Central University of Punjab

M.Sc. Chemistry (Theoretical and Computational Chemistry)

Batch: 2025

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,

1. Understand the fundamentals and application of modern chemical and scientific theories in all branches of Chemical sciences.
2. Apply Mathematics and Computer Science to solve various complex chemical problems that are of interest in various interdisciplinary areas such as protein & drug modeling, material designing, energy surface, reaction pathway prediction, and computational tool development.
3. Apply the knowledge, competence, and computational skills needed in the industry, consultancy, education, research, or public administration.
4. Examine the complex information from the available scientific literature, identify the knowledge gap, shortlist attainable objectives, design comprehensive methodology, and successfully carry out research assignment and projects, both independently and in collaboration with others.

Therefore, the graduates of M.Sc. Chemistry (Theoretical and Computational Chemistry) would be a technically competing professional and can secure employment in academic/ research/ industry by undertaking this programme.

Course Structure of the Programme

SEMESTER I							
S.No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MPCP.401	Mathematics for Computational Sciences	CC	3	0	0	3
2	MCCC.516	Numerical Methods	CC	3	0	0	3
3	MCCC.523	Numerical Methods Lab (Practical)	SBC	0	0	4	2
4	MCCC.517	Quantum Chemistry	CC	3	0	0	3
5	MCCC.518	Statistical Mechanics	CC	3	0	0	3
6	MPCP.402	Python Programming Lab	SBC	0	0	4	2
		Individualized Education Plan/ Tutorial		0	2	0	0
Choose any one of these courses							
7	MCCC.520	Inorganic Chemistry	DE	3	0	0	3
8	MCCC.521	Organic Chemistry	DE	3	0	0	3
9	MCCC.522	Physical Chemistry	DE	3	0	0	3
				15	**2**	**8**	**19**

SEMESTER II							
S.No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MCCC.526	Fundamentals of Molecular Simulations	CC	3	0	0	3
2	MPCP.525	Physics and Chemistry of Solids	CC	3	0	0	3
3	MPCP.526	Computational Condensed Matter Lab	SBC	0	0	4	2
4	MPCP.527	Atomic and Molecular Spectroscopy	CF	2	0	0	2
5	MCCC.531	Molecular Simulations Lab (Lab)	SBC	0	0	4	2
6	MCCC.527	Electronic Structure Theory	CC	3	0	0	3
7	MCCC.530	Electronic Structure Theory Lab (Lab)	SBC	0	0	4	2
8	XXX.XXX	Interdisciplinary course	IDC	2	0	0	2
9	MPCP.511	Research Methodology	VAC	2	0	0	2

		Individualized Education Plan/ Tutorial		0	2	0	0
				15	**2**	**12**	**21**

SEMESTER III							
S.No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MCCC.599-1	Dissertation Part-I	SBE	0	0	40	20

SEMESTER IV							
S.No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MCCC.599-2	Dissertation Part-II	SBE	0	0	40	20

Semester	**L**	**T**	**P**	**Credits**
I	15	2	8	19
II	15	2	12	21
III	0	0	40	20
IV	0	0	40	20
Total	30	4	100	80

L: Lectures; T: Tutorial; P: Practical
CC: Core Course, DE: Discipline Elective, CF: Compulsory Foundation, IDE: Inter-Disciplinary Elective, SBC: Skill-based Core, DEC: Discipline Enrichment Course, SBE: Skill- based Elective, VAC: Value Added Courses

Total Credits Distribution:

S.No	**Types of Courses**	**No. of courses (Total credits)**			
		Sem-I	Sem-II	Sem-III	Sem-IV
1	Discipline Specific Core	4 (12)	3 (9)		
2	Skill enhancement (Practical, Dissertation/Internship)	2 (4)	3 (6)	1 (20)	1 (20)
3	Discipline Elective	1 (3)			
4	Interdisciplinary/ Multidisciplinary Course		1 (2)		
5	Foundation Course (Ability Enhancement / Compulsory Foundation)		1 (2)		
6	Value based		1 (2)		

One non-credit hour (two contact hours) for tutorial will be added for remedial teaching to cater to the learning needs of all the learners. The objective of this class is to facilitate the students to understand the concepts better and absorb and assimilate the content more effectively during extra hours.

MOOC: MOOCs may be taken up to 40% of the total credits (excluding dissertation credits). MOOC may be taken in lieu of any course, but the content of that course should match a minimum of 70%. The department will do mapping, and students will be informed accordingly.

Students will have an option to carry out dissertation work in industry, national institutes or Universities in the top 100 NIRF ranking.

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

Examination pattern and evaluation:

Formative Evaluation: Internal assessment shall be 25 marks using any two or more of the given methods: tests, open book examinations, assignments, term paper, etc. The Mid-semester test shall be a descriptive type of 25 marks, including short answer and essay type. The number of questions and distribution of marks shall be decided by the teachers.

Summative Evaluation: The End semester examination (50 marks) with descriptive type (up to 100%) and objective type (up to 30%) shall be conducted at the end of the semester. The objective type shall include one-word/sentence answers, fill-in-the-blanks, MCQs', and matching. The descriptive type shall include short answer and essay-type questions. The number of questions and distribution of marks shall be decided by the teachers. Questions for exams and tests shall be designed to assess course learning outcomes along with the focus on knowledge, understanding, application, analysis, synthesis, and evaluation.

The evaluation for IDC, VAC and entrepreneurship, innovation and skill development courses shall include MST (50 marks) and ESE (50 marks). The pattern of examination for both MST and ESE shall be the same as ESE described above for other courses.

Evaluation of dissertation proposal in the III semester shall include 50% weightage by supervisor and 50% by HoD and senior-most faculty of the department. The evaluation of the dissertation in the IV semester shall include 50% weightage for continuous evaluation by the supervisor/co-supervisor for regularity in work, mid-term evaluation, report of the dissertation, presentation, and final viva-voce; 50% weightage based on average assessment scores by an external expert. The distribution of marks is based on the report of dissertation (25), Presentation (10), Novelty/originality (5) and Final viva-voce (10). The external expert may attend the final viva-voce through offline or online mode.

Examination pattern from 2025-26 session onwards

Core, Discipline Elective, and Compulsory Foundation Courses			IDC, VAC, Entrepreneurship, Innovation and Skill Development Courses (<2 credits) or any other theory course of <2 credits	
	Marks	Evaluation	Marks	Evaluation
Internal Assessment	25	Various methods	-	-
Mid-semester test (MST)	25	Descriptive	50	Descriptive (up to 100%) Objective (up to 30%)
End-semester exam (ESE)	50	Descriptive (up to 100%) Objective (up to 30%)	50	Descriptive (up to 100%) Objective (up to 30%)

Dissertation Proposal (Third Semester)			Dissertation (Fourth Semester)		
	Marks	Evaluation		Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation	Supervisor / Co-Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce
HoD and senior-most faculty of the department	50	Dissertation proposal and presentation	External expert	50	Report of dissertation (25), Presentation (10), Novelty /originality (5) and Final viva-voce (10).

Marks for internship shall be given by the supervisor/internal mentor and external mentor.

Some Guidelines for Internal Assessment:

1. The components/pattern of internal assessment/evaluation should be made clear to students during the semester.
2. The results of the internal assessment must be shown to the students.
3. The question papers and answers to the internal assessment should be discussed in class.
4. The internal assessment shall be transparent and student-friendly, and free from personal bias or influence.

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

***Multiple entry and exit*:** As per UGC guidelines, students who exit after the first year of M.Sc. Bioinformatics shall be awarded the PG Diploma in Bioinformatics, provided the candidate fulfils the following eligibility.

