### M.Sc. Chemistry (Computational Chemistry) for 2019-21 batch

#### Semester I

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Choose any one of these courses:

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Interdisciplinary course offered for other centres:

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<tr>
<td>12</td>
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<td>Chemistry without test tube</td>
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Total: 23 Credits 575

#### Semester II

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Choose any one of these courses:

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Total: 24 Credits 600

**Mode of Transaction**

Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning.

**Evaluation Criteria**

As per UGC guidelines on adoption of CBCS.
### Semester III

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**Mode of Transaction**
Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning.

**Evaluation Criteria**
- As per UGC guidelines on adoption of CBCS.
  - **a:** Continuous Assessment: Subjective by enlarge
  - **b:** Mid-Term Test-1: Based on Objective Type & Subjective Type Test
  - **c:** Mid-Term Test-2: Based on Objective Type & Subjective Type Test
  - **d:** Surprise Test - 1: Based on Objective Type Test
  - **e:** Surprise Test – 2: Based on Objective Type Test
  - **f:** End-Term Exam (Final): Based on Objective Type Tests
  - **g:** Total Marks

M.Sc. Chemistry (Computational Chemistry) Course Structure

SEMESTER- I

<table>
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<th>Course Title: Basics of Biochemistry</th>
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<td>Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.</td>
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<tr>
<td>Course Objective: By the end of the course, students will have gained a fundamental understanding of Biochemistry. Biochemistry is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics ranging from sub-cellular to large systems.</td>
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<td>Learning Outcomes: The outcomes of the subject is to ensure that a student comprehends the following:</td>
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<td>a. The structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles.</td>
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<td>b. The energy metabolism by cellular components in cells and the process of mitotic cell division.</td>
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<td>c. Influences of changes or losses in cell function; including the responses to environmental or physiological changes, or alterations of cell function brought about by mutation.</td>
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<tr>
<td>Unit 1 Principles of biophysical chemistry Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc.</td>
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<td>Unit 2 Composition, structure, function and metabolism of Carbohydrates, Lipids.</td>
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<td>Unit 3 Composition, structure, function and metabolism of Amino Acids and Nucleotides.</td>
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<td>Unit 4 Enzymology: Classification, Principles of catalysis, Mechanism of enzyme catalysis, Enzyme kinetics, Enzyme regulation, Isozymes.</td>
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<td>Suggested Reading:</td>
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Course Title: Mathematics for Chemists

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<tr>
<td>Learning Outcomes: At the end of the course, the students will be able to:</td>
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<td>• identify and describe the basic mathematical techniques that are commonly used by chemist.</td>
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<td>• develop skills in vectors, matrices, differential calculus, integral calculus and probability.</td>
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<td>• apply the principles to a number of simple problems that have analytical solutions.</td>
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<td>• design different methods to problems related to chemistry.</td>
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Unit I: Vectors, matrices and determinants
Vectors: Vectors, dot, cross and triple products etc. the gradient, divergence & curl, vector calculus. Applications: Two body problem, center of mass and relative coordinates, Potentials. Matrix algebra: addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (symmetric, skew symmetric, hermitian, skew hermitian, unit, diagonal, unitary etc) and their properties, matrix equations: homogeneous, non homogeneous linear equations and conditions for the solution, linear dependence and independe, introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants, introduction to tensors. Applications: Slater determinants, Huckel Molecular Orbital Theory, Polarizability and Magnetic Susceptibility.

Unit II: Differential calculus:
Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials with their applications to thermodynamic properties. Applications: Maximally populated rotational energy levels, Bohr’s radius and most probable velocity from Maxwell distribution.

Unit III: Integral calculus:
basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations. Applications: Cartesian to spherical polar, curve sketching.

Unit IV: Elementary differential equations:
variables-separable and exact first-order differential equations, homogeneous, exact and linear equations, solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and legendre equation etc, spherical harmonics, second order differential equations and their solutions. Applications: chemical kinetics, secular equilibria, quantum chemistry etc,
Permutation and probability: permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, example from the kinetic theory of gases etc, curve fitting (including least squares fit etc) with a general polynomial fit. Statistics: mean, median, mode, standard deviations, and Correlation coefficient, student t-test.

Suggested Readings:

Course Title: Scientific Programming
Paper Code: CCC.508
Total Lectures: 60
Course Type: CF

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.
Learning Outcomes: At the end of the course, the students will be able to:
• identify and describe the basic art of scientific programming related to Fortran 95/2003.
• concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
• develop skills to write programs related to standard problems and as well as to chemistry.

Unit I
Introduction to Computers and Fortran language: History and evolution of Fortran language, Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program.

Unit II
Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit III
Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types. Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran.

Unit IV

Suggested Readings:
4. Parallel Programming in C with MPI and OpenMP by M J Quinn (2003).
Course Title: Programming I  
Paper Code: LBI.502  
Semester: I  
Total Hours: 30  
Course Type: CF  
Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Course Objective
By the end of the course, students will have gained a fundamental understanding of programming in Python by creating a variety of scripts and applications for the Web and for systems development. Python is a versatile programming language, suitable for projects ranging from small scripts to large systems. This course emphasizes best practices such as version control, unit testing and recommended styles and idioms. Students will explore the large standard library of Python 3, which supports many common programming tasks.

Learning Outcomes:
Upon successfully completing this course, students will be able to “do something useful with Python”.

• Identify/characterize/define a problem
• Design a program to solve the problem
• Create pseudo executable code
• Read most of the basic Python code

Syllabus
Unit 1: 8 Hrs  
Introduction, gitHub, Functions, Booleans and Modules, Sequences, Iteration and String Formatting, Dictionaries, Sets, and Files

Unit 2: 8 Hrs  
Exceptions, Testing, Comprehensions, Advanced Argument Passing, Lambda -- functions as objects

Unit 3: 7 Hrs  
Object Oriented Programming, More OO -- Properties, Special methods

Unit 4: 7 Hrs  
Iterators, Iterables, and Generators, Decorators, Context Managers, Regular Expressions, and Wrap Up

Suggested Reading and resources:
• Core Python Programming (http://corepython.com/): Only available as a dead trees version, but if you like to have book to hold in your hands anyway, this is the best textbook style introduction out there. It starts from the beginning, but gets into the full language. Published in 2009, but still in print, with updated appendixes available for new language features. In the third edition, “the contents have been cleaned up and retrofitted w/Python 3 examples paired w/their 2.x friends.”
• Dive Into Python 3 (http://www.diveinto.org/python3/): This book offers an introduction to Python aimed at the student who has experience programming in another language.
• Python for You and Me (http://pymbook.readthedocs.org/en/latest/): Simple and clear. This is a great book for absolute newcomers, or to keep as a quick reference as you get used to the language. The latest version is Python 3.
• Think Python (http://greenteapress.com/thinkpython/): Methodical and complete. This book offers a very "computer science"-style introduction to Python. It is really an intro to Python in the service of Computer Science, though, so while helpful for the absolute newcomer, it isn’t quite as “pythonic” as it might be.
• Python 101 (http://www.blog.pythonlibrary.org/2014/06/03/python-101-book-published-today/) Available as a reasonably priced ebook. This is a new one from a popular Blogger about Python. Lots of practical examples. Also available as a Kindle book: http://www.amazon.com/Python-101-Michael-Driscoll-ebook/dp/B00KQTFHNK
• Problem Solving with Algorithms and Data Structures (http://interactivepython.org/runestone/static/pythonds/index.htmlLinks to an external site.))Links to an external site.)
• Python Course (http://www.python-course.eu/python3_course.phpLinks to an external site.))Links to an external site.)

References for getting better, once you know the basics
• Python Essential Reference (http://www.dabeaz.com/per.html): The definitive reference for both Python and much of the standard library.
• Hitchhikers Guide to Python (http://docs.python-guide.org/en/latest): Under active development, and still somewhat incomplete, but there is good stuff.
• Writing Idiomatic Python (https://www.jeffknupp.com/writing-idiomatic-python-ebook): Focused on not just getting the code to work, but how to write it in a really "Pythonic" way.
• **Fluent Python** ([http://shop.oreilly.com/product/0636920032519.do](http://shop.oreilly.com/product/0636920032519.do)): All python3, and focused on getting the advanced details right. Good place to go once you've got the basics down.

• **Python 3 Object Oriented Programming** ([https://www.packtpub.com/application-development/python-3-object-oriented-programming](https://www.packtpub.com/application-development/python-3-object-oriented-programming)): Nice book specifically about Object Oriented programming structure, and how to do it in Python. From local Author and founder of the Puget Sound Programming Python (PuPy) meetup group, Dusty Phillips.

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**Course Title:** Scientific Programming Lab (Practical)

**Paper Code:** CCC.513

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**Total Lectures:** 90

**Course Type:** CC

**Transactional Modes:** Laboratory based practicals; Problem solving; Self-learning.

**Learning Outcomes:** The objective of this course is to introduce students to the art of scientific programming. The practical aspects of scientific programming languages Fortran and C will be taught to students in this course. The students after completion of this course will be able to:

- Identify/characterize/define a computational problem
- Design a fortran program to solve the problem
- Create pseudo executable code
- Read most of the basic fortran code

**Unit I**

Structure of a Fortran Program, compiling, linking and executing the Fortran programs. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

**Unit II**

Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.

**Unit III**

Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran. Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination.

**Unit IV**

What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting

**Suggested Readings:**

4. Parallel Programming in C with MPI and OpenMP by M J Quinn
5. Introduction to Parallel Computing by Ananth Grama, George Karypis, Vipin Kumar, and Anshul Gupta.

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**Course Title:** Physical Chemistry I

**Paper Code:** CCC.506

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**Total Lectures:** 45

**Course Type:** DSE

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Learning Outcomes:** At the end of the course, the students will be able to:

- Understand the thermodynamics, phase transition, fugacity, solid and liquid transitions.
- identify and describe thermodynamical properties of a system.
- apply thermodynamical properties for various systems.
- use the knowledge of phase equilibria for various systems.
- understand how the computational techniques can be applied to study problems in advanced physical chemistry.

**Unit 1**


**Unit 2**
**Partial Molar Properties and Fugacity:** Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs-Duhem equation, real gases, fugacity, its importance and determination, standard state for gases.

**Phase transition:** Phase rule, water, CO₂ phase transition, binary and ternary component phase transitions. Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

### Unit 3

**Thermodynamics of Simple Mixtures:** Thermodynamic functions for mixing of perfect gases. Chemical potential of liquids. Raoult’s law, thermodynamic functions for mixing of liquids (ideal solutions only). Real solutions and activities.

**Solid-Liquid Solutions:** Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point.

### Unit 4

**Statistical Thermodynamics:** Thermodynamic probability and entropy, Maxwell-Boltzmann, Bose-Einstein and Dermer-Dirac statistics. Partition function, molar partition function, thermodynamic properties in term of molecular partition function for diatomic molecules, monoatomic gases, rotational, translational, vibrational and electronic partition functions for diatomic molecules, calculation of equilibrium constants in term of partition function, monoatomic solids, theories of specific heat for solids.

**Suggested Readings:**


### Course Title: Inorganic Chemistry I

**Paper Code:** CCC.509

**Total Lectures:** 45

**Course Type:** DSE

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Course Objective and Learning Outcomes:** The objective of this course is that students learn the metal-ligand equilibrium, transition metal complexes, ligand field theory, and crystal field theory, which are the fundamental branches of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

### Unit 1

**Metal-Ligand Equilibria in Solution**

Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by spectrophotometry and potentiometric (pH) methods.

### Unit 2

**Reaction Mechanisms of Transition Metal Complexes**

Introduction, potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere, Berry pseudorotation.

### Unit 3

**Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties of transition metal ions and free ions preservative, effects of L-S coupling on magnetic properties, temperature independent paramagnetism (TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), quenching of orbital angular momentum by crystal fields in complexes in terms of term splitting, effect of spin-orbit coupling and A, E & T states mixing.

### Unit 4
Crystal Fields Splitting
Spin-spin, orbital-orbital and spin orbital coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of \( p^2 \), \( d^6 \) ions, determination of the ground state terms for \( p^2 \), \( d^6 \), \( p^6 \) ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters \( \lambda \) energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. Splitting patterns of and G, H and I terms. Strong field configurations, transition from weak to strong crystal fields, selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths.

Suggested Readings:

Course Objective and Learning Outcomes:
The objective of this course is that students learn the reaction mechanism and its intermediates, aromaticity, different sets of aliphatic nucleophilic reaction, aromatic nucleophilic and electrophilic reaction, elimination reaction, addition reaction, which are the fundamental branches of organic chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in computational organic chemistry.

Unit 1
Reaction mechanism, structure and reactivity: Types of reaction and mechanisms, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, methods of determining mechanisms, isotope effects, effect of structure on reactivity: Hammet equation, Taft equation.

Reactive intermediates: Generation, structure and reactions of carbenoids, carbanions, free radicals, carbenes, nitrenes and benzynes. Neighbouring group participation, classical and non-classical carbenoids, phenonium ions and norbornyl system.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity, homoaromatic compounds.

Unit 2
Aliphatic nucleophilic substitution reaction: The \( S^2 \), \( S^1 \), mixed \( S^2 \) and \( S^1 \) and SET mechanism, the \( S^1 \) mechanism. nucleophilic substitution at an allylic, aliphatic and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition between \( S^2 \) and \( S^1 \) mechanisms.

Aromatic nucleophilic substitution: The \( S^1 \), bimolecular displacement mechanism and benzene mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles.

Unit 3
Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation, and hydroxylation.
Unit 4


Suggested Readings:

Course Title: Statistics for Chemical and Biochemical Applications

Paper Code: CCC.511

Total Lecture: 45
Course Type: DSE
Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Course Objective and Learning Outcomes: This course will introduce the basic aspects of various industry based statistical methods to Masters students.

Unit I
Overview of Biostatistics: Difference between parametric and non-parametric statistics, Univariate and multivariate analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Unit II
Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit III
Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

Unit IV
Inferential Statistics: Student’s t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal-Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, χ² test. Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Suggested Readings:

Course Title: Physical Organic Chemistry

Paper Code: CCC.512

Total Lecture: 45
Course Type: DSE
Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.
This course on Physical Organic Chemistry will provide conceptual understanding of chemical bonding, aromaticity, structure and stereochemistry, steric and conformational properties, chemical reactivity, correlation of structure with reactivity, Hammond postulates, solvent effects, acidity, nucleophilicity, electrophilicity, studying reaction mechanisms, isotope effects Woodward Hoffmann rules.

**Unit-I**

Chemical bonding: Covalency and molecular structure, approximate molecular orbital theory, properties of covalent bonds, intermolecular forces, aromaticity, structure. Woodward Hoffmann rules.

**Unit-II**

Correlation of structure with reactivity: Electronic demands, the Hammett equation, substituent constants $\sigma$, theories of substituent effects, interpretation of $\sigma$-values, reaction constants, $\rho$, deviations from the Hammett equation, dual-parameter correlations, molecular orbital considerations, cross-interaction terms

**Unit-III**

Steric and conformational properties: Origins of steric strain, examples of steric effects upon reactions, measurement of steric effects upon rates.

Solvation effects: structure of liquids, solutions, solvation, thermodynamic measures of solvation, effects of solvation on reaction rates and equilibria, empirical indexes of solvation, use of solvation scales in mechanistic studies.

**Unit-IV**

Kinetic isotope effects: isotopic substitution, theory of isotopic effects, transition-state geometry, secondary kinetic isotope effects, heavy atom isotope effects, tunnel effect

Acids and bases, nucleophiles and electrophiles: acid-base dissociation, the strengths of oxygen and nitrogen acids, linear free-energy relationships, rates of proton transfers, structural effects on amine protonation, factors that influence carbon acidity, theories of proton transfer, nucleophilicity and electrophilicity and their measurement.

**Recommended Readings:**

Suggested Readings:

Course Title: Quantum Chemistry-I

Paper Code: CCC.525

Total Lecture: 60

Transaction Modes: Lecture; Tutorial; Problem solving; Self-learning.

Course Type: CC

Learning Outcomes: At the end of the course, the students will be able to:

- identify and describe the basic concepts of quantum mechanics.
- the connection of quantum mechanical operators to observables.
- identify the characteristics of quantum mechanics in chemistry.
- apply the principles to a number of simple problems that have analytical solutions.
- analyze basic ideas on solving problems related to atomic and molecular structure, which will, in turn, prepare them to take the next advanced level course of Electronic Structure Theory.

Unit I (16)

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor. Angular momentum, eigenvalues of angular momentum operator. Particle on a Ring, Hydrogen Atom.

Unit II (14)


Unit III (14)

Symmetry Point Groups: Determination of point group of a molecule, representations, the great orthogonality theorem, character table, construction of character tables for c2v and c3v groups, symmetry adapted atomic basis sets, construction of molecular orbitals. The direct product representation.

Unit IV (16)


Suggested Readings:


Course Title: Statistical Mechanics I

Paper Code: CCC.524

Total Lectures: 60

Course Type: CC

Transaction Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- apply the classical laws of thermodynamics and their application, mathematical review of classical mechanics
- learn the postulates of statistical mechanics, Liouville's Theorem, and statistical interpretation of thermodynamics
- identify the microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function, elementary probability theory, distributions and fluctuations
- learn the methods of statistical mechanics and their use to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases

After completion of this course will help the students to apply the principles and techniques from statistical mechanics to a range of modern day research based problems.

Unit I: (16)

Mathematical Review of Classical Mechanics:
Lagrangian Formulation, Hamiltonian Formulation, Poisson Brackets and Canonical Transformations
Classical approach to Ensembles:
Ensembles and Phase Space, Liouville's Theorem, Equilibrium Statistical Mechanics and it's ensembles

Unit II: (16)
Elementary Probability Theory
Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem
Distributions & Fluctuations:
Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable

Unit III: (14)

Unit IV: (14)

Suggested Readings:

Course Title: Physical Chemistry II
Paper Code: CCC.523
Total Lectures: 45
Course Type: CC

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:
• apply thermodynamical properties for various systems.
• interpret various electrochemical phenomena.
• identify and describe differential rate laws, integrated rate laws, temperature dependence of reaction rates, and reaction mechanisms and parallel and consecutive reactions
• knowledge about catalysts and catalyzed reactions.
• gain depth knowledge in this fundamental branch of chemistry.
• understand how the computational techniques can be applied to study problems in advanced physical chemistry.

Unit 1 (10)

Electrochemical Cells: Nernst equation, redox systems, electrochemical cells, application of electrochemical cell, concentration cells with and without liquid junction, thermodynamics of reversible electrodes and reversible cells, and potentiometric titration.

Unit 2 (10)
Reaction Kinetics: Introduction, rates of chemical reactions, complex reactions, steady state approximation, determination of mechanisms of chemical reactions, temperature dependence of rate constant, Arrhenius and Eyring equations and their applications, collision and transition state theories of rate constant, treatment of unimolecular reactions, stearic factor, ionic reactions: salt effect.

Unit 3 (12)
Photochemical Reactions and Processes: Laws of photochemistry and kinetics of photochemical reactions, measurement of fluorescence and phosphorescence lifetimes and photoinduced electron transfer rates.

