Central University of Punjab, Bathinda

M. Sