Central University of Punjab

M. Sc. Physics (Computational Physics)

Batch: 2025-2027

Department of Computational Sciences

School of Basic Sciences

Graduate Attributes

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

- Understand various areas of Physics, the knowledge in Mathematics and scientific programming for different branches of Physics.
- Apply the Computational techniques to solve Physics problems which are of interest in different interdisciplinary domains such as materials science, drug design, chemical and biological sciences.
- Apply the knowledge, general competence, and analytical skills on an advanced level, needed in industry, consultancy, education, research, or public administration.
- Examine the complex information from the concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology, and successfully carry out research assignment and projects, both independently and in collaboration with others.

Therefore, graduated students of M.Sc. Physics (Computational Physics) would be a valuable asset for nation by virtue of his/her scientific abilities. The student can expect gainful employment in academic/research/industry by undertaking this programme.

Course Structure of the Programme

SEMESTER – I							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	L	T	P	Cr
1	MPCP.401	Mathematics for Computational Sciences	CC	3	0	0	3
2	MPCP.516	Classical Mechanics	CC	3	0	0	3
3	MPCP.402	Python programming (Lab)	SBC	0	0	4	2
4	MPCP.517	Quantum Mechanics	CC	3	0	0	3
5	MCCC.518	Statistical Mechanics	CC	3	0	0	3
6	MCCC.523	Numerical Methods (Lab)	SBC	0	0	4	2
7	×××.×××	Discipline Elective	DE	3	0	0	3
8		Individualized Education Plan/ Tutorial		0	2	0	0
Total credits				**15**	**2**	**8**	**19**

List of Discipline Electives (Choose anyone)							
S. No.	**Course code**	**Course name**	**Course type**	**L**	**T**	**P**	**Cr**
1	MPCP.518	Introduction to Computational Physics	DE	3	0	0	3
2	MPCP.519	Electromagnetic Theory	DE	3	0	0	3
3	MPCP.520	Nuclear and Particle Physics	DE	3	0	0	3
4	MPCP.521	Quantum Computation	DE	3	0	0	3

SEMESTER – II							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MPCP.525	Physics and Chemistry of Solids	CC	3	0	0	3
2	MPCP.526	Computational Condensed Matter Lab	SBC	0	0	4	2
3	MPCP.527	Atomic and Molecular Spectroscopy	CF	2	0	0	2
4	MPCP.528	Electronics	CC	3	0	0	3
5	MCCC.530	Electronic Structure Theory (Lab)	SBC	0	0	4	2
6	MCCC.527	Electronic Structure Theory	CC	3	0	0	3
7	MCCC.531	Molecular Simulation (Lab)	SBC	0	0	4	2
Interdisciplinary and Value-Added Courses							
8	XXX.XXX	IDC offered by other departments	IDC	2	0	0	2
9	MPCP.511	Research Methodology	VAC	2	0	0	2
10		Individualized Education Plan/ Tutorial		0	2	0	0
Total credits				**15**	**2**	**12**	**21**

SEMESTER – III							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MPCP.599-1	Dissertation part-I	SBC	0	0	40	20
Total credits				**0**	**0**	**40**	**20**

SEMESTER – IV							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	MPCP.599-2	Dissertation part-II	SBC	0	0	40	20
Total credits				**0**	**0**	**40**	**20**

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

L: Lectures; T: Tutorial; P: Practical

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

Total Credits Distribution:

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

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

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

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

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

Examination pattern and evaluation:

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

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

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

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

Examination pattern from 2025-26 session onwards

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

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

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

Some Guidelines for Internal Assessment:

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

Evaluation Criteria for Practical Courses:

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

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

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

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

SEMESTER-I

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

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):

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

CLO1: Develop understanding of linear algebra for new cutting-edge areas of computational sciences such as machine learning.
CLO2: Familiarization to the concepts of probability, statistics and optimization problem.
CLO3: Calculate the complex functions as Delta, Gamma, and Beta Functions,
CLO4: Calculate the second-order partial differential equations

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	**Matrices:** Basic matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors, system of linear equations, particular and general solution, elementary transformations. Cholesky Decomposition, Eigen decomposition and Diagonalization. **Vector Calculus:** Vector spaces, linear dependence and basis. Inner product, orthogonality of vectors. Basis functions. Differentiation of univariate function, partial differentiation and gradients, Gradients and gradients of matrices. Higher order derivatives. Linearization and multi-variate Taylor series. **Learning Activities**: Peer discussion, Brain-storming and Problem Solving	CLO1
II 11 Hours	**Probability and distribution:** Construction of probability space, discrete and continuous probabilities, Sum rule, product rule and Baye's theorem. Summary statistic and independence, Gaussian distribution, Conjugacy and exponential family. Change of variables, inverse transformation. **Continuous optimization:** Optimization using gradient descent, constrained optimization, Lagrange's multipliers, convex optimization. **Learning Activities**: Brain-storming, group discussions and Problem Solving	CLO2
III 11 Hours	**Delta, Gamma, and Beta Functions:** Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions. **Learning Activities**: Brain-storming and Problem Solving	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 too
Suggested Readings

1. Marc Peter Deisenroth, A. Aldo Faisal and Cheng Soon Ong *Mathematics for Machine Learning* https://mml-book.com (2024)
2. E. Kreyszig. (2017). *Advanced Engineering Mathematics* Wiley India Pvt. Ltd., New Delhi, India.
3. B.S. Rajput, (2020). *Mathematical Physics* Pragati Prakashan
4. L. A. Pipes. (1985). *Applied Mathematics for Engineers and Physicist* McGraw-Hill, Noida, India.
5. D. G. Zill. (2012). *Advanced Engineering Mathematics* Jones & Barlett Learning, Massachusetts, USA.
6. P. K. Chattopadhyay. (2000). *Mathematical Physics* New Age International (P) Ltd., New Delhi.
7. E.Steiner. (2008). The chemistry Mathematics Book, Oxford University Press.
8. F. Daniels. (1959). Mathematical for Physical Chemistry: Mc. Graw Hill.
9. Tebbutt. (1994). Basic Mathematics for Chemists, Wiley.
10. G. Arfken, H. Weber and F. Harris. (2012). *Mathematical Methods for Physicists* Elsevier Academic Press, Massachusetts, USA.

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 Code: MPCP.516
Course Title: Classical Mechanics
Course type: Core Course
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: A quick overview of Special Theory of Relativity and its significance
CLO2: Exploring the Lagrangian and Hamiltonian Formalism of Mechanics
CLO3: Significance of Canonical Transformations and Hamilton - Jacobi theory,
CLO4: Understanding the dynamics of rigid body and its applications

Units/Hours	Contents	Mapping with CLO
I 8 Hours	**Special Theory of Relativity:** Lorentz transformations and its consequences, Relativistic kinematics and mass energy equivalence, Relativistic Lagrangian and Hamiltonian, Four vectors, Covariant formulation of Lagrangian and Hamiltonian. **Learning Activities**: Brain-storming and Problem Solving	CLO1
II 7 Hours	**Lagrangian Formalism:** Newton's laws, Classification of constraints, D'Alembert's principle and its applications, Generalized coordinates, Lagrange's equation for conservative, non-conservative and dissipative systems and problems, **Hamiltonian Formalism:** Variational principle, Principle of least action, Hamilton's principle, Hamilton's equation of motion, Lagrange and Hamilton equations of motion from Hamilton's principle, Hamilton's principle to non-conservative and non-holonomic systems. **Learning Activities**: Brain-storming and Problem Solving	CLO2
III 8 Hours	**Canonical Transformations and Hamilton - Jacobi theory:** Canonical transformation and problems, Poisson brackets, Canonical equations in terms of Poisson bracket, Integral invariants of Poincare, Infinitesimal canonical transformation and generators of symmetry, Relation between infinitesimal transformation and Poisson bracket, Hamilton–Jacobi equation for Hamilton's principal function, Linear harmonic oscillator problem by Hamilton-Jacobi method, Action angle variables, Application to Kepler's problem. **Learning Activities**: Brain-storming and Problem Solving	CLO3
IV 7 Hours	**Rigid Body Dynamics**: Euler's angles, Euler's theorem, Moment of inertia tensor, Non-inertial frames and pseudo forces: Coriolis force, Foucault's pendulum, Formal properties of the transformation matrix, Angular velocity and momentum, Equations of motion for a rigid body, Torque free motion of a rigid body - Poinsot solutions, Motion of a symmetrical top under the action of gravity, Two Body Problems. **Learning Activities**: Brain-storming and Problem Solving	CLO4

Transaction Mode: Lecture delivery using White Board and PPT, Problem Solving through Assignments, Online tool.

Suggested Readings

1. S.T. Thornton and J.B. Marion, (2013). *Classical Dynamics of Particles and Systems,* Cengage Learning, Boston/Massachusetts, United States.
2. J. Safko, H. Goldstein and C. P. Poole (2011) *Classical Mechanics* Pearson, New Delhi, India.
3. Jon Magne Leinass (2020). *CLASSICAL MECHANICS AND ELECTRODYNAMICS*, World Scientific Publishing, Singapore
4. G. Walter, (2010). *Systems of Particles and Hamiltonian Dynamics* Springer, New York, USA.
5. P.S. Joag and N.C. Rana, (1991). *Classical Mechanics* Tata McGraw-Hill, Noida, India.
6. S.T. Thornton and J.B. Marion, (2013). *Classical Dynamics of Particles and Systems* Cengage Learning, Boston/Massachusetts, United States.
7. J. Safko, H. Goldstein and C. P. Poole, (2011). *Classical Mechanics* Pearson, New Delhi, India.
8. G. Walter, (2010). *Systems of Particles and Hamiltonian Dynamics* Springer, New York, USA.
9. P.S. Joag and N.C. Rana, (1991). *Classical Mechanics* Tata McGraw-Hill, Noida, India.

e-learning resources

1. https://ocw.mit.edu/courses/8-01sc-classical-mechanics-fall-2016/

L	T	P	Cr
0	0	4	2

Course Code: MPCP.402
Course Title: Python Programming (Lab)
Course type: Discipline Elective
Total Hours: 60
Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Install the package for python programming, write, compile and run programs
CLO2: Perform various arithmetic and logical operations using python
CLO3: Apply conditioning and looping statements in python for different scientific problems
CLO4: Understand and employ different data structures and file operations to write elegant python programs

Course Content

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

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

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

Suggested Readings

1. S. Gowrishankar, A. Veena, (2019). *Introduction to Python Programming*, 1st Edition, CRC Press/Taylor & Francis.
2. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press
3. J. Vander Plas, (2016). *Python Data Science Handbook: Essential Tools for Working with Data*, 1st Edition, O'Reilly Media.
4. Aurelien Geron, (2019). *Hands-On Machine Learning with Scikit-Learn and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems*, 2nd Edition, O'Reilly Media.
5. Wesley J Chun, (2015). Core *Python Applications Programming* 3rd Edition, Pearson Education India.

e-learning resources

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

Course Code: MPCP.517
Course Title: Quantum Mechanics
Course type: Core Course
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: Understand the Mathematical Formulations and Postulates of Quantum Mechanics,
CLO2: Understand the quantum mechanical counterparts of angular momenta
CLO3: Explore various approximation methods for quantum mechanical solutions
CLO4: Understand the of addition of Angular momenta in terms of C-G coefficients,
CLO5: Understand scattering in quantum systems

Units/ Hours	Contents	Mapping with CLO
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**: Brain-storming and Problem Solving	CLO1
II 11 Hours	**Angular Momentum:** eigenvalues and eigen vectors of orbital angular momentum, Angular momentum algebra and commutation relations, Matrix representation of angular momentum, Spin angular momentum: Pauli matrices and their properties. **Approximation methods:** Stationary perturbation theory for non-degenerate and degenerate systems with examples, time-dependent perturbation theory, **Learning Activities**: Brain-storming and Problem Solving	CLO2 CLO3
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	CLO4
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**: Brain-storming and Problem Solving	CLO5

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

e-learning resources

1. https://www.edx.org/course/quantum-mechanics
2. https://www.coursera.org/learn/quantum-physics
3. https://ocw.mit.edu/courses/8-04-quantum-physics-i-spring-2016/

L	T	P	Cr
3	0	0	3

Course code: MCCC.518
Course Title: Statistical Mechanics
Course type: Core Course
Total Lectures: 45

Course Learning Outcomes (CLO):

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: Apply the principles and techniques from statistical mechanics to a range of modern-day research-based problems.

Units/ Hours	Contents	Mapping with CLO
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**: Brain-storming 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**: Brain-storming and Problem Solving	CLO3
IV 11 Hours	**Bose-Einstein distribution:** Einstein condensation. Thermodynamic properties of ideal BE gas. **Fermi-Dirac distribution:** Degenerate Fermi gas. Electron in metals. Magnetic susceptibility. **Learning Activities**: Brain-storming and Problem Solving	CLO4

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

Suggested Readings

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

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 code: MCCC.523
Course Title: Numerical Methods Lab
Course type: Skill Based Core
Total Hours: 60

L	T	P	Cr
0	0	4	4

Learning Outcomes:

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

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

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

Course Content

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

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

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

Suggested Readings

1. Y. Kirani Singh and B.B. Chaudhuri, (2007). *MATLAB Programming*, Prentice-Hall India.
2. Rudra Pratap, (2006). *Getting Started with Matlab 7*, Oxford, Indian University Edition.
3. E. Balaguruswamy, (2017). *Numerical Methods*, Tata McGraw Hill.
4. V. Rajaraman, (2018). *Computer oriented numerical methods*, PHI Learning Pvt. Ltd.
5. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press

Course Code: MPCP.518
Course Title: Introduction to Computational Physics
Course type: Discipline Elective
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: write computer programs for physics problems
CLO2: Generate, test and employ the random numbers for numerical integration
CLO3: Apply Monte-Carlo simulations to understand the 2D Ising lattice.
CLO4: Solve differential equations numerically.
CLO5: Apply the knowledge to interdisciplinary topics.