Fast Reaction Kinetics: Introduction to time-resolved techniques for absorption and emission measurements, relaxation method, study of kinetics of fast reactions by millisecond stopped-flow, nanosecond flash photolysis techniques, detection and kinetics of reactive intermediates.

Unit 4 (13)

Suggested Readings:
Course Title: Computational Methods

Power Code: CCC.526

Total Hours: 60

Course Type: CC

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to solve:

- the large scale systems of linear, non-linear and simultaneous equations
- the matrix and determinants, interpolations, polynomial and spline interpolation
- the numerical differentiation and integration
- complex curve fitting methods, explicit schemes to solve differential equations
- the simple optimisation, vectorisation.

After, completion of this course will help the students to apply numerical methods to obtain approximate solutions of complex mathematical problems.

Unit I:

Linear and Non-linear Equations:
Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basic principles-Formulæ-algorithms.

Simultaneous equations:

Unit II:

Matrix and Determinants:
Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

Unit III:

Interpolations:
Concept of linear interpolation-Finite differences-Newton’s and Lagrange’s interpolation formulæ-principles and Algorithms

Numerical differentiation and integration:

Curve Fit:
least square, straight line and polynomial fits.

Unit IV:

Numerical Solution of Differential Equations:

Suggested Readings:

Course Title: Computational Methods lab

Paper Code: CCC.527

Total Hours: 90

Course Type: CC

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- learn computer code for the large scale systems of transcendental and polynomial equations
- understand numerical strategies to write a computer code for the solution of matrix and determinants, interpolations, polynomial and spline interpolation
- learn the computer code for numerical differentiation and integration, differential equations, complex curve fitting, and simple optimisation

After, completion of this course will help the students to apply numerical methods to obtain approximate solutions of complex mathematical problems.

Jacobi Method of Matrix Diagonalization, Solution of transcendental or polynomial equations by the Newton Raphson method, Linear curve fitting and calculation of linear correlation coefficient, Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination, Finding Eigen values and eigenvectors, Matrix factorizations Curve Fitting – Polynomial curve fitting on the fly,

Suggested Readings:

Course Title: Density Functional Theory
Paper Code: CCC.528
Course Type: DSE
Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.
Total Lecture: 45

Objective and Learning Outcomes: This is a specialization course for students of Computational Chemistry. The objective of this course is to make the students understand the basics of Density Functional Theory (DFT), which is a popular electronic structure method. With the increasing power of computers, DFT-based calculations are emerging as a useful tool to characterize the properties of molecules and materials. This course will review the various theories/approximations necessary to understand most popular framework of modern DFT.

Unit-I

Unit-II

Unit-III
Practical Implementation of Density Functional Theory (DFT): Kohn-Sham formulation: Plane waves and pseudopotentials, Janak’s theorem, Ionization potential theorem, Self consistent field (SCF) methods, Understanding why LDA works, Consequence of discontinuous change in chemical potential for exchange-correlation, Strengths and weaknesses of DFT.

Unit-IV

Suggested Readings:
5. C. Kittel, Introduction to Solid State Physics (Wiley India (P) Ltd., New Delhi, India) 2007

Course Title: Introduction to Quantum Dynamics
Paper Code: CCC.529
Total Lecture: 45
Course Type: DSE
Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:
• learn systematic theoretical validations of the separation of electronic and nuclear motions
• gain the knowledge about the basic aspects of time dependent quantum wavepacket dynamics
• understand various numerical methods for solving the TDSE

Unit I
Separation of electronic and nuclear motions: adiabatic representation, Born-Oppenheimer approximation, Hellmann-Feynman theory, diabatic representation, transformation between two representations, crossing of adiabatic potentials.
TDSE: separation of variables and reconstitution of the wavepacket, expectation values, free-particle wavepacket: centre and dispersion of the wavepacket.

**Unit II**

(11)

Gaussian wavepacket: Gaussian free particle, general properties of Gaussian wavepackets, Gaussian in a quadratic potential. Correspondence between Classical and Quantum Dynamics: Ehrenfest’s Theorem, Bohmian Mechanics and the Classical limit.

**Unit III**

(11)

Spectra as Fourier transforms of wavepacket correlation functions. 1D barrier scattering: wavepacket formulation of reflection and transmission coefficients, cross-correlation function and S-matrix.

**Unit IV**

(11)

Numerical methods for solving the TDSE: spectral projection and collocation, pseudospectral basis, gaussian quadrature, representation of the hamiltonian in the reduced space, discrete variable representation, Fourier method, time propagation.

**Suggested Readings:**


**Course Title:** Seminar -I

**Paper Code:** CCC.542

The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literalual knowledge.

The evaluation criteria shall be as follows:

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**Course Title:** Inorganic Chemistry II

**Paper Code:** CCC.521

**Total Lectures:** 45

**Course Type:** DSE

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Learning Outcomes:** At the end of the course, the students will be able to:

- learn the advanced topics in inorganic chemistry, eg symmetry operation and group theory, metal complexes, inorganic rings and cages
- understand how the computational techniques can be applied to study problems in inorganic chemistry

**Unit 1**

(12)

**Symmetry**

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination,

**Unit 2**

(12)

**Group theory**

Determination of reducible and irreducible representations, character tables, construction of character tables for C_2V, C_3V, use of symmetry in obtaining symmetry of orbitals in molecules.

