Central University of Punjab

M. Sc. Physics (Computational Physics)

Session: 2021-23

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 in various areas of Computational Physics, advanced knowledge in Mathematics, and knowledge in applied fields like Computer Science. Further, they apply the knowledge, general competence, and analytical skills on an advanced level, needed in industry, consultancy, education, research, or public administration. 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	CCC.515	Scientific Programming (Practical)	SBC	0	0	4	2
4	PCP.507	Classical Mechanics	CC	3	0	0	3
5	PCP.527	Quantum Mechanics	CC	3	0	0	3
6	CCC.524	Statistical Mechanics	CC	3	0	0	3
7	PCP.519	Python Programming	CC	3	0	0	3
8	PCP.520	Entrepreneurship	CF	1	0	0	1
9	XXX.XXX	Interdisciplinary Course	IDC	2	0	0	2
Total				**21**	**0**	**4**	**23**

SEMESTER – II							
Sr. No	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	PCP.525	Solid State Physics	CC	3	0	0	3
2	CCC.554	Fundamentals of Molecular Simulations	CC	3	0	0	3
3	CCC.556	Electronic Structure Theory	CC	3	0	0	3
4	CCC.525	Computational Methods	CC	3	0	0	3
5	PCP.557	Atomic and Molecular Spectroscopy	CC	3	0	0	3
6	XXX.XXX	Value Added Course	VAC	2	0	0	2
Choose any one of these courses/MOOC							
7	PHY.552	Nuclear and Particle Physics	DE	3	0	0	3
8	PHY.578	Particle Physics	DE	3	0	0	3
9	PHY.574	Introduction to Mesoscopic	DE	3	0	0	3

		Physics					
10	CCC.521	Machine Learning and Data Science	DE	3	0	0	3
Total				**20**	**0**	**0**	**20**

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	PCP.526	Computational Solid State Physics Lab (Practical)	SBC	0	0	4	2
3	CCC.528	Computational Methods Lab (Practical)	SBC	0	0	4	2
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.569	Enrichment Course-I	DEC	2	0	0	2
7	PCP.600	Research Proposal	SBE	0	0	8	4
Choose any two of these courses/MOOC							
8	PCP.573	Electronics	DE	3	0	0	3
9	PCP.570	Introduction of Density Functional Theory	DE	3	0	0	3
10	PHY.576	Nanostructured Materials	DE	3	0	0	3
11	PHY.577	Materials Characterization	DE	3	0	0	3
12	PHY.524	Electromagnetic Theory	DE	3	0	0	3
13	PHY.554	Advanced Solid State Physics	DE	3	0	0	3
Total				**11**	**0**	**24**	**23**

SEMESTER – IV							
Sr. No	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	PCP.600	Dissertation	SBE	0	0	40	20
Total				**0**	**0**	**40**	**20**

Grand Total	86 Credits

L: Lectures; T: Tutorial; P: Practical

MOOCs may be taken upto 40% of the total credits (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match a minimum 70%. Mapping will be done by the department and students will be informed accordingly.

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

Evaluation Criteria for Theory Courses

A. Continuous Assessment (Course wise): [25 Marks]
Two or more of the given methods (Surprise Tests, in-depth interview, unstructured interview, Jigsaw method, Think-Pair Share, Students Teams Achievement Division (STAD), Rubrics, portfolios, case based evaluation, video based evaluation, Kahoot, Padlet, Directed paraphrasing, Approximate analogies, one sentence summary, Pro and con grid, student generated questions, case analysis, simulated problem solving, media assisted evaluation, Application cards, Minute paper, open book techniques, classroom assignments, homework assignments, term paper).

B. Mid Semester Test: Based on Subjective Type Test [25 Marks]

C. End Semester Test: Based on Subjective (70%) and Objective (30%) Type Test [50 Marks]

The objective type will include one word answers, fill-in the blank, sentence completion, true/false, MCQs', and matching, analogies. The subjective type will include a very short answer (1-2 lines), short answer (one paragraph), essay type with restricted response, and essay type with extended response.

Core, Discipline Elective, Compulsory Foundation, Value Added and Interdisciplinary Courses			Discipline Enrichment Course		Entrepreneurship Course	
	Marks	Evaluation	Mark s	Evaluation	Marks	Evaluation
Internal	25	Various	-	-	-	-

Assessment						
Mid-semester test (MST)	25	Subjective	50	Objective	25	Objective
End-semester test (EST)	50	Subjective (70%) Objective (30%)	50	Objective	25	Subjective

Evaluation Criteria for Practical Courses:

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

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

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

SEMESTER I

Course Code: PCP.506
Course Title: Mathematics for Computational Sciences
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcome: The course on Mathematical Physics is introduced to familiarize the students with the idea about transformation of coordinates and complex functions, special functions, group theory, and tensors which will be useful in understanding theoretical treatment and for developing a strong background to pursue research in theoretical physics.

Course Content

Unit I **12 hours**

Matrices & Vector Calculus: matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors

Differential calculus: Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials

Unit II **11 hours**

Integral calculus: basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations

Fourier Transforms: Fourier series, Dirichlet condition, General properties of Fourier series, Fourier transforms, their properties and applications,

Unit III **11 hours**

Delta, Gamma, and Beta Functions: Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions.

Unit IV **11 hours**

Differential Equations Solutions of Hermite, Legendre, Bessel and Laugerre Differential equations, basics properties of their polynomials, and associated Legendre polynomials,

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

Suggested Readings

1. E. Kreyszig. (2011). *Advanced Engineering Mathematics* Wiley India Pvt. Ltd., New Delhi, India.
2. L. A. Pipes. (1985). *Applied Mathematics for Engineers and Physicist* McGraw-Hill, Noida, India .
3. D. G. Zill. (2012). *Advanced Engineering Mathematics* Jones & Barlett Learning, Massachusetts, USA.
4. P. K. Chattopadhyay. (2000). *Mathematical Physics* New Age International (P) Ltd., New Delhi.
5. E.Steiner. (2008). The chemistry Mathematics Book, Oxford University Press .
6. F. Daniels. (1959). Mathematical for Physical Chemistry : Mc. Graw Hill.
7. Tebbutt. (1994). Basic Mathematics for Chemists, Wiley.
8. G. Arfken, H. Weber and F. Harris. (2012). *Mathematical Methods for Physicists* Elsevier Academic Press, Massachusetts, USA.
9. B.S. Rajput, (2016). *Mathematical Physics* Pragati Prakashan

Paper Code: CCC.508
Course Title: Scientific Programming
Total Lectures: 45

L	T	P	Cr
3	0	0	3

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

- identify and describe the basic art of scientific programming related to Fortran 95/2003.
- demonstrate concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
- develop skills to write programs related to standard problems and as well as to chemistry.

Course Content

Unit 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

Unit II **12 Hours**

Intrinsic functions, Program design and branching structures, loop and character manipulation. Basic I/O concepts, Formatted READ and WRITE statements,

Unit III **13 Hours**

Introduction to File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatableattays in procedures, derived data types.

Unit IV **10 Hours**

What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation,

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

Suggested Readings

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

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

L	T	P	Credits
0	0	4	2

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

- 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 a Files.
6. Introduction to Arrays and procedures, Additional features of arrays and procedures.
7. Pointers and dynamic data structures using pointers in assignment statements.
8. Matrix summation, subtraction and multiplication, Matrix inversion.

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

Suggested Readings

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

Course Code: PCP.507
Course Title: Classical Mechanics
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcome: The overall goal of this course is to provide tools and applications of classical mechanics that student can use these in various branches of physics. Students who have completed this course have a deep understanding of solid understanding of classical mechanics (Newton's laws, Lagrangian mechanics, conservation principles, Hamiltonian formalism, Hamilton - Jacobi theory, central force, scattering, rigid body dynamics, small oscillations and special relativity). Establish firm physics and math foundation on which student can build a good carrier in physics**.**

Course Content

Unit I **12 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.

Unit II **11 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.

Unit III **11 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

Unit IV **11 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.

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 State.
2. J. Safko, H. Goldstein and C. P. Poole (2011) *Classical Mechanics* Pearson, New Delhi, India.
3. G. Walter, (2010). *Systems of Particles and Hamiltonian Dynamics* Springer, New York, USA.
4. P.S. Joag and N.C. Rana, (1991). *Classical Mechanics* Tata McGraw-Hill, Noida, India.
5. S.T. Thornton and J.B. Marion, (2013). *Classical Dynamics of Particles and Systems* Cengage Learning, Boston/Massachusetts, United State.
6. J. Safko, H. Goldstein and C. P. Poole, (2011). *Classical Mechanics* Pearson, New Delhi, India.
7. G. Walter, (2010). *Systems of Particles and Hamiltonian Dynamics* Springer, New York, USA.
8. P.S. Joag and N.C. Rana, (1991). *Classical Mechanics* Tata McGraw-Hill, Noida, India.

L	T	P	Cr
3	0	0	3

Course Code: PCP.527
Course Title: Quantum Mechanics
Total Hours: 45

Learning Outcome: At the end of course, students will be able to apply mathematical formulation of quantum mechanics and Schrodinger's equation to solve eigen value problems such as box potential, harmonic oscillator, hydrogen atom and quantum mechanical tunneling. Students will also be able to apply: angular momentum algebra to find out C G coefficients; WKB method to describe bound states of potentials well and quantum scattering theory to calculate scattering amplitude.

Course Content

Unit 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

Unit 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,

Unit 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.

Unit 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

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. E. Merzbacher, (2011). *Quantum Mechanics* Wiley India Pvt. Ltd., New Delhi, India.
3. L.I. Schiff, (2010). *Quantum Mechanics* Tata McGraw-Hill Education, Noida, India.
4. K. Venkatesan, (2010). P.M. Mathews, *A Textbook of Quantum Mechanics* Tata McGraw - Hill Education, Noida, India.
5. J. J. Sakurai, (2009). *Modern Quantum Mechanics* Pearson Education, India.

6. D. J. Griffiths, (2015). *Introduction to Quantum Mechanics* Pearson Education, India.
7. G. D. Mahan, (2009). *Quantum Mechanics in a Nutshell Princeton* University Press
8. V.K. Thankappan, (2016). *Quantum Mechanics* New Age Pub. N. Delhi.

Paper Code: CCC.524
Course Title: Statistical Mechanics
Total Lectures: 45

L	T	P	Cr
3	0	0	3

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

- apply the classical laws of thermodynamics and their application, mathematical review of classical mechanics
- learn the postulates of statistical mechanics, Liouville's Theorem, and statistical interpretation of thermodynamics
- identify the microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function, elementary probability theory, distributions and fluctuations
- learn the methods of statistical mechanics and their use to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases
- After, completion of this course will help the students to apply the principles and techniques from statistical mechanics to a range of modern day research based problems.

Course Content

Unit I **13 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.

Unit II **12 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

Unit III **10 Hours**

Basic Thermodynamics: Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function

Unit IV **10 Hours**

Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas.

Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

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

Suggested Readings

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

Course Code: PCP.519
Course Title: Python Programming
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course students will be able to explain and learn Python Programming to build applications intheir core domain. Python is becoming popular in artificial intelligence and machine learning. Micro Pythonis sub-set of Python Programming useful to port in hardware for embedded and IoT applications.

Course Content

Unit 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

Unit 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

Unit III **11 hours**

Python Functions and Modules: Defining custom functions, Organising 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

Unit 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.

Transaction Mode: Lecture, tutorial, problem solving

Suggested Readings

1. S. Gowrishankar, A. Veena, (2018). *Introduction to Python Programming*, 1st Edition, CRC Press/Taylor & Francis.
2. J. Vander Plas, (2016). *Python Data Science Handbook: Essential Tools for Working with Data*, 1st Edition, O'Reilly Media.
3. 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.
4. Wesley J Chun, (2015). Core *Python Applications Programming* 3rd Edition, Pearson Education India.

Course Code: PCP.520
Course Title: Entrepreneurship
Total Hours: 15

L	T	P	Cr
1	0	0	1

Learning Outcomes: On the completion of this course, students will be able
a. To absorb an entrepreneurial mind-set.
b. To learn what is entrepreneurship and its impact
c. To develop understanding about problems and prospects in entrepreneurship.
d. To gain insights about entrepreneurial behaviour and skills.
e. To develop understanding about writing business plan/project proposals & managing start-up issues.

UNIT I **4 Hours**

Introduction:

- The concept of entrepreneurship, the history of entrepreneurship
- Entrepreneurial Structure; Nature, Characteristics, functions and its role in economic development
- Entrepreneurship- problems and prospects in India

UNIT II **4 Hours**

The Entrepreneur

- Entrepreneurial Behaviour and Skills
- The entrepreneurial decision process
- The skill gap analysis, role models
- The entrepreneurial success stories

Unit III **3 Hours**

E-Cell

- The concept of E-cells
- The significance, and activities conducted by E-cell
- Benefits of Joining E-Cells

Unit IV **4 Hours**

- Role of industries/entrepreneur's associations and self-help groups
- Funding opportunities for start-ups. Basic start-up problems
- Contents of business plan/ project proposal
- Barriers and gateways to communication, the ability of personal selling and negotiation.

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

Suggested Readings

1. G. K. Varshney, (2012). *Fundamentals of Entrepreneurship*, Sahitya Bhawan Publications.
2. R. Roy, (2011). *Entrepreneurship* 2nd Edition, Oxford.
3. B. K. Mehta, (2018). *Entrepreneurship and Small Business* SBPD Publishing House,

SEMESTER II

Paper Code: PCP.525

Course Title: Solid State Physics

L	T	P	Credits
3	0	0	3

Total Lecture: 45

Learning Outcomes: The course on Solid State Physics is to provide the student with a clear and logical presentation of the basic and advanced concepts and principles of the physics for solid state.

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

- learn the various types of crystal structure, and x-ray diffraction methods
- interpret the lattice vibrations and band theory of solids
- gain deep knowledge on magnetic properties of solids, defects, superconductivity

which will help them to apply these techniques in investigating the aspects of the matter in condensed phase.

Course Content

Unit I **12 hours**

Crystal Structure: Bravais lattices, Crystal structures, Reciprocal lattices, Ewald sphere, Lattice parameter determination, Atomic and crystal structure factors

X-ray diffraction: X-ray diffraction, Bragg law, Laue equations, Concept of reciprocal lattice and Ewald's construction. Experimental diffraction methods: Laue rotating crystal method and powder method.

Unit II **11 hours**

Electronic properties and band theory: Electronic structure of solids- band theory,Refinement of simple band theory- k-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, p-n junctions, Defects in solids

Unit III **11 hours**

Magnetic Properties: Behavior of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

Unit IV **11 hours**

Superconductivity: Meissner effect, Type-I and type-II superconductors; BCS theory, Flux quantization, Coherence, AC and DC Josephson effect, Superfluity, High TC superconductors and their applications.

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

Suggested Readings

1. J. Ziman, (2011). *Principles of the Theory of Solids,* Cambridge University Press, Cambridge, U.K..
2. C. Kittel, (2007). *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi, India.
3. R.J. Singh, (2011). *Solid State Physics,* Pearson, New Delhi, India.
4. A.J. Dekker, (2012). *Solid State Physics* Macmillan, London, U.K.
5. N. W. Ashcroft and N. D. Mermin, (2003). *Solid State Physics,* Thomson Press.
6. A.R. Verma and O.N. Srivatava, (2012). *Crystallography Applied to Solid state physics,* New Age International).

Paper Code: CCC.554
Course Title: Fundamentals of Molecular Simulations
Total Lecture: 45

L	T	P	Credits
3	0	0	3

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

- learn the modelling of small to large molecular environments
- understand various force field for biomoleculra simulation in details
- learn different methods for simulating large systems
- gain the knowledge about different molecular simulation techniques
- understand the dynamics of the structural transitions

which will help them use the techniques of molecular simulations in their further potential careers in academia and industry.

Course Content

Unit I **11 Hours**

Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.

Force Fields and Molecular Representation – (a) Intramolecular Interactions, (b) Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, (c) Hydrogen Bonds, (d) Constraints and Restraints, (e) United Atom and Other Coarse-Grained Approaches, (f) Non-pairwise Interactions, (g) How accurate are force fields?
Example: Protein, Nucleic Acid, Small Molecule Force Field, Water Models.

Unit 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

Unit III **12 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

Unit 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

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). *MolecularModeling Principles and applications*. II edition, Prentice Hall.
4. S. Alavi, (2020). *Molecular Simulations: Fundamentals and Practice* 1st Edition, Wiley-VCH.

Paper Code: CCC.556
Course Title: Electronic Structure Theory
Total Hours: 45

L	T	P	Credits
3	0	0	3

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

- identify and define basic terms and concepts which are needed for this specialized corse.
- describe the HF SCF method.
- choose the basis sets.
- compare post-HF methods.
- identify how to apply quantum chemistry to study chemical and biochemical problems.

Course Content

Unit 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,

Unit II **12 Hours**

Second-Quantized Operators and Matrix Elements. The Fock Operator, HF Equations, Roothaan Equations, SCF Procedure.

Unit II **10 Hours**

Polyatomic Basis sets, Minimal, Double zeta, triple zeta and Polarized basis sets.

Unit IV **11 Hours**

Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method.

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.

Paper Code: CCC.525

Course Title: Computational Methods

L	T	P	Credits
3	0	0	3

Total Hours: 45

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

- the large scale systems of linear, non-linear and simultaneous equations
- the matrix and determinants, interpolations, polynomial and spline interpolation
- the numerical differentiation and integration
- complex curve fitting methods, explicit schemes to solve differential equations
- the simple optimisation, vectorisation.

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

Course Content

Unit I **11 Hours**

Introduction: Errors, Siccessive 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.

Unit II **11 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

Unit III **13 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.

Unit IV **10 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.

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.

Paper Code: PCP.557
Course Title: Atomic and Molecular Spectroscopy
Total Lectures: 45

L	T	P	Credit
3	0	0	3

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

- gain the knowledge about various spectroscopic techniques, such as, electronic, microwave, vibrational, raman, nuclear magnetic resonance, and laser spectroscopy
- understand, how spectroscopic transitions come into picture in molecular quantum mechanics
- learn various spectroscopic selection rules and their applications

Course Content

Unit 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.

Unit II **11 hours**

Molecular Spectra: Molecular potential, Separation of electronic and nuclear wave functions, Born-Oppenheimer approximation, Electronic, Vibrational and rotational spectrum of diatomic molecules, Selection rules, Frank-Condon principle,

Unit III **11 hours**

Molecular Spectroscopy: Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO2), FT-IR instrumentation

Unit IV **11 hours**

Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines, Vibrational spectroscopy of diatomic molecules, Franck-Condon factor,rotational fine structure.

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

Suggested Readings

1. J. M. Hollas, (2004). *Modern Spectroscopy* John Wiley & Sons, Ltd.

2. G. M. Barrow, (1962). *Introduction to Molecular Spectroscopy* McGraw-Hill.
3. C. N. Banwell and E.M. Mc Cash, (1994). *Fundamentals of Molecular Spectroscopy* Tata McGraw Hill, New Delhi.
4. L. R. Lakowicz, (2012). *Principle of Fluorescence Spectroscopy*, Springer.
5. A. Carrington and A. D. Mc Lachlan, (1979). *Introduction to Magnetic Resonance* Chapman and Hall, London.
6. R. K. Harris, Addison Wesley, (1986). *Nuclear Magnetic Resonance Spectroscopy* Longman Ltd, London.
7. C. N. Banwell and E. M. Mc Cash, (2012). *Fundamentals of Molecular Spectroscopy*, Tata, McGraw Hill Publishing Company Limited.
8. C.J. Foot, (2005). *Atomic Physics,* Oxford University Press, Oxford, U. K.

Course Code: PHY.552
Course Title: Nuclear and Particle Physics
Total Hours: 60

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course students will be able to explain basics of nuclear properties, nuclear interactions, nuclear decay, nuclear models, detectors, nuclear reactions and elementary particles.

Course Content

Unit I **12 hours**

Basic Nuclear Properties: Nuclear size, shape and charge distribution, Form factor, Mass and binding energy, Saturation of nuclear force, Abundance of nuclei, Spin, Isospin, Mirror nuclei, Parity and symmetry, Magnetic dipole moment and electric quadrupole moment.

Unit II **11 hours**

Nuclear Models: Evidence of shell structure, Single particle shell model, its validity and limitations, Rotational spectra, Shell model, Liquid drop model, Collective model, Semi empirical mass formula. Exchange force model.Double beta decay.

Nuclear Decay: Different kinds of particle emission from nuclei, Alpha decay Fine structure of α spectrum, 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.

Unit III **11 hours**

Nuclear Reactions: Types of Nuclear Reactions and conservation laws, Energetic of Nuclear reactions, Isospin, Reaction Cross sections, Coulomb Scattering, Optical model, Compound nucleus reactions, Direct Reactions, Resonance reactions, Heavy Ion reactions,

Unit IV **11 hours**

Elementary Particle Physics: Classification of particles: Fermions and bosons, Elementary Particles and antiparticles, Quarks model, baryons, mesons and leptons, Classification of fundamental forces: Strong, Electromagnetic, Weak and Gravitational.Conservation laws of momentum, energy, Angular momentum, Parity non conservation in weak interaction, Pion parity, Isospin, Charge conjugation, Time reversal invariance, CPT invariance.Baryon and Lepton numbers, Strangeness, charm and other additive quantum numbers, Gell Mann Nishijima formula.

Transaction Mode: Lecture, tutorial, problem solving

Suggested Readings

1. B. Martin, (2011). *Nuclear & Particle Physics* an Introduction, John Wiley & Sons, Inc., New Jersey, USA.
2. K.S. Krane, (2008). *Introductory Nuclear Physics,* John Wiley & Sons, Inc., New Jersey, USA.
3. C.A. Bertulani, (2007). *Nuclear Physics in a Nutshell,* Princeton University Press, Princeton, USA.
4. S.S.M. Wong, (2008). *Introductory Nuclear Physics,* John Wiley & Sons, Inc., New Jersey, USA.
5. K. Heyde, (2004). *Basic Ideas and Concepts in Nuclear Physics* An Introductory approach, CRC Press, London, U. K.
6. B. Povh, K. Rith, C. Scholz, (2012). *Particles and Nuclei: An Introduction to the Physical Concepts* Springer, New York, USA.
7. D.H. Perkin, (2009). *Introduction to High Energy Physics,* Cambridge University Press, Cambridge, U.K.
8. I.S. Hughes, (1991). *Elementary Particles*, Cambridge University Press, Cambridge, U.K.
9. W.R. Leo, (2009). *Techniques for Nuclear and Particle Physics Experiments,* Springer, New York, USA.
10. T. Stefan, (2010). *Experimental Techniques in Nuclear and Particle Physics,* Springer, New York, USA.
11. D.J. Griffiths, (2008). *Introduction to Elementary Particles,* Wiley-VCH Verlag GmbH, Germany.

Course Code: PHY.578
Course Title: Particle Physics
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: After a successful completion of the course, students will be able to explain the basic properties of elementary particles, various fundamental interactions (Strong, weak and electromagnetic and gravity), kinematics of decay and scattering, symmetries, and various aspects of quark models.

Course Content

Unit I **12 hours**

Particles and Forces: Production and basic properties of elementary particles in cosmic rays and accelerators experiments, mass spectra and decays of elementary particles, Fundamental interactions: basic properties of Strong, weak and electromagnetic and gravity. Yukawa theory of pion exchange.

