Central University of Punjab

M.Sc. Chemistry (Theoretical and Computational Chemistry)

Batch: 2023

Department of Computational Sciences

School of Basic Sciences

Graduate Attributes

In line with the syllabus of M.Sc. Chemistry (Theoretical and Computational Chemistry) it is expected that a student graduating after successful completion of the course shall be able to,

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.	**Paper Code**	**Course Title**	**Course Type**				
				L	T	P	Cr
1	PCP.506	Mathematics for Computational Sciences	CF	3	0	0	3
2	CCC.508	Scientific Programming	CF	3	0	0	3
3	CCC.515	Scientific Programming Lab (Practical)	SBC	0	0	4	2
4	PCP.527	Quantum Mechanics	CC	3	0	0	3
5	CCC.524	Statistical Mechanics	CC	3	0	0	3
6	PCP.519	Python Programming	CC	3	0	0	3
7	XXX	Tutorial		0	2	0	0
Choose any one of these courses							
1	BIM.511	Protein Engineering	DE	3	0	0	3
2	CCC.509	Inorganic Chemistry	DE	3	0	0	3
3	CCC.510	Organic Chemistry	DE	3	0	0	3
4	CCC.517	Physical Chemistry	DE	3	0	0	3
Total				18	2	4	20

SEMESTER – II							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	CCC.525	Numerical Methods	CC	3	0	0	3
2	CCC.554	Fundamentals of Molecular Simulations	CC	3	0	0	3
3	PCP.525	Solid State Physics	CC	3	0	0	3
4	CCC.528	Numerical Methods Lab (Practical)	SBC	0	0	4	2
5	PCP.526	Computational Solid State Physics Lab (Practical)	SBC	0	0	4	2
6	XXX.XXX	Interdisciplinary course (offered by other departments)	IDC	2	0	0	2
7	XXX	Tutorial		0	2	0	0
Interdisciplinary course offered for other departments							
	CCC.516	Chemistry without test tube	IDC	2	0	0	2
Choose any Two of these courses							
1	BIM.521	Big Data Analytics in Bioinformatics and Healthcare	DE	3	0	0	3
2	BIM.522	Cheminformatics	DE	3	0	0	3
3	BIM.523	Molecular Evolution	DE	3	0	0	3
4	CCC.526	Biomolecular Structure Modelling and Drug Designing	DE	3	0	0	3
5	CCC.514	Physical Organic Chemistry	DE	3	0	0	3
6	CCC.513	Statistics for Chemical and Biochemical Applications	DE	3	0	0	3
Total				17	2	8	21

SEMESTER – III							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	CCC.551	Research Methodology	CC	3	0	0	3
2	CCC.529	Density Functional Theory	CC	3	0	0	3
3	CCC.556	Electronic Structure Theory	CC	3	0	0	3
4	PCP.557	Atomic and Molecular Spectroscopy	CC	3	0	0	3
5	CCC.573	Electronic Structure Theory Lab (Practical)	SBC	0	0	4	2
6	CCC.555	Molecular Simulations Lab (Practical)	SBC	0	0	4	2
7	PCP.520	Entrepreneurship	CF	2	0	0	2
8	PCP.600	Dissertation Part-I	SBE	0	0	8	4
9	XXX.XXX	Value Added Course offered by other departments	VAC	2	0	0	2
10	XXX	Tutorial		0	2	0	0
Value Added Course offered for other departments							
	XXX.XXX	Introduction to Molecular Docking	VAC	2	0	0	2
Total				16	2	16	24

SEMESTER IV							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCC.601	Dissertation Part-II	SBE	0	0	40	20
Total				**0**	**0**	**40**	**20**
Grand Total				**85 Credits**			

Semester	L	T	P	C
I	18	2	4	20
II	17	2	8	21
III	16	2	16	24
IV	0	0	40	20
Total	**51**	**6**	**68**	**85**

L: Lectures; T: Tutorial; P: Practical

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.

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 70% descriptive type and 30% objective type 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 third 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 fourth semester shall include 50% weightage for continuous evaluation by the 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, HoD and senior-most faculty of the department. The distribution of marks is based on the report of the dissertation (30%), presentation (10%), and final viva-voce (10%). The external expert may attend the final viva-voce through offline or online mode.

Examination pattern from 2022-23 session onwards

Core, Discipline Elective, and Compulsory Foundation Courses			IDC, VAC, and Entrepreneurship, Innovation and Skill Development Courses	
	Marks	Evaluation	Marks	Evaluation
Internal Assessment	25	Various methods	-	-
Mid-semester test (MST)	25	Descriptive	50	Descriptive (70%) Objective (30%)
End-semester exam (ESE)	50	Descriptive (70%) Objective (30%)	50	Descriptive (70%) Objective (30%)

Dissertation Proposal (Third Semester)			Dissertation (Fourth Semester)		
	Marks	Evaluation		Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation	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, HoD and senior-most faculty of the department	50	Dissertation report (30), presentation (10), final viva-voce (10)

Marks for internship shall be given by the supervisor, HoD and senior-most faculty of the department.

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

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

L: Lecture, T: Tutorial, P: Practical

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

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.