**Unit 3**

(14)

**Metal Complexes**

Organic-transition metal chemistry, complexes with π-acceptor and σ-donor ligands, 18-electron and 16-electron rules, isolobal analogy, structure and bonding. Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygencomplexes, tertiary phosphine as ligand. Metallocenes, metal cluster compounds, metal-metal bond, carbonyl and non-carbonyl clusters, fluxional molecules.

**Unit 4**

(16)
Inorganic chains, rings and cages

a) Chains: Catenation, heterocatenation, isopolyanions and heteropolyanions.

b) Rings: Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.

c) Cages: Cage compounds having phosphorus, oxygen, nitrogen and sulphur: boron cage compounds, boranes, carboranes and metallocenecarboranes.

Suggested Readings:

Course Title: Organic Chemistry II

Paper Code: CCC.522

Total Lectures: 45

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- learn the advanced topics in organic chemistry eg. stereochemistry, photochemistry, pericyclic and cycloaddition reaction, sigmatropic rearrangements.

- gain the knowledge of different computational techniques and its application to study problems in advanced organic reactions.

Unit 1 (12)

Stereochemistry: Elements of symmetry, chirality, projection formulae, configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, D/L, R/S, E/Z and cis/trans configurational notations, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus, conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2, 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on reactivity, conformation of sugars.

Unit 2 (12)

Photochemistry: Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di π– methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.

Unit 3 (16)

Pericyclic chemistry:

Introduction, Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl cation, allyl radical, pentadienyl cation and pentadienyl radical.


Cycloaddition reactions: Suprafacial and antarafacial interactions. \( \pi^2 + \pi^2 \) and \( \pi^4 + \pi^2 \) cycloadditions and stereochemical aspects. Diels-Alder reaction. Woodward-Hoffmann Selection rules. Explanation for the mechanism by (i) Conservation of orbital symmetry and correlation diagrams (ii) FMO theory

Sigmatropic reactions: \([1,j]\) and \([i,j]\) shifts; suprafacial and antarafacial, selection rules for \([l, j]\) shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Introduction to chelotropic reactions and the explanation of mechanism by FMO theory.

Unit 4 (14)

Rearrangements: General mechanistic considerations—nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Neber,
Beckmann, Hofmann, Curtius, Schmidt, Carroll, Claisen, Cope, Gabriel–Colman, Smiles and Sommelet–Hauser rearrangements.

**Selective Name Reactions:** Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Hofmann-Löffler Fretag, Chichibabin reaction.

**Suggested Readings:**

Course Title: Electronic Structure Theory

Paper Code: CCC.556

Total Hours: 60

Course Type: CC

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- identify and define basic terms and concepts which are needed for this specialized course.
- describe the HF SCF method.
- choose the basis sets.
- compare post-HF methods.
- identify and define the concept of DFT.
- identify how to apply quantum chemistry to study chemical and biochemical problems.

Objective and Learning Outcomes: This is an advanced course for students who specialize in Computational Chemistry. The objective of this course is that students learn the techniques of molecular quantum chemistry (eg. Hartree-Fock SCF and Roothaan-Hartree-Fock method, CI Interaction, CCSD, CCSD(T), Kohn-Sham equations) and apply them to study chemical and biochemical problems.

Unit I

Review of molecular structure calculations, Hartree-Fock SCF method for molecules

Unit II

Roothaan-Hartree-Fock method, selection of basis sets.

Unit III


Unit IV

Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

Suggested Readings:

Course Title: Fundamentals of Molecular Simulations

Paper Code: CCC.554

Total Lecture: 60

Course Type: CC

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- learn the modelling of small to large molecular environments
- understand various force field for biomolecular simulation in details
- learn different methods for simulating large systems
- gain the knowledge about different molecular simulation techniques
- understand the dynamics of the structural transitions

which will help them use the techniques of molecular simulations in their further potential careers in academia and industry.

Unit I

Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.

Force Fields and Molecular Representation – (a) Intramolecular Interactions, (b) Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, (c) Hydrogen Bonds, (d) Constraints and Restraints, (e) United Atom and Other Coarse-Grained Approaches, (f) Non-pairwise Interactions, (g) How accurate are force fields?

Example: Protein, Nucleic Acid, Small Molecule Force Field, Water Models.

Unit II

Methods for Simulating Large Systems
(a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists, (b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary, (c) Long-range Interactions – The Ewald Sum, The Reaction Field Method

Unit III

Energy Minimization and Related Analysis Techniques
(a) Steepest Descent, (b) Conjugate Gradient, (c) Newton-Raphson, (d) Comparison of Methods, (e) Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, (f) What's the big deal about the minimum? Introduction to Equilibrium Statistical Mechanics

23
(a) Phase space, Ergodicity, and Liouville's theorem, (b) Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles (c) Statistical Mechanics of Fluids

Unit IV (15)

Simulation Methods:
Monte Carlo: (a) MC integration and Markov chains, (b) The Metropolis method, (c) Biased MC


Free Energy: (a) Perturbation Methods, (b) TI (Thermodynamic Integration)
Brownian dynamics and the Langevin Equation.

