Central University of Punjab



M.Sc. Chemistry
(Theoretical and Computational Chemistry)

Batch: 2026-2028

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	MCCC.515	Computational Methods for Molecular Structure Analysis	CF	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
10	MPCP.401	Mathematics for Computational Sciences	DE	3	0	0	3
11	MCCC.510	AI in Molecular Modeling	DE	3	0	0	3
12	MCCC.511	Machine Learning in 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	MCCC.528	Advanced Statistical Mechanics and Molecular Reaction Dynamics	CC	3	0	0	3
5	MCCC.531	Molecular Simulations Lab (Prac)	SBC	0	0	4	2
6	MCCC.527	Electronic Structure Theory	CC	3	0	0	3
7	MCCC.530	Electronic Structure Theory Lab (Prac)	SBC	0	0	4	2
8	XXX.XXX	Interdisciplinary course	IDC	2	0	0	2
9	MPCP.529	Research Methodology	VAC	2	0	0	2
		Individualized Education Plan/ Tutorial		0	2	0	0
				16	**2**	**12**	**22**

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	16	2	12	22
III	0	0	40	20
IV	0	0	40	20
Total	31	4	100	81

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	3 (9)	4 (12)		
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 (3)			
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. Chemistry (Theoretical and Computational Chemistry) shall be awarded the PG Diploma in Theoretical and Computational Chemistry, provided the candidate fulfils the following eligibility.

Eligibility: Successfully completing the first year (two semesters) courses of M.Sc. Chemistry (Theoretical and Computational Chemistry) 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: Computational Methods for Molecular Structural sAnalysis
Course Code: CCC.526
Total Hours: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):

On completion of this course, students will be able to:
CLO1: Describe the hierarchical organization of protein, nucleic acid, and small-molecule structures, and explain the physical forces governing their three-dimensional architecture.
CLO2: Interpret and analyze standard structural file formats and critically evaluate associated metadata for deposited structures.
CLO3: Apply the principles of X-ray diffraction, Fourier transformation, phase determination, and crystal symmetry, and interpret unit cell and crystallographic parameters.
CLO4: Apply structural superposition methods and perform quantitative comparative analysis of related molecular structures.
CLO5: Identify, classify, and quantitatively characterize non-covalent interactions in protein–ligand, protein–protein, and crystal-packing contexts.
CLO6: Assess macromolecular structure quality using geometric, stereochemical, and crystallographic validation metrics; interpret validation reports; and integrate these analyses to critically appraise structures in drug discovery and functional studies.

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	**Introduction to Molecular Structure and Data:** Hierarchy of Molecular Structure- Proteins, Nucleic acids and small molecules. Proteins: primary sequence, secondary structure motifs, tertiary fold, quaternary assembly. Nucleic acids: A, B, and Z-DNA helical parameters; RNA secondary motifs. Small molecules: constitutional isomers, stereoisomers, conformational isomers. Physical Forces Governing Molecular Structure: Covalent bonding, Electrostatic interactions, Van der Waals interactions, Hydrogen bonds, Hydrophobic effect, Pi-pi stacking. Three-dimensional Structure File Formats**:** PDB file format, mmCIF / PDBx format, Small molecule formats: MDL MOL/SDF, SMILES notation, InChI and InChIKey, MOL2, XYZ formats. Electron density map formats: CCP4 and MTZ reflection file structure. Structural Databases: RCSB PDB, Cambridge Structural Database (CSD), PubChem, ChEMBL, ZINC databases, Electron microscopy data bank (EMDB), AlphaFold DB.	CLO1 and CLO2
II 11 Hours	**Structure Determination: Methods and Mathematical Basis:** X-ray Crystallography: Physical Principles, Crystal lattice, unit cell, and the concept of periodicity, Bragg's law, Structure factors, Phase problem. Crystallographic Refinement and Data Quality: R-factor and R-free, Resolution and its effect on interpretability, B-factor, Occupancy refinement. NMR Spectroscopy for Structural Determination: Basics of the NMR experiment relevant to structure, quality metrics. Cryo-Electron Microscopy: Electron scattering from biological specimens, Single-particle analysis workflow, Comparison of X-ray, NMR and cryo-EM structural methods.	CLO3

