Central University of Punjab

M.Sc. Chemistry (Theoretical and Computational Chemistry)

Session: 2021-2023

Department of Computational Sciences

School of Basic Sciences

Graduate Attributes

In line with the syllabus of M.Sc. Chemistry (Theoretical and Computational Chemistry) it is expected that a student graduating after successful completion of the course shall be able to understand in various areas of Theoretical and Computational Chemistry, advanced knowledge in Mathematics, and knowledge in applied fields like Computer Science. Further, they apply the knowledge, general competence, and analytical skills on an advanced level, needed in industry, consultancy, education, research, or public administration. Therefore graduated students of M.Sc. Chemistry (Theoretical and Computational Chemistry) would be a valuable asset for nation by virtue of his/her scientific abilities. The student can expect gainful employment in academic/research/industry by undertaking this programme.

Course Structure of the Programme

SEMESTER I							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	PCP.506	Mathematics for Computational Sciences	CF	3	0	0	3
2	CCC.508	Scientific Programming	CF	3	0	0	3
3	CCC.515	Scientific Programming Lab (Practical)	SBC	0	0	4	2
4	PCP.527	Quantum Mechanics	CC	3	0	0	3
5	CCC.524	Statistical Mechanics	CC	3	0	0	3
6	PCP.519	Python Programming	CC	3	0	0	3
7	PCP.520	Entrepreneurship	CF	1	0	0	1
Choose any one of these courses/MOOC							
8	CCC.506	Introduction to Biochemistry	DE	3	0	0	3
9	CCC.509	Inorganic Chemistry	DE	3	0	0	3
10	CCC.510	Organic Chemistry	DE	3	0	0	3
11	XXX.XXX	Interdisciplinary Course	IDC	2	0	0	2
Total				**21**	**0**	**4**	**23**

SEMESTER II							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCC.556	Electronic Structure Theory	CC	3	0	0	3
2	CCC.554	Fundamentals of Molecular	CC	3	0	0	3

		Simulations					
3	CCC.525	Computational Methods	CC	3	0	0	3
4	PCP.525	Solid State Physics	CC	3	0	0	3
5	PCP.557	Atomic and Molecular Spectroscopy	CC	3	0	0	3
6	XXX.XXX	Value Added Course	VAC	2	0	0	2
Choose any two of these courses/MOOC							
7	CCC.521	Machine Learning and Data Science	DE	3	0	0	3
8	LBI.524	Molecular Evolution	DE	3	0	0	3
9	LBI.526	Biomolecular Structure Modelling and Drug Designing	DE	3	0	0	3
10	CCC.517	Physical Chemistry	DE	3	0	0	3
11	CCC.514	Physcal Organic Chemistry	DE	3	0	0	3
12	CCC.513	Statistics for Chemical and Biochemical Applications	DE	3	0	0	3
Total				**23**	**0**	**0**	**23**

SEMESTER III							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCC.551	Research Methodology	CC	3	0	0	3
2	CCC.529	Density Functional Theory	CC	3	0	0	3
3	CCC.528	Computational Methods Lab (Practical)	SBC	0	0	4	2
4	PCP.526	Computational Solid State	SBC	0	0	4	2

		Physics Lab (Practical)					
5	CCC.555	Molecular Simulations Lab (Practical)	SBC	0	0	4	2
6	CCC.573	Electronic Structure Theory Lab (Practical)	SBC	0	0	4	2
7	CCC.570	Enrich in Chemistry	DEC	2	0	0	2
8	CCC.600	Research Proposal	SBC	0	0	8	4
Total				**8**	**0**	**24**	**20**

SEMESTER IV							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCC.600	Dissertation	SBC	0	0	40	20
Total				**0**	**0**	**40**	**20**
Grand Total				**86 Credits**			

L: Lectures; T: Tutorial; P: Practical

MOOCs may be taken upto 40% of the total credits (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match a minimum 70%. Mapping will be done by the department and students will be informed accordingly.

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

Evaluation Criteria for Theory Courses

A. Continuous Assessment (Course wise): [25 Marks]

Two or more of the given methods (Surprise Tests, in-depth interview, unstructured interview, Jigsaw method, Think-Pair Share, Students Teams Achievement Division (STAD), Rubrics, portfolios, case based evaluation, video based evaluation, Kahoot, Padlet, Directed paraphrasing, Approximate analogies, one sentence summary, Pro and

con grid, student generated questions, case analysis, simulated problem solving, media assisted evaluation, Application cards, Minute paper, open book techniques, classroom assignments, homework assignments, term paper).

B. Mid Semester Test: Based on Subjective Type Test [25 Marks]

C. End Semester Test: Based on Subjective (70%) and Objective (30%) Type Test [50 Marks]

The objective type will include one word answers, fill-in the blank, sentence completion, true/false, MCQs', and matching, analogies. The subjective type will include a very short answer (1-2 lines), short answer (one paragraph), essay type with restricted response, and essay type with extended response.

Core, Discipline Elective, Compulsory Foundation, Value Added and Interdisciplinary Courses			Discipline Enrichment Course		Entrepreneurship Course	
	Marks	Evaluation	Marks	Evaluation	Marks	Evaluation
Internal Assessment	25	Various	-	-	-	-
Mid-semester test (MST)	25	Subjective	50	Objective	25	Objective
End-semester test (EST)	50	Subjective (70%) Objective (30%)	50	Objective	25	Subjective

Evaluation Criteria for Practical Courses:

Evaluation	Marks
Maintaining the lab records/notebooks	10
Continuous assessment	20
Attendance	10
Final practical examination	50
Viva-voce	10

CF: Compulsory Foundation, CC: Core Course, DE: Discipline Elective, DEC: Discipline Enrichment Course, IDE: Inter-Disciplinary Elective, SBC: Skill-based Core, SBE: Skill-based Elective, VAC: Value Added Courses

L: Lecture, T: Tutorial, P: Practical

* Every student has to take 1 IDE (Inter-Disciplinary Elective) course of 2 credits from other disciplines in 1st semester of the program.

SEMESTER- I

Course Title: Mathematics for Computational Sciences

L	T	P	Cr
3	0	0	3

Paper Code: PCP.506
Total Lectures: 45

Learning Outcome: The course on Mathematical Physics is introduced to familiarize the students with the idea about transformation of coordinates and complex functions, special functions, group theory, and tensors which will be useful in understanding theoretical treatment and for developing a strong background to pursue research in theoretical physics.

Course Content

Unit I **12 hours**

Matrices & Vector Calculus: matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors

Differential calculus: Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials

Unit II **11 hours**

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

Fourier Transforms: Fourier series, Dirichlet condition, General properties of Fourier series, Fourier transforms, their properties and applications,

Unit III **11 hours**

Delta, Gamma, and Beta Functions: Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions.

