Central University of Punjab

M. Sc. Physics (Computational Physics)

Batch: 2024

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 Computational Physics, advanced knowledge in Mathematics, and knowledge in applied fields like Computer Science.
- 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	PCP.506	Mathematics for Computational Sciences	CF	3	0	0	3
2	CCC.508	Scientific Programming	CF	3	0	0	3
3	PCP.507	Classical Mechanics	CC	3	0	0	3
4	PCP.527	Quantum Mechanics	CC	3	0	0	3
5	CCC.524	Statistical Mechanics	CC	3	0	0	3
6	CCC.515	Scientific Programming (Practical)	SBC	0	0	4	2
7		DE-I	DE	3	0	0	3
8		Individualized Education Plan/ Tutorial		0	2	0	0
Total credits				**18**	**2**	**4**	**20**

List of courses for discipline elective (DE-I)							
S. No.	**Course code**	**Course name**	**Course type**	**L**	**T**	**P**	**Cr**
1	PCP.519	Python Programming	DE	3	0	0	3
2	PCP.508	Waves and Optics	DE	3	0	0	3
3	PCP.509	Introduction to Computational Physics	DE	3	0	0	3

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	PHY.522	Electromagnetic Theory	CC	3	0	0	3
5	CCC.528	Numerical Methods Lab (Practical)	SBC	0	0	4	2
6	PCP.526	Computational Solid State Physics Lab (Practical)	SBC	0	0	4	2
7		Interdisciplinary course (offered by other departments)	IDC	2	0	0	2
8		DE-II	DE	3	0	0	3
9		Individualized Education Plan/ Tutorial		0	2	0	0
Total credits				**20**	**2**	**4**	**21**

List of courses for discipline elective (DE-II)							
S. No.	**Course code**	**Course name**	**Course type**	**L**	**T**	**P**	**Cr**
1	PCP.573	Electronics	DE	3	0	0	3
2	BIM.514	Biomolecular Simulations Modelling and Drug Designing	DE	3	0	0	3
3	BIM.515	Data Mining and Machine learning	DE	3	0	0	3
4	PCP.558	Quantum Computation	DE	3	0	0	3

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.556	Electronic Structure Theory	CC	3	0	0	3
3	PCP.557	Atomic and Molecular Spectroscopy	CC	3	0	0	3
4	CCC.555	Molecular Simulations Lab (Practical)	SBC	0	0	4	2
5	CCC.573	Electronic Structure Theory Lab (Practical)	SBC	0	0	4	2
6	PCP.520	Entrepreneurship	CF	2	0	0	2
7	PCP.600	Dissertation (Part-I)	SBE	0	0	8	4
8		Value Added Course offered by other departments	VAC	2	0	0	2
9		DE-III	DE	3	0	0	3
10		Individualized Education Plan/ Tutorial		0	2	0	0
Total credits				**13**	**2**	**20**	**24**

List of courses for discipline elective (DE-III)							
S. No.	**Course code**	**Course name**	**Course type**	**L**	**T**	**P**	**Cr**
1	PCP.570	Introduction to Density Functional Theory	DE	3	0	0	3
2	PHY.555	Advanced Solid-State Physics	DE	3	0	0	3
3	PHY.552	Nuclear and Particle Physics	DE	3	0	0	3

SEMESTER – IV							
Sr. No.	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	PCP.601	Dissertation (Part-II)	SBE	0	0	40	20
Total credits				**0**	**0**	**40**	**20**
Grand Total				**51**	**0**	**68**	**85**

	Core courses	Elective courses			Foundation courses		Total Credit
		DE	ID	SB	CF	EF/VB	
Sem I	3 (9 Cr)	1 (3 Cr)	--	1 (2 Cr)	2 (6 Cr)	--	**20**
Sem II	4 (12 Cr)	1 (3 Cr)	1 (2 Cr)	2 (4 Cr)			**21**
Sem III	3 (9 Cr)	1 (3 Cr)	--	2 (4 Cr) 1 (4 Cr Dissertation)	1 (2 Cr Entre.)	1 (2 Cr)	**24**
Sem IV	--	--	--	01 (20 Cr Dissertation)	--	--	**20**
Total Credit	**30**	**9**	**2**	**34**	**8**	**2**	**85**

L: Lectures; T: Tutorial; P: Practical

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

* 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.

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.