III 12 Hours	**Computational Structural and Interaction Analysis:** Structural Superposition and Comparison: Rigid-body superposition, Root Mean Square Deviation, TM-score and MaxSub score, Multiple structure alignment. Geometric Analysis of Macromolecular Structures: Solvent-accessible surface area, Molecular volume, Cavity and pocket detection, Electrostatic surface potential calculation, B-factor profiles as measures of atomic mobility, Normal mode analysis. Non-Covalent Interaction Analysis: Hydrogen bonds, Salt bridges and ionic interactions, Hydrophobic contacts, Pi-pi stacking, Cation-pi interactions, Metal coordination, 2D interaction diagrams. Protein-Protein and Crystal Packing Interfaces: Interface area and its biological significance, Hot spot residues, Crystal contact analysis, Protein-nucleic acid interfaces, Molecular interaction networks.	CLO4 CLO5
IV 10 Hours	**Structure Validation, Quality Assessment and Applications:** Geometric and Stereochemical Validation: Ideal bond lengths and angles, Ramachandran plot analysis, Rotamer outliers and libraries, Clash score, Omega angle distribution, Cbeta deviation, MolProbity percentile score Crystallographic Quality Metrics: R-free/R-factor ratio, Local ligand validation, B-factor analysis, Completeness of diffraction data. Cryo-EM and NMR Validation: Q-score, EMRinger score, Map-model Fourier Shell Correlation. NMR validation: backbone completeness, side-chain assignment, restraint violation statistics. Small Molecule Structure Validation: Geometry Validation against Cambridge Structural Database, R-factor expectations for small molecule crystal structures, Disorder in small molecule crystals. Applications and Case Studies: Drug-receptor structural analysis, Crystal engineering and small molecule solid-state design, AI/ML methods in structural analysis of small and macromolecules.	CLO6

Transactional Modes: Lectures; project-based learning; seminars; group discussions; flipped classroom; team teaching; and self-directed learning.

Suggested Readings

1. Desiraju, G. R., Vittal, J. J. and Ramanan, A. (2012) Crystal Engineering: A Textbook., World Scientific Pub Co Inc, 1e
2. Klostermeier, D. and Rudolph, M. G. (2025) Biophysical Chemistry, CRC Press, 2e.
3. Blow, D. (2002) Outline of Crystallography for Biologists, Oxford University Press.
4. Lesk, A. M. (2014) Introduction to Bioinformatics, Oxford University Press, 4e.
5. Pal, S. (2020) Fundamentals of Molecular Structural Biology, Academic Press. ISBN: 9780128148556.
6. Lisacek, F. (2024) Protein Bioinformatics (Methods in Molecular Biology, Vol. 2836), Humana Press, New York, NY.
7. Timir Tripathi, Vikash Dubey, (2022) Advances in Protein Molecular and Structural Biology Methods, Academic Press, 1e.
8. Rupp, B. (2009) Biomolecular Crystallography: Principles, Practice, and Application to

Structural Biology, Garland Science.
9. Gu, J. and Bourne, P. E. (2009) Structural Bioinformatics, John Wiley & Sons, 2e.
10. Liljas, A., Liljas, L., Piskur, J., Lindblom, G., Nissen, P. and Kjeldgaard, M. (2016) Textbook of Structural Biology, World Scientific Publishing Co.
11. Branden, C. and Tooze, J. (1999) Introduction to Protein Structure, Garland Publishing Inc., 2e.
12. Kessel, A. and Ben-Tal, N. (2018) Introduction to Protein Structure, Function, and Motion, Chapman & Hall/CRC Press, 2e.

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: Develop understanding of linear algebra for new cutting-edge areas of computational sciences such as machine learning.

CLO2: Familiarization to the concepts of probability, statistics and optimization problem.

CLO3: Calculate the complex functions and the solutions of second-order partial differential equations.

CLO4: Calculate the Fourier and Laplace Transform and develop the understanding of computational Physics applications.

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	**Matrices:** Basic matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors, system of linear equations, particular and general solution, elementary transformations. Cholesky Decomposition, Eigen decomposition and Diagonalization. **Vector Calculus:** Vector spaces, linear dependence and basis. Inner product, orthogonality of vectors. Basis functions. Differentiation of univariate function, partial differentiation and gradients, Gradients and gradients of matrices. Higher order derivatives. Linearization and multi-variate Taylor series. **Learning Activities**: Peer discussion, Brain-storming and Problem Solving	CLO1
II 11 Hours	**Probability and distribution:** Construction of probability space, discrete and continuous probabilities, Sum rule, product rule and Baye's theorem. Summary statistic and independence, Gaussian distribution, Conjugacy and exponential family. Change of variables, inverse transformation. **Continuous optimization:** Optimization using gradient descent, constrained optimization, Lagrange's multipliers, convex optimization. **Learning Activities**: Brain-storming, group discussions 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. 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	CLO3
IV 11 Hours	**Fourier and Laplace transforms:** Definition, Existence Conditions (exponential order), Laplace of elementary functions. Periodic functions, Dirichlet's conditions, Odd & Even functions, Half-range Sine/Cosine series.	CLO4

	Computational Physics Applications: Harmonic oscillator (numerical, Damped oscillator, Nonlinear Pendulum, Projectile motion with air resistance, Potential well problem, Electric field computation **Learning Activities**: Brain-storming and Problem Solving	

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: Artificial Intelligence in Molecular Modeling
Paper Code: MCCC.510
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: Understand the basics of AI/ML
CLO2: Apply AI/ML techniques to chemical and biological systems
CLO3: Build predictive and generative models
CLO4: Work on real-world drug design problems

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 10 Hours	**Basics of Artificial Intelligence and Machine Learning:** AI overview and problem-solving approaches, Supervised vs unsupervised learning, Regression, classification, clustering, Neural networks and deep learning basics, Model evaluation and validation **Learning Activities**: Brain-storming and Problem Solving	CLO1
II 11 Hours	**Data Handling and Machine Learning in Molecular Modeling:** Molecular datasets (PDB, PubChem, ChEMBL), Feature engineering (descriptors, fingerprints), Data preprocessing and normalization, Dimensionality reduction (PCA, t-SNE), QSAR/QSPR modeling, Property prediction (toxicity, solubility, binding affinity), Classification of bioactive compounds, Model building using: (a) Random Forest; (b) SVM (c) Neural Networks **Learning Activities**: Peer discussion, and Problem Solving	CLO2
III 11 Hours	**Deep Learning for Molecular Systems:** Graph Neural Networks (GNNs), Convolutional Neural Networks (CNNs) in chemistry, Sequence-based models (RNNs, Transformers), Molecular embeddings and latent space **Learning Activities**: Group discussions, and Class Quiz	CLO3
IV 13 Hours	**Generative AI for Drug Design:** Virtual screening, Molecular docking + AI scoring, Binding affinity prediction, Lead optimization and ADMET prediction, SMILES-based generative models, Variational Autoencoders (VAE), GANs for molecule generation, Diffusion models, Reinforcement learning for drug design. **Advanced Topics:** Explainable AI (XAI) in chemistry, AI-assisted MD simulations, Cryo-EM structure prediction with AI, Materials modeling using AI, Python for molecular AI, Libraries: (a) RDKit, (b) TensorFlow / PyTorch, (c) Scikit-learn, Workflow automation and pipelines **Learning Activities**: Brain-storming and Problem Solving	CLO4

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

Suggested Readings

1. R. A. Devi, A. K. Saran, K. L. Mounika, D. Kanchana. (2026). *AI and Generative AI for Beginners.* Publisher Leilani Katie Publication and Press.
2. A. R. Leach. (2001). *Molecular Modelling: Principles and Applications.* Prentice Hall.
3. Editors: Manish Kumar Gupta, Sanjay Kumar, Krishna Misra. (2026). *The AI Frontier in Molecular Modelling and Drug Designing.* Academic Press.
4. Editors: Abhirup Khanna, May El Barachi, Sapna Jain, Manoj Kumar, Anand Nayyar. (2024). *Artificial Intelligence and Machine Learning in Drug Design and Development.* Wiley.

Course Title: Machine Learning in Chemistry
Paper Code: MCCC.511
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:
On completion of this course, students will be able to understand:
CLO1: The basics of ML and related mathematical basics
CLO2: Apply ML techniques for chemical data interpretation
CLO3: Deep learning for chemistry and applications
CLO4: The real-world chemical industry-based problems

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 10 Hours	**Foundations of Machine Learning, Mathematical and Statistical Basics :** Types of learning: supervised, unsupervised, reinforcement, Regression vs classification, Model evaluation (accuracy, RMSE, cross-validation), Overfitting and bias–variance trade-off Linear algebra (vectors, matrices, eigenvalues), Probability and statistics (distributions, Bayesian methods), Optimization techniques (gradient descent) **Learning Activities**: Brain-storming and Problem Solving	CLO1
II 10 Hours	**Chemical Data Representation and Common ML Algorithms in Chemistry:** Molecular descriptors (topological, geometric, electronic), Molecular fingerprints (e.g., Morgan fingerprints), SMILES and graph-based representations, Feature engineering for chemical datasets Linear & logistic regression, Decision trees and random forests, Support Vector Machines (SVM), k-Nearest Neighbors (k-NN), Clustering (k-means, hierarchical) **Learning Activities**: Peer discussion, and Problem Solving	CLO2
III 11 Hours	**Deep Learning for Chemistry:** Basics of neural networks, Convolutional Neural Networks (CNNs), Graph Neural Networks (GNNs) for molecules, Recurrent Neural Networks (RNNs) for sequence data **Applications in Chemistry:** Quantitative Structure–Activity Relationship (QSAR) modelling, Drug discovery and design, Predicting chemical properties (solubility, toxicity), Materials discovery, Reaction prediction and synthesis planning **Learning Activities**: Group discussions, and Class Quiz	CLO3
IV 14 Hours	**Programming and Tools:** Python programming, Libraries: (a) NumPy, Pandas (b) Scikit-learn (c) TensorFlow / PyTorch, Cheminformatics tools (e.g., RDKit) **Model Interpretation:** Explainable AI in chemistry, Feature importance and SHAP values, Data bias and reproducibility **Advanced Topics:** Transfer learning, Integration with quantum chemistry **Learning Activities**: Brain-storming and Problem Solving	CLO4

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning, Online tool.
Suggested Readings
1.R. U. Kumar, M. Sreenivasulu, A. Jain, S. Sharma. (2022). *Machine Learning for Absolute Beginners.* Book Rivers.
2.A. R. Leach. (2001). *Molecular Modelling: Principles and Applications.* Prentice Hall.
3.Editors: Manish Kumar Gupta, Sanjay Kumar, Krishna Misra. (2026). *The AI Frontier in Molecular Modelling and Drug Designing.* Academic Press.
4.Editor: H. M. Cartwright (2020). *MACHINE LEARNING IN CHEMISTRY: THE IMPACT OF ARTIFICIAL INTELLIGENCE: VOLUME 17 (Theoretical and Computational Chemistry Series),* Royal Society of Chemistry.
5. Editor: J. B. Ghasemi. (2022). *Machine Learning and Pattern Recognition Methods in Chemistry.*

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: identify and describe the basic art of scientific programming related to Fortran 95/2003.
CLO2: demonstrate concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
CLO3: develop skills to write programs related to standard problems and as well as to chemistry/physics.
CLO4: Solve large-scale systems of linear, non-linear and simultaneous equations.
CLO5: Apply numerical differentiation and integration
CLO6: Apply complex curve fitting methods, explicit schemes to solve differential equations.