Unit IV **11 hours**

Differential Equations Solutions of Hermite, Legendre, Bessel and Laugerre Differential equations, basics properties of their polynomials, and associated Legendre polynomials,

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

Suggested Readings

1. E. Kreyszig. (2011). *Advanced Engineering Mathematics* Wiley India Pvt. Ltd., New Delhi, India.
2. L. A. Pipes. (1985). *Applied Mathematics for Engineers and Physicist* McGraw-Hill, Noida, India .

3. D. G. Zill. (2012). *Advanced Engineering Mathematics* Jones & Barlett Learning, Massachusetts, USA.
4. P. K. Chattopadhyay. (2000). *Mathematical Physics* New Age International (P) Ltd., New Delhi.
5. E.Steiner. (2008). The chemistry Mathematics Book, Oxford University Press .
6. F. Daniels. (1959). Mathematical for Physical Chemistry : Mc. Graw Hill.
7. Tebbutt. (1994). Basic Mathematics for Chemists, Wiley.
8. G. Arfken, H. Weber and F. Harris. (2012). *Mathematical Methods for Physicists* Elsevier Academic Press, Massachusetts, USA.

Course Title: Scientific Programming

L	T	P	Cr
3	0	0	3

Paper Code: CCC.508
Total Hours: 45

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.
- demonstrate 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.

Course Content

Unit I **10 Hours**

Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program. Constants and variables, assignment statements and arithmetic calculations

Unit II **12 Hours**

Intrinsic functions, Program design and branching structures, loop and character manipulation. Basic I/O concepts, Formatted READ and WRITE statements,

Unit III **13 Hours**

Introduction to 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 IV **10 Hours**

What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation,

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

Suggested Readings

1. Chapman, (2006). Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York.
2. V. Rajaraman, (1997). Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi .
3. M. Metcalf, J. Reid, and M. Cohen, (2005). Fortran 95/2003 Explained, OUP .
4. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996). Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press .
5. M. J. Quinn, (2003). Parallel Programming in C with MPI and OpenMP.
6. A. Grama, G. Karypis, V. Kumar, and A. Gupta, (2003). Introduction to Parallel Computing .

Course Title: Scientific Programming Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: CCC.515
Total Hours: 60

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, will be taught to students in this course. The students after completion of this course will be able to

1. identify/characterize/define a computational problem
2. design a fortran program to solve the problem
3. create pseudo executable code
4. read most of the basic fortran code

Course Content

1. Compiling, linking and executing the Fortran programs.
2. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions,
3. Program design and branching structures, loop and character manipulation.
4. Basic I/O concepts, Formatted READ and WRITE statements,
5. Read/write of a Files.
6. Introduction to Arrays and procedures, Additional features of arrays and procedures.
7. Pointers and dynamic data structures using pointers in assignment statements.
8. Matrix summation, subtraction and multiplication, Matrix inversion.

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

Suggested Readings

1. Chapman, (2006). Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York.
2. V. Rajaraman, (1997). Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi .
3. M. Metcalf, J. Reid, and M. Cohen, (2005). Fortran 95/2003 Explained, OUP .
4. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996). Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press .
5. M. J. Quinn, (2003). Parallel Programming in C with MPI and OpenMP.
6. A. Grama, G. Karypis, V. Kumar, and A. Gupta, (2003). Introduction to Parallel Computing .

Course Title: Quantum Mechanics

L	T	P	Cr
3	0	0	3

Paper Code: PCP.527
Total Lectures: 45

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 charecteristics 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 Elctronic Structure Theory.

Course Content

Unit I **12 hours**

Mathematical Formulation and Postulates of Quantum Mechanics: Limitations of Classical Mechanics and foundation of Quantum Mechanics, Matrix representations of kets, bras and operators, Change of basis, Basic postulates of quantum mechanics, Schrödinger wave equation (time dependent and time independent), Expectation values, Commutation relations.

Unit II **11 hours**

Angular Momentum: eigenvalues and eigen vectors of orbital angular momentum, Angular momentum algebra and commutation relations, Matrix representation of angular momentum, Spin angular momentum: Pauli matrices and their properties.

Approximation methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples, time-dependent perturbation theory,

Unit III **11 hours**

Addition of Angular Momenta: Addition of two angular momenta. Transformation between bases: Clebsch-Gordan Coefficients, Eigenvalues of J^2 and Jz, Coupling of orbital and spin angular momenta.

Unit IV **11 hours**

Scattering Theory: Scattering Theory: Quantum Scattering theory, Scattering cross-section and scattering amplitude, Born scattering formula, Central force problem, Partial wave analysis, Bound states and resonances.

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

Suggested Readings

1. I.N. Levine, (2000). Quantum Chemistry, Pearson Educ., Inc. New Delhi .
2. D. A. McQuarrie, and J. D. Simon, (2011). Physical Chemistry: A Molecular Approach, Viva Books .
3. J.N. Murrell, S.F.A. Kettle and J. M. Tedder, (1965). Valence Theory, John Wiley .
4. A.K. Chandra, 4th Edition, (1994). Introductory Quantum Chemistry, Tata Mcgraw Hill.
5. N. Zettili, (2009). *Quantum Mechanics-Concepts and Applications*, John Wiley & Sons Ltd., Sussex, U.K.
6. E. Merzbacher, (2011) *Quantum Mechanics,* Wiley India Pvt. Ltd., New Delhi, India.
7. J. J. Sakurai, (2009) *Modern Quantum Mechanics,* Pearson Education, India.
8. D. J. Griffiths, (2015). *Introduction to Quantum Mechanics*, Pearson Education, India.
9. G. D. Mahan,(2009). Quantum Mechanics in a Nutshell , Princeton University Press.
10. J. P. Lowe, and Peterson, K., (2005). Quantum Chemistry, Academic Press.

Course Title: Statistical Mechanics

L	T	P	Cr
3	0	0	3

Paper Code: CCC.524

Total Hours: 45

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

- demonstrate the classical laws of thermodynamics and their application, mathematical review of classical mechanics
- discuss 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
- execute 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.

Course Content

Unit I **13 Hours**

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

Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

Unit II **12 Hours**

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 **10 Hours**

Basic Thermodynamics: Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function

Unit IV **10 Hours**

Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas.

Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

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

Suggested Readings

1. K. Haung (2008). Statistical Mechanics, Wiley.
2. R. K. Pathria and P. D. Beale, (2011). Statistical mechanics, Elsevier.
3. D. A. Mcquarrie, (2018). Statistical Mechanics, Viva Books.
4. D. Chandler, (1987). Introduction to Statistical Mechanics, Oxford University Press.

Course Title: Python Programming

L	T	P	Cr
3	0	0	3

Course Code: PCP.519
Total Hours: 45
Learning Outcomes: At the end of the course students will be able to explain and learn Python Programming to build applications intheir core domain. Python is becoming popular in artificial intelligence and machine learning. MicroPythonis sub-set of Python Programming useful to port in hardware for embedded and IoT applications.