SEMESTER- I

Course Title: Mathematics for Computational Sciences

Paper Code: PCP.506
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: Calculate the Integral calculus and Fourier Transforms
CLO3: Calculate the complex functions like Delta, Gamma, and Beta Functions
CLO4: 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. (2017). *Advanced Engineering Mathematics* Wiley India Pvt. Ltd., New Delhi, India.
2. B.S. Rajput, (2020). *Mathematical Physics* Pragati Prakashan
3. L. A. Pipes. (1985). *Applied Mathematics for Engineers and Physicist* McGraw-Hill, Noida, India.
4. D. G. Zill. (2012). *Advanced Engineering Mathematics* Jones & Barlett Learning, Massachusetts, USA.
5. P. K. Chattopadhyay. (2000). *Mathematical Physics* New Age International (P) Ltd., New Delhi.
6. E.Steiner. (2008). The chemistry Mathematics Book, Oxford University Press.
7. F. Daniels. (1959). Mathematical for Physical Chemistry: Mc. Graw Hill.
8. Tebbutt. (1994). Basic Mathematics for Chemists, Wiley.
9. G. Arfken, H. Weber and F. Harris. (2012). *Mathematical Methods for Physicists* Elsevier Academic Press, Massachusetts, USA.
10. A. Prudil, BJ Lewis (2021) Advanced Mathematics for Engineering Students: The Essential Toolbox, Butterworth-Heinemann Inc

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc21_ma27/preview
2. https://www.edx.org/course/mathematical-and-computational-methods
3. http://web.mit.edu/al24406/www/mathmeth.html

Course Title: Scientific Programming
Paper Code: CCC.508
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 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.

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 10 Hours	Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program. Constants and variables, assignment statements and arithmetic calculations **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 Hours	Intrinsic functions, Program design and branching structures, loop and character manipulation. Basic I/O concepts, Formatted READ and WRITE statements, **Learning Activities**: Peer discussion, Problem based learning.	CLO2
III 13 hours	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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO2 CLO3
IV 10 Hours	What is parallel programming, Why use parallel programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, **Learning Activities**: Peer discussion on various parallel algorithms, problem solving.	CLO2 CLO3

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

Suggested Readings

1. Chapman, (2006). Fortran 95/2003 for Scientists and Engineers, McGraw-Hill International Edition, New York.
2. N. Singh, (2017). *Computational Methods for Physics and Mathematics*, Narosa Publications.
3. V. Rajaraman, (1997). Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi.
4. M. Metcalf, J. Reid, and M. Cohen, (2005). Fortran 95/2003 Explained, OUP.

5. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996). Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press.
6. M. J. Quinn, (2003). Parallel Programming in C with MPI and OpenMP.
7. A. Grama, G. Karypis, V. Kumar, and A. Gupta, (2003). Introduction to Parallel Computing.
8. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press

Course Title: Scientific Programming Lab (Practical)
Paper Code: CCC.515
Total Hours: 60

L	T	P	Cr
0	0	4	2

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

1. Identify/Characterize/Define A Computational Problem
2. Design A Fortran Program to Solve the Problem
3. Create Pseudo Executable Code
4. Read Most of The Basic Fortran Code

Course Content

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

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

Suggested Readings

1. Chapman, (2006). Fortran 95/2003 for Scientists and Engineers, McGraw-Hill International Edition, New York.
2. N. Singh, (2017). *Computational Methods for Physics and Mathematics*, Narosa Publications.
3. V. Rajaraman, (1997). Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi.
4. M. Metcalf, J. Reid, and M. Cohen, (2005). Fortran 95/2003 Explained, OUP.
5. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996). Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press.
6. M. J. Quinn, (2003). Parallel Programming in C with MPI and OpenMP.
7. A. Grama, G. Karypis, V. Kumar, and A. Gupta, (2003). Introduction to Parallel Computing.
8. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press

Course Title: Quantum Mechanics
Paper Code: PCP.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: Apply the Mathematical Formulation and Postulates of Quantum Mechanics,
CLO2: Apply the theories of angular momenta and approximations methods,
CLO3: Apply the theory of addition of Angular momenta in the terms of C-G coefficient,
CLO4: Better understanding about different types of scattering theory of quantum mechanics,

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 12 Hours	**Mathematical Formulation and Postulates of Quantum Mechanics:** Limitations of Classical Mechanics and foundation of Quantum Mechanics, Matrix representations of kets, bras and operators, Change of basis, Basic postulates of quantum mechanics, Schrödinger wave equation (time dependent and time independent), Expectation values, Commutation relations **Learning Activities**: Peer discussion, Student seminars on recent developments	CLO1
II 11 Hours	**Angular Momentum:** eigenvalues and eigenvectors of orbital angular momentum, Angular momentum algebra and commutation relations, Matrix representation of angular momentum, Spin angular momentum: Pauli matrices and their properties. **Approximation methods:** Stationary perturbation theory for non-degenerate and degenerate systems with examples, time-dependent perturbation theory. **Learning Activities**: Problem Solving, research paper discussion.	CLO2
III 11 Hours	**Addition of Angular Momenta:** Addition of two angular momenta. Transformation between bases: Clebsch-Gordan Coefficients, Eigenvalues of J^2 and Jz, Coupling of orbital and spin angular momenta. **Learning Activities**: Brain-storming and Problem Solving	CLO3
IV 11 Hours	**Scattering Theory:** Scattering Theory: Quantum Scattering theory, Scattering cross-section and scattering amplitude, Born scattering formula, Central force problem, Partial wave analysis, Bound states and resonances **Learning Activities**: Peer discussion, and Problem Solving	CLO4

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

Suggested Readings

1. N. Zettili, (2009). *Quantum Mechanics-Concepts and Applications* John Wiley & Sons Ltd., Sussex, U.K.
2. R. L. Liboff (2011). *Introductory Quantum Mechanics* Pearson Education India
3. E. Merzbacher, (2011). *Quantum Mechanics* Wiley India Pvt. Ltd., New Delhi, India.
4. L.I. Schiff, (2010). *Quantum Mechanics* Tata McGraw-Hill Education, Noida, India.
5. K. Venkatesan, (2010). P.M. Mathews, *A Textbook of Quantum Mechanics* Tata McGraw - Hill Education, Noida, India.
6. J. J. Sakurai, (2009). *Modern Quantum Mechanics* Pearson Education, India.
7. D. J. Griffiths, (2015). *Introduction to Quantum Mechanics* Pearson Education, India.
8. G. D. Mahan, (2009). *Quantum Mechanics in a Nutshell Princeton* University Press
9. V.K. Thankappan, (2016). *Quantum Mechanics* New Age Pub. N. Delhi.
10. Albert Maxwell (2021) *QUANTUM PHYSICS* ISBN: 979-8472288415