Eligibility: Successfully completing the first year (two semesters) courses of M.Sc. Bioinformatics degree programme and earning 4 credits from any of the following skill development / Experiential learning options.

- Completion of Skill based course(s) from MO0C (approved in CDDC/AAC)
- Mini Project in the proposed specialized area of the PG Diploma
- Industrial training or Internship in the relevant domain

SEMESTER- I

Course Title: Mathematics for Computational Sciences
Paper Code: MPCP.401
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:

On completion of this course, students will be able to:
CLO1: Estimate the Matrices, Vector Calculus and Differential Calculus
CLO2: Lean to calculate the Integral calculus and Fourier Transforms
CLO3: Lean to calculate the complex functions as like Delta, Gamma, and Beta Functions
CLO4: Lean to calculate the second order partial differential equations

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 12 Hours	**Matrices & Vector Calculus:** matrix algebra, Cayley-Hamilton theorem, Eigenvalues and Eigenvectors **Differential calculus:** Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials **Learning Activities**: Brain-storming and Problem Solving	CLO1
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, coordinate transformations **Fourier Transforms:** Fourier series, Dirichlet condition, General properties of Fourier series, Fourier transforms, their properties and applications **Learning Activities**: Peer discussion, and Problem Solving	CLO2
III 11 Hours	**Delta, Gamma, and Beta Functions:** Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions. **Learning Activities**: Group discussions, and Class Quiz	CLO3
IV 11 Hours	Differential Equations Solutions of Hermite, Legendre, Bessel and Laguerre Differential equations, basics properties of their polynomials, and associated Legendre polynomials, **Learning Activities**: Brain-storming and Problem Solving	CLO4

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

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 .D. G. Zill. (2012). *Advanced Engineering Mathematics* Jones & Barlett Learning, Massachusetts, USA.
3. P. K. Chattopadhyay. (2000). *Mathematical Physics* New Age International (P) Ltd., New Delhi.

4. E.Steiner. (2008). The chemistry Mathematics Book, Oxford University Press .
5. F. Daniels. (1959). Mathematical for Physical Chemistry : Mc. Graw Hill.
6. Tebbutt. (1994). Basic Mathematics for Chemists, Wiley.
7. G. Arfken, H. Weber and F. Harris. (2012). *Mathematical Methods for Physicists* Elsevier Academic Press, Massachusetts, USA.
8. B.S. Rajput, (2016). *Mathematical Physics* Pragati Prakashan

Course Title: Numerical Methods
Paper Code: MCCC.516
Total Hours: 45

L	T	P	Cr
3	0	0	3

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

CLO1: Solve large-scale systems of linear, non-linear and simultaneous equations
CLO2: Solve matrix and determinants, interpolations, polynomial and spline interpolation
CLO3: Apply numerical differentiation and integration
CLO4: Apply complex curve fitting methods, explicit schemes to solve differential equations
CLO5: apply numerical methods to obtain approximate solutions of complex mathematical problems.

Units/ Hours	Contents	Mapping with CLO
I 13 Hours	**Introduction:** Errors, Successive 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. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 Hours	**System of Linear Algebraic Equations:** System of Linear Equations, Gauss Elimination Method, Importance of Diagonal Dominance, Gauss Seidel Iteration Method, Matrix Inversion Method: Gauss-Jordan's Matrix-Inversion Method **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
III 10 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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	**Numerical Solution of Differential Equations:** Picard's Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4 CLO5

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.
6. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press.

Course Title: Numerical Methods Lab (Practical)
Paper Code: MCCC.523
Total Hours: 60

L	T	P	Cr
0	0	4	2

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

1. Demonstrate computer code for the large- scale systems of transcendental and polynomial equations
2. Execute numerical strategies to write a computer code for the solution of matrix and determinants, interpolations, polynomial and spline interpolation
3. Construct the computer code for numerical differentiation and integration, differential equations, complex curve fitting, and simple optimisation
4. Apply numerical methods to obtain approximate solutions of complex mathematical problems.