Course Content

Unit I **12 hours**

Introduction, Data Types and Operators: Installation and working with Python, Variables and data types in python, Perform computations and create logical statements using Python's operators: Arithmetic, Assignment, Comparison, Logical, Membership, Identity, Bitwise operators, list, tuple and string operations

Unit II **11 hours**

Python Decision making and Loops: Write conditional statements using If statement, if …else statement, elif statement and Boolean expressions, While loop, For loop, Nested Loop, Infinite loop, Break statement, Continue statement, Pass statement, Use for and while loops along with useful built-in functions to iterate over and manipulate lists, sets, and dictionaries. Plotting data, Programs using decision making and loops

Unit III **11 hours**

Python Functions and Modules: Defining custom functions, Organising Python codes using functions, Create and reference variables using the appropriate scope, Basic skills for working with lists, tuples, work with dates and times, get started with dictionaries, Importing own module as well as

external modules, Programming using functions, modules and external packages

Unit IV **11 hours**

Python File Operations: An introduction to file I/O, use text files, use CSV files, use binary files, Handle a single exception, handle multiple exceptions, Illustrative programs.

Transaction Mode: Lecture, tutorial, problem solving

Suggested Readings

1. Gowrishankar S, Veena A, (2018). "Introduction to Python Programming", 1st Edition, CRC Press/Taylor & Francis,.
2. Jake VanderPlas, (2016). "Python Data Science Handbook: Essential Tools for Working with Data", 1st Edition, O'Reilly Media,.
3. Aurelien Geron, (2019). "Hands-On Machine Learning with Scikit-Learn and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems", 2nd Edition, O'Reilly Media.
4. Wesley J Chun, (2015)."Core Python Applications Programming", 3rd Edition, Pearson Education India.

Course Code: PCP.520

L	T	P	Cr
1	0	0	1

Course Title: Entrepreneurship

Total Hours: 15

Learning Outcomes: On the completion of this course, students will be able

a. To absorb an entrepreneurial mind-set.

b. To learn what is entrepreneurship and its impact

c. To develop understanding about problems and prospects in entrepreneurship.

d. To gain insights about entrepreneurial behaviour and skills.

e. To develop understanding about writing business plan/project proposals & managing start-up issues.

UNIT I **4 Hours**

Introduction:

- The concept of entrepreneurship, the history of entrepreneurship
- Entrepreneurial Structure; Nature, Characteristics, functions and its role in economic development
- Entrepreneurship- problems and prospects in India

UNIT II **4 Hours**

The Entrepreneur

- Entrepreneurial Behaviour and Skills
- The entrepreneurial decision process
- The skill gap analysis, role models
- The entrepreneurial success stories

Unit III **3 Hours**

E-Cell

- The concept of E-cells
- The significance, and activities conducted by E-cell
- Benefits of Joining E-Cells

Unit IV **4 Hours**

- Role of industries/entrepreneur's associations and self-help groups
- Funding opportunities for start-ups. Basic start-up problems
- Contents of business plan/ project proposal
- Barriers and gateways to communication, the ability of personal selling and negotiation.

Transactional Modes: Videos and quizzes through the on-line LMS; Classroom learning (Videos, In-class Activities); Assignments and Projects; and Practical Experiences including challenges.

Suggested Readings

1. G. K. Varshney, (2012). *Fundamentals of Entrepreneurship*, Sahitya Bhawan Publications, .

2. R. Roy, (2011). *Entrepreneurship*, 2nd Edition, Oxford, .

3. B. K. Mehta, (2018). *Entrepreneurship and Small Business*, SBPD Publishing House.

Course Title: Introduction to Biochemistry

L	T	P	Cr
3	0	0	3

Course Code: CCC.506
Total Hours: 45

Learning Outcomes: The outcomes of the subject is to ensure that a student comprehends the following:

1. The structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles.
2. The energy metabolism by cellular components in cells and the process of mitotic cell division.
3. 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.

Course Content

Unit I **15 Hours**

Principles of biophysical chemistry Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc.

Unit II **12 Hours**

Composition, structure, function and metabolism of Carbohydrates, Lipids. Bioenergetics and metabolism of Carbohydrates, Lipids

Unit III **8 Hours**

Composition, structure, function and metabolism of Amino Acids and Nucleotides.

Unit IV **10 Hours**

Enzymology: Classification, Principles of catalysis, Mechanism of enzyme catalysis, Enzyme kinetics, Enzyme regulation, Isozymes.

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

Suggested Readings

1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). *Biochemistry.* W.H. Freeman & Company. USA.
2. Brown, T.A. (2006). *Gene Cloning and DNA analysis: In Introduction*. Blackwell Publishing Professional. USA.
3. Nelson, D. and Cox, M.M. (2013). *Lehninger Principles of Biochemistry*. BI publications Pvt. Ltd. Chennai, India.
4. Ochiai, E. (2008). *Bioinorganic chemistry: A survey.* Academic Press. Elsevier, India.
5. Shukla AN (2009). *Elements of enzymology.* Discovery Publishing. New Delhi, India.
6. Voet, D. and Voet, J.G. (2014). *Principles of biochemistry*. CBS Publishers & Distributors. New Delhi, India.

Course Title: Inorganic Chemistry

L	T	P	Cr
3	0	0	3

Paper Code: CCC.509
Total Lectures: 45

Learning Outcomes: At the end of the course, the students will be able to:
1. identify the metal-ligand equilibrium, transition metal complexes, ligand field theory, and crystal field theory, which are the fundamental branches of Chemistry.
2. understand how the computational techniques can be applied to study problems in inorganic chemistry.

Course Content

Unit I **11 Hours**

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.

Unit II **11 Hours**

Reaction Mechanisms of Transition Metal Complexes

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.

Unit III **13 Hours**

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 presentive, effects of L-S coupling on magnetic properties, temperature independent paramagnetism(TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT).

Unit IV **12 Hours**

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^n, d^n ions, determination of the ground state terms for p^n, d^n, f^n 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 (λ) 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.

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

Suggested Readings

1. Cotton, F.A. and Wilkinson G. Advanced Inorganic Chemistry, 2007, John Wiley& Sons.
2. Huheey, J. E. (2006). Inorganic Chemistry: Principles of Structure and Reactivity,, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. (2005). Chemistry of the Elements, (reprinted),Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. (1984). Inorganic Electronic Spectroscopy, Elsevier Science Publishers B.V.

5. Carlin, R. L. and Van Duyneveldt, A.J. (1977). Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, SpringerverlagNew York Inc.
6. Miessler,G. L.and Tarr, D. A. (2011). Inorganic Chemistry,4thedition, Pearson Education.
7. Figgis,B.N. (1966). Introduction to Ligand Field, Wiley Eastern.
8. Drago,R.S. (1965) Physical Method in Chemistry, W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. (2010) Inorganic Chemistry, Oxford University Press.
10. Earnshaw, A. Introduction to Magnetochemistry, (1968) Academic Press.
11. Dutta, R.L.; Syanal, A. (1993) Elements of Magnetochemistry, Affiliated East West Press.
12. Drago, R. S. (1992) Physical Methods for Chemists, Saunders College Publishing.

Course Title: Organic Chemistry

L	T	P	Cr
3	0	0	3

Paper Code: CCC.510

Total Hours: 45

Learning Outcomes: The outcomes of this course is that students will be able to:

1. identify the reaction mechanism and its intermediates, aromaticity, different sets of aliphatic nucleophilic reaction, aromatic nucliophilic and electrophilic reaction, elimination reaction, addition reaction, which are the fundamental branches of organic chemistry.
2. understand how the computational techniques can be applied to study problems in computational organic chemistry.

Course Content

Unit I **12 Hours**

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: Hammett equation.

Reactive intermediates: Generation, structure and reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzynes. Neighbouring group participation, classical and non-classical carbocations.

Unit II **13 Hours**

Aliphatic nucleophilic substitution reaction: The S_N2, S_N1, mixed S_N2 and S_N1 and SET mechanism, the S_Ni 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 betweenS_N2 and S_N1 mechanisms.

Aromatic nucleophilic substitution: The S_NAr, bimolecular displacement mechanism and benzyne 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 III **10 Hours**

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures.

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 IV **10 Hours**

Addition to carbon-hetero multiple bonds: Structure and reactivity of carbonyl group towards nucleophilic addition: addition of CN, ROH, RSH, H_2O, hydride ion, ammonia derivatives, $LiAlH_4$, $NaBH_4$, organozinc and organolithium reagents to carbonyl and conjugated carbonyl compounds, Arndt-Eistert synthesis. Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Dieckmann, Mannich, Benzoin, Perkin and Stobbe reactions..

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

Suggested Readings

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012) Organic Chemistry, Oxford University Press.
2. Finar, I.L. (2012) Organic Chemistry Volume 1, Pearson Education UK.

3. McMurry J. (2011) Organic Chemistry, Asian Book Pvt. Ltd, New Delhi
4. Smith, M. B. March's (2013) Advanced Organic Chemistry: Reactions, Mechanisms and Structure, John Wiley & Sons.
5. Ahluwalia, V. K. and Parashar R. K. (2011) Organic Reaction Mechanism, Narosa Publishing House (P) Ltd., New Delhi.
6. Bansal, R. K. (2010) A text book of Organic Chemistry, New Age International (P) Ltd., New Delhi.
7. Bansal R.K. (2010) Organic Reaction Mechanism, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S. (2010) Organic Reactions and Their Mechanisms. New Age International, New Delhi.
9. Kalsi, P.S. (2010) Stereochemistry: Conformation and Mechanism, New Age International Ltd, New Delhi.
10. Lowry, T. H. and Richardson K. S. (1998) Mechanism and Theory in Organic Chemistry, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T. and Boyd, R.N. (2011) Organic Chemistry, Prentice-Hall of India, New Delhi.
12. Mukherjee, S.M. and Singh, S.P. (2009) Reaction Mechanism in Organic Chemistry. Macmillan India Ltd., New Delhi.
13. Robert, J. D. and Casereo, M.C. (1977) Basic principle of Organic Chemistry, Addison-Wesley.
14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A. (2013) Organic Chemistry. John Wiley and Sons, Inc.
15. Sykes, P. A (1997) Guide Book to Mechanism in Organic Chemistry, 1997, Prentice Hall.
16. Eliel, E. L. and Wilen, S. H. (1994) Stereochemistry of Organic Compounds, John Wiley & Sons.

SEMESTER II

Course Title: Electronic Structure Theory

L	T	P	Cr
3	0	0	3

Paper Code: CCC.556
Total Hours: 45

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 corse.
- describe the HF SCF method.
- select the basis sets.
- compare post-HF methods.
- devlop how to apply quantum chemistry to study chemical and biochemical problems.

Course Content

Unit I **13 Hours**

Review of molecular structure calculations and Hückel Molecular Orbital Theory, Hartree products and Hartree-Fock Approximation. One and Two-Electron Integrals, General Rules, Coulomb and Exchange Integrals,

Unit II **12 Hours**

Second-Quantized Operators and Matrix Elements. The Fock Operator, HF Equations, Roothaan Equations, SCF Procedure.

Unit II **10 Hours**

Polyatomic Basis sets, Minimal, Double zeta, triple zeta and Polarized basis sets.

Unit IV **11 Hours**

Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method.

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

Suggested Readings

1. F. Jensen, (2006) Introduction to Computational Chemistry, Wiley-Blackwell.
2. P. W. Atkins and R. S. Friedman, (1997) Molecular Quantum Mechanics, OUP, Oxford.
3. H. Eyring, J. Walter and G.E. Kimball, (1944) Quantum Chemistry, John Wiley, New York (1944).
4. I.N. Levine, (2000) Quantum Chemistry, Pearson Educ., Inc., New Delhi.

5. A. Szabo and N. S. Ostlund, (1982) Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, Dover, New York (1982).

Course Title: Fundamentals of Molecular Simulations

L	T	P	Cr
3	0	0	3

Paper Code: CCC.554
Total Lectures: 45

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

- explain the modelling of small to large molecular environments
- execute various force field for biomoleculra simulation in details
- demonstrate different methods for simulating large systems
- distinguish the knowledge about different molecular simulation techniques
- describe 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.

Course Content

Unit I **11 Hours**

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 **11 Hours**

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 **12 Hours**

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

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

Unit IV **11 Hours**

Simulation Methods:

Monte Carlo: The Metropolis method

Molecular Dynamics: (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method (f) Pressure Control: Andersen's Method.

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

Suggested Readings

1. M.P. Allen and D.J. Tildesley, (2017) Computer Simulation of Liquids 2nd Edition, Oxford University Press.

2. D. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.

3. A. R. Leach, (2001) Molecular Modelling Principles and Applications 2nd Edition. Pearson.

4. S. Alavi, (2020) Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.

Course Title: Computational Methods

L	T	P	Cr
3	0	0	3

Paper Code: CCC.525

Total Hours: 45

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

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

Course Content

Unit I **11 Hours**

Introduction: Errors, Siccessive Approximation, Taylor's Series, Polynomial Evaluation

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

Unit II **11 Hours**

System of Linear Algebraic Equations: System of Linear Equations, Guass Elimination Method, Importance of Diagonal Dominance, Gauss Seidel Iteration Method, Matrix Inversion Method: Gauss-Jordan's Matrix-Inversion Method

Unit III **13 Hours**

Interpolations: Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms

Numerical differentiation and integration: Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor's series, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration.

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

Unit IV **10 Hours**

Numerical Solution of Differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

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

Suggested Readings

1. V. Rajaraman, (1993) Computer Oriented Numerical Methods, PHI.
2. E. Balaguruswamy, (2017) Numerical Methods, Tata McGraw Hill.
3. F.Acton, (1997) Numerical Methods that Work, Harper and Row.
4. S. D. Conte and C.D.Boor, (2005) Elementary Numerical Analysis, McGraw Hill.
5. S. S. Shastri, (2012) Introductory Methods of Numerical Analysis, PHI.

Course Title: Solid State Physics

L	T	P	Cr
3	0	0	3

Paper Code: PCP.525
Total Lectures: 45

Learning Outcomes: The course on Solid State Physics is to provide the student with a clear and logical presentation of the basic and advanced concepts and principles of the physics for solid state.
At the end of the course, the students will be able to:

- learn the various types of crystal structure, and x-ray diffraction methods
- interpret the lattice vibrations and band theory of solids
- gain deep knowledge on magnetic properties of solids, defects, superconductivity

which will help them to apply these techniques in investigating the aspects of the matter in condensed phase.

Course Content

Unit I **12 hours**

Crystal Structure: Bravais lattices, Crystal structures, Reciprocal lattices, Ewald sphere, Lattice parameter determination, Atomic and crystal structure factors

X-ray diffraction: X-ray diffraction, Bragg law, Laue equations, Concept of reciprocal lattice and Ewald's construction. Experimental diffraction methods: Laue rotating crystal method and powder method.

Unit II **11 hours**

Electronic properties and band theory: Electronic structure of solids-band theory, Refinement of simple band theory- k-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, p-n junctions, Defects in solids

Unit III **11 hours**

Magnetic Properties: Behavior of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

Unit IV **11 hours**

Superconductivity: Meissner effect, Type-I and type-II superconductors; BCS theory, Flux quantization, Coherence, AC and DC Josephson effect, Superfluity, High TC superconductors and their applications.

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

Suggested Readings

1. J. Ziman, (2011) *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, U.K.).
2. C. Kittel, (2007) *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India).
3. R.J. Singh, (2011) *Solid State Physics* (Pearson, New Delhi, India).
4. A.J. Dekker, (2012) *Solid State Physics* (Macmillan, London, U.K.).
5. N. W. Ashcroft and N. D. Mermin, (2003) *Solid State Physics* (Thomson Press).
6. A.R. Verma and O.N. Srivatava, (2012) *Crystallography Applied to Solid state physics* (New Age International).

Course Title: Atomic and Molecular Spectroscopy

L	T	P	Cr
3	0	0	3

Paper Code: PCP.557
Total Lectures: 45

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 Content

Unit I **12 hours**

Atomic Spectra: Revision of quantum numbers, electron configuration, Hund's rule etc. origin of spectral lines, LS & JJ coupling , selection rules, Spectrum of hydrogen, helium and alkali atoms, X-ray spectra, fine spectra, hyperfine structure, Width of spectrum lines.

Unit II **11 hours**

Molecular Spectra: Molecular potential, Separation of electronic and nuclear wave functions, Born-Oppenheimer approximation, Electronic, Vibrational and rotational spectrum of diatomic molecules, Selection rules, Frank-Condon principle,

Unit III **11 hours**

Molecular Spectroscopy: Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO2), FT-IR instrumentation

Unit IV **11 hours**

Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines, Vibrational spectroscopy of diatomic molecules, Franck-Condon factor, rotational fine structure.

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

Suggested Readings

1. J. M. Hollas, (2004) Modern Spectroscopy, John Wiley & Sons, Ltd. .
2. G. M. Barrow, (1962) Introduction to Molecular Spectroscopy, McGraw-Hill .
3. C. N. Banwell and E.M. Mc Cash, (1994) Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, New Delhi .
4. L. R. Lakowicz, (2006) Principle of Fluorescence Spectroscopy 3rd Edition, Springer.
5. A. Carrington and A. D. Mc Lachlan, (1979) Introduction to Magnetic Resonance Chapman and Hall, London.
6. R. K. Harris, (1986) Nuclear Magnetic Resonance Spectroscopy, Addison Wesley, Longman Ltd, London .
7. C.J. Foot, (2005) Atomic Physics (Oxford University Press, Oxford, U. K.

Course Title: Machine learning and Data Science

L	T	P	Cr
3	0	0	3

Course Code: CCC.521
Total Lectures: 45

Learning Outcomes: On completion of the course the student should be able to:

- learn the data cleaning, cross-validation, and application of regression analysis
- gain knowledge about distance matrices, various methods of clustering as well as dimensionality reduction
- apply several techniques for information retrieval and text mining

Course Content

Unit I **10 Hours**

Introduction: Overview of Machine Learning field, terminology alert: true positive, false positive, Confusion matrix, Bias and variance

Unit II **12 Hours**

Unsupervised Methods: Clustering: Distance Metrics, K-Means, leader, Jarvis-Patrick, hierarchical clustering; Dimensionality Reduction: Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA)

Unit III **12 Hours**

Supervised Methods: Classification: k-nearest neighbors algorithm (K-NN), naïve Bayes, decision trees, boosting and bagging

Unit IV **11 Hours**

Classification: Ensemble methods, random Forests; Support vector machines Neural networks, Recommendation systems; Outlier detection.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Helder I., N. (Ed.). (2021). Bioinformatics. Exon Publications.
2. Alonso-Betanzos, A., & Bolón-Canedo, V. (2018). Big-Data Analysis, Cluster Analysis, and Machine-Learning Approaches. Advances in experimental medicine and biology, 1065, 607–626. https://doi.org/10.1007/978-3-319-77932-4_37
3. Max Kuhn and Kjell Johnson, (2013). Applied Predictive Modeling.
4. James, Witten, Hastie, Tibshirani, (2014). An Introduction to Statistical Learning and Applications in R.
5. Wes McKinney, (2013). Python for Data Analysis.
6. Han, Kamber, and Pei, (2011) Data Mining: Concepts and Techniques, 3rd Edition.

Course Title: Molecular Evolution

L	T	P	Cr
3	0	0	3

Course Code: LBI.524

Total Hours: 45

Learning Outcomes: After completing the course the student should be able to

- describe evolutionary processes that give rise to variation in sequences and genomes and how these influence the architecture of the genome, contents and variation in base composition
- explain and justify different models for sequence and genome evolution
- choose, apply and evaluate bioinformatics methods for studying genetic variation in and between species.

Course Content

Unit I **12 Hours**

Comparison of DNA sequences to calculate gene distance; Convergent and

divergent evolution; Mutation Vs. Substitution-Rate of Molecular Evolution. Jukes Cantor Correction and evolutionary distance

Unit II **12 Hours**

Genome evolution, RNA structure and evolution, Compensatory substitutions and the
comparative method, Fitting evolutionary models to sequence data, The influence of thermodynamics on RNA sequence evolution

Unit III **10 Hours**

Molecular clock- Concepts and significance-molecular mechanisms of molecular clock- Neutral theory -gene family organization. Applications of molecular phylogenetics

Unit IV **11 Hours**

Paralogy and Orthology- coordination expression in evolution-genome: content, structure and evolution. Molecular evolution of recently diverged species - Databases of Molecular evolution.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Darwin, C.R. (1911). On the origin of species by means of natural Selection, or preservation of favoured races in the struggle for life. Hurst Publishers, UK.
2. Dawkins, R. (1996). The Blind Watchmaker, W.W. Norton & Company Jones and Bartlett Publishers.
3. Futuyma, D.J. (2009). Evolution. Sinauer Associates Inc. USA
4. Bromham, L. (2016). An Introduction to Molecular Evolution and phylogenetics. OUP Oxford.
5. Warnow, T.(2019) Bioinformatics and Phylogenetics.Springer International Publishing, ISBN 978-3-030-10836.