<u>Examination pattern from 2024-25 session onwards</u>

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

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

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

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

SEMESTER-I

Course Title: Mathematics for Computational Sciences Paper Code: PCP.506
Total Lectures: 45
Course type: CF

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, Eigendecomposition 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: CCC.508
Course Title: Scientific Programming
Course type: Compulsory Foundation
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Couse Learning Outcomes (CLO):
At the end of this course, students will be able to:

CLO1: Demonstrate 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: Write programs related to standard problems and as well as to chemistry/physics.

Units/ Hours	**Contents**	**Mapping with CLO**
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. Expression writing and translating scientific formulae into FORTRAN expressions. **Learning Activities**: Brain storming 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, control statements in FORTRAN: IF-ELSE and IF-ELSEIF, DO loop. **Learning Activities**: Brain storming and problem solving.	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. Manipulating vector and matrix operations using FORTRAN. **Learning Activities**: Brain storming 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**: Brain storming and problem solving, modelling and scaffolding.	CLO2 CLO3

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

Suggested Readings

1. Chapman, (2007). *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. Alex Gezerlis (2020). *Numerical Methods in Physics with Python* Cambridge University Press
4. V. Rajaraman, (1997). Computer *Programming in Fortran 90 and 95*, PHI Learning Pvt. Ltd, New Delhi.
5. M. Metcalf, J. Reid, and M. Cohen, (2005). *Fortran 95/2003 Explained*, OUP.

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

Course Code: PCP.507
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/

Course Code: PCP.527
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/

Course code: CCC.524
Course Title: Statistical Mechanics
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 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: CCC.515
Course Title: Scientific Programming (Practical)
Course type: Skill Based Course
Total Lectures: 60

L	T	P	Cr
0	0	4	2

Course Learning Outcomes (CLO):

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:

- Identify/characterize/define a computational problem
- Design a Fortran program to solve the problem
- Create pseudo executable code
- Read most of the basic Fortran code

Course Content

1. Compiling, linking and executing the Fortran programs.
2. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions,
3. Program design and branching structures, loop and character manipulation.
4. Basic I/O concepts, Formatted READ and WRITE statements,
5. Read/write of Files in FORTRAN.
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*, Mc Graw-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 Code: PCP.519
Course Title: Python Programming
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: Learn the Introductions of various types of programming languages,
CLO2: Apply the theories of Python Decision making and Loops,
CLO3: Apply the theories of Python Functions and Modules,
CLO4: Apply the theories of Python File Operations,

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**: Brain storming and problem solving.	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**: Brain storming and problem solving.	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**: Brain storming and problem solving, modelling and scaffolding.	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**: Brain storming and problem solving, modelling and scaffolding.	CLO4

Transaction Mode: Lecture, tutorial, problem solving

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: PCP.508
Course Title: Waves and optics
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: Identify the vibration and wave natures of representative systems in daily life.
CLO2: Identify the wave properties in optics.
CLO3: Apply the basic concepts and theories on the wave formations and propagations in media to explain and predict phenomena in daily life.
CLO4: Recognize the disasters caused due to the improper use of vibrations and waves.

Units/Hours	Contents	Mapping with CLO
I 12 Hours	**Geometrical optics:** Fermats principle, reflection and refraction at plane interface, Matrix formulation of geometrical Optics, Cardinal points and Cardinal planes of an optical system, Idea of dispersion, Application to thick Lens and thin Lens, Ramsden and Huygens eyepiece. Wave Optics: Electromagnetic nature of light. Definition and properties of wave front Huygens Principle. Temporal and Spatial Coherence. **Learning Activities**: Brain storming and problem solving.	CLO1
II 11 Hours	**Wave Motion:** Plane and Spherical Waves, Longitudinal and Transverse Waves, Plane Progressive (Traveling) Waves, Wave Equation, Particle and Wave Velocities, Differential Equation, Pressure of a Longitudinal Wave, Energy Trans- port, Intensity of Wave. Superposition of two perpendicular Harmonic Oscillations: Graphical and Analytical Methods, Lissajous Figures and their uses, Superposition of Anharmonic waves. **Learning Activities**: Brain storming and problem solving.	CLO2
III 11 Hours	**Interference:** Division of amplitude and wave front, Youngs double slit experiment, Lloyds Mirror and Fresnels Bi-prism, Phase change on reflection: Stokes treatment, Interference in Thin Films: parallel and wedge-shaped films, Fringes of equal inclination (Haidinger Fringes), Fringes of equal thickness (Fizeau Fringes), Newtons Rings: Measurement of wavelength and refractive index. Interferometer: Michelsons Interferometer, Idea of form of fringes, Determination of Wavelength, Wavelength Difference, Refractive Index, Visibility of Fringes, Fabry-Perot interferometer **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	**Fraunhofer diffraction:** Single slit, Circular aperture, Resolving Power of a telescope, Double slit, Multiple slits, Diffraction grating, Resolving power of grating. Fresnel Diffraction: Fresnels Assumptions, Fresnels Half-Period Zones for Plane Wave, Explanation of Rectilinear Propagation	CLO4

	of Light, Theory of a Zone Plate: Multiple Foci of a Zone Plate, Fresnels Integral, Fresnel diffraction pattern of a straight edge. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	