Unit II **11 hours**

Kinematics: Kinematics of decay and scattering, Scattering in lab and centre of mass frames, Two and Three body decay phase space, Dalitz plot.

Unit III **12 hours**

Quark Model:- Quark structure of strange and nonstrange hadrons, need of colour quantum number. observation of new flavour states, charm, bottom hadrons, higher symmetries (brief description). Application of quark model for electromagnetic decays of vector mesons.

Unit IV **10 hours**

Weak Interactions: Classification of weak Interactions; Leptonic Semi-Leptonic and Non- Leptonic Decay, Tau- Theta Puzzle, Parity Violation in Weak Decays Selection Rules Semileptonic Decays, and nonleptonic decays, Universality of Weak Interactions, Fermi Theory of weak interactions, Intermediate Vector – Boson Hypothesis, Helicity of Neutrino, Two Component Theory of Neutrino, K0-K0bar Mixing and CP Violation.

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

1. R. Leo, (2009). *Techniques for Nuclear and Particle Physics Experiments,* Springer, New York, USA.
2. D.H. Perkin, (2000). *Introduction to High Energy Physics,* Cambridge Univ. Press, U.K.
3. D.J. Griffiths, (2008). *Introduction to Elementary Particles,* Wiley-VCH GmbH, Germany.
4. I.S. Hughes, (1991). *Elementary Particles,* Cambridge University Press, Cambridge, U.K.
5. M.P. Khanna, (2013). *Particle Physics*, Prentics Hall. Pub., N. Delhi.
6. M.P. Khanna, (1999). *Quantum Mechanics*, Har Anand Pub. N. Delhi.
7. T. Stefan, (2010). *Experimental Techniques in Nuclear and Particle Physics,* Springer, New York, USA.
8. V.K. Mittal, R.C. Verma& S.C. Gupta, (2015). *Nuclear & Particle Physics*, Prentics Hall Pub. N. Delhi, 3rd edition,
9. W.E. Burcham and M. Jobes, (2014). *Nuclear Physics,* Addison Wesley. Pub.

Course Code: PHY.574
Course Title: Introduction to Mesoscopic Physics
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: After a successful completion of the course, students will be able to explain the transition regime between macroscopic and microscopic object. They will be able to demonstrate the knowledge for quantum transport with illustrative examples showing how conductors evolve from the atomic to the ohmicregime as they get larger. In this regard, they will be able to explain various phenomenon such as, quantization of electrical conductance in nanoscale conductors, Coulomb Blockade, quantum capacitance and etc.

Course Content

Unit I **12 hours**

Introduction, Why Electrons Flow, Conductance Formula, Ballistic Conductance, Diffusive Conductance, Connecting Ballistic to Diffusive, Dispersion Relation, Drude Formula.

Unit II **11 hours**

Counting States, Density of States, Number of Modes, Electron Density, Conductivity vs. Electron Density, Quantum Capacitance, What and Where is the Voltage, A New Boundary Condition, Current from Quasi-Fermi Levels, Electrostatic Potential.

Unit III **11 hours**

Boltzmann Equation, SemiclassicalModel,Quantum Model, Landauer Formulas, NEGF Equations, Self-Energy, Surface Green's Function, Current Operator, Scattering Theory, Transmission, Golden Rule, Quantum Master Equations.

Unit IV **11 hours**

Electronic Spin-Orbit Coupling, Spin Hamiltonian, Spin Density/Current, Spin Voltage, Spin Circuits, Seebeck Coefficient, heat Current, One-level Device, Second Law, Entropy.

Transaction Mode: Lecture, demonstration, PPT .

Suggested Readings

1. S. Datta, (2010). *Quantum Transport Atom to Transistor*, CAMBRIDGE.
2. S. Datta, (2009). *Lessons from Nanoelectronics: A New Perspective on Transport: Volume 1 & 2*, World Scientific.
3. D.A. Ryndyk, *Theory of Quantum Transport at Nanoscale: An Introduction*, Springer.
4. Yuli V. Nazarov and Yaroslav M. Blanter, *Quantum Transport: Introduction to Nanoscience,* CAMBRIDGE.

L	T	P	Cr
3	0	0	3

Course Code: CCC.521
Course Title: Machine Learning and Data Science
Total Lecture: 45

Learning Outcomes: On completion of the course the student should be able to:

10. learn the data cleaning, cross-validation, and application of regression analysis
11. gain knowledge about distance matrices, various methods of clustering as well as dimensionality reduction
12. apply several techniques for information retrieval and text mining

Course Content

Unit I **11 Hours**

Introduction: Overview of Machine Learning field, terminology alert: true positive, false positive, Confusion matrix, Bias and variance

Unit II **12 Hours**

Unsupervised Methods: Clustering: Distance Metrics, K-Means, leader, Jarvis-Patrick, hierarchical clustering; Dimensionality Reduction: PCA, LDA, Sammon's

Unit III **11 Hours**

Supervised Methods: Classification: K-NN, naïve Bayes, decision trees, boosting and bagging

Unit IV **11 Hours**

Classification: Ensemble methods, random Forests; Support vector machines Neural networks, Recommendation systems; Outlier detection.

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

Suggested Readings

1. Han, Kamber and Pei, (2011). *Data Mining: Concepts and Techniques, Third Edition*
2. Christopher Bishop, (2007). Pattern Recognition and Machine Learning
3. Max Kuhn and Kjell Johnson, (2013). *Applied Predictive Modeling*
4. James, Witten, Hastie, Tibshirani, (2014). *An Introduction to Statistical Learning and Applications in R*
5. Wes McKinney, (2013). *Python for Data Analysis*,

SEMESTER III

Course Code: CCC.551
Course Title: Research Methodology
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: The course Research Methodology has been framed to introduce basic concepts of Research Methods. The course covers preparation of research plan, reading and understanding of scientific papers, scientific writing, research proposal writing, ethics, plagiarism, computer laboratory safety issues etc.

Course Content

Unit 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.

Unit II **12 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.

Unit 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.

