:

- **Introduction**  
The rate constant - History and current view. What are molecular reaction dynamics? [2]
- **Theoretical methods i**  
Transition State Theory (TST), RRKM Theory.
- **Theoretical Methods ii**  
Rate and cross-section, Classical scattering theory, Quantum scattering theory (reactive and non-reactive), Connection to TST and RRKM.
- **Experimental methods**  
Newton's diagrams, Molecular Beams, State-resolved spectroscopic techniques, Imaging techniques.
- **Applications**  
Photoselective chemistry - photodissociation and photoisomerization dynamics, Dynamics in real time (ps, fs and attosecond regimes), Molecular energy transfer, Control of chemical reactions, Condensed phase dynamics, Dynamics of gas-surface reactions. [15]

### Course Outcomes:

- Apply transition state theory and RRKM theory to compute rate constants
- Understand the theory of classical and quantum scattering phenomena
- Learn, how to follow the dynamics of chemical reactions experimentally and theoretically

### References:

1. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press, NY 2005
2. J. Steinfield, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall Inc., NJ, 1999.

## CHE664: Theory of Molecular Spectroscopy (45L+15T)

Coordinators: Prof. U. Lourderaj  
u.lourderaj@niser.ac.in

### Course Details:

- **Recap**  
Introduction and review of basic quantum mechanics, Molecular symmetry.
- **Rovibronic Hamiltonian - Coordinates and Momenta**  
Euler angles, Axis systems, Rotational and vibrational angular momentum, Normal and internal coordinates, the g matrix, the gF matrix.
- **Rovibronic Wavefunctions**  
Classification of rotational, Vibrational, Rotation-Vibration, and electronic wave functions, Hund's cases.
- **Energy Levels and Interaction**  
Rotation-vibration interactions, Vibronic and rovibronic interactions, Renner-Teller and Jahn-Teller effect, Rydberg states, Spin effects.
- Transition intensities and optical selection rules, Electric – magnetic dipole electric quadrupole transitions, Multiphoton processes and Raman effect.
- **Advanced topics**  
Spectroscopy at high energies, Intramolecular vibrational energy redistribution (IVR), Wave-packet approach to spectroscopy.

### Course Outcomes:

- Separate the molecular motion into translations, rotations, and vibrations components
- Transform between internal and normal mode coordinates
- Understand the rovibronic spectroscopy of molecules
- Understand multiphoton processes and their application in modern spectroscopy

### References:

1. Billmeyer Jr. F. W. Textbook of Polymer Science Wiley-interscience
2. P. R. Bunker and P. Jensen, Molecular Symmetry and Spectroscopy, NRC Research Press, Ottawa.
3. J. D. Graybeal, Molecular Spectroscopy, McGraw-Hill.
4. P. F. Bernath, Spectra of Atoms and Molecules, Oxford University press, NY, 1995.
5. E. B. Wilson, J. C. Decius and P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover, NY, 1955.

## CHE665: Advanced Organic Chemistry (45L+15T)

Coordinators: Dr. Rajkumar Misra  
rajkumarmisra@niser.ac.in

### Course Details:

- Review of basic bonding concepts; Conformational analysis; Stereochemistry; Kinetics and Thermodynamics of Organic Reactions; Reaction Mechanisms and Conformational Effects on Reactivity; Oxidation Reactions; Reductions Reactions; Enolate Chemistry; Metalation Reactions; Key Ring Forming Reactions; Olefin Synthesis; Conjugate Additions; Synthetic analysis and Design; Total Synthesis of natural products; Asymmetric Synthesis; Combinatorial Chemistry. [42]

### Course Outcomes:

- Understanding of important organic transformations with advanced mechanisms.
- Learning the recent advances in organic chemistry
- Enhanced ability to connect the learned topics with current research problem and envisage new research projects.

### References:

1. E. V. Anslyn, D. A. Dougherty, "Modern Physical Organic Chemistry" California University Science Books, 2006.
2. E. L. Eliel, S. H. Wilen, "Stereochemistry of Organic Compounds" Wiley-interscience, 1994.
3. R. Bruckner, "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
4. F. A. Carey, R. J. Sundberg, "Advanced Organic Chemistry Parts A & B: Structure and Mechanisms" 5th Edn., Springer, 2007.
5. B. Smith, J. March "Advanced Organic Chemistry" 6th Edn., Wiley-VCH, 2007.
6. E. J. Corey, X.-M. Cheng, "The Logic of Chemical Synthesis" Wiley-interscience, 1995.
7. T. Hudlicky, J. W. Reed, "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley-VCH, 2007.
8. P. Wyatt, S. Warren, "Organic Synthesis: Strategy and Control" Wiley, 2007.
9. Christmann, S, BraseEds "Asymmetric Synthesis- The Essentials" 2nd Edn., Wiley-VCH, 2008.
10. K. C. Nicolaou, R. Hanks, W. HartwigEds. "Handbook of Combinatorial Chemistry", VCH-Wiley, Weinheim, 2002.