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

Suggested Readings

1. R. A. Serway, (2018). *Physics for Scientists and Engineers*, Saunders
2. F. W. Sears, M. W. Zemansky and H. D. Young, (2014). *University Physics,* Addison-Wesley
3. I. G. Main, (2019). *Vibrations and Waves in Physics*, Cambridge U Press
4. A. P. French, (2017). *Vibrations and Waves*, Van Nostrand Reinhold
5. M. N. Avadhanulu and T. V. S. Arun Murthy (2022). *Waves and Optics* S. Chand Publications

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc19_ph18/preview
2. https://www.mooc-list.com/course/waves-optics-edx

Course Code: PCP.509
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

SEMESTER-II

Course code: CCC.525
Course Title: Numerical Methods
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: 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**: Brain storming and problem solving.	CLO1 CLO2
II 12 Hours	**System of Linear Algebraic Equations:** System of Linear Equations, Guass Elimination Method, Importance of Diagonal Dominance, Gauss Seidel Iteration Method, Matrix Inversion Method: Gauss-Jordan's Matrix-Inversion Method **Learning Activities**: Brain storming 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**: Brain storming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	**Numerical Solution of Differential Equations:** Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method. **Learning Activities**: Brain storming 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

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc19_ma21/preview
2. https://onlinecourses.swayam2.ac.in/cec20_ma11/preview
3. https://ocw.mit.edu/courses/18-335j-introduction-to-numerical-methods-spring-2019/

Course code: CCC.554
Course Title: Fundamentals of Molecular Simulations
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: 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 CLO
I 12 Hours	**Molecular Modeling and Structure** - molecular modeling today: overview of problems, tools, and solution analysis, mini- tutorials 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
II 11 Hours	**Methods for Simulating Large Systems** a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary c) Long-range Interactions – The Ewald Sum, The Reaction Field Method **Learning Activities**: Brain-storming and Problem Solving	CLO2
III 11 Hours	**Energy Minimization and Related Analysis Techniques** (a) Steepest Descent, (b) Conjugate Gradient, (c) Newton-Raphson, (d) Comparison of Methods, (e) Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, (f) What's the big deal about the minimum? Introduction to Equilibrium Statistical Mechanics (a) Phase space, Ergodicity, and Liouville's theorem, (b) Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3

IV 11 Hours	**Simulation Methods:** **Monte Carlo:** The Metropolis method **Molecular Dynamics:** (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method (f) Pressure Control: Andersen's Method **Learning Activities**: Brain-storming and Problem Solving	CLO4 CLO5

Transactional Modes: Lecture; Tutorial; 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 461. F86.
3. Andrew R. Leach, (2001). *Molecular Modeling Principles and applications*. II edition, Prentice Hall.
4. S. Alavi, (2020). *Molecular Simulations: Fundamentals and Practice* 1st Edition, Wiley-VCH.

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc22_ch30/preview
2. https://www.edx.org/course/from-atoms-to-materials-predictive-theory-and-simu

L	T	P	Cr
3	0	0	3

Course code: PCP.525
Course Title: Solid State Physics
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. **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 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: PCP.573
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: CCC.528
Course Title: Numerical Methods 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 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 Rung-Kutta method,
10. Monte Carlo integration.

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

Suggested Readings

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

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

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: PHY.522
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 Title: Biomolecular Simulations and Drug Design
Course Code: BIM.514
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: Describe the modelling of small to large molecular environments
CLO2: Describe the concept of molecular mechanics force fields and select an appropriate energy function/force field for a given problem
CLO3: Choose an appropriate energy minimization method for the required simulation study.
CLO4: Apply different methods for simulating large molecular systems
CLO5: Describe a pharmacophore model from a set of drug molecule and quantify the structure-activity relationship
CLO6: Perform and evaluate different virtual screening methods using large datasets

Units/ Hours	Contents	Mapping with CLO
I 11 Hours	**Molecular Modeling and Structure** Introduction to Molecular modelling, Coordinate systems, potential energy surfaces for simple molecules. mini tutorials with protein and nucleic acid structure as examples. The simple molecular mechanics force field; general features of molecular mechanics force fields. Force Fields and Molecular Representation – Intramolecular Interactions, Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, Hydrogen Bonds, Constraints and Restraints, United Atom and Other Coarse-Grained Approaches, Non-pairwise Interactions, accuracy of the force fields. **Learning Activities**: Peer discussion, Demonstration using physical and computer model, Problem based learning, Analysing Experimental data.	CLO1 & CLO2
II 12 Hours	**Energy Minimization and Related Analysis Techniques** Steepest Descent, Conjugate Gradient, Newton- Raphson, Comparison of Methods, Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, What's the big deal about the minimum? Phase space, Ergodicity, and Liouville's theorem, Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles **Learning Activities**: Hands-on training, Peer discussion, Research paper presentation	CLO3

III 11 Hours	**Methods for Simulating Large Systems** Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists. Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary. Long-range Interactions – The Ewald Sum, The Reaction Field Method Molecular dynamics using simple models, Molecular dynamics with continuous potentials, finite difference and predictor-corrector integration methods, choosing the time step. Calculating properties by integration; implementation of the Metropolis Monte Carlo method; Monte Carlo simulation of rigid and flexible molecules; Lattice and continuous polymer models. **Learning Activities**: Hands-on training on simulation, Peer discussion, Case studies, research paper discussion.	CLO4
IV 11 Hours	**Drug design** 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, Artificial intelligence in drug discovery and development **Learning Activities**: Peer discussion, Case studies, research papers, Hands-on training on drug deigning	CLO5 & CLO6

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

Suggested Readings

1. Leach R. (2001). Molecular Modelling Principles and Applications 2nd Edition. Pearson.
2. Frenkel D. and Smit B. (2001). Understanding Molecular Simulation 2nd Edition, Academic Press.
3. Buschmann, H., & Holenz, J. (2018). Biomolecular Simulations in Structure- Based Drug Discovery. Germany: Wiley. ISBN:9783527342655
4. Alavi S. (2020). Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.
5. Bhatt, T. K., & Nimesh, S. (Eds.). (2021). The design and development of novel drugs and vaccines: Principles and protocols. Academic Press. ISBN: 9780128214718.
6. Renaud, J. P. (Ed.). (2020). Structural biology in drug discovery: Methods, Techniques, and Practices. John Wiley & Sons. ISBN: 9781118900406.
7. Allen, M. P., & Tildesley, D. J. (2017). Computer Simulation of Liquids 2nd Edition, Oxford University Press.
8. Stromgaard, K., Krogsgaard-Larsen, P., & Madsen, U. (2016). Textbook of Drug Design and Discovery. CRC Press, 5e, 2016.

Course Title: Data Mining and Machine Learning Course
Code: BIM.515
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: Perform data cleaning, cross-validation, and application of regression analysis
CLO2: Use various methods of clustering and dimensionality reduction for data analysis
CLO3: Explain classification as a tool to develop predictive platform
CLO4: Apply SVM and Neural network methods data analysis.

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	**Introduction:** Overview of Machine Learning field, Artificial intelligence Vs Machine learning, Regression and classification problem, cross validation, Terminology in ML: true positive, false positive, Specificity, Sensitivity, Accuracy, Recall, Precision, AUC-ROC curves, Confusion matrix, Errors in ML: Bias and variance. **Learning Activities**: Demonstration using random dataset, Problem based learning,	CLO1
II 12 Hours	**Unsupervised Methods:** Clustering: Distance Metrics, K-Means, leader, Jarvis-Patrick, hierarchical clustering; Dimensionality Reduction: Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Partial Least Squares – Discriminant Analysis (PLS-DA). **Learning Activities:** Peer discussion, Problem based learning, Analysing Experimental data for unsupervised model training.	CLO2
III 12 Hours	**Supervised Methods:** Univariate and multivariate linear regression: Model representation and cost function; Classification: k-nearest neighbors' algorithm (K-NN), naïve Bayes, decision trees, boosting and bagging **Learning Activities:** Case study, Peer discussion, brainstorming and Problem Solving.	CLO3
IV 11 Hours	**Other ML algorithms:** Ensemble methods, random Forests; Support vector machines, Neural networks, Recommendation systems; Outlier detection. Bonferroni Correction. **Learning Activities:** Problem Solving, case study, Peer discussion on various classification methods, brainstorming discussion	CLO4

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

Suggested Readings

1. Helder I., N. (2021). Bioinformatics. Exon Publications.
2. Alonso-Betanzos, A., & Bolón-Canedo, V. (2018). Big-Data Analysis, Cluster Analysis, and Machine-Learning Approaches. Advances in experimental medicine and biology, 1065, 607–626.
3. Applied Predictive Modeling by Max Kuhn and Kjell Johnson; 2013.
4. James, G., Witten, D., Hastie, T., & Tibshirani, R. (2014). An introduction to statistical learning: With applications in R.
5. McKinney, W. (2013). Python for data analysis
6. Han, J., Kamber, M., & Pei, J. (2011). Data Mining: Concepts and Techniques, Third Edition.

e-learning resources

1. https://onlinecourses.nptel.ac.in/noc20_cs29/preview
2. https://onlinecourses.nptel.ac.in/noc23_cs11/preview
3. https://openlearninglibrary.mit.edu/courses/course-v1:MITx+6.036+1T2019/about

Course Title: Quantum Computation
Code: PCP.558
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-III

Course Code: CCC.551
Course Title: Research Methodology
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: The course Research Methodology has been framed to introduce basic concepts of Research Methods.

CLO2: The course covers the preparation of a research plan, reading and understanding of scientific papers, scientific writing, research proposal writing, ethics, plagiarism, computer laboratory safety issues, etc.

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**: Brain storming and problem solving.	CLO1
II 11 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**: Brain storming and problem solving.	CLO1
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. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO2
IV 11 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**: Brain storming and problem solving, modelling and scaffolding.	CLO2

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

1. R. Kumar, (2012). *Research Methodology*, SAGE Publications India Pvt. Ltd., New Delhi, India.
2. S. Gupta, (2005). *Research Methodology and Statistical techniques*, Deep and Deep Publications (P) Ltd. New Delhi, India.

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

4. Standard /Reputed Journal authors' instructions.

e-learning resources

1. https://onlinecourses.swayam2.ac.in/cec20_hs17/preview
2. https://onlinecourses.nptel.ac.in/noc22_ge08/preview
3. https://www.edx.org/course/quantitative-and-qualitative-research-for-beginners

Course code: CCC.556
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 concepts, which are needed for this specialized core.
CLO2: Describe the HF SCF method.
CLO3: Select the basis sets.
CLO4: Compare post-HF methods.
CLO5: Develop and apply quantum chemistry to study chemical and biochemical problems.

Units/ Hours	Contents	Mapping with CLO
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**: Brain storming 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**: Brain storming and problem solving.	CLO1 CLO2
III 10 hours	Polyatomic Basis sets, Minimal, Double zeta, triple zeta and Polarized basis sets. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method. **Learning Activities**: Brain storming 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: 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. 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: CCC.555
Course Title: Molecular Simulations Lab (Practical)
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 code: CCC.573
Course Title: Electronic Structure Theory Lab (Practical)
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%20Chemistry%20With%20Electronic%20Structure%20Methods.pdf
3. Gaussian 09/16 website or manual.

Course code: PCP.570
Course Title: Introduction to Density Functional Theory
Course type: Discipline Elective
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: Learn basics of Density Functional Theory (DFT),
CLO2: Understand most popular framework of modern DFT,
CLO3: Characterize the properties of molecules and materials,
CLO4: Use different functional appropriately for different problems,

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	Schrödinger equation for many particles system, Hartree theory, Identical particles and spin, Hartree-Fock theory, Antisymmetric wavefunctions and Slater determinant, Koopmans' theorem. **Learning Activities**: Brain storming 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**: Brain storming 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**: Brain storming 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**: Brain storming 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. N. T. Hung, Ahmad R. T. Nugraha, R. Saito (2022), *Quantum ESPRESSO Course for Solid-State Physics* Jenny Stanford Publishing.
3. Robert G. Parr and Weitao Yang, (1994). *Density Functional Theory of Atoms and Molecules*, Oxford University Press.
4. David S. Sholl and Janice A. Steckel, (2009). *Density Functional Theory: A Practical Introduction*, John Wiley and Sons.
5. June Gunn Lee, (2011). *Computational Materials Science: An Introduction*, CRC Press.
6. C. Kittel, (2007). *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi.