Units/ Hours	Contents	Mapping with CLO
I 13 Hours	Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program. Constants and variables, assignment statements and arithmetic calculations Intrinsic functions, Program design and branching structures, loop and character manipulation. Basic I/O concepts, Formatted READ and WRITE statements, **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 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, What is parallel programming, Why use paralle programming, Parallel Architecture, **Learning Activities**: Brainstorming and problem solving.	CLO2 CLO3
III 10 hours	**Introduction:** Errors, Successive Approximation, Taylor's Series, Polynomial Evaluation. **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, modelling and scaffolding.	CLO4
IV 11 Hours	**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. Curve Fit: least square, straight line and polynomial fits. **Numerical Solution of Differential Equations:** 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.	CLO5 CLO6

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.

L	T	P	Cr
3	0	0	3

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

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.

Course Title: Python Programming Lab
Course Code: MPCP.402
Course type: CC
Total Hours: 45

L	T	P	Cr
3	0	0	3

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

CLO1: Describe Python Programming to build applications in their core domain.
CLO2: Write python scripts by using decision making command and loops
CLO3: Apply functions, modules and external packages in Programming
CLO4: Write programs by calling inputs and write specific output files

Units/ Hours	Contents	Mapping with CLO
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	CLO1
	Learning Activities: Peer discussion, brainstorming and Problem based learning sessions, Class quiz	
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	CLO2
	Learning Activities: Peer discussion on different code designing, Decoding quiz	
III 11 Hours	**Python Functions and Modules:** Defining custom functions, Organizing 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	CLO3
	Learning Activities: Brainstorming and Problem Solving code designing.	
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.	CLO4
	Learning Activities: Problem Solving code practice based on CSV files.	

Transaction Mode: Lecture, tutorial, problem solving

Suggested Readings

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

Course Title: Inorganic Chemistry

Paper Code: MCCC.520

Total Lectures: 45

L	T	P	Cr
3	0	0	3

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. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
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. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
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,	CLO1 CLO2

	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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO1 CLO2

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. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2 CLO3 CLO4
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

L	T	P	Cr
3	0	0	3

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

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	Credits
3	0	0	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Learn the various types of crystal structure, and x-ray diffraction methods,
CLO2: Apply the theories of lattice vibrations and band theory of solids,
CLO3: Learn about the magnetism corresponding their theories,
CLO4: Better understanding about superconductivity,

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: Advanced Statistical Mechanics and Molecular Reaction Dynamics

Paper Code: MCCC.528

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: identify and define basic terms and concepts of Phase transitions
CLO2: describe the Non-equilibrium dynamics
CLO3: learn the behavior of systems not far from equilibrium
CLO4: create potential energy surfaces for different small molecules
CLO5: explain the energetics of transition states of reactions

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 13 Hours	Review of Statistical Mechanical concepts, Phases & Phase Transitions: The Ising Model : Stability of Thermodynamics Phases, First-order Phase transitions, Interfaces, The Ising Model, Lattice Gas, Broken Symmetry, Mean Field Theory. **A brief introduction to Liquid Theory:** Averages, Distribution Functions, Reversible Work Theorem, Radial distribution function, Molecular liquids **Atomic and continuum models of liquids:** The Lennard-Jones Fluid, Molecular dynamics simulation, Correlation functions and measurements, elements of linear response theory, Linear models (a) Langevin equations (diffusion, friction and memory). (b) Gaussian fields (Debye-Huckel and beyond), The hard sphere model, WCA theory, Chemical equilibrium and relaxation. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 10 Hours	**Non-equilibrium systems:** Fluctuation-Dissipation Theorem, Onsager's Regression Hypothesis Brownian Motion, Friction and the Langevin Equation, Transport, Time Correlation Functions. **Special topics:** Free energy perturbation, The Jarzynski Equality, Electron transfer--quantum rare events--golden rule--Marcus theory, Path integrals, Tunneling—instantons, Ising model / Quantum correspondence, Monte Carlo and Biased Monte Carlo methods. **Learning Activities**: Brainstorming and problem solving.	CLO3
III 10 Hours	**Potential Energy Surfaces:** Long-range Potentials, Empirical Intermolecular Potentials, Molecular Bonding Potentials, Internal Coordinates and Normal Modes of Vibration, Ab Initio Calculation of Potential Energy Surfaces, Analytic Potential Energy Functions, Details of the Reaction Path. **Dynamics of Bimolecular Collisions:** Simple Collision Models, Two-Body Classical Scattering, Complex	CLO4