Course Content

Computer Program design and branching structures, loop and character manipulation. Basic I/O concepts, formatted READ and WRITE statements, compiling, linking and executing the program. Introduction to file processing, introduction to arrays and procedures, additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable arrays in procedures, derived data types.

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 Eigenvalues 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 Runge-Kutta method,
10. Monte Carlo integration.

Transactional Modes: Laboratory based practical; 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.
5. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press

Course Title: Quantum Chemistry
Paper Code: MCCC.517
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:

On completion of this course, students will be able to:

CLO1: Apply the Schrödinger Equation for simple one particle systems,
CLO2: Apply the Schrödinger Equation for multi electron systems,
CLO3: Apply the Group Theory to solve the Schrödinger Equation,
CLO4: Apply Molecular Orbital Theory and HMO for molecules.

Units/Hours	Contents	Mapping with Course Learning Outcome
I 12 Hours	**Solving Schrödinger Equation for Simple Systems:** Free particle in 1D, particle in a box (1D, 3D), particle in a ring, scattering of particle in 1D. Harmonic oscillator, angular momentum, rigid rotor, Hydrogen like atom. **Learning Activities**: Peer discussion, Student seminars on recent developments	CLO1
II 11 Hours	**Approximation methods, many electron atoms:** Time-independent perturbation theory and applications. Variation method and applications. Time-dependent perturbation theory. Many electron atoms, Slater determinants and the Pauli principle, vector model of the atom. **Learning Activities**: Problem Solving, research paper discussion.	CLO2
III 11 Hours	**Group Theory:** Symmetry operations, Point groups, determination of point group of a molecule, representations of groups, the character, irreducible representations and their characters. **Learning Activities**: Brain-storming and Problem Solving	CLO3
IV 11 Hours	**Molecular Orbital Theory for Some Systems:** H2+, H2. Hückel method and applications. **Learning Activities**: Peer discussion, and Problem Solving	CLO4

Transaction Mode: Lecture, demonstration, tutorial, problem solving, online tools

Suggested Readings

1. I. N. Levine (2016), *Quantum Chemistry*, Pearson, India.
2. D. A. Mcquairre and J. D. Simon (2019), *Physical Chemistry: A Molecular Approach*, Viva Student Edition, India.
3. A. K. Chandra (2017), *Introductory Quantum Chemistry*, McGraw Hill Education, India.
4. H. Eyring, J. Walter, J. Walter (2022), *Quantum Chemistry*, Legare Street Press, India.
5. D. J. Griffiths (2015). *Introduction to Quantum Mechanics* Pearson Education, India.
6. V. K. Thankappan (2016). *Quantum Mechanics* New Age Pub. New Delhi.
7. J. J. Sakurai (2009). *Modern Quantum Mechanics* Pearson Education, India.

Course Title: Statistical Mechanics
Paper Code: MCCC.518
Total Hours: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:

On completion of this course, students will be able to:

CLO1: learn the postulates of statistical mechanics, Liouville's Theorem and statistical interpretation of thermodynamics

CLO2: identify the microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function, elementary probability theory, distributions and fluctuations

CLO3: learn the methods of statistical mechanics and their use to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases

CLO4: 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.

Units/ Hours	**Contents**	**Mapping with Course Learning Outcome**
I 12 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. **Learning Activities**: Brain-storming and Problem Solving	CLO1
II 11 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 **Learning Activities**: Peer discussion, and Problem Solving	CLO2
III 11 Hours	**Basic Thermodynamics:** Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function **Learning Activities**: Problem based learning sessions, Class quiz.	CLO3
IV 11 Hours	**Bose-Einstein distribution:** Einstein condensation. Thermodynamic properties of ideal BE gas. **Fermi-Dirac distribution:** Degenerate Fermi gas. Electrons in metals. Magnetic susceptibility. **Learning Activities**: Peer Discussion, and Research paper presentation.	CLO4

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

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.