Web Resources

1. http://www.bioinf.wits.ac.za/software/fire/evodb/
2. https://www.megasoftware.net/

Web Resources

https://www.youtube.com/playlist?list=PLblh5JKOoLUICTaGLRoHQDuF_7q2GfuJF
https://www.youtube.com/playlist?list=PLblh5JKOoLUKxzEP5HA2d-Li7IJkHfXSe

Course Title: Biomolecular Structure Modelling and Drug Designing

L	T	P	Cr
3	0	0	3

Course Code: LBI.526
Total Hours: 45

Learning Outcomes: On completion of the course the student should be able to:

1. describe different types of protein–ligand interactions and characterise binding pockets
2. use different search methods to find compounds with specific properties in large compound databases
3. set up, perform and evaluate different virtual screening methods using large datasets
4. account for and set up molecular dynamics simulations and free energy calculations

Course Content

Unit I **10 Hours**

Basics of Biomolecules: Principles of protein and nucleic acid structure: Primary, Secondary, Tertiary structure and Quaternary structure. Protein secondary structure: Introduction, Hydrogen bond, Defining a secondary structure element, Methods for predicting secondary structure

Unit II **12 Hours**

Protein tertiary structure modeling: Basic concepts, Protein folding

and Energetics, Comparative modeling, Threading, Ab initio modeling, Modeling protein sidechains, CASP: A blind protein structure prediction competition, CAPRI, Protein Structure Initiative (PSI).

Unit III **12 Hours**

Introduction to drug designing, ADMET, drug metabolism, toxicity and pharmacokinetics. lipinski rule of 5, Identification and validation strategies. Drug Target classification, Concept of Pharmacophore, Functional group considered as pharmacophore, Structure-based drug design, docking, QSAR

Unit IV **11 Hours**

Modelling macromolecular structure: Homology modeling, *ab-initio* structure modeling; Molecular Recognition: Prediction of Protein-ligand interaction sites, Prediction of Protein-protein interaction sites, Prediction of Protein-membrane interaction sites, Prediction of Protein-nucleic acid interaction sites

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Hybrid Biomolecular Modeling. (2019). (n.p.): Frontiers Media SA. ISBN:9782889456994
2. Biomolecular Modelling and Simulations. (2014). United Kingdom: Elsevier Science.ISBN:9780128007891
3. Molecular Modeling of Proteins. (2017). United States: Springer New York. ISBN:9781493954919
4. Biomolecular Simulations in Structure-Based Drug Discovery. (2019). Germany: Wiley. ISBN:9783527342655
5. Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo Molecular design : concepts and applications Weinheim: Wiley-VCH, c2008
6. Andrew R.Leach Molecular Modelling Principles and applications. (2001) II ed. Prentice Hall.

Course Title: Physical Chemistry

L	T	P	Cr
3	0	0	3

Paper Code: CCC.517
Total Hours: 45

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

- undestand 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.
- investigate how the computational techniques can be applied to study problems in advanced physical chemistry.
- 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.

Course Content

Unit I **12 Hours**

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 II **10 Hours**

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, CO_2 phase transition, binary and ternary component phase transitions. Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

Unit III **12 Hours**

Electrochemistry: Ionic equilibria, electrolytic conductance –Kohlrausch's Law, Activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law, and conductometric titrations.

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 IV **11 Hours**

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.

Adsorption and Catalysis: Colloids and their stability, Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm, Langmuir and Fredulich Isotherms. Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Kinetics of catalytic reactions.

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

Suggested Readings

1. Barrow, G. M. (2007) Physical Chemistry, Tata McGraw-Hill.
2. Kapoor, K. L. (2011) Text Book of Physical Chemistry, Volume 2-3,5, Macmillan.
3. Atkins, P. and De Paula, J. Atkins' (2009) Physical Chemistry. Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. (1998) Physical Chemistry: A Molecular Approach, Viva Books.
5. Moore, J. W. and Pearson, R. G. (1981) Kinetics and Mechanism, John Wiley and Sons.
6. Engel, T., Reid, P. and Hehre, W. (2012) Physical Chemistry, Pearson Education.
7. Rastogi, R. P. and Mishra, R. R. (2013) An Introduction to Chemical Thermodynamics, Vikas Publishing
8. Rajaram, J. and Kuriacose, J. C. (2013) Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics, Pearson Education.
9. Laurendeau N. M. (2005) Statistical Thermodynamics: Fundamentals and Applications, Cambridge University Press.
10. Nash, L. K. (2012) Elements of Statistical Thermodynamics, Dover Publication Inc.
11. Hill, T. L. (1986) An Introduction to Statistical Thermodynamics, Dover Publications Inc.

Course Title: Physical Organic Chemistry

L	T	P	Cr
3	0	0	3

Paper Code: CCC.514
Total Lectures: 45

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

- identify chemical bonding, aromaticity, structure and stereochemistry, steric and conformational properties, chemical reactivity, correlation of structure with reactivity, Hammond postulates, solvent effects, acidity, nucleophilicity, electrophilicity.
- demonstarte reaction mechanisms, isotope effects Woodward Hoffmann rules.

Course Content

Unit I **10 Hours**

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

Unit II **13 Hours**

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

Unit III **10 Hours**

Steric and conformational properties: Origins of steric strain, examples of steric effects upon reactions, measurement of steric effects upon rates.
Solvent 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 **12 Hours**

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.

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

Suggested Readings

1. Neil S. Isaacs, (1995) *Physical Organic Chemistry*, PHI.
2. E. V. Anslyn & D. A. Dougherty, (2005) *Modern Physical Organic Chemistry*, Illustrated Edition,University Science Books.
3. Francis A. Carey and Richard J. Sundberg, (2007) *Advanced Organic Chemistry*, Part A, Structure and Mechanisms, Springer.
4. Jerry March, (1999) *Advanced Organic Chemistry, Reactions, Mechanims and Structure*, John-Wiley.
5. Thomas H. Lowry, Kathleen S. Richardson, (1981) *Mechanism and Theory in Organic Chemistry*, Harper & Row.
6. S. P. Gupta, (2011) *QSAR and Molecular Modeling*, Anamaya Publishers.

Course Title: Statistics for Chemical and Biochemical Applications

L	T	P	Cr
3	0	0	3

Paper Code: CCC.513
Total Lectures: 45

Learning Outcomes: This course will introduce the basic aspects of various industry based statistical methods to students which will be used to compare different results.

Course Content

Unit I **10 Hours**

Overview of Biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Unit II **12 Hours**

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

Unit III **10 Hours**

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

Unit IV **12 Hours**

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, χ^2 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.