Course Title: Statistical Mechanics
Paper Code: CCC.524
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 tool

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.
5. Müller-Kirsten, Harald J.W. (2022). Basics of Statistical Physics, 3rd ed. World Scientific

e-learning resources

1. https://ocw.mit.edu/courses/8-333-statistical-mechanics-i-statistical-mechanics-of-particles-fall-2013/video_galleries/video-lectures/
2. https://www.coursera.org/learn/statistical-mechanics
3. https://www.edx.org/course/chemical-thermodynamics-i

Course Title: Python Programming
Course Code: PCP.519
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 **Learning Activities**: Peer discussion, brainstorming and Problem based learning sessions, Class quiz	CLO1
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 **Learning Activities**: Peer discussion on different code designing, Decoding quiz	CLO2
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 **Learning Activities**: Brainstorming and Problem-Solving code designing.	CLO3
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. **Learning Activities**: Problem Solving code practice based on CSV files.	CLO4

Transaction Mode: Lecture, tutorial, problem solving

Suggested Readings

1. Gowri Shankar, S., Veena, A. (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. VanderPlas, J. (2016). Python Data Science Handbook: Essential Tools for Working with Data, 1st Edition, O'Reilly Media.
4. 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.
5. Chun, W. J. (2015). Core Python Applications Programming, 3rd Edition, Pearson Education India.
6. Romano F, Kruger H. (2023) Learn Python Programming: An in-depth introduction to the fundamentals of Python, Packt Publishing Limited

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

Course Title: Protein Engineering
Course Code: BIM.511
Course type: DE
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 protein folding process, mechanism and its importance.
CLO2: Choose a suitable experimental technique to introduce desired amino acid modifications to wild type proteins
CLO3: Design and modify sequence for a protein with a desired structure and/or property
CLO4: Design the protein molecules with the desired bonded and non-bonded interactions using computational methods

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	**Protein Folding and stability:** Protein structural features, protein structure-function relationship, Protein Folding: Theory and Experiment-Protein Renaturation, Determinants of Protein Folding, Folding Pathways, Folding Accessory Proteins. Introduction to Conformational Diseases. Protein stabilising factors, Protein Denaturation, Explaining the Stability of Thermostable Proteins **Learning Activities**: Peer discussion, demonstration using physical and computer models on folding process, Student seminars	CLO1
II 13 Hours	**Strategies for Protein Design:** Introduction to protein expression and mutagenesis. Protein engineering using unnatural amino acids- methodologies; applications-enhanced stability, tuning catalytic activity, tuning selectivity, enzyme design Protein design; strategies for the design of structure - self-assembly - ligand-induced assembly - assembly via covalent cross-linking - assembly of peptides on a synthetic template. Strategies for the design of function- novel functions by retrofitting natural proteins - incorporation of binding sites into *de novo* proteins - design of catalytically active proteins - membrane proteins and ion channels - design of new materials. **Learning Activities**: Peer discussion, Case studies, research paper discussion, Problem based learning	CLO2
III 10 Hours	**Computational Protein Design:** Methods of Computational Protein Design, core and full repacking, predicting native protein core sequences; altering protein folds. Geometry and stereochemistry-	CLO3

	based design, Case studies on Computationally Designed Proteins. **Learning Activities**: Problem based learning, demonstration using and computer models and experimental evidence, Classroom presentation	
IV 12 Hours	Engineering artificial metalloenzymes, engineered cytochromes P450 for Biocatalysis, Application of engineered biocatalysts for the synthesis of active pharmaceutical ingredients, Engineering antibody-based therapeutics: progress and opportunities, Development of novel cellular imaging tools using protein engineering. **Learning Activities**: Peer discussion, Case studies, research paper discussion, Problem based learning	CLO4

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

Suggested Readings

1. Zhao,H. (2021) Protein Engineering: Tools and Applications, Wiley-VCH Verlag GmbH & Co
2. Park, S.J., and Cochran, J.R. (2010). Protein Engineering and Design, 1/e, Taylor and Francis Inc., CRC Press, USA.
3. Carey, P.R. (1996) Protein Engineering and Design, 1/e, Academic Press Inc, USA.
4. Samish,I. (2017). Computational Protein Design, 1/e, Humana Press, New York.
5. Branden, C. I., & Tooze, J. (1999)., Introduction to Protein Structure, 2/e, Garland Science, USA.
6. Stefan, L. and Uwe, T.B. (Eds), (2012) Protein Engineering Handbook: Volume 3, 1/e, Wiley-VCH Verlag GmbH & Co.

Web resources:

1. https://onlinecourses.nptel.ac.in/noc21_cs100/preview
2. https://onlinecourses.nptel.ac.in/noc21_bt14/preview
3. https://ocw.mit.edu/courses/biology/7-344-antibiotics-toxins-and-protein- engineering-spring-2007/
4. https://ocw.mit.edu/courses/biology/7-91j-foundations-of-computational- and-systems-biology-spring-2014/video-lectures/leture-12-introduction-to-protein-structure-structure-comparison-and-classification/

Course Title: Inorganic Chemistry
Paper Code: CCC.509
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 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). **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO1 CLO2
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: CCC.510
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 computational techniques can be applied to study problems in computational organic chemistry.

Units/ Hours	Contents	Mapping with CLO
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 SN^2, SN^1, mixed SN^2 and SN^1 and SET mechanism, the SN^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 between SN^2 and SN^1 mechanisms. **Aromatic nucleophilic substitution:** The SN^{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.	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	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, H2O, hydride ion, ammonia derivatives, LiAlH4, NaBH4, 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.