Unit IV **10 hours**

Research and Academic Integrity: Plagiarism, Copyright issues, Ethics in research, and case studies. Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials.

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.
3. R. Kothari, (2008). *Research Methodology*, New Age International, New Delhi, India.
4. Standard /Reputed Journal authors' instructions.
5. Web resources: www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.
6. Web resources: www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

Paper Code: PCP.526
Course Title: Computational Solid State Physics Lab (Practicals)
Total Hours: 60

L	T	P	Credits
0	0	4	2

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

- learn the computational methods for CSCl crystal structure determination
- carry out the geometry optimization of molecular crystals
- measure the Infrared spectra of crystals, and Raman spectra
- interpret the dispersion relation and cut-off frequency for the mono-atomic lattice

which will enhance their employability in their further potential careers in academia and industry.

Course Content

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

1. Determine the crystal structure of CsCl using Gaussian package.
2. Geometry optimization of crystals using Gaussian package.
3. Determination of Infrared spectra of crystals using Gaussian package.
4. X-ray diffraction refinement using ICSD data.

5. Obtaining the structure of NaCl crystal system using Diamond software package.
6. Determination of Raman spectra using Gaussian package.
7. To determine magneto resistance of a bismuth crystal as a function of magnetic field.
8. Determination of critical temperature of high temperature superconductor and Meissner effect for a high Tc superconductor.
9. Determination of ferromagnetic to paramagnetic phase transition temperature (TC = Curie temperature).
10. Determination of dielectric constant of solids.
11. Study of the dispersion relation and cut-off frequency for the mono-atomic lattice. Study of the dispersion relation for the di-atomic lattice – 'acoustical mode' and 'optical mode' and energy gap.
12. Study of thermal expansion pf solids.
13. Study of thermal conductivity of solids.
14. Study of specific heat of solids.

Transactional Modes: Computation work, Experimentation and Viva-voce..

Suggested Readings

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

Paper Code: CCC.528
Course Title: Computational Methods lab (Practical)
Total Hours: 60

L	T	P	Credits	
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 optimisation

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, 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.

Paper Code: CCC.555
Course Title: Molecular Simulations Lab (Practical)
Total Lecture: 90

L	T	P	Credits	
0	0	4	2	

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

- learn the basics of Linux environment
- use the remote computing as a tool for high performance computation
- use different energy minimization techniques
- create molecular model from scratch, and high definition images using various graphics tools
- gain the practical in-hand experience of various modeling and classical simulation tools
- learn the use of different insilico techniques for biomolecular simulations

which will enhance their employability in their further potential carrers 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. Review of Molecular Dynamics Principles

Transactional Modes: Laboratory based practicals; 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). *MolecularModeling Principles and applications*. II edition, Prentice Hall.
4. S. Alavi, (2020). *Molecular Simulations: Fundamentals and Practice* 1st Edition, Wiley-VCH.

Paper Code: CCC.573
Course Title: Electronic Structure Theory Lab (Practical)
Total Hours: 60

L	T	P	Credits
0	0	4	2

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

Following experiments will be carried out in the lab.

1. Introduction to electronic structre 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 suface 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 practicals; Problem solving; Self-learning.

Suggested Readings

1. David S. Sholl and Janice A. Steckel, (2009). *Density Functional Theory: A Practical Introduction*, John Wiley and Sons.
2. http://blogs.cimav.edu.mx/daniel.glossman/data/files/Libros/Exploring%20Chemistry%20With%20Electronic%20Structure%20Methods.pdf

3. Gaussian 09/16 website or manual.

Paper Code: PCP.569
Course Title: Enrichment Course-I
Total Lecture: 30

L	T	P	Credits	
2	0	0	2	

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

- learn systematic Knowledge of different type of competitive examination
- Gain the knowledge about the basic aspects higher studies.

Course Content

Unit I **8 hours**

Mathematical Methods of Physics: Elements of complex analysis, analytic functions; Taylor & Laurent series; poles, residues and evaluation of integrals, Elementary probability theory, random variables, binomial, Poisson and normal distributions, Central limit theorem.

Unit II **7 hours**

Quantum Mechanics: Hydrogen atom, Stern-Gerlach experiment, Identical particles, Pauli exclusion principle, spin-statistics connection,Wave-function in coordinate and momentum representations,Commutators and Heisenberg uncertainty principle, Dirac notation for state vectors.

Unit III **8 hours**

Thermodynamics: Laws of thermodynamics and their consequences. Thermodynamic potentials, Maxwell relations, chemical potential, phase equilibria. Phase space, micro- and macro-states.

Unit IV **7 hours**

Experimental Electronics: Microprocessor and microcontroller basics, High frequency devices (including generators and detectors),Data interpretation and analysis, Precision and accuracy, Error analysis, propagation of errors, Least squares fitting, filtering and noise reduction, shielding and grounding.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning, online tools, online lecture series, online study materials.

Suggested Readings

1. D. J. Tannor, (2006). *Introduction to Quantum Mechanics: A Time-dependent Perspective*, University Science Books.
2. R. E. Wyatt and J. Z. H. Zhang, (1996). *Dynamics of Molecules and Chemical Reactions*, CRC Press.
3. K. C. Kulander, (1991). *Time-dependent Methods for Quantum Dynamics*, Elsevier Science.

Paper code: PCP.600
Course Title: Research Proposal
Invested Hours: 120

L	T	P	Cr
0	0	8	4

Course Objective and Learning Outcomes:

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

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

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

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

Evaluation Criteria:

Dissertation 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: Laboratory based practicals; Problem solving; Self-learning.

Paper Code: PCP.573
Course Title: Electronics
Hours Invested: 60

		L	T	P	Credits	
		3	0	0	3	

Learning Outcomes: The course on Electronics and Digital Electronics Circuits Theory is introduced to familiarize the students with the idea of electronic devices, circuits, operations, signal processing and their applications.

Course Content

Unit 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, derivation of β, α and various parameters, loadline analysis, Operating point, voltage-divider bias, transistor switching networks, bias stabilization, working of CE amplifier. Construction, working and characteristics of JFET and MOSFET.