## CHE666: Reaction Mechanisms and Applications (45L+15T)

Coordinators: Prof. C. Gunanathan  
gunanathan@niser.ac.in

### Course Details:

- **Introduction to Catalysis**  
Fundamental concepts.
- **Survey of Ligands**  
Characteristics of the transition-metal in the complexes; Elementary steps.
- **Reaction Mechanisms and Applications**  
Carbonylation, Hydroformylation, Hydrogenation, metathesis reactions, Oxidation reactions, Isomerization reactions, Cross- Coupling reactions, and C–H functionalization reactions.
- Examples of synthetic and industrial applications.

### Course Outcomes:

- Understanding the principles of catalysis.
- Key concepts of various elementary steps which are important in catalytic cycle.
- Understanding the development of various catalysts in many important catalytic reactions.
- Implications and applications of catalysis in industry and academia.

### References:

1. The Organometallic Chemistry of the Transition Metals. R. H. Crabtree, John Wiley & Sons, 2005.
2. Industrial Catalysis. J. Hagen, Wiley-VCH, 2006.
3. Homogeneous Catalysis. P. W. N. M. van Leeuwen, Kluwer Academic Publishers, 2004.
4. Homogeneous Catalysis. S. Bhaduri, D. Mukesh, John Wiley & Sons, 2000.
5. Metal-Catalyzed Cross-Coupling Reactions A. De Meijere, F. Diederich (Eds.), 2004.
6. Catalysts for Fine Chemical Synthesis. S. M. Roberts, G. Poignant, John Wiley & Sons, 2002.
7. Catalysis of Organic Reactions, S.R. Schmidt, CRC press, 2007.

## CHE667: Advanced Main Group Chemistry (45L+15T)

Coordinators: Prof. Sharanappa Nembenna  
snembenna@niser.ac.in

### Course Details:

- **Direct Bonds Between Metal Atoms**  
Mg and Ca compounds with metal-metal bonds (b) Multiple bonded group 13, 14 and 15 elements: Synthesis, reactivity and bonding. [12]
- NHC stabilized low oxidation state main group metal complexes. [4]
- Low Oxidation State Main Group Metal Hydrides
- **NHCs Analogues with Low Valent Group 13 and 14 Elements**  
Synthesis, structure and reactivity studies; (a) Boron (i), Aluminium (i), Gallium (i), Indium (i) and Thallium (i) Heterocycles; (b) Silicon (ii), Germanium (ii), Tin (ii), and Lead (ii) Heterocycles. [8]
- Role of main group compounds in catalysis, organic synthesis and medicinal chemistry
- **Inorganic New Materials**  
Nanomaterials, Polymers and chemical sensors

### Course Outcomes:

- Understanding the structure and bonding aspects of metal-metal single or multiple bond of main group elements
- Soluble main group metal hydrides: synthesis and their reactivity studies.
- Group 13 and Group 14 low valent metallacycles: synthesis and reactivity studies
- Application of Main group compounds in homogeneous catalysis

### References:

1. Inorganic Chemistry-Principles of Structure and Reactivity. 4th Edn. Huheey, J. E.; Keiter, E. A.; and Keiter, R. L. Harper-Collins, NY, 1993.
2. Concepts and Models of Inorganic Chemistry. 3rd Edn. Douglas, B.; McDaniel, D.; and Alexander, J. John Wiley, New York. 1993.
3. Chemistry of the Elements. 2nd Edn. Greenwood, N. N.; and Earnshaw, A. Pergamon, Oxford, 1989.
4. Organometallics: A Concise Introduction, C. Elschenbroich and a. Salzer, 3rd Edn. 1999.
5. Inorganic and Organometallic Polymers. Chandrasekhar, V. Springer-Verlag, Heidelberg, 2005