Course Code: PHY.552
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. **Learning Activities:** Group discussions, Application based peer thinking, and Problem Solving	CL04

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 Code: PHY.555
Course Title: Advanced Solid-State Physics
Course Type: Discipline Elective
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: Explain Fermi surfaces and their construction and the experimental methods used for the detection of Fermi surfaces.
CLO2: Explain the theories of magnetism.
CLO3: Explain Plasmon, color centers, excitons, Raman Effect, luminescence and optical properties of solids.
CLO4: Outline the theory of dielectrics and ferroelectrics.

Units/ Hours	Contents	Mapping with CLO
I 11 Hours	**Fermi Surfaces:** Zone schemes, Construction of Fermi surfaces, Electron, Hole and open orbits, Harrison's method of constructing Fermi surfaces in two dimensions for monovalent, divalent, and tetravalent metal, Fermi surfaces in metals for SC, BCC, and FCC, Fermi surface of Cu and Al, Experimental methods in Fermi surface studies: De Haas-van Alphen Effect, Anomalous skin effect and cyclotron resonance, Extremal orbits, Magnetic breakdown, Calculation of energy bands: Wigner-Seitz Method, Pseudopotential Method. **Learning Activities**: Problem Solving	CLO1
II 11 Hours	**Magnetic Properties of Solids:** Classical and quantum theory of diamagnetism and paramagnetism, Pauli paramagnetism, Landau diamagnetism, Cooling by adiabatic demagnetization, Weiss theory of ferromagnetism, Curie-Weiss law, Heisenberg's model and molecular field theory, Domain structure and Bloch wall, Neel model of anti-ferromagnetism and ferrimagnetism, Ferrites, Spin waves (Magnons in ferro and anti-ferromagnets), Bloch $T^{3/2}$ law, brief discussion of Kondo effect. **Learning Activities:** Group discussions, Application based peer thinking, and Problem Solving.	CLO2
III 12 Hours	**Optical Processes, Exciton, Color Centre's and Luminescence:** Connection between optical and dielectric constants, Optical reflectance, Optical properties of metals, Color centers: Types (Electronic and Hole centers), F' centers, Production and properties, NV center's in diamond and applications in quantum computation and quantum cryptography, Excitons (Frenkel, Mott-Wannier), Excitonic insulators, Experimental studies of excitons in alkali halide, molecular crystals and carbon nanostructures, Free Excitons at High Densities, Raman effect in crystal, Types of luminescent systems: Electroluminescence, Triboluminescence, Mechanism of luminescence, Thermo luminescence, mechanism and applications in dosimetry and dating. **Learning Activities:** Group discussions, Application based peer thinking, and Problem Solving.	CLO3

IV 11 Hours	**Dielectrics and Ferroelectrics:** Local field, Clausius-Mossotti relation, Components of polarizability: Electronic, Ionic, Orientational, Measurements of dielectric constant, Pyroelectric and ferroelectric crystals and classification, Electrostatic screening, Plasma oscillations (Plasmons), Transverse optical modes in plasma, Interaction of EM waves with optical modes: Polaritons, LST relation, Electron-electron interaction, Electron-phonon interactions: Polarons. **Learning Activities:** Group discussions, Application based peer thinking, and Problem Solving.	CLO4

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

Suggested Readings:

1. Ziman J.M. (2018). *Principles of the Theory of Solids.* Cambridge University Press, India.
2. Kittel C. (2019). *Introduction to Solid State Physics.* New Delhi, India: Wiley India (P) Ltd.
3. Singh R.J. (2011). *Solid State Physics.* New Delhi, India: Pearson.
4. Dekker A.J. (2012). *Solid State Physics.* London, U.K: Macmillan.
5. Ashcroft N.W and Mermin N. D. (2003). *Solid State Physics*. Cengage, India.
6. Pillai S.O. (2020), *Solid State Physics,* New Age International Private Limited, India.
7. Wahab M.A. (2015), *Solid State Physics,* Narosa Publishing House Pvt. Ltd. - New Delhi, *India.*
8. Wahab M.A. (2011), Numerical Problems in *Solid State Physics,* Alpha Science International Ltd, India.
9. Wahab M.A. (2021), Numerical Problems in Crystallography, Springer Nature, Singapore Pte. Ltd., Singapore.

Course code: PCP.600
Course Title: Dissertation (Part-I)
Course type: Skill Based Elective
Invested Hours: 120

L	T	P	Cr
0	0	8	4

Course Objective and Learning Outcomes:

- Critically analyse, 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 Proposal (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: PCP.600
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