L	T	P	Cr
0	0	4	2

Course Code: MPCP.402
Course Title: Python Programming (Lab)
Course type: Discipline Elective
Total Hours: 60

Course Learning Outcomes (CLO):

On completion of this course, students will be able to:

CLO1: Install the package for python programming, write, compile and run programs
CLO2: Perform various arithmetic and logical operations using python
CLO3: Apply conditioning and looping statements in python for different scientific problems
CLO4: Understand and employ different data structures and file operations to write elegant python programs

Course Content

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

1. Installation and basic demonstration of python package: PyCharm/IDLE
2. To understand different data types in Python: Variables, identifiers.
3. To perform basic arithmetic and logical operations in Python.
4. To understand and apply Python's operators: Arithmetic, logical, membership, Identity, Bitwise operators.
5. To understand and apply lists, tuples and string operations in python.
6. To understand and apply conditional statements using *If*, *if ...else* and *if-elif* statements.
7. To understand and apply looping statements in python: *For loop, nested loops, continue and break statements*
8. To employ and explore various built-in functions and modules in Python.
9. Writing own functions and modules in python.
10. To explore and apply different file processing options in python.
11. Writing Python Code with AI Chatbots.

Transactional Modes: Computation work, Programming, Problem Solving and Viva-voce.

Suggested Readings

1. S. Gowrishankar, A. Veena, (2019). *Introduction to Python Programming*, 1st Edition, CRC Press/Taylor & Francis.
2. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press
3. J. Vander Plas, (2016). *Python Data Science Handbook: Essential Tools for Working with Data*, 1st Edition, O'Reilly Media.
4. 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.
5. Wesley J Chun, (2015). Core *Python Applications Programming* 3rd Edition, Pearson Education India.

e-learning resources

1. https://www.edx.org/course/cs50s-introduction-to-programming-with-python
2. https://onlinecourses.swayam2.ac.in/cec22_cs20/preview
3. https://www.coursera.org/specializations/python

L	T	P	Cr
3	0	0	3

Course Title: Inorganic Chemistry

Paper Code: MCCC.520

Total Lectures: 45

Learning Outcomes:

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

CLO1: identify the metal-ligand equilibrium, transition metal complexes, ligand field theory, and crystal field theory, which are the fundamental branches of Chemistry.

CLO2: understand how the computational techniques can be applied to study problems in inorganic chemistry.

Units/ Hours	Contents	Mapping with Course Learning Outcome
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. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
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. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
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).	CLO1 CLO2
	Learning Activities: Brainstorming and problem solving, modelling and scaffolding.	

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	CLO1 CLO2
	fields, selection rules of electronic transitions in transition metal complexes. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	

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,4th edition, 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
Paper Code: MCCC.521
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: The outcomes of this course are that students will be able to:
CLO1: identify 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.
CLO2: understand how the computational techniques can be applied to study problems in computational organic chemistry.

Units/ Hours	Contents	Mapping with Course Learning Outcome
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.	CLO1 CLO2
	Learning Activities: Brainstorming and problem solving.	
II 13 Hours	**Aliphatic nucleophilic substitution reaction:** The S_N^2, S_N^1, mixed S_N^2 and S_N^1 and SET mechanism, the S_N^i 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_N^2 and S_N^1 mechanisms.	CLO1 CLO2
	Aromatic nucleophilic substitution: The S_N^{Ar}, 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. **Learning Activities**: Brainstorming and problem solving.	
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	CLO1 CLO2

	reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	
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.	CLO1 CLO2
	Learning Activities: Brainstorming and problem solving, modelling and scaffolding.	

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 textbook 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) GuideBook to Mechanism in Organic Chemistry, 1997, Prentice Hall.
16. Eliel, E. L. and Wilen, S. H. (1994) Stereochemistry of Organic Compounds, John Wiley & Sons.

Course Title: Physical Chemistry
Paper Code: MCCC.522
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes:
At the end of this course, students will be able to
CLO1: understand the thermodynamics, phase transition, fugacity, solid and liquid transitions.
CLO2: identify and describe thermodynamic properties of a system.
CLO3: apply thermodynamic properties for various systems.
CLO4: use the knowledge of phase equilibria for various systems.
CLO5: interpret various electrochemical phenomena.
CLO6: identify and describe differential rate laws, integrated rate laws, temperature dependence of reaction rates, and reaction mechanisms and parallel and consecutive reactions
CLO7: knowledge about catalysts and catalysed reactions.

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 12 Hours	Thermodynamics: The Zeroth Law of Thermodynamics, The First Law of Thermodynamics, Entropy and the Second Law of Thermodynamics, Entropy and the Third Law of Thermodynamics. Helmholtz and Gibbs Energies, Phase Equilibria. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2 CLO3 CLO4
II 10 Hours	Chemical Equilibrium: Gibbs energy is a minimum with respect to the extent to the extent of reaction, Equilibrium constant is a function of temperature, Standard Gibbs energies of formation is used to calculate Equilibrium constant, Direction of reaction spontaneity, Van't Hoff equation, Molecular partition functions and related thermodynamic data.	CLO1 CLO2 CLO3 CLO4
	Learning Activities: Brainstorming and problem solving.	
III 12 hours	Liquid-Liquid Solutions: Partial molar quantities, Gibbs-Duhem equation, Raoult's and Henry's law. 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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO5

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, steric factor, ionic reactions: salt effect. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO6 CLO7

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

Suggested Readings

1. D. W. Ball (2017), Physical Chemistry, Cengage India Pvt.
2. G. M. Barrow (2007), Physical Chemistry, Tata McGraw-Hill.
3. P. Atkins, and J. De Paula (2009), Physical Chemistry. Oxford University Press.
4. D. A. McQuarrie, and J. D. Simon (1998), Physical Chemistry: A Molecular Approach, Viva Books.
5. T. Engel, P. Reid, and W. Hehre (2012), Physical Chemistry, Pearson Education.
6. J. Rajaram, and J. C. Kuriacose (2013), Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics, Pearson Education.

SEMESTER II

Course Title: Electronic Structure Theory
Paper Code: MCCC.527
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes:

At the end of this course, students will be able to

CLO1: Identify and define basic terms and concepts which are needed for this specialized course.
CLO2: describe the HF SCF method.
CLO3: Select the basis sets.
CLO4: Learn basics of Density Functional Theory.
CLO5: develop how to apply quantum chemistry to study chemical and biochemical problems.

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 13 Hours	Hartree products and Hartree- Fock Approximation. One and Two-Electron Integrals, General Rules, Coulomb and Exchange Integrals, Configuration Interaction, Coupled Cluster Method. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 Hours	Second-Quantized Operators and Matrix Elements. The Fock Operator, HF Equations, Roothaan Equations, SCF Procedure. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
III 10 hours	Polyatomic Basis sets, Minimal, Double zeta, triple zeta and Polarized basis sets. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	Electron density, Thomas Fermi model, Hohenberg-Kohn theorems, Approximations for exchange-correlation: Local density approximation, Gradient expansion and generalized gradient approximation, Hybrid functionals and meta-GGA approaches. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4 CLO5

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
Paper Code: MCCC.526
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:
On completion of this course, students will be able to:
CLO1: learn the modelling of small to large molecular environments
CLO2: understand various force field for biomolecular simulation in details,
CLO3: learn different methods for simulating large systems,
CLO4: gain the knowledge about different molecular simulation techniques,
CLO5: understand the dynamics of the structural transitions

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 13 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. **Learning Activities**: Brain-storming and Problem Solving	CLO1 CLO2
II 10 Hours	**Methods for Simulating Large Systems** Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary Long-range Interactions – The Ewald Sum, The Reaction Field Method **Learning Activities**: Brain-storming and Problem Solving	CLO3
III 10 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? **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4
IV 12 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)	CLO5

	Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method (f) Pressure Control: Andersen's Method **Learning Activities**: Brain-storming and Problem Solving	

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: Physics and Chemistry of Solids
Paper Code: MPCP.525
Total Lecture: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):

On completion of this course, students will be able to:
CLO1: Identify and describe various types of crystal structure, and x-ray diffraction methods,
CLO2: Apply the band theory of solids and understand physical origin of band formation,
CLO3: Understand and describe magnetism and corresponding theories,
CLO4: Understand the phenomenon of superconductivity and different superconducting materials.

Units/ Hours	Contents	Mapping with CLO
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. **Learning Activities**: Brain-storming and Problem Solving	CLO1
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 **Learning Activities**: Brain-storming and Problem Solving	CLO2
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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO3
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. **Learning Activities**: Brain-storming and Problem Solving	CLO4

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. Srivastava, (2012). *Crystallography Applied to Solid state physics,* New Age International).

Course Title: Atomic and Molecular Spectroscopy
Paper Code: MPCP.527
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:
On completion of this course, students will be able to:
CLO1: Learn the various types of atomic spectra and corresponding their features,
CLO2: Learn the various types of Molecular spectra and corresponding their features
CLO3: Gain the knowledge about various molecular spectroscopic techniques,
CLO4: Apply the theories of molecular spectroscopy,

Units/ Hours	Contents	Mapping with Course Learning
		Outcome
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 spectral lines.	CLO1
	Learning Activities: Brainstorming and problem solving.	
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	CLO2
	Learning Activities: Brainstorming and problem solving.	
III 11 Hours	Molecular Spectroscopy: Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO2), FT-IR instrumentation	CLO3
	Learning Activities: Brainstorming and problem solving.	
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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4

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. McCash, (1994). *Fundamentals of Molecular Spectroscopy*
4. Tata McGraw Hill, New Delhi.

5. L. R. Lakowicz, (2012). *Principle of Fluorescence Spectroscopy*, Springer.
A. Carrington and A. D. Mc Lachlan, (1979). *Introduction to Magnetic Resonance*
6. Chapman and Hall, London.
7. R. K. Harris, Addison Wesley, (1986). *Nuclear Magnetic Resonance Spectroscopy*
8. Longman Ltd, London.
B. N. Banwell and E. M. McCash, (2012). *Fundamentals of Molecular Spectroscopy*, Tata, McGraw Hill Publishing Company Limited.
9. C.J. Foot, (2005). *Atomic Physics,* Oxford University Press, Oxford, U. K

Course Title: Computational Condensed Matter (Lab)
Paper Code: MPCP.526
Total Hours: 60

L	T	P	Cr
0	0	4	2

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

1. learn the computational methods for CSCl crystal structure determination
2. carry out the geometry optimization of molecular crystals
3. measure the Infrared spectra of crystals, and Raman spectra
4. 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

Students have to perform any of ten experiments from the following experiments.

1. Determine the crystal structure of CsCl using the 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 of 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

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

Course Title: Molecular Simulations Lab (Practical)
Paper Code: MCCC.531
Total Hours: 60

L	T	P	Cr
0	0	4	2

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
- Ddesign molecular model from scratch, and high- d e f i n i t i o n images using various graphics tools
- Execute the practical in-hand experience of various modeling and classical simulation tools
- Construct the use of different in silico techniques for biomolecular simulations which will enhance their employability in their further potential careers in academia and industry

Course Content

1. Linux basics and remote computing
2. Coordinate generations and interconversions of small molecules
3. Energy minimizations and optimization
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
6. Secondary Structure Prediction, Fold Recognition
7. Molecular Dynamics
    a. Water structure and dynamics
    b. Binary Mixtures
    c. HP36 in Water
    d. Serotonin 1A 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. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.
3. 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)
Paper Code: MCCC.530
Total Hours: 60

L	T	P	Cr
0	0	4	2

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 structure 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
3. Gaussian 09/16 website or manual.