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

Suggested Readings

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley, USA.

2. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc. USA.

3. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials.* 3/e (with SPSS). Decker Inc. USA.

4. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*. W.H. Freeman publishers, USA.

5. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley, USA.

SEMESTER III

Course Code: CCC.551

Course Title: Research Methodology

L	T	P	Cr
3	0	0	3

Total Hours: 45

Learning Outcomes: The course Research Methodology has been framed to introduce basic concepts of Research Methods. The course covers preparation of research plan, reading and understanding of scientific papers, scientific writing, research proposal writing, ethics, plagiarism, computer laboratory safety issues etc.

Course Content

Unit I **12 hours**

Introduction: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Hypothesis formulation and development of research plan, Art of reading and understanding scientific papers, Literature survey, Interpretation of results and discussion.

Unit II **12 hours**

Library: Classification systems, e-Library, Reference management, Web-based literature search engines, Intellectual property rights (IPRs). **Entrepreneurship and Business Development:** Importance of entrepreneurship and its relevance in career growth, Types of enterprises and ownership.

Unit III **11 hours**

Scientific and Technical Writing: Role and importance of communication, Effective oral and written communication, Scientific writing, Research paper writing, Technical report writing, Making R and D proposals, Dissertation/Thesis writing, Letter writing and official correspondence, Oral and poster presentation in meetings, Seminars, Group discussions, Use of modern aids; Making technical presentations.

Unit IV **10 hours**

Research and Academic Integrity: Plagiarism, Copyright issues, Ethics in research, and case studies. Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials.

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

1. R. Kumar, *Research Methodology*, (2012), SAGE Publications India Pvt. Ltd., New Delhi, India.

2. S. Gupta, *Research Methodology and Statistical techniques*, (2005), Deep and Deep Publications (P) Ltd. New Delhi, India.

C. R. Kothari, *Research Methodology*, (2008) New Age International, New Delhi, India.

4. Standard /Reputed Journal authors' instructions.

5. Web resources: www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.

6. Web resources: www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

Course Title: Density Functional Theory

L	T	P	Cr
3	0	0	3

Paper Code: CCC.529
Total Lectures: 45

Learning Outcomes: This is a specialization course for students of Computational Chemistry. At the end of the course, the students will be able to:

- identify basics of Density Functional Theory (DFT)
- discuss most popular framework of modern DFT.
- characterize the properties of molecules and materials
  After completion of this course, it will help the students to use different functional appropriately for different problems.

Course Content

Unit I **11 Hours**

Schrödinger equation for many particles system, Hartree theory, Identical particles and spin, Hartree-Fock theory, Antisymmetric wavefunctions and Slater determinant, Koopmans' theorem.

Unit II **12 Hours**

Idea of functional, Functional derivatives, Electron density, Thomos Fermi model, Hohenberg-Kohn theorems, Approximations for exchange-correlation: Local density approximation (LDA) and local spin density approximation (LSDA), Gradient expansion and generalized gradient approximation (GGA), Hybrid functionals and meta-GGA approaches.

Unit III **11 Hours**

Kohn-Sham formulation: Plane waves and pseudopotentials, Janak's theorem, Ionization potential theorem, Self consistent field (SCF) methods, Strengths and weaknesses of DFT.

Unit IV **11 Hours**

Free electron theory, Band theory of solids, Tight-binding method, Semiconductors, Band structure, Density of states. Interpretation of Kohn-Sham eigenvalues in relation with ionization potential, Fermi surface and band gap.

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

Suggested Readings

1. R. M. Martin, (2004) Electronic Structure: Basic Theory and Practical Methods, Cambridge University Press.
2. R. G. Parr and W. Yang, (1994) *Density Functional Theory of Atoms and Molecules*, Oxford University Press.
3. D. S. Sholl and J. A. Steckel, (2009) *Density Functional Theory: A Practical Introduction* (John Wiley and Sons.
4. J. G. Lee, (2011) *Computational Materials Science: An Introduction*, CRC Press.
5. C. Kittel, (2007) *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi, India.
6. W. Koch, M. C. Holthausen, (2001) A Chemist's Guide to Density Functional Theory, 2nd Ed. Wiley-VCH.

Course Title: Computational Methods Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: CCC.528
Total Hours: 60

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

- demonstrate computer code for the large scale systems of transcendental and polynomial equations
- execute numerical strategies to write a computer code for the solution of matrix and determinants, interpolations, polynomial and spline interpolation
- construct 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.

Course Content

To write and execute computer programs in Fortran/Python language for the following problems:

1. Solution of transcendental or polynomial equations by the Newton Raphson method.
2. Matrix summation, subtraction and multiplication.
3. Matrix inversion using Gauss-Jordan's Matrix-Inversion Method.
4. Solution of Simultaneous Linear Equations: Gaussian Elimination, Gauss Seidel Iteration Method.
5. Finding Eigen values and Eigenvectors.
6. Newton/Lagrange interpolation based on given input data.
7. Numerical first order differentiation of a given function.
8. Numerical integration using Trapezoidal, Simpson's 1/3, Gaussian Quadrature methods.
9. Solution of first order differential equations using the Rung-Kutta method,
10. Monte Carlo integration.

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

Suggested Readings

1. Y.Kirani Singh and B.B.Chaudhuri, (2007) MATLAB Programming, Prentice-Hall India.
2. Rudra Pratap, (2006) Getting Started with Matlab 7, Oxford, Indian University Edition.
3. E. Balaguruswamy, (2017) Numerical Methods, Tata McGraw Hill.
4. V. Rajaraman, (2018) Computer oriented numerical methods, PHI Learning Pvt. Ltd.

Course Title: Computational Solid State Physics Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: PCP.526

Total Hours: 60

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

17. learn the computational methods for CSCl crystal structure determination
18. carry out the geometry optimization of molecular crystals
19. measure the Infrared spectra of crystals, and Raman spectra
20. interpret the dispersion relation and cut-off frequency for the mono-atomic lattice

which will enhance their employability in their further potential careers in academia and industry

Course Content

Student has to perform any of ten experiments from the following experiments.

1. Determine the crystal structure of CsCl using Gaussian package.
2. Geometry optimization of crystals using Gaussian package.
3. Determination of Infrared spectra of crystals using Gaussian package.
4. X-ray diffraction refinement using ICSD data.
5. Obtaining the structure of NaCl crystal system using Diamond software package.
6. Determination of Raman spectra using Gaussian package.
7. To determine magneto resistance of a bismuth crystal as a function of magnetic field.
8. Determination of critical temperature of high temperature superconductor and Meissner effect for a high Tc superconductor.
9. Determination of ferromagnetic to paramagnetic phase transition temperature (TC = Curie temperature).
10. Determination of dielectric constant of solids.
11. Study of the dispersion relation and cut-off frequency for the mono-atomic lattice. Study of the dispersion relation for the di-atomic lattice – 'acoustical mode' and 'optical mode' and energy gap.
12. Study of thermal expansion pf solids.
13. Study of thermal conductivity of solids.
14. Study of specific heat of solids.