## CHE668: Advanced Fluorescence Spectroscopy (45L+15T)

Coordinators: Prof. Moloy Sarkar  
msarkar@niser.ac.in

### Course Details:

- **Phenomena of Fluorescence and Instrumentation for Fluorescence Spectroscopy**  
Introduction, Jablonski Diagram, Characteristics of Fluorescence Emission, Fluorescence Lifetimes and Quantum Yields, Spectrofluorometers, Light Sources, Monochromators, Optical Filters, Photomultiplier Tubes, Polarizers.
- **Fluorophores**  
Intrinsic or Natural Fluorophores; Fluorescence Enzyme Cofactors, Extrinsic Fluorophores; Protein-Labeling Reagents, Membrane probes, Red and near-infrared (NIR) Dyes, DNA probes, Chemical sensing probes, Viscosity probes, Green fluorescent proteins, Long-lifetime probes, Quantum dots.
- **Life-Time measurements**  
Time-Domain and Frequency-Domain Measurements, Time-Correlated Single-photon Counting, Principle and instrumentation, Alternative Methods for Time-Resolved Measurements; Streak Cameras, Up conversion Methods, Data analysis. [6]
- **Some important Photo-processes**  
Dynamics of Solvent and Spectral Relaxation: Measurement of Time-Resolved Emission Spectra (TRES), Theory for Time-Dependent Solvent Relaxation, Fluorescence Quenching: Theory, Fractional Accessibility to Quenchers, Applications of Quenching to Proteins; Fluorescence Anisotropy: Origin of the Definitions of Polarization and Anisotropy, Measurement of Fluorescence anisotropies, Causes of Depolarization, Biochemical Applications. Energy Transfer: Theory of Energy Transfer for a Donor acceptor pair, Distance Measurements Using Resonance Energy Transfer (RET), Biochemical applications of RET.
- **Multiphoton Excitation**  
Introduction to Multiphoton Excitation, Two-photon Absorption Spectra, Cross Section for Multiphoton Absorption. [3]
- **Single-molecule Detection (SMD)**  
Detectability of Single Molecules, Instrumentation for SMD, Single-Molecule photophysics, Biochemical applications of SMD. [3]
- **Fluorescence Correlation Spectroscopy (FCS)**  
Principles of Fluorescence Correlation Spectroscopy, Theory of FCS, Examples of FCS Experiments. [3]
- **Fluorescence-Lifetime imaging microscopy (FLim)**  
Early Methods for Fluorescence-Lifetime imaging, Laser Scanning TCSpCFLiM, Lifetime imaging of Cellular Biomolecules.

▪ **Radiative Decay engineering**

Introduction to Radiative Decay Engineering, Review of Metal Effects on Fluorescence Surface Plasmon-Coupled Emission (SPCE), Applications of Metal-Enhanced Fluorescence, Application of SPCE.

**Course Outcomes:**

- Describes basic principles and application of fluorescence spectroscopy.
- To learn, how fluorescence spectroscopy is used for frequency and time domain studies of important chemical process.
- To learn to use fluorescence spectroscopy in biological related molecules.
- It also introduces fluorescence imaging.

**References:**

1. Principles of Fluorescence Spectroscopy, Joseph R. Lakowicz, 3rd Edn., Springer, 2006.
2. Advanced Time-correlated Single Photon Counting Techniques, W. Becker, Springer, 2005.
3. Molecular Fluorescence Principles and Applications, B. Valeur, WILEY-VCH, 2002.
4. Single-Molecule Detection in Solution. Methods and Applications, C. Zander, R. A. Keller, and J. Enderlein, WILEY- VCH, 2001.

## CHE669: Bio macromolecules (45L+15T)

Coordinators: Dr. C. S. Purohit  
purohit@niser.ac.in

### Course Details:

- Buffers (their use in study of biomolecules), pH, pKa of amino acids, D and L amino acid nomenclature. [1]]
- Biophysical techniques to purify and study proteins: Dialysis, Salting out and precipitation by organic solvents, Ion exchange, Gel filtration, Reversed phase, Affinity chromatography, Ultracentrifugation, Gel electrophoresis. [3]
- **Proteins**  
Protein sequencing by chemical and mass & NMR spectroscopic methods, Use of spectroscopic tools in studying biomolecules. Primary (single letter amino acid codes), Ramachandran plot, Secondary structures like helices, parallel- and antiparallel-sheets, Circular Dichroism of secondary structures, Tertiary (motifs and domains: some important motifs like Rossmann fold, helix turn helix, 4 helix bundles, beta barrel), Quaternary structure (Haemoglobin and Myoglobin) and Enzymes.
- **Nucleic acids**  
A, B and Z-DNA structures, Method of replication, Sequencing of nucleic acids (Chemical, dideoxy and fluorescence), Transcription, Translation, Genetic code, Genomes, Genes, overexpression of recombinant proteins, Mutagenesis (random and site directed); Polymerase Chain Reaction (PCR). [9]
- Carbohydrates and glycoproteins, Proteoglycans, Membranes and lipids, Bacterial cell wall synthesis and mechanism of some important antibiotics like Penicillin, Antibiotic resistance.
- **Metabolism**  
Photosynthesis, Calvins cycle, Glycolysis, Krebs cycle, Electron transport, Cofactors.