Course Title: Research Methodology
Course Code: MPCP.511
Course type: VAC
Total Hours: 30

L	T	P	Cr
2	0	0	2

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Perform a Literature survey, critically analyse the scientific problem and develop a research plan
CLO2: Use reference management systems and perform literature reviews using online resources
CLO3: Describe the importance of IPR and develops interest in entrepreneurship
CLO4: Write a good technical report, manuscripts, and scientific proposals
CLO5: Appreciate the importance of Research and Academic Integrity and follow safety protocols

Units/ Hours	Contents	Mapping with CLO
I 8 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. **Learning Activities**: Research paper presentation, Writing and Evaluation of research proposals, Peer discussion.	CLO1
II 7 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. **Learning Activities**: Concept built with real examples, case studies, Student presentation Perform literature survey, Research paper presentation and group discussion.	CLO2, CLO3
III 8 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, Thesis writing, Oral and poster presentation, Seminars, Group discussions, Use of modern aids. **Learning Activities**: Project report /research article preparation as a group activity, Research paper presentation	CLO4
IV 7 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. **Learning Activities:** Case studies, Peer discussion, brainstorming, spontaneous quizzes	CLO5

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

1. Kumar, R. (2012). Research Methodology, SAGE Publications India Pvt. Ltd., New Delhi, India.
2. Gupta, S. (2005). Research Methodology and Statistical techniques, Deep and Deep Publications (P) Ltd. New Delhi, India.
3. Kothari, C.R. (2008). Research Methodology, New Age International, New Delhi, India.
4. Standard /Reputed Journal authors' instructions.
5. Denisova-Schmidt, E. (2021). Book Review: A Roadmap to the Future of Academic Integrity Research. Academy of Management Learning & Education.
6. Sutherland-Smith, W. (2008). Plagiarism, the Internet, and student learning: Improving academic integrity. Routledge.
7. Bretag, T. (Ed.). (2020). A research agenda for academic integrity. Edward Elgar Publishing.

Gould, J. R. (2020). Directions in Technical Writing and Communication. Routledge.

Semester III

Course Title: Dissertation
Course Code: MCCC.599-1
Course type: SBC
Total Hours: 600

L	T	P	Cr
0	0	40	20

Course Learning Outcomes (CLO):
On completion of this course, students will be able to,

CLO1: Demonstrate an in-depth knowledge of scientific research about the area of study
CLO2: Demonstrate experimental/theoretical research capabilities based on rigorous hands-on training
CLO3: Critically analyse, interpret, and present the data considering existing scientific knowledge to arrive at specific conclusions
CLO4: 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 (25), Presentation (10%), Novelty /originality (5) and Final viva-voce (10). The final viva-voce will be through offline or online mode.

Dissertation (Third Semester)		
	Marks	Evaluation
Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce
HoD and senior-most faculty of the department	50	Report of dissertation (25), Presentation (10%), Novelty /originality (5) and Final viva-voce (10).

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

Semester IV

Course Title: Dissertation
Course Code: MCCC.599-2
Course type: SBC
Total Hours: 600

L	T	P	Cr
0	0	40	20

Course Learning Outcomes (CLO):
On completion of this course, students will be able to,

CLO1: Demonstrate an in-depth knowledge of scientific research about the area of study
CLO2: Demonstrate experimental/theoretical research capabilities based on rigorous hands-on training
CLO3: Critically analyse, interpret, and present the data considering existing scientific knowledge to arrive at specific conclusions
CLO4: 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 (25), Presentation (10%), Novelty /originality (5) 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	50	Report of dissertation (25), Presentation (10%), Novelty /originality (5) and Final viva-voce (10).

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