Transactional Modes: Computation work, Experimentation and Viva-voce..

Suggested Readings

- J. Ziman, (2011) *Principles of the Theory of Solids,* Cambridge University Press, New Delhi.
- J. P. Srivastava, (2011) *Elements of Solid State Physics,* PHI Learning, New Delhi, India.
- R. J. Singh, (2011) *Solid State Physics,* Pearson, New Delhi, India.
- C. Kittel, (2014) *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi, India.

Course Title: Molecular Simulations Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: CCC.555
Total Hours: 60

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

- discuss the basics of Linux environment
- use the remote computing as a tool for high performance computation
- solve different energy minimization techniques
- design molecular model from scratch, and high definition images using various graphics tools
- execute the practical in-hand experience of various modeling and classical simulation tools
- construct the use of different insilico techniques for biomolecular simulations

which will enhance their employability in their further potential carrers in academia and industry

Course Content

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
6. Secondary Structure Prediction, Fold Recognition
7. Molecular Dynamics with GROMACS
    a. Water structure and dynamics
    b. Binary Mixtures
    c. HP36 in Water
    d. Serotonin1A in Membrane Bilayers
8. Review of Molecular Dynamics Principles

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

Suggested Readings

1. M.P. Allen and D.J. Tildesley, (2017) Computer Simulation of Liquids 2nd Edition, Oxford University Press.

2. D. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.
3. A. R. Leach, (2001) Molecular Modelling Principles and Applications 2nd Edition. Pearson.
4. S. Alavi, (2020) Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.

Course Title: Electronic Structure Theory Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: CCC.573
Total Hours: 60

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.

- Introduction to electronic structre calculations.
- Basis set dependency.
- HF and DFT methods related calculations.
- Carrying of conformational analysis of small molecules.
- MO and charge distribution calculations.
- Vibrational spectra calculations.
- 2D potential energy suface generation.
- Transition state calculations.
- Absorption spectra study.
- Calculations using solvent.
- Thermochemistry study.
- Post-HF based calculations
- Studying potential energy surface.
- Carrying of conformational analysis of large systems.
- Model chemistry.
- Study of NMR spectra
- QM/MM study.

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

Suggested Readings

1. David S. Sholl and Janice A. Steckel, (2009) *Density Functional Theory: A Practical Introduction,* John Wiley and Sons.

2. http://blogs.cimav.edu.mx/daniel.glossman/data/files/Libros/Exploring%20Chemistry%20With%20Electronic%20Structure%20Methods.pdf

3. Gaussian 09/16 website or manual.

Course Title: Enrich in Chemistry

L	T	P	Cr
2	0	0	2

Paper Code: CCC.570
Total Hours: 30

Course Content

Unit I **8 Hours**

Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.

Unit II **7 Hours**

Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

Unit III **8 Hours**

Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.

Unit IV **7 Hours**

Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis. Polymer chemistry: Molar masses; kinetics of polymerization.

Transactional Modes: Lectures; Problem solving; Self-learning.

Suggested Readings

1. Barrow, G. M. (2007) Physical Chemistry, Tata McGraw-Hill.

2. Kapoor, K. L. (2011) Text Book of Physical Chemistry, Volume 2-3,5, Macmillan.
3. Atkins, P. and De Paula, J. (2009) Atkins' Physical Chemistry. Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. (1998) Physical Chemistry: A Molecular Approach, Viva Books.
5. Moore, J. W. and Pearson, R. G. (1981) Kinetics and Mechanism, John Wiley and Sons.
6. Engel, T., Reid, P. and Hehre, W. (2012) Physical Chemistry, Pearson Education.
7. Rastogi, R. P. and Mishra, R. R. (2013) An Introduction to Chemical Thermodynamics, Vikas Publishing
8. Rajaram, J. and Kuriacose, J. C. (2013) Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics, Pearson Education.
9. Laurendeau N. M. (2005) Statistical Thermodynamics: Fundamentals and Applications, Cambridge University Press.
10. Nash, L. K. (2012) Elements of Statistical Thermodynamics, Dover Publication Inc.
11. Hill, T. L. (1986) An Introduction to Statistical Thermodynamics, Dover Publications Inc.

Course Title: Research Proposal

L	T	P	Cr
0	0	8	4

Paper Code: CCC.600
Total Hours: 120

Learning outcomes:

- Critically analyze, interpret, synthesize existing scientific knowledge based on literature review
- Demonstrate an understanding of the selected scientific problem and identify the knowledge gap
- Formulate a hypothesis and design an experimental/theoretical work

Students will prepare a research proposal based on literature review and extensive student-mentor interactions involving discussions, meetings and presentations. Each student will submit a research/dissertation proposal of the research work planned for the M.Sc. dissertation with origin of the

research problem, literature review, hypothesis, objectives, methodology to carry out the planned research work, expected outcomes and bibliography.

Students will have an option to carry out dissertation work in industry, national institutes or Universities in the top 100 NIRF ranking. Group dissertation may be opted, with a group consisting of a maximum of four students. These students may work using a single approach or multidisciplinary approach. Research projects can be taken up in collaboration with industry or in a group from within the discipline or across the discipline.

Evaluation Criteria:

The evaluation of the dissertation proposal will carry 50% weightage by supervisor and 50% by HoD and senior-most faculty of the department.

Dissertation Proposal (Third Semester)		
	Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation
HoD and senior-most faculty of the department	50	Dissertation proposal and presentation

Modes of transaction

Group discussions and presentations; Self-Learning; Experimentation

SEMESTER IV

Course Title: Dissertation

L	T	P	Cr
0	0	40	20

Paper Code: CCC.600
Total Hours: 600

Learning outcomes:

- Demonstrate an in-depth knowledge of scientific research pertaining to the area of study
- Demonstrate experimental/theoretical research capabilities based on rigorous hands-on training
- Critically analyze, interpret and present the data in light of existing scientific knowledge to arrive at specific conclusions
- Develop higher order thinking skills required for pursuing higher studies (Ph.D.)/research oriented career options

Students will carry out their research work under the supervision of a faculty member. Students will interact with the supervisors through meetings and presentations on a regular basis. After completion of the research work, students will complete the dissertation under the guidance of the supervisor. The dissertation will include literature review, hypothesis, objectives, methodology, results, discussion, and bibliography.

Evaluation Criteria:

The evaluation of dissertation in the fourth semester will be as follows: 50% weightage for continuous evaluation by the supervisor which includes regularity in work, mid-term evaluation, report of dissertation, presentation, and final viva-voce; 50% weightage based on average assessment scores by an external expert, HoD and senior-most faculty of the department. Distribution of marks will be based on report of dissertation (30%), presentation (10%), and final viva-voce (10%). The final viva-voce will be through offline or online mode.

Dissertation (Fourth Semester)

	Marks	Evaluation
Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce
External expert, HoD and senior-most faculty of the department	50	Dissertation report (30), presentation (10), final viva-voce (10)

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.