### Course Outcomes:

- Basic understanding of biomolecules with respect to their structure
- Structure and function relation of biologically important molecules
- In-depth understanding of various biological processes such as DNA replication, protein synthesis

### References:

1. Voet, D; Voet, J. G; Pratt, C. W., Fundamentals of Biochemistry: Life at the Molecular Level, 2nd Edn., 2006
2. Berg J. M, Tymoczko J. L. and Stryer L., Biochemistry, 6th Edn., 2007.
3. Creighton, T. E., Proteins: Structure and Molecular Properties, 2nd Edn., 1993.
4. Lewin B., Genes IX, 2008
5. Branden C and Tooze J., Introduction to Protein Structure, 2nd Edn., 1999.
6. Fersht A., Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding, 1999.

## CHE670: Advanced Heterocyclic Chemistry (45L+15T)

Coordinators: Dr. N. K. Sharma  
nagendra@niser.ac.in

### Course Details:

- Heterocyclic Chemistry; Introduction to heterocycles: Nomenclature, Spectral characteristics, Reactivity and Aromaticity. [2]
- Synthesis and reactivity of three and four membered heterocycles e.g., Aziridine, Azirine, Azetidine, Oxiranes, Thiarines, Oxetenes and Thietanes.
- Synthesis and reactivity of five membered rings with two heteroatoms: Pyrazole, Imidazole, Oxazole, Thiazole, Isothiazole and Benzofusedanalogs; Benzo-fused five membered heterocycles with one heteroatom, e.g., Indole, Benzofuran, Benzothiophene.
- Synthesis and reactivity of benzofused six membered rings with one, two and three heteroatoms: Benzopyrans, Quinolines, Isoquinoline, Quinoxaline, Acridine, Phenoxazine, Phenothiazine, Benzotriazine, Pteridines.
- Synthesis and reactivity of seven and large membered heterocycles: Azepines, Oxepines, Thiepinines; Spiro-heterocycles; Bicyclic compounds containing one or more heteroatoms
- Recent methods of C-H functionalization/activations of heterocyclic derivatives.

### Course Outcomes:

- Introduction of Heterocyclic Chemistry: Nomenclature, spectral characteristics, reactivity and aromaticity of heterocycles (three- and four-membered)
- Synthesis and reactivity of five-membered rings, benzo-fused six-membered rings with one, two and three heteroatoms, seven and large membered
- Recent methods of C–H functionalization/activations of heterocyclic derivatives
- Beneficial to synthesized therapeutic drugs

### References:

1. Carey, F. A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B., Plenum: U.S., 2004
2. Thomas. L. Gilchrist, Heterocyclic Chemistry, (3rd Edn.), 1997.
3. Joules, J.A; Mills, K.; Smith, G.F. Heterocyclic Chemistry, 3rd Edn.
4. Advances in Heterocyclic Chemistry, Book Series Elsevier Edited by Alan Katritzky.
5. Branden C and Tooze J., Introduction to Protein Structure, 2nd Edn., 1999.

## CHE671: Statistical Mechanics (45L+15T)

Coordinators: Dr. B. L. Bhargava  
bhargava@niser.ac.in

### Course Details:

- Basic assumptions, Concept of microscopic and macroscopic states, Ensembles and averages; Calculation of distribution functions in canonical ensemble and the canonical partition function; Relations between the canonical partition function and thermodynamic functions; Calculations in other ensembles like microcanonical and grand canonical ensembles. Calculations of fluctuations and equivalence of ensembles.
- Calculations of partition functions and thermodynamic properties for ideal systems of monatomic and diatomic molecules. Calculations of fluctuations and equivalence of ensembles
- Calculation of heat capacity of solids, Einstein and Debye theories, Study of chemical equilibrium in terms of partition functions.
- **Quantum Statistics**  
Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. Systems of Fermions and Bosons in weak and strong degenerate limits.
- **Classical Statistical Mechanics**  
Partition functions as integrals over phase space coordinates, Systems of interacting particles, imperfect gases, concept of radial distribution functions of liquids and applications to ionic solutions using Debye-Huckel theory.
- **Non-equilibrium Statistical Mechanics**  
Onsager regression hypothesis and fluctuation-dissipation theorem, Calculations of transport coefficients like Diffusion and Conductivity.

### Course Outcomes:

- Understanding the concepts of ensembles, energy partition and probability distribution
- Learning of classical and quantum statistical mechanics
- Application of statistical mechanics to study the thermodynamic properties of simple gases and solids

### References:

1. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon, Viva Books, New Delhi, 1998.
2. Statistical Mechanics, D.A. McQuarrie, University Science Books, 2nd Edn., 2000.
3. Introduction to Modern Statistical Mechanics, D. Chandler, Oxford Univ. Press, 1987.
4. Statistical Thermodynamics of Non-Equilibrium Processes, J. Kaizer, Springer, 1st Edn., 1987.
5. Statistical Physics II: Non-Equilibrium Statistical Mechanics, R. Kubo, M. Toda and N. Hashitsume, Springer, 2003