L	T	P	Cr
3	0	0	3

Course Title: Physical Chemistry
Paper Code: CCC.517
Total Hours: 45

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 of Simple Mixtures:** Thermodynamic functions for mixing of perfect gases. chemical potential of liquids. Raoult's law, thermodynamic functions for mixing liquids (ideal solutions only). Real solutions and activities. **Solid-Liquid Solutions:** Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2 CLO3 CLO4
II 10 Hours	**Partial Molar Properties and Fugacity:** Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs-Duhem equation, real gases, fugacity, its importance and determination, a standard state for gases. **Phase transition**: Phase rule, water, CO2 phase transition, binary and ternary component phase transitions. Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria. **Learning Activities:** Brainstorming and problem-solving.	CLO1 CLO2 CLO3 CLO4
III 12 hours	**Electrochemistry:** Ionic equilibria, electrolytic conductance Kohlrausch's Law, Activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law, and conductometric titrations.	CLO5

	Electrochemical Cells: Nernst equation, redox systems, electrochemical cells, application of electrochemical cells, concentration cells with and without liquid junction, thermodynamics of reversible electrodes and reversible cells, and potentiometric titration. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	
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. **Adsorption and Catalysis:** Colloids and their stability, Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm, Langmuir and Freundlich Isotherms. Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Kinetics of catalytic reactions. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO6 CLO7

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

Suggested Readings

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

SEMESTER II

Course Title: Fundamentals of Molecular Simulations
Paper Code: CCC.554
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** a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary c) Long-range Interactions – The Ewald Sum, The Reaction Field Method **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) 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	CLO5

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. 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: Numerical Methods
Paper Code: CCC.525
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: the large-scale systems of linear, non-linear and simultaneous equations
CLO2: the matrix and determinants, interpolations, polynomial and spline interpolation
CLO3: the numerical differentiation and integration
CLO4: 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 code: PCP.525
Course Title: Solid State Physics
Course type: Core Course
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	**Fundamentals of Crystalline Materials:** Periodic array of atoms, Lattice translation vectors, unit cells: primitive and conventional unit cells, basis and lattice, Different types of Bravais lattices, Crystal structure examples: perovskite structure, CsCl, NaCl, diamond and zinc blende structures. 2D lattices, Honeycomb lattice and graphene, some popular 2D crystals (germanene, silicene, transition metal dichancogenides, Janus monolayers). **Reciprocal lattice and Bragg's law:** Diffraction of waves by crystal, Bragg's law and Lattice parameter determination, Fourier series and Concept of reciprocal lattice, Diffraction condition in reciprocal space and concept of Brillouin zones, Laue equations, Ewald construction and Ewald's sphere. Fourier analysis of basis and crystal structure factors. Experimental diffraction methods: Laue rotating crystal method and powder method. **Learning Activities**: Brain-storming and Problem Solving, Software visualization of real and reciprocal space structures	CLO1
II 11 Hours	**Electronic properties and band theory:** Elements of Drude and Sommerfeld Free electron theory, concept of Fermi energy, density of states, band structure for free electron gas. Electrical and thermal conductivity of metals, Wiedemann-Franz law. Failures of Free electron theory: Concept and origin of bandgap, Hall effect and concept of electrons and holes, effective mass and heavy fermions. Empty lattice approximation and different zone schemes, Free electron dispersions in different zone schemes. Nearly free electron theory, Bloch theorem and Kronig-Penney model, Fourier series representation of periodic potential, Born-von-Kerman boundary conditions. Central equation and its solution. Some standard examples of band structures: 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, magnetic susceptibility and classification of magnetic materials. Langevin theory of diamagnetic and ferromagnetic materials. Curie and Curie-Weiss law, origin of magnetic moment. Exchange interaction and Heisenberg model and for ferromagnetic, antiferromagnetic ordering. Concept of super-exchange. Magnetic anisotropic energy (MAE), Domain walls and	CLO3

	formation of magnetic domains. Hysteresis loop and its explanation. Pauli paramagnetism. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	
IV 11 Hours	**Superconductivity:** Discovery and fundamental properties of superconductors. Concept of zero resistivity and Meissner effect. Type-I and type-II superconductors, Flux quantization. Isotope effect and electron-phonon coupling for Cooper pair formation, overview BCS theory. McMillan formula for superconducting transition temperature. Coherence length, AC and DC Josephson effect, two-fluid model for superconductivity and London equations. Superconductivity beyond electron-phonon coupling: High T_C cooperate superconductors, iron-based superconductors. Near room temperature superconductivity: high pressure hydrides. Some applications of superconductivity. **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. N. T. Hung, Ahmad R. T. Nugraha, R. Saito (2022), *Quantum ESPRESSO Course for Solid-State Physics* Jenny Stanford Publishing.
3. C. Kittel, (2007). *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi, India.
4. R.J. Singh, (2011). *Solid State Physics,* Pearson, New Delhi, India.
5. A.J. Dekker, (2012). *Solid State Physics* Macmillan, London, U.K.
6. N. W. Ashcroft and N. D. Mermin, (2003). *Solid State Physics,* Thomson Press.
7. A.R. Verma and O.N. Srivatava, (2012). *Crystallography Applied to Solid state physics,* New Age International).
8. Lilia Boeri (2018) "*Understanding Novel Superconductors with Ab Initio Calculations*" W. Andreoni, S. Yip (eds.), *Handbook of Materials Modeling*, Springer International Publishing https://doi.org/10.1007/978-3-319-50257-1_21-1
9. Lilia Boeri et al (2022) "*The 2021 room-temperature superconductivity roadmap*" J. Phys.: Condens. Matter 34 183002

e-learning resources

1. https://ocw.mit.edu/courses/8-231-physics-of-solids-i-fall-2006/pages/syllabus/
2. https://onlinecourses.nptel.ac.in/noc21_ph21/preview

Course Title: Numerical Methods Lab (Practical)
Paper Code: CCC.528
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:

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

Course Content

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

1. Solution of transcendental or polynomial equations by the Newton Raphson method.
2. Matrix summation, subtraction and multiplication.
3. Matrix inversion using Gauss-Jordan's Matrix-Inversion Method.
4. Solution of Simultaneous Linear Equations: Gaussian Elimination, Gauss Seidel Iteration Method.
5. Finding 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 code: PCP.526
Course Title: Computational Solid State Physics Lab (Practical)
Course type: Skill Based Core
Total Hours: 60

L	T	P	Cr
0	0	4	2

Learning Outcomes:
At the end of the computational Solid State Physics laboratory, the students will be able to:
- Create and visualize crystal structure of various substances using different softwares such as VESTA, Gaussian, XCRYSDEN
- Compute total energy and lattice parameters of crystals using ab-initio density functional theory
- Use Gaussian package to compute various properties of crystals
- Use ELK code 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 any of ten experiments from the following experiments.