Suggested Readings:

Course Title: Molecular Simulations Lab (Practical)
Paper Code: CCC.555
Total Lecture: 90
Course Type: CC

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:
- learn the basics of Linux environment
- use the remote computing as a tool for high performance computation
- use different energy minimization techniques
- create molecular model from scratch, and high definition images using various graphics tools
- gain the practical in-hand experience of various modeling and classical simulation tools
- learn the use of different in silico techniques for biomolecular simulations
which will enhance their employability in their further potential careers in academia and industry

1. Linux basics and remote computing
2. Coordinate generations and inter-conversions of small molecules
3. Energy minimizations and optimization, ab initio methods
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
7. Molecular Dynamics with GROMACS
   a. Water liquid structure and dynamics
   b. Simulation of Ionic Solutions
   c. Simulation of Protein in Water
   d. Simulation of Membrane Proteins
   e. Simulations of DNA
8. Review of Molecular Dynamics Principles

Suggested Readings:

Course Title: Molecular Spectroscopy
Paper Code: CCC.557
Total Lectures: 60

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:
- gain the knowledge about various spectroscopic techniques, such as, electronic, microwave, vibrational, raman, nuclear magnetic resonance, and laser spectroscopy
- understand, how spectroscopic transitions come into picture in molecular quantum mechanics
- learn various spectroscopic selection rules and their applications

Course Type: CC
Objective and Learning Outcomes: This is a fundamental course for students who specialize in Physical/Computational Chemistry. The objective of this course is that students learn the basic concepts of molecular spectroscopy from a fundamental point of view. The course will help students to understand how spectroscopic transitions come into picture in molecular quantum mechanics.

Unit I


Microwave Spectroscopy: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, applications.

Unit II

Vibrational Spectroscopy: Instrumentation and applications of infrared spectroscopy, simple harmonic oscillator, vibrational energies of diatomic molecules, anharmonicity, vibration-rotation spectroscopy, P, Q, R branches, vibrations of polyatomic molecules, overtones, hot bands and applications.

Raman Spectroscopy - Classical and quantum theories of Raman Effect, pure rotational, vibrational and vibrational-rotational Raman spectra, mutual exclusion principle, resonance Raman Spectroscopy, surface enhanced Raman spectroscopy, coherent anti stokes Raman spectroscopy.

Unit III

Nuclear Magnetic Resonance (NMR) Spectroscopy: Basic principles, instrumentation, magnetization vector and relaxation, NMR transitions, Bloch equation, relaxation effects and mechanism, double resonance and spin tickling, effect of quadrupole nuclei, nuclear overhauser effect (NOE), multiple pulse methods, NMR in medical diagnostics.

Unit IV


Suggested Readings:

Course Title: Electronic Structure Theory Lab-I (Practical)
Paper Code: CCC.558
Total Hours: 60
Course Type:CC

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Course Learning Outcomes: This course will provide practical experience to the students through use of important Computational Chemistry softwares related to electronic structure theory.
Following experiments will be carried out in the lab.
1. Introduction to electronic structure calculations.
2. Basis set dependency.
3. HF and DFT methods related calculations.
5. MO and charge distribution calculations.
6. Vibrational spectra calculations.
7. 2D potential energy surface generation.
8. Transition state calculations.
9. Absorption spectra study.
11. Thermochemistry study.

Suggested Readings:

Course Title: M.Sc. Dissertation I
Paper Code: CCC.599
Invested Hours: 180
Course Type:SBE
Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Course Objective and Learning Outcomes: The objective of dissertation part I would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

The Evaluation criteria shall be multifaceted as detailed below:

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Criteria</th>
<th>Marks allotted</th>
</tr>
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<tbody>
<tr>
<td></td>
<td><strong>Theoretical work</strong></td>
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</tr>
<tr>
<td>1.</td>
<td>Review of literature and Bibliography</td>
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</tr>
<tr>
<td>2.</td>
<td>Identification of gaps in knowledge</td>
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</tr>
<tr>
<td>3.</td>
<td>Objective formulation</td>
<td>15</td>
</tr>
<tr>
<td>4.</td>
<td>Methodology</td>
<td>35</td>
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<tr>
<td>5.</td>
<td>Presentation</td>
<td>35</td>
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<tr>
<td></td>
<td><strong>Experimental Work</strong></td>
<td></td>
</tr>
<tr>
<td>6.</td>
<td>Continuous evaluation by guide</td>
<td>25</td>
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<tr>
<td></td>
<td><strong>Total</strong></td>
<td><strong>150</strong></td>
</tr>
</tbody>
</table>