	Scattering Process. **Learning Activities**: Brainstorming and problem solving.	
IV 12 Hours	**Transition State Theory:** Basic Postulates and Derivation of Transition State Theory, Dynamical Derivation of Transition State Theory, Quantum Mechanical Effects in Transition State Theory, Thermodynamic Formulation of Transition State Theory, Applications of Transition State Theory.Unimolecular **Reaction Dynamics:** The Lindmann-Hinshelwood Mechanism, Statistical Energy-dependent Rate Constant, RRKM Theory, Applications of RRKM Theory to Thermal Activation. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4

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

Suggested Readings

1. Kerson Haung, Statistical Mechanics, Wiley, (2008).
2. R. K. Pathria and P. D. Beale, Statistical mechanics, Elsevier, (2011).
3. B. K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi (1998).
4. D. A. Mcquarrie, Statistical Mechanics, University Science Books (2011).
5. D. Chandler, Introduction to Statistical Mechanics, Oxford University Press (1987).
6. B. Widom, Statistical Mechanics- A concise Introduction for Chemists, Cambridge University Press (2002).
7. Terrell L. Hill, Statistical mechanics: principles and selected applications, Courier DoverPublications (1987).
8. J. I. Steinfeld, J. S. Francisco, and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall (1998).
9. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press (2009).
10. N. E. Henriksen F. Y. Hansen, Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics, Oxford University Press, USA (2012).
11. M. Brouard, Reaction Dynamics, Oxford Chemistry Primers (1998).
12. P. L. Houston, Chemical Kinetics and Reaction Dynamics, Dover Publications (2012).
13. S. K. Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer (2006).
14. K. J. Laidler, Chemical Kinetics, Pearson (2008).
15. A. H. Zewail, Femtochemistry-Ultrafast Dynamics of the Chemical Bond, World Scientific, New Jersey (1994).

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

L	T	P	Cr
0	0	4	2

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

- Create and visualize crystal structure of various substances using different software such as VESTA, Gaussian, XCRYSDEN
- Compute total energy and lattice parameters of crystals using ab initio density functional theory by using ELK and Quantum Espresso code
- Use open-source ELK & Quantum Espresso codes for computing different properties such as lattice parameters, electronic band structure, density of states, magnetic moment, phonon dispersions, specific heat and superconducting transition temperature.

Course Content

Student has to perform following computational experiments from the following experiments.

1. Creating the crystal structure, calculating the bond length and X-ray diffraction pattern for various crystals using VESTA software (NaCl, Diamond, CsCl, ZnS, Perovskite structures).
2. Compiling and installing ELK code and understanding the basic structure of ELK input file.
3. To understand the importance of convergence with respect to different computational parameters
4. To compute lattice parameters of different cubic (SC, FCC, BCC) crystals using ELK package.
5. To compute the electronic band structure and density of states (DOS) for simple crystals (Al, Cu, Si, Diamond, NaCl, GaAs) using ELK package.
6. To compute magnetic moment and spin resolved band structure and DOS for BCC iron and FCC Ni.
7. To compute the phonon dispersions and obtain various thermal properties using ELK code.
8. To compute the superconducting transition temperature of any material (Nb) within the McMillan formula using the ELK package.
9. Identify at least one research paper published in last 5 years and reproduce the results of the publication by employing ELK/Quantum Espresso code.

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-definition 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.

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