1. Creating the crystal structure, calculating bond length and X-ray diffraction pattern for various crystals using VESTA software (NaCl, Diamond, CsCl, ZnS, Perovskite structures).
2. Determine the crystal structure of CsCl using Gaussian package.
3. Geometry optimization of crystals using Gaussian package.
4. Determination of Infrared spectra of crystals using Gaussian package.
5. X-ray diffraction refinement using ICSD data.
6. Determination of Raman spectra using Gaussian package.
7. To compute lattice parameters of different cubic (SC, FCC, BCC) crystals using ELK package.
8. To compute the electronic band structure and density of states (DOS) for simple crystals (Al, Cu, Si, Diamond, NaCl, GaAs) using ELK package.
9. To compute magnetic moment and spin resolved band structure and DOS for BCC iron and FCC Ni.
10. To compute the phonon dispersions and obtain various thermal properties using ELK code.
11. To compute superconducting transition temperature of any material (Nb) within McMillan formula using ELK package.

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.
5. N. T. Hung, Ahmad R. T. Nugraha, R. Saito (2022), *Quantum ESPRESSO Course for Solid-State Physics* Jenny Stanford Publishing.

Course Title: Big Data Analytics in Bioinformatics and Healthcare
Course Code: BIM.521
Course type: DE
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: Discuss the fundamental concepts of big data
CLO2: Explain the methods used for large scale biological data handling
CLO3: Describe various approaches to generate protein big data
CLO4: Outline role of big data analytics in genomic research
CLO5: Explain the importance of big data analytics in healthcare

Units/ Hours	Contents	Mapping with CLO
I 11 Hours	**Fundamentals in Big Data** Introduction to Big data and big data in bioinformatics. Techniques for handling big data- Data management, Data analytics. Map-Reduce Fundamentals, Technologies for handling big data- Vertical and Horizontal scaling techniques- Foundations of the Hadoop Ecosystem, Apache Spark **Learning Activities**: Group discussion, hands-on training in data handling, Peer discussion and student presentations	CLO1 & CLO2
II 12 Hours	**Big Data Analytics in Protein Bioinformatics** Protein Structure Alignment and Similarity Searching, functional assignment. Prediction of intrinsically disordered proteins using cloud computing. Mass spectrometry and NMR data analysis using inferential structure determination, low resolution crystallographic data analysis using probabilistic, Bayesian methods from SAXS and SANS data. **Learning Activities**: Hands-on training on biological data analysis, student presentations, research paper discussion	CLO3
III 11 Hours	**Big Data Analytics in Genomics** Challenges of Handling Genomic and Clinical Data, Big Data on the Cloud, Big data in NGS Read Alignment, Big Data Analytics in Calling Variants, Statistical Analysis of Genomic Data, Data mining using RNA seq data, Analysis of Genomic and Clinical Data. **Learning Activities**: Hands-on training on biological data analysis, student presentations, research paper discussion	CLO4
IV 11 Hours	**Big Data Analytics in Health Research:** Case studies on big data analytics for preventive and personalized medicine. Mining Massive Genomic Data for Therapeutic Biomarker Discovery in Cancer, Medical image processing and its role in healthcare data analysis. Big Data analytics-based models for various stages in healthcare.	CLO5

	Learning Activities: Classroom presentation on real world application and peer discussion, Case studies, research paper discussion.	

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

Suggested Readings

1. Mrozek, D. (2018). Scalable Big Data Analytics for Protein Bioinformatics. Springer Press.
2. Hurwitz, J. S., Nugent, A., Halper, F., & Kaufman, M. (2013). Big data for dummies. John Wiley & Sons.
3. Elmasri, R. (2021). Fundamentals of database systems seventh edition.
4. Lytras, M. D., & Papadopoulou, P. (Eds.). (2017). Applying big data analytics in bioinformatics and medicine. IGI Global.
5. Mrozek, D. (2018). Scalable big data analytics for protein bioinformatics. Computational Biology.
6. Li, S. (Ed.). (2020). Computational methods and data analysis for metabolomics. Totowa, NJ, USA:: Humana Press.
7. Wong, K. C. (2016). Big data analytics in genomics. Springer. Springer Press, 1st ed. 2016
8. Wong, K. C. (Ed.). (2016). Big data analytics in genomics. Springer.
9. Dey, N., Das, H., Naik, B., & Behera, H. S. (2019). Big data analytics for intelligent healthcare management. Academic Press. 1st ed.

Web resources

1. https://doi.org/10.3390/ijms18020412
2. https://doi.org/10.1016/j.copbio.2019.03.004
3. https://doi.org/10.1007/s00521-019-04095-y

NPTEL

1. https://onlinecourses.nptel.ac.in/noc20_bt10/preview
2. https://onlinecourses.nptel.ac.in/noc20_cs92/preview
3. https://onlinecourses.nptel.ac.in/noc22_bt20/preview

Course Title: Cheminformatics
Course Code: BIM.522
Course type: DE
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: Decode the molecular structure from various structural representations retrieved from the database
CLO2: Identify specific descriptors for small molecular compounds
CLO3: Develop a pharmacophore model from a set of drug molecule and quantify the structure activity relationship
CLO4: Virtual screening tools and efficiency assessments

Units/ Hours	**Contents**	**Mapping with CLO**
I 12 Hours	Cheminformatics as a theoretical chemistry discipline: definition, main concepts and areas of application. Representing chemical structures on computers. Molecular graphs. Connectivity tables. Adjacency and distance matrices. Linear representations SMILES and SMIRKS. Hashed fingerprints. Exchange formats for chemical structures (MOL, SDF) and reactions (RXN et RDF). Chemical Databases. Different types of searching structures in the databases: exact match, sub-structural, super-structural and by similarity. **Learning Activities**: Classroom presentation and discussion on the topic, hands-on training in the chemical structure file formats and databases	CLO1
II 11 Hours	Molecular descriptors. Definition and main requirements. Different types of descriptors: constitutional, topological indices, geometry-based, surface based, substructural fragments, lipophilicity, etc. Development and validation of QSAR/QSPR models. Data preparation. Statistical parameters assessing models performance. Cross-validation. Models applicability domain. Ensemble modeling. **Learning Activities**: Problem based learning, Improved discussion, research paper discussion	CLO2
III 11 Hours	Molecular Interaction Fields. 3D QSAR. Molecular fields' similarity Pharmacophore approach Pharmacophore features. Ligand- and structure-based pharmacophores. Merged and shared pharmacophores. Pharmacophore-based virtual screening	CLO3

	Learning Activities: Peer discussion, Seminars on application of Pharmacophores, real world application, Problem Solving.	
IV 11 Hours	Chemical Space concept. Graph-based chemical space: scaffolds, frameworks and R-groups. Scaffold tree approach. Descriptor-based chemical space: distance and similarity metrics. Data visualization: Generative Topographic Mapping. Network-like similarity graphs. Activity landscapes. Bioisosteres. Activity cliffs. Virtual screening workflow. Drug-likeness filters and structural alerts. Parameters of screening efficiency. **Learning Activities**: small group projects, Case studies, research paper and peer discussion	CLO4

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

Suggested Readings

1. Leach, A. R., & Gillet, V. J. (2017) .An Introduction to Cheminformatics, Springer,
2. Varnek, A.(2017). Tutorials in cheminformatics. John Wiley & Sons.
3. Engel, T., & Gasteiger, J. (2018). Chemoinformatics: basic concepts and methods. John Wiley & Sons.
4. Sharma, N., Ojha, H., Raghav, P., & Goyal, R. K. (2021). Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences. Elsevier.
5. Stromgaard, K., Krogsgaard-Larsen, P., & Madsen, U. (2009). Textbook of drug design and discovery. CRC press. ISBN: 9780429111242.

Course Title: Molecular Evolution
Course Code: BIM.523
Course type: DE
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 evolutionary processes that give rise to variation in sequences and genomes
CLO2: Describe the architecture of the genome, contents and variation in base composition
CLO3: Outline the molecular level mechanisms of the various models in genome evolution
CLO4: Apply bioinformatics methods for studying genetic variation in and between species.

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	Comparison of DNA sequences to calculate gene distance; Convergent and divergent evolution; Mutation Vs. Substitution-Rate of Molecular Evolution. Jukes Cantor Correction and evolutionary distance **Learning Activities**: Peer discussion, brainstorming, Case studies, research paper discussion.	CLO1
II 12 Hours	Genome evolution, RNA structure and evolution, Compensatory substitutions and the comparative method, Fitting evolutionary models to sequence data, The influence of thermodynamics on RNA sequence evolution **Learning Activities**: Classroom presentation and discussion on the topic, Problem based learning.	CLO2
III 10 Hours	Molecular clock- Concepts and significance-molecular mechanisms of molecular clock- Neutral theory -gene family organization. Applications of molecular phylogenetics **Learning Activities**: Discussion on each topic in a learner centric manner through term paper presentation, real world problems.	CLO3
IV 11 Hours	Paralogy and Orthology- coordination expression in evolution-genome: content, structure and evolution. Molecular evolution of recently diverged species - Databases of Molecular evolution. **Learning Activities**: Research paper presentation, Problem based learning sessions, Class quiz.	CLO4

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

Suggested Readings

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

Web Resources

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

Course Title: Biomolecular Structure Modelling and Drug Designing
Course Code: CCC.526
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: Find relationships between similar kinds of multiple sequences (in MSA) and sequence conservation pattern, conserved structural motifs etc.
CLO2: use different search methods to find compounds with specific properties in large compound databases
CLO3: explain and make a use of different types of protein–ligand interactions and characterize binding pockets
CLO4: set up, perform and evaluate different virtual screening methods using large datasets

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	Basics of Biomolecules: Principles of protein and nucleic acid structure: Primary, Secondary, Tertiary structure and Quaternary structure. Protein secondary structure: Introduction, Hydrogen bond, Defining a secondary structure element, Methods for predicting secondary structure **Learning Activities:** Peer discussion, problem solving, Quiz.	CLO1
II 12 Hours	Protein tertiary structure modeling: Basic concepts, Protein folding and Energetics, Comparative modeling, Threading, Ab initio modeling, Modeling protein side chains, CASP: A blind protein structure prediction competition, CAPRI, Protein Structure Initiative (PSI). **Learning Activities:** Peer discussion, problem solving, Quiz.	CLO2
III 12 Hours	Introduction to drug designing, ADMET, drug metabolism, toxicity and pharmacokinetics. lipinski rule of 5, Identification and validation strategies. Drug Target classification, Concept of Pharmacophore, Functional group considered as pharmacophore, Structure-based drug design, docking, QSAR. **Learning Activities:** Peer discussion, problem solving, Quiz.	CLO3
IV 11 Hours	Modelling macromolecular structure: Homology modeling, *ab-initio* structure modeling; Molecular Recognition: Prediction of Protein-ligand interaction sites, Prediction of Protein-protein interaction sites, Prediction of Protein-membrane interaction sites, Prediction of Protein-nucleic acid interaction sites. **Learning Activities:** Peer discussion, problem solving, Quiz.	CLO4

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

Suggested Readings

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

Web Resources

https://www.uniprot.org/
bioinformatics.org/molvis/phipsi/

Course Title: Physical Organic Chemistry
Paper Code: CCC.514
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 chemical bonding, aromaticity, structure and stereochemistry, steric and conformational properties, chemical reactivity, correlation of structure with reactivity, Hammond postulates, solvent effects, acidity, nucleophilicity, electrophilicity.
CLO2: demonstrate reaction mechanisms, isotope effects Woodward Hoffmann rules.

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	**Chemical bonding:** Covalency and molecular structure, approximate molecular orbital theory, properties of covalent bonds, intermolecular forces, aromaticity, structure. Woodward Hoffmann rules. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 10 Hours	**Correlation of structure with reactivity:** Electronic demands, the Hammett equation, substituent constants σ, theories of substituent effects, interpretation of σ- values, reaction constants, ρ, deviations from the Hammett equation, dual-parameter correlations, molecular orbital considerations, cross-interaction terms **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
III 10 hours	Steric and conformational properties: Origins of steric strain, examples of steric effects upon reactions, measurement of steric effects upon rates. Solvent effects: structure of liquids, solutions, solvation, thermodynamic measures of solvation, effects of solvation on reaction rates and equilibria, empirical indexes of solvation, use of solvation scales in mechanistic studies. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO1
IV 11 Hours	**Kinetic isotope effects:** isotopic substitution, theory of isotopic effects, transition-state geometry, secondary kinetic isotope effects, heavy atom isotope effects, tunnel effect **Acids and bases, nucleophiles and electrophiles:** acid-base dissociation, the strengths of oxygen and nitrogen acids, linear free-energy relationships, rates of proton transfers, structural effects on amine protonation, factors that influence carbon acidity, theories of proton transfer, nucleophilicity and electrophilicity and their measurement. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO1 CLO2

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

Suggested Readings

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

Course Title: Statistics for Chemical and Biochemical Applications
Paper Code: CCC.513
Total Lectures: 45

L	T	P	Cr
3	0	0	3

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

Course Content

Unit I **10 Hours**
Overview of Biostatistics: Difference between parametric and non-parametric statistics, Univariate and multivariate analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Unit II **12 Hours**
Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit III **10 Hours**
Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

Unit IV **13 Hours**
Inferential Statistics: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, x^2 test. Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

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

Suggested Readings

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley, USA.
2. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc. USA.
3. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials.* 3/e (with SPSS). Decker Inc. USA.
4. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research.* W.H. Freeman publishers, USA.
5. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley, USA.

SEMESTER III

Course Title: Research Methodology
Course Code: CCC.551
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: Perform Literature survey, critically analyze 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 to 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 12 Hours	Introduction: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Hypothesis formulation and development of research plan, Art of reading and understanding scientific papers, Literature survey, Interpretation of results and discussion. **Learning Activities**: Research paper presentation, Writing and Evaluation of research proposals, Peer discussion.	CLO1
II 12 Hours	Library: Classification systems, e-Library, Reference management, Web-based literature search engines, Intellectual property rights (IPRs). **Learning Activities**: Perform literature survey, Research paper presentation and group discission.	CLO2
	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 and group discussion.	CLO3
III 11 Hours	Scientific and Technical Writing: Role and importance of communication, Effective oral and written communication, Scientific writing, Research paper writing, technical report writing, Making R and D proposals, Dissertation/Thesis writing, Letter writing and official correspondence, Oral and poster presentation in meetings, Seminars, Group discussions, Use of modern aids; Making technical presentations.	CLO4

	Learning Activities: Project report /research article preparation as a group activity, Research paper presentation	
IV 10 Hours	Research and Academic Integrity: Plagiarism, Copyright issues, Ethics in research, and case studies. Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials. **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.
8. Gould, J. R. (2020). Directions in Technical Writing and Communication. Routledge.

Paper Code: CCC.529
Course Title: Density Functional Theory
Total Lecture: 60

L	T	P	C
3	0	0	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: learn basics of Density Functional Theory (DFT),
CLO2: understand most popular framework of modern DFT,
CLO3: characterize the properties of molecules and materials,
CLO4: to use different functional appropriately for different problems,

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	Schrödinger equation for many particle systems, Hartree theory, Identical particles and spin, Hartree-Fock theory, Antisymmetric wave functions and Slater determinant, Koopmans' theorem. **Learning Activities**: Brainstorming and problem solving.	CLO1
II 11 Hours	Idea of functional, Functional derivatives, Electron density, Thomas Fermi model, Hohenberg-Kohn theorems, Approximations for exchange-correlation: Local density approximation (LDA) and local spin density approximation (LSDA), Gradient expansion and generalized gradient approximation (GGA), Hybrid functionals and meta-GGA approaches. **Learning Activities**: Brainstorming and problem solving.	CLO2
III 11 Hours	Kohn-Sham formulation: Plane waves and pseudopotentials, Janak's theorem, Ionization potential theorem, Self consistent field (SCF) methods, Strengths and weaknesses of DFT. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	Free electron theory, Band theory of solids, Tight-binding method, Semiconductors, Band structure, Density of states. Interpretation of Kohn-Sham eigenvalues in relation with ionization potential, Fermi surface and band gap. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4

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

Suggested Readings

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

Course Title: Electronic Structure Theory
Paper Code: CCC.556
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: compare post-HF methods.
CLO5: develop how to apply quantum chemistry to study chemical and biochemical problems.