The final presentation shall be evaluated by a three membered committee consisting of

a. HOD/OHOD of the department
b. VC nominee
c. Supervisor (and Co-supervisor if applicable)

*of as recommended by School Board.
Course Title: Advanced Statistical Mechanics and Molecular Reaction Dynamics

Paper Code: CCC.572
Total Lecture: 60
Course Type: CC

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- identify and define basic terms and concepts of Phase transitions
- describe the Non-equilibrium dynamics
- learn the behavior of systems not far from equilibrium
- create potential energy surfaces for different small molecules
- explain the energetics of transition states of reactions

Unit I


A brief introduction to Liquid Theory: Averages, Distribution Functions, Reversible Work Theorem, Radial distribution function, Molecular liquids

Atomic and continuum models of liquids: The Lennard-Jones Fluid, Molecular dynamics simulation, Correlation functions and measurements, elements of linear response theory, Linear models (a) Langevin equations (diffusion, friction and memory). (b) Gaussian fields (Debye-Huckel and beyond), The hard sphere model, WCA theory, Chemical equilibrium and relaxation.

Unit II

Non-equilibrium systems: Fluctuation-Dissipation Theorem, Onsager's Regression Hypothesis Brownian Motion, Friction and the Langevin Equation, Transport, Time Correlation Functions.

Special topics: Free energy perturbation, The Jarzynski Equality, Electron transfer--quantum rare events--golden rule--Marcus theory, Path integrals, Tunneling—instantons, Ising model / Quantum correspondence, Monte Carlo and Biased Monte Carlo methods.

Unit III


Unit IV


Books Recommended:

Course Title: Advanced Molecular Simulation Lab

Paper Code: CCC.571
Total Lectures: 90
Course Type: CC

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:
- learn various tools for protein structure prediction
- learn the homology and comparative modeling techniques
- understand the effect of sequence on the molecular model building
- learn the structure based drug designing
- gain the knowledge about various advanced molecular modeling techniques

1. Introduction to protein structure prediction
2. Homology or comparative modeling using MODELLER
3. Effect of sequence on model accuracy (eg. FABP)
   a. Select template structures
   b. How to validate protein structure
   c. Validate homology model and compare with x-ray structure
4. Homology Modeling and MD Refinement
5. Molecular Recognition
   a. Prediction of Protein-ligand interaction sites
   b. Prediction of Protein-nucleic acid interaction sites
   c. Prediction of Protein-protein interaction sites
6. Structure based Drug Designing
   a. Molecular Docking
   b. De Novo Ligand Design
   c. Virtual Screening
   Ligand based Drug Design
   a. Pharmacophore Identification
   b. QSAR
7. Special Topic: (a) Umbrella Sampling
   (b) Free Energy Calculations
   (c) Multicomponent Systems

Books Recommended:

Course Title: Electronic Structure Theory Lab - II (Practical)
Paper Code: CCC.558
Total Hours: 120
Course Type: CC

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.
Learning Outcomes: This course will provide practical experience to the students through use of important Computational Chemistry softwares related to electronic structure theory. Following experiments will be carried out in the lab.

1. Post-HF based calculations
2. Studying potential energy surface.
3. Carrying of conformational analysis of large systems.
4. Model chemistry.
5. Study of NMR spectra
6. Fluorescence and photoelectron spectra.
7. Modeling chemical reactions using classical dynamics.
8. Electronic circular dichroism study.
10. Pseudopotential generation and testing of Si atom.
11. QM/MM study.
12. Inclusion of Relativistic effects.

Suggested Readings:
Course Title: Two Value Added Courses  
Paper Code: XXX.XXX

Semester: IV  
Total Hours:  
Course Type: VAC  
Transactional Modes: Lectures; Problem solving; Self-learning.

Course Type:EF  
Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Course Title: Credit Seminar -II  
Paper Code: CCC.544

<table>
<thead>
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<td>1</td>
<td>25</td>
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The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Criteria</th>
<th>Marks</th>
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<tbody>
<tr>
<td>1</td>
<td>Content</td>
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<tr>
<td>2</td>
<td>Presentation Skills</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>Handling of queries</td>
<td>05</td>
</tr>
</tbody>
</table>

Course Title: M.Sc. Dissertation II  
Paper Code: CCC.599  
Course Type:SBE  
Hours Invested: 240  
Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Course Objective and Learning Outcomes: The objective of dissertation part II would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

The Evaluation criteria shall be multifaceted as detailed below:

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Criteria</th>
<th>Total marks 150*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Report Writing</td>
<td>50</td>
</tr>
<tr>
<td>2.</td>
<td>Presentation and defense of research work</td>
<td>50</td>
</tr>
<tr>
<td>3.</td>
<td>Continuous evaluation of student by Guide</td>
<td>50</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>150</td>
</tr>
</tbody>
</table>

The final presentation shall be evaluated by a three membered committee consisting of:
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*of as recommended by School Board.