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	**FORTRAN Programming:** A Brief Introduction To Input/Output Statements, Fortran Constants, Variables And Expression Writing, Control Statements And Loops, Arrays, Format Statements. File Processing in Fortran. **Random number generation and testing:** True and pseudo random numbers, different Random number generators, testing random numbers. **Numerical Integration:** Deterministic (Trapezoidal method) and stochastic methods (Monte-Carlo) for numerical integration. **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
II 11 Hours	**Lattice Monte-Carlo Simulations:** Metropolis algorithm, Ising model to understand phase transitions and role of kinetic energy barriers, finite size effects and thermal fluctuations. Principle of detailed balance, calculating thermodynamical averages. Determining transition temperature using Binders cumulant. **Learning Activities**: Brain storming and problem solving.	CLO3
III 11 Hours	**Solving differential equations:** Linear, non-linear, coupled differential equations. Numerical solution of Schrodinger's equation using Shooting matching method, Numerov's and variational algorithms. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO4
IV 11 Hours	**Interdisciplinary topics:** Protein folding: lattice model for protein folding and Monte-Carlo simulation of the same. Earthquake and self-organized criticality: Mass-spring model to simulate earthquake. Neural networks and the brain. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO5

Transaction Mode: Lecture delivery using White Board and PPT, Problem Solving through Assignments.

Suggested Readings

1. V. Rajaraman, (1997) *Computer Programming in FORTRAN 90 & 95*, PHI Learning
2. N. Singh, (2017). *Computational Methods for Physics and Mathematics*, Narosa Publications
3. Nicholas J. Giordano and Hasio Nakanishi (2006), *Computational Physics* Pearson Addison-Wesley
4. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press
5. Jos Thijssen, (1997) *Computational Physics,* Cambridge University Press
6. R. C. Verma, P. K. Ahluwalia, K. C. Sharma, (2005) *Computational Physics: An Introduction* New Age Publishers
7. P. L. DeVries and J. Hasbun, (2010) *A first course in Computational Physics* John Wiley and Sons

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc19_ph16/preview
2. https://www.mooc-list.com/course/waves-optics-edx

Course Code: MPCP.519
Course Title: Electromagnetic Theory
Total Hours: 45
Course type: Discipline Elective

L	T	P	Cr
3	0	0	3

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

CLO1: Theory and calculation of electrical parameters,
CLO2: Estimation of Electric and magnetic fields of the electrical system,
CLO3: Application of theories in the technology development,
CLO4: Skill to modify the existing formula for the modern technology

Units/ Hours	Contents	Mapping with CLO
I 11 Hours	**Electrostatics:** Review of Gauss's law and its applications, Work and energy in electrostatics, Electrostatic potential energy, Electric Fields and Boundary Condition, Poisson and Laplace equations, Uniqueness theorem I & II, Method of Images, Solution of Laplace's equation, Multipole expansion, Boundary condition with dielectrics. **Learning Activities**: Brain storming and problem solving	CLO1
II 11 Hours	**Magnetostatics:** Biot-Savart law, Ampere's theorem and its applications, Lorentz Force, Magnetic scalar and Vector potential. **Magnetic Fields and Boundary Condition:** Magnetic dipole and Magnetization, Field of a magnetized object, Magnetic susceptibility and permeability, Dia, para and Ferro-magnetic materials, Boundary condition on B and H, **Learning Activities**: Brain storming and problem solving	CLO2
III 11 Hours	**Maxwell Equations:** Faraday's Law, Maxwell's equations in free space and linear isotropic media. Time Varying Fields and Conservation Laws: Scalar and vector potentials, Gauge invariance, Lorentz gauge and Coulomb gauge, Poynting theorem and conservations of energy and momentum for a system of charged particles **Learning Activities**: Brain storming and problem solving, Research paper presentation	CLO3
IV 12 Hours	**Plane Electromagnetic Waves and wave equations:** EM wave in free space, Dispersion characteristics of dielectrics, Waves in a conducting and dissipative media, Skin effect, Transmission lines and wave guides, TE mode, TM mode, Cut off frequency, Retarded potentials. **Radiation from Moving Point Charges and Dipoles:** Lienard-Wiechert potentials, Radiation from a moving point charge and oscillating electric and magnetic dipoles. **Learning Activities**: Brain storming and problem solving, Peer discussion, Research paper presentation	CLO4

Transaction Mode: Lecture, Demonstration, Power point Presentations.

Suggested Readings:

1. Heald M.A and Marion J.B. (2012). *Classical Electromagnetic Radiation* New York, USA: Dover Publications.
2. Griffiths D.J. (2012). *Introduction to Electrodynamics*. New Delhi: Prentice Hall of India Pvt.Ltd.
3. Zangwill A. (2012). *Modern Electrodynamics.* Cambridge, U.K: Cambridge University Press.
4. Jackson J.D. (2004). *Classical Electrodynamics.* New Delhi, India: Wiley India (P) Ltd.
5. Lifshitz E.M, Landau L.D and PitaevskiiL. P. (1984). *Electrodynamics of Continuous Media.* New York, USA: Elsevier.
6. Matthew N. O. Sadiku (2015). *Principles of Electromagnetics*, Oxford University Press
7. Arnab Rai Choudhary (2023). *Advanced Electromagnetic Theory*, Springer Nature Singapore

Course Code: MPCP.520
Course Title: Nuclear and Particle Physics
Total Hours: 45
Course Type: Discipline Elective

L	T	P	Cr
3	0	0	3

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

CL01: Understand nuclear properties, and various models related to the existence of the nucleus and nuclear force.
CL02: Understand nuclear potential, Scattering and its characteristics
CL03: Understand the basics of nuclear force to implement it to designing of nuclear structure
CL04: Understand the nature and properties of fundamental elementary particles

Unit /hours	Contents	Mapping with CLO
I 11 Hours	**Introduction to Nuclear Properties:** Review of Nuclear size and shape, charge distribution, empirical formula of radius, Magnetic Moment, Electric Quadrupole, Mass and binding energy, semi-empirical mass formula. **Learning Activities:** Brain storming and problem solving, Group discussions, Application based peer thinking.	CL01
II 11 Hours	**Two Nucleon Problems:** Nature of nuclear forces, Deuteron problem, Spin, Parity, Magnetic moment and electric quadrupole moment of deuteron, scattering cross-section, n-p scattering, phase shifts and Scattering length. **Learning Activities:** Brain storming, Group discussions, Application based peer thinking, and Problem Solving	CL02
III 12 Hours	**Nuclear Model:** Liquid drop model, Evidence of shell structure, Shell model, Single particle shell model, its validity and limitations, Collective model, Vibrational and Rotational spectra, Exchange force model. **Learning Activities:** Group discussions, Application based peer thinking, and Problem Solving	CLO3
	Nuclear Decay: Different kinds of particle emission from nuclei, Alpha, Beta and Gamma decay and their selection rules. Fermi's theory of allowed beta decay, Selection rules for Fermi and Gamow-Teller transitions. Double beta decay. **Learning Activities:** Group discussions, Application based peer thinking, and Problem Solving	
IV 11 Hours	**Elementary Particle Physics:** Elementary Particles and antiparticles, Quarks model, baryons, mesons and leptons, Classification of fundamental forces, Parity non-conservation in weak interaction, CPT invariance. Baryon and Lepton numbers, Strangeness, charm and other additive quantum numbers, Gell Mann Nishijima formula.	CL04

	Learning Activities: Group discussions, Application based peer thinking, and Problem Solving	

Transaction Mode:
Lecture, tutorial, problem solving.

Suggested Readings:

1. Martin B. (2011). Nuclear & Particle Physics an Introduction. New Jersey, USA: John Wiley & Sons.
2. Krane K.S. (2008). Introductory Nuclear Physics. New Jersey, USA: John Wiley & Sons, Inc.
3. Bertulani C.A. (2007). Nuclear Physics in a Nutshell. Princeton, USA: Princeton University Press.
4. Wong S.S.M. (2008). Introductory Nuclear Physics. New Jersey, USA: John Wiley & Sons, Inc.
5. Povh B, Rith K, Schol C. (2012). Particles and Nuclei: An Introduction to the Physical Concepts. New York, USA: Springer.
6. Perkin D.H. (2000). Introduction to High Energy Physics. Cambridge, U.K: Cambridge University Press.
7. Hughes I.S. (1991). Elementary Particles. Cambridge, U.K: Cambridge University Press.
8. Stefan T. (2010). Experimental Techniques in Nuclear and Particle Physics. New York, USA: Springer.

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc22_ph41/preview
2. https://www.edx.org/course/understanding-nuclear-energy
3. https://www.coursera.org/learn/particle-physics

Course Title: Quantum Computation
Code: MPCP.521
Course type: Discipline Elective
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: Basic idea of quantum computation, Qbits and related concepts
CLO2: Appreciate the Quantum Logic gates and their role in quantum computing.
CLO3: Understand density operators and their significance in quantum computing
CLO4: Understand basic components of quantum circuits.

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	**Introduction:** Overview of Quantum mechanics, significance of quantum computation. Classical vs Quantum computing. Basic working idea of quantum computer. Idea of Q-bits, Matrix and Bloch sphere representation of Q-bits. Multi Qbit states, No-cloning theorem, super dense coding, pure states, bell states, Bell inequalities. **Learning Activities**: Peer discussion, brainstorming, problem solving, Online tutorials,	CLO1
II 10 Hours	**Quantum logic gates:** Universal quantum gates, rotation operators, phase shift gates, CNOT, Clifford set gate, Toffoli gate, NAND - FANOUT - Walsh Hadamard, Deutsch gate **Measurement:** Projective operators, Projective and positive operator-valued measure (POVM) measure. **Learning Activities:** Peer discussion, brainstorming, problem solving, Online tutorials.	CLO2
III 10 Hours	**Ensemble:** Density operators, pure and mixed ensembles, time evolution, post measure density operator. **Composite systems:** Partial trace, Reduced density operator, Schmidt decomposition, Purification, bipartite entanglement. **Learning Activities:** Peer discussion, brainstorming and Problem Solving, Online tutorials.	CLO3
IV 15 Hours	**Quantum computing and circuits:** Serially wired gates: Exponents of Quantum states, parallel gates: Hadamard transform, application on entangled states, Unitary inversion gates. Classical computing using qubits, Quantum parallelism, Deutsch's algorithm, Deutsch Josza algorithm. Basic gates, ABC decomposition, Gray codes, Universal gates, Principle of deferred and implicit measurements, Quantum Fourier transform, applications: phase estimation, order finding, factoring, discrete logarithm and hidden subgroup	CLO4

	problems, Role of prime factoring in classical cryptography, search algorithms. **Learning Activities:** Problem Solving, Peer discussion, brainstorming, Online tutorials	

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

Suggested Readings

1. Chuck Easttom, *Quantum computing fundamentals* Pearson Education (2022)
2. M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press (2010).
3. Asher Peres, *Quantum Theory: Concepts and Methods*, Kluwer Academic Publishers (2002)

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc21_cs103/preview
2. https://onlinecourses.nptel.ac.in/noc19_cy31/preview

SEMESTER-II

L	T	P	Cr
3	0	0	3

Course code: MPCP.525
Course Title: Physics and Chemistry of Solids
Course type: Core Course
Total Lecture: 45

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.	CLO2

	Learning Activities: Brain-storming and Problem Solving	
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 formation of magnetic domains. Hysteresis loop and its explanation. Pauli paramagnetism. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3
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 code: MPCP.526
Course Title: Computational Condensed Matter (Lab)
Course type: Skill-Based Core
Total Hours: 60

L	T	P	Cr
0	0	4	2

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

- Create and visualize crystal structure of various substances using different software such as VESTA, Gaussian, XCRYSDEN
- Compute total energy and lattice parameters of crystals using ab initio density functional theory
- Use the 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.

12. Creating the crystal structure, calculating the bond length and X-ray diffraction pattern for various crystals using VESTA software (NaCl, Diamond, CsCl, ZnS, Perovskite structures).
13. Compiling and installing ELK code and understanding the basic structure of ELK input file.
14. To understand the importance of convergence with respect to different computational parameters
15. To compute lattice parameters of different cubic (SC, FCC, BCC) crystals using ELK package.
16. To compute the electronic band structure and density of states (DOS) for simple crystals (Al, Cu, Si, Diamond, NaCl, GaAs) using ELK package.
17. To compute magnetic moment and spin resolved band structure and DOS for BCC iron and FCC Ni.
18. To compute the phonon dispersions and obtain various thermal properties using ELK code.
19. To compute the superconducting transition temperature of any material (Nb) within the McMillan formula using the 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.

Course code: MPCP.527
Course Title: Atomic and Molecular Spectroscopy
Course type: Core Course
Total Lectures: 30

L	T	P	Cr
2	0	0	2

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 8 Hours	**Atomic Spectra:** Revision of quantum numbers, electron configuration, origin of spectral lines, LS & JJ coupling, selection rules, Spectrum of hydrogen, alkali atoms, X-ray spectra. **Learning Activities**: Brain storming and problem solving.	CLO1
II 7 Hours	**Molecular Spectra (Pure Rotational Spectra):** Types of molecular spectra, 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 8 Hours	**Vibrational - Rotational Spectra:** Salient features of vibrational-rotational spectra, molecule as a harmonic oscillator, an-harmonic oscillator, isotope effect on vibrational level, fine structure of Infrared (IR) bands. **Learning Activities**: Brain storming and problem solving.	CLO3
IV 7 Hours	**Raman Spectra:** Nature of Raman effect, Raman spectra and Molecular structure, classical and quantum theory of Raman effect. **Electronic Spectra:** Formation of electronic spectra, 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. C. N. Banwell and E. M. Mc Cash, (2012). *Fundamentals of Molecular Spectroscopy*, Tata, McGraw Hill Publishing Company Limited.
7. C.J. Foot, (2005). *Atomic Physics,* Oxford University Press, Oxford, U. K.

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc23_ph16/preview
2. https://www.edx.org/course/atoms-molecules-and-bonding

Course Code: MPCP.528
Course Title: Electronics
Course type: Core Course
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: Apply the theories of basic electronics and semiconductor diodes,
CLO2: Demonstrate basics knowledge about the circuits,
CLO3: Apply the theories of the operational amplifier and their operations,
CLO4: Apply the theories of combinational and sequential logic circuits,

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	**Semiconductor Diode:** construction, operation, characteristics, application of p-n diode and Zener diode, Bipolar Junction Transistors- construction, operation, common-emitter configuration, common-base configuration, common-collector configuration, load line analysis, Operating point, voltage-divider bias, transistor switching networks, bias stabilization, working of CE amplifier. Construction, working and characteristics of JFET and MOSFET. **Learning Activities**: Brain storming and problem solving.	CLO1
II 11 Hours	**Field Effect Transistor (FET):** Construction, working and characteristics of JFET and MOSFET. CS and CD amplifiers at low frequencies, Biasing the FET, CS and CD amplifiers at high frequencies. **Optoelectronic Devices and Transducers:** Solar cell, Photo detector and LEDs, Transducers, Measurement and control, Shielding and grounding. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO2
III 11 Hours	**Operational Amplifier-** Introduction, ideal characteristics, voltage follower circuit, inverting amplifier, non-inverting amplifier, Op-Amp parameters- input and output voltage, common mode and supply rejection, offset voltages and currents, input and output impedances, slew rate. Op-Amps as summing amplifier, difference amplifier, differentiator and integrator. Active filters: Types, specifications, filter transfer function, first order and second order low pass and high pass filters, band pass and band reject filters. Signal generator: Basic principles, phase shift oscillator, Wien bridge oscillator, triangular/ rectangular wave generators. A/D and D/A conversion circuits. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3

IV 11 Hours	**Combinational logic circuits-** Number systems-binary, octal, decimal and hexadecimal, number base conversions, binary arithmetic, 1's and 2's complement, Binary codes- BCD, 8421, Excess-3, reflected code, alpha-numeric codes, logic gates analysis-AND, OR, NOT, NAND, NOR, Boolean Algebra-theorems and properties, Boolean functions- Canonical and Standard forms, AND-OR and NAND-NOR implementation and simplification of Boolean expressions, Karnaugh map (up to four variables). Adder, Parallel binary adder, subtractor, comparator, decoders, BCD to seven segment decoder, encoders, code converter, multiplexers and demultiplexers. **Sequential logic circuits:** Flip flops-SR, JK, D, T and master-slave JK flip flops, Edge triggered flip flops, Registers, shift register, ripple counters, synchronous counters. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO4

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

Suggested Readings

1. J. Millman, C. Halkias and C. Parikh, (2009). *Integrated Electronics: Analog and Digital Circuits and Systems,* Tata McGraw - Hill Education, Noida, India.
2. R.L. Boylestad and L. Nashelsky, (2009). *Electronic Devices and Circuit Theory,* Pearson, New Delhi, India.
3. B. L. Theraja, (2010). *Basic Electronics: Solid State*, S. Chand & Company Ltd., New Delhi, India.
4. D. Chattopadhyay and P. C.Rakshit, (2008). and Applications, NewAge International, New Delhi, India.
5. G. Saha, A.P. Malvino and D.P. Leach, (2011). *Digital Principles and Applications*, Tata McGraw - Hill Education, Noida, India.
6. P. Malvino and J.A. Brown, (2011). *Digital Computer Electronics*, Tata McGraw - Hill Education, Noida, India.

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc21_ee55/preview
2. https://www.edx.org/course/circuits-and-electronics-1-basic-circuit-analysi-2

Course code: MCCC.527
Course Title: Electronic Structure Theory
Course type: Core Course
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: Identify and define basic terms and concepts which are needed for this specialized course.
CLO2: describe the HF SCF method.
CLO3: Select the basis sets.
CLO4: Learn basics of Density Functional Theory.
CLO5: develop how to apply quantum chemistry to study chemical and biochemical problems.

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

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

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.
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.

Course code: MCCC.530
Course Title: Electronic Structure Theory (Lab)
Course type: Skill Based Core
Total Hours: 60

L	T	P	Cr
0	0	4	2

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

Following experiments will be carried out in the lab.

1. Introduction to electronic structure calculations.
2. Basis set dependency.
3. HF and DFT methods related calculations.
4. Carrying of conformational analysis of small molecules.
5. MO and charge distribution calculations.
6. Vibrational spectra calculations.
7. 2D potential energy surface generation.
8. Transition state calculations.
9. Absorption spectra study.
10. Calculations using solvent.
11. Thermochemistry study.
12. Post-HF based calculations
13. Studying potential energy surface.
14. Carrying of conformational analysis of large systems.
15. Model chemistry.
16. Study of NMR spectra
17. QM/MM study.

Transactional Modes: Laboratory based practical; 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 code: MCCC.531
Course Title: Molecular Simulations (Lab)
Course type: Skill Based Core
Total Lecture: 60

L	T	P	Cr
0	0	4	2

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

- Apply the remote computing as a tool for high performance computation
- Apply different energy minimization techniques
- Create molecular model from scratch, and high-definition images using various graphics tools
- Apply various modeling and classical simulation tools
- 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 inter-conversions of small molecules
3. Energy minimizations and optimization, *ab initio methods*
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
6. Secondary Structure Prediction, Fold Recognition
7. Molecular Dynamics with GROMACS
    a. Water structure and dynamics
    b. Binary Mixtures
    c. HP36 in Water
    d. Serotonin1A in Membrane Bilayers
8. Analysis of Molecular Dynamics data

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

Suggested Readings

1. M.P. Allen and D.J. Tildesley, (1992). Computer Simulation of Liquids, QC 145.2.A43.
2. Daan Frenkel and Berend Smit, (1996). Understanding molecular simulation, QD
3. 461. F86.
4. Andrew R. Leach, (2001). Molecular Modeling Principles and applications. II edition, Prentice Hall.
5. S. Alavi, (2020). Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH

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

L	T	P	Cr
2	0	0	2

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

Units/ Hours	Contents	Mapping with CLO
I 8 Hours	Introduction: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Hypothesis formulation and development of research plan, Art of reading and understanding scientific papers, Literature survey, Interpretation of results and discussion. **Learning Activities**: Research paper presentation, Writing and Evaluation of research proposals, Peer discussion.	CLO1
II 7 Hours	Library: Classification systems, e-Library, Reference management, Web-based literature search engines, Intellectual property rights (IPRs). Entrepreneurship and Business Development: Importance of entrepreneurship and its relevance in career growth, Types of enterprises and ownership. **Learning Activities**: Concept built with real examples, case studies, Student presentation Perform literature survey, Research paper presentation and group discussion.	CLO2, CLO3
III 8 Hours	Scientific and Technical Writing: Role and importance of communication, Effective oral and written communication, Scientific writing, Research paper writing, technical report writing, Making R and D proposals, Thesis writing, Oral and poster presentation, Seminars, Group discussions, Use of modern aids. **Learning Activities**: Project report /research article preparation as a group activity, Research paper presentation	CLO4
IV 7 Hours	Research and Academic Integrity: Plagiarism, Copyright issues, Ethics in research, and case studies. Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials. **Learning Activities:** Case studies, Peer discussion, brainstorming, spontaneous quizzes	CLO5

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

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

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

SEMESTER-III

L	T	P	Cr
0	0	40	20

Course code: MPCP.599-1
Course Title: Dissertation Part-I
Course type: Skill Based Elective
Invested Hours: 600
Course Objective and 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.

Evaluation Criteria:

Dissertation Part-1 (Third Semester)		
	Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation
HoD and senior-most faculty of the department	50	Dissertation proposal and presentation

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

SEMESTER-IV

L	T	P	Cr
0	0	40	20

Course code: MPCP.599-2
Course Title: Dissertation Part-II
Course type: Skill Based Elective
Total Hours: 600

Course Objective and Learning Outcomes:

1. Demonstrate an in-depth knowledge of scientific research pertaining to the area of study
2. Demonstrate experimental/theoretical research capabilities based on rigorous hands-on training
3. Critically analyze, interpret and present the data in light of existing scientific knowledge to arrive at specific conclusions
4. 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 the 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