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 13 Hours	Review of molecular structure calculations and Hückel Molecular Orbital Theory, Hartree products and Hartree-Fock Approximation. One and Two-Electron Integrals, General Rules, Coulomb and Exchange Integrals, **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	Configuration Interaction, Multi-Configuration Self-Consistent Field, Multireference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method. **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 code: PCP.557
Course Title: Atomic and Molecular Spectroscopy
Course type: Core Course
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):

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 CLO
I 12 Hours	Atomic Spectra: Revision of quantum numbers, electron configuration, Hund's rule etc. origin of spectral lines, LS & JJ coupling, selection rules, Spectrum of hydrogen, helium and alkali atoms, X-ray spectra, fine spectra, hyperfine structure, Width of spectrum lines. **Learning Activities**: Brain storming and problem solving.	CLO1
II 11 Hours	**Molecular Spectra (Pure Rotational Spectra):** Types of molecular spectra, Born-Oppenheimer approximation, molecular energy states, salient features of rotational spectra, requirement for rotational spectra, molecule as a rigid rotator, Non-rigid rotator, isotope effect on rotational spectra. **Learning Activities**: Brain storming and problem solving.	CLO2
III 11 Hours	**Vibrational - Rotational Spectra:** Salient features of vibrational-rotational spectra, molecule as a harmonic oscillator, an-harmonic oscillator, Vibrational frequency and force constant, isotope effect on vibrational level, fine structure of Infrared (IR) bands, thermal distribution of IR spectra. **Learning Activities**: Brain storming and problem solving.	CLO3
IV 11 Hours	**Raman Spectra:** Nature of Raman effect, Raman spectra and Molecular structure, classical and quantum theory of Raman effect, vibrational Raman Spectrum, pure rotational Raman spectrum. **Electronic Spectra:** Formation of electronic spectra, electronic band system in emission and absorption mode, Fine structure of electronic bands, Intensity distribution, Franck-Condon Principle. **Learning Activities**: Brain storming 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. Mc Cash, (1994). *Fundamentals of Molecular Spectroscopy* Tata McGraw Hill, New Delhi.
4. L. R. Lakowicz, (2012). *Principle of Fluorescence Spectroscopy*, Springer.
5. A. Carrington and A. D. Mc Lachlan, (1979). *Introduction to Magnetic Resonance* Chapman and Hall, London.
6. R. K. Harris, Addison Wesley, (1986). *Nuclear Magnetic Resonance Spectroscopy* Longman Ltd, London.
7. C. N. Banwell and E. M. Mc Cash, (2012). *Fundamentals of Molecular Spectroscopy*, Tata, McGraw Hill Publishing Company Limited.
8. C.J. Foot, (2005). *Atomic Physics,* Oxford University Press, Oxford, U. K.

L	T	P	Cr
2	0	0	2

Course Title: Entrepreneurship
Course Code: PCP.520
Course type: CF
Total Hours: 30

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Describe the nature of entrepreneurship and their role in economic development.
CLO2: Outline the behaviour and skills of an entrepreneur
CLO3: Explain the role of E-Cells in entrepreneurial development
CLO4: Write business plan/project proposals & managing start-up issues.

Units/ Hours	Contents	Mapping with CLO
I 7 Hours	The concept of entrepreneurship, the history of entrepreneurship**.** Entrepreneurial Structure; Nature, Characteristics, functions and its role in economic development**.** Entrepreneurship- problems and prospects in India **Learning Activities:** Students Teams, Student generated test questions, role playing	CLO1
II 7 Hours	Entrepreneurial behavior and skills, The entrepreneurial decision process, The skill gap analysis, role models, The entrepreneurial success stories **Learning Activities:** Case studies, Concept mapping, spontaneous quizzes	CLO2
III 8 Hours	Examination of emerging trends in the types of Computational sciences data being generated, The way it is managed and possibilities for new directions. Profiling the Computational entrepreneur. **Learning Activities**: Comparison debate, group discussion.	CLO3
IV 8 Hours	Funding opportunities for start-ups. Schemes of the Department of Science and Technology. Strategy and conduct of computational research. Understanding Business Models based on scientific computing and Managing Risk **Learning Activities**: Comparison debate, brainstorming, group discussion, student presentations.	CLO4

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

Suggested Readings

1. G. K. Varshney, (2012). Fundamentals of Entrepreneurship, Sahitya Bhawan Publications.
2. R. Roy, (2011). Entrepreneurship, 2nd Edition, Oxford
3. B.K. Mehta, (2018). Entrepreneurship and Small Business, SBPD Publishers.
4. Craig Shimasaki, (2020) Biotechnology Entrepreneurship Leading, Managing and Commercializing Innovative Technologies, 2nd Edition, Academic Press 2020
5. G.M. Javie, K. Li (2021) Chemistry Entrepreneurship, John Wiley & Sons, Inc.

Course Title: Molecular Simulations Lab (Practical)
Paper Code: CCC.555
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
- Design molecular model from scratch, and high-definition images using various graphics tools
- Execute the practical in-hand experience of various modeling and classical simulation tools
- Construct the use of different 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. Analysis of Molecular Dynamics data

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: CCC.573
Total Hours: 60

L	T	P	Cr
0	0	4	2

Course Learning Outcomes: This course will provide practical experience to the students using important Computational Chemistry software related to electronic structure theory.

The 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 surface generation.
- Transition state calculations.
- Absorption spectra study.
- Calculations using a 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%20 Chemistry%20With%20Electronic%20Structure%20Methods.pdf
3. Gaussian 09/16 website or manual.

Course Title: Dissertation Part I
Paper Code: CCC.600
Total Hours: 120

L	T	P	Cr
0	0	8	4

Learning outcomes:

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

Students will prepare a research proposal based on literature review and extensive student-mentor interactions involving discussions, meetings and presentations. Each student will submit a research/dissertation proposal of the research work planned for the M.Sc. dissertation with origin of the research problem, literature review, hypothesis, objectives, methodology to carry out the planned research work, expected outcomes and bibliography.

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

Evaluation Criteria:

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

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

Modes of transaction

Group discussions and presentations; Self-Learning; Experimentation

SEMESTER IV

Course Title: Dissertation Part II
Paper Code: CCC.601
Total Hours: 600

L	T	P	Cr
0	0	40	20

Learning outcomes:

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

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

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

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

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