Unit II **11 hours**

Optoelectronic Devices and Transducers: Solar cell, Photo detector and LEDs, Transducers, Measurement and control, Shielding and grounding.
Field Effect Transistor: Field effect transistor and its small signal model, CS

and CD amplifiers at low frequencies, Biasing the FET, CS and CD amplifiers at high frequencies.

Unit 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.

Unit 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 (upto 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.

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). *Electronics: Fundamentals andApplications*, 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.

Paper Code: PCP.570
Course Title: Introduction of Density Functional Theory
Total Lecture: 45

L	T	P	Credits	
3	0	0	3	

Learning Outcomes: This is a specialization course for students of Computational Chemistry. At the end of the course, the students will be able to:

- learn basics of Density Functional Theory (DFT)
- understand most popular framework of modern DFT.
- characterize the properties of molecules and materials
  After completion of this course, it will help the students to use different functional appropriately for different problems.

Course Content

Unit I **11 Hours**
Schrödinger equation for many particles system, Hartree theory, Identical particles and spin, Hartree-Fock theory, Antisymmetricwavefunctions and Slater determinant, Koopmans' theorem.

Unit II **12 Hours**
Idea of functional, Functional derivatives, Electron density, Thomos 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.

Unit 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.

Unit 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.

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

Suggested Readings

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

Course Code: PHY.576
Course Title: Nanostructured Materials
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: After the completion of this course student will have solid understandings of nanomaterials, their properties, synthesis via different methods, applications of nanomaterials and different characterization tools that are used to probe the nanomaterials.

Course Content

Unit I **12 hours**

Nanomaterials, Their Properties and Applications: Low-dimensional materials: Qunatum dot, tube and well, Some special nanomaterials: Synthesis, properties and applications of Fullerenes, Carbon Nanotubes (SWCNT and MWCNT) and Nanowires, Graphene, Porous materials: Porous silicon, Aerogel, Quantum size effect, Self assembly of Nanomaterials, Structural, Electrical, optical, mechanical, chemical, and magnetic properties at nanoscale, Applications and benefits of nanotechnology, Nanotechnology Ethics and Environment, Challenges and Future of nanotechnology.

Unit II **11 hours**

Synthesis of Nanomaterials: Fabrication methods i.e. top-down and bottom-up approach, Synthesis of nanomaterials by Physical, Chemical and Biological methods, Thin Film nanomaterials, Electrolytic deposition, Thermal evaporation, Spray pyrolysis, Sputtering, Pulse laser deposition, LB, Spin coating, Dip coating, Solution cast, Tape casting, Sol gel, Chemical vapour deposition, Molecular beam epitaxy, Cluster beam evaporation, Ion beam deposition, Chemical bath deposition with capping techniques.

Unit III **11 hours**

Microscopy: Light Microscopy (Bright field, dark field, phase contrast), Fluorescence (wide-field, confocal, 2-photon) microscopy, Field Emission Scanning Electron Microscopy (FESEM), Energy-dispersive X-ray spectroscopy (EDS), Transmission Electron Microscopy (TEM), High resolution TEM, Selected area electron diffraction (SAED).

Surface Probe Analysis: Atomic Force Microscope (AFM), Scanning Tunnelling Microscope (STM), spectroscopy, X-ray photoemission spectroscopy (XPS).

UNIT IV **11 hours**

Diffraction Methods: Generation and detection of X-rays, Diffraction of X-rays, X-ray diffraction techniques, Electron diffraction.

Spectroscopy: IR Spectroscopy, FTIR, UV-Visible spectroscopy, Raman Spectroscopy, Auger Spectroscopy, Impedance Spectroscopy, Dielectric Spectroscopy.

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

Suggested Readings

1. S. B. Ogale, T. V. Venkatesan, and M. G. Blamire, (2013) *Functional Metal Oxides: New Science and Novel Applications*, Wiley-VCH.
2. R. W. Chan and P. Hassen, (1983). *Physical Metallurgy, Vol. 1 and Vol. 2* North Holland Publishing Company, New York.
3. R. E. Smallman, (1999). *Modern Physical Metallurgy and Materials Engineering 6th Edition* Butterworth-Heinemann.
4. Greg Haugstad, (2012). *Atomic Force Microscopy: Understanding Basic Modes and Advanced Applications* John Wiley & Sons.
5. B.S Murty, P.Shankar, B. Raj, B. B. Rath, and J. Murday, (2013). *Textbook of Nanoscience and Nanotechnology,* Springer.
6. Klaus D. Sattler, (2010). *Handbook of Nanophysics*, CRC press.

7. Claudia Gutirrez-Wing, Jos Luis Rodrguez-Lpez, Olivia A. Graeve, and Milton Muoz-Navia, (2013). *Nanostructured Materials and Nanotechnology*, Cambridge University Press.

Course Code: PHY.577
Course Title: Materials Characterizations
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, students would be able to know the basic characterizations used for the different information and purpose of the prepared nanomaterials/thin films.

Course Content

Unit I **12 hours**

Microscopy: Optical Microscopy, Scanning Electron Microscopy (SEM), Field Emission Scanning Electron Microscopy (FESEM), Energy-dispersive X-ray spectroscopy (EDS), Transmission Electron Microscopy (TEM), High resolution TEM, Selected area electron diffraction (SAED).

Diffraction Methods: Generation and detection of X-rays, Diffraction of X-rays, X-ray diffraction techniques, Electron diffraction.

Unit II **11 hours**

Surface Probe Analysis: Atomic Force Microscope (AFM), Scanning Tunneling Microscope (STM), X-ray photoemission spectroscopy (XPS), Angle Resolved XPS (ARPS), Rutherford Back Scattering, Carbon Dating, Ion Beam (Low energy and high energy) irradiation.

UNIT III **11 hours**

Spectroscopy: IR Spectroscopy, FTIR, UV-Visible spectroscopy, Raman Spectroscopy, Auger Spectroscopy, Impedance Spectroscopy (Nyquist Plot, Bode Plot, Electrical {: electronic, ionic, cationic} conductivity estimation, ac conductivity and Jonscher Power law), Dielectric Spectroscopy (Cole-Cole Plot,Cole-Davidson plot, Debye Plot, loss tangent, sigma representation, relaxation time), Modulus spectroscopy.

Unit IV **11 hours**

Thermal Analysis: Thermogravimetric analysis, Differential thermal analysis, Differential Scanning calorimetry, Modulated DSC, Dynamic Thermal Analysis, Universal tensile testing.

Transport Number Analysis: Transference Number (Electron, ion, cation transport measurement) Analysis, IV characteristics, Activation Energy Estimation (VTF and Arrhenius), Transport Parameters analysis.

Transaction Mode: Lecture, demonstration, PPT

Suggested Readings

1. Yang Leng, (2013). *Materials Characterization: Introduction to Microscopic and Spectroscopic Methods*, 2nd Edition WILEY.
2. Greg Haugstad, (2012). *Atomic Force Microscopy: Understanding Basic Modes and Advanced Applications*, WILEY.
3. C. Julian Chen, (1993). *Introduction to Scanning Tunneling Microscopy*, Oxford University.
4. John F. Watts and John Wolstenholme, (2003). *An Introduction to Surface Analysis by XPS and AES*, WILEY.

Course Code: PHY.524
Course Title: Electromagnetic Theory
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, students will able to explain various concepts of electrostatics and magnetostatics. Students will also solve the boundary value problems and will explain the propagation of electromagnetic waves in dielectrics, metals and plasma. This course will also inculcate the knowledge of the motion of relativistic and non- relativistic charged particles in electrostatic and magnetic fields.

Unit I **12 hours**

Electrostatics: Gauss's law and its applications, Displacement current, Energy density and capacitance. Gauss's law in the presence of dielectric, Electrostatic energy in dielectric media.

Unit II **11 hours**

Magnetostatics: Biot-Savart law and Ampere's theorem, Electromagnetic induction, Vector potential and magnetic induction for a circular current loop, Magnetic fields of a localized current distribution, Boundary condition on B and H, Uniformly magnetized sphere.

Unit III **11 hours**

Maxwell's Equations: Maxwell's equations in free space and linear isotropic media, Boundary conditions on the fields at interfaces. 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, EM fields.

Unit IV **11 hours**

Plane Electromagnetic Waves and Wave Equations: EM wave in free space, Dispersion characteristics of dielectrics, Waves in a conducting and dissipative media, Reflection and refraction, Polarization, Fresnel's law, Skin effect, Transmission lines and wave guides, TE mode, TM mode, Cut off wavelength

Transaction Mode: Lecture, Demonstration, Power point Presentations

Suggested Readings:

1. D.J. Griffiths, (2012). *Introduction to Electrodynamics*, Prentice Hall of India Pvt.Ltd., New Delhi.
2. A. Zangwill, (2012). *Modern Electrodynamics,* Cambridge University Press, Cambridge, U.K.
3. J. D. Jackson, (2004). *Classical Electrodynamics,* Wiley India (P) Ltd., New Delhi, India.
4. E. M. Lifshitz, L. D. Landau and L. P. Pitaevskii, (1984). *Electrodynamics of Continuous Media,* Elsevier, New York, USA.

Course Code: PHY.554
Course Title: Advanced Solid State Physics
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: The purpose of this course is to introduce students to the fundamental and advanced concepts of solid state physics. After the completion of this course the students will have solid understandings of the topics include Fermi surfaces and its determinations, band gap in semiconductor, Plasmons, Dielectric, Ferroelctrics and optical processes in crystalline and amorphous solids.

Unit I **12 hours**

Fermi Surfaces and Metals: Zone schemes, Construction of Fermi surfaces, Electron orbits, Hole orbits and open orbits, Calculation of energy bands: Wigner-seitz Method, Pseuopotential Method, Experimental methods in Fermi surface studies: De Haas-van Alphen Effect, Fermi Surface of Cu and Au, Magnetic Breakdown.

Unit II **11 hours**

Semiconductor Crystals: Direct and indirect band gap, Equation of motion, Intrinsic and extrinsic semiconductors, Physical interpretation of effective mass, Effective masses in semiconductors, Cyclotron resonance, Intrinsic carrier concentration, Fermi level and electrical conductivity, Metal-metal contacts, Thermoelectric effects: Diode and transistors.

Unit III **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, Transverse optical modes in plasma, Interaction of EM waves with optical modes: Polaritons, LST relation, Electron-electron interaction, Electron-phonon interactions: Polarons.

Unit IV **11 hours**

Plasmons and Optical Processes: Connection between optical and dielectric constants,Optical reflectance, Optical properties of metals, Luminescence, Types of luminescent systems, Electroluminescence, Color centers, Production and properties, Types of color centers, Excitons (Frenkel, Mott-Wannier), Experimental studies (alkali halide and molecular crystals), Raman effect in crystals, Diffraction pattern and low energy excitations in amorphous solids

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

Suggested Readings

1. J. Ziman, (2011). *Principles of the Theory of Solids,* Cambridge University Press, Cambridge, U.K.
2. C. Kittel, (2007). *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi, India.
3. R.J. Singh, (2011). *Solid State Physics,* Pearson, New Delhi, India.
4. A.J. Dekker, (2012). *Solid State Physics,* Macmillan, London, U.K.
5. N. W. Ashcroft and N. D. Mermin, (2003). *Solid State Physics,* Thomson Press.

SEMESTER IV

Paper Code: PCP.600
Course Title: Dissertation
Total Hours: 600

L	T	P	Cr
0	0	40	20

Course Objective and Learning Outcomes:

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

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

***Evaluation Criteria:**

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

Dissertation (Fourth Semester)		
	Marks	Evaluation
Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report,

		presentation, final viva-voce
External expert, HoD and senior-most faculty of the department	50	Dissertation report (30), presentation (10), final viva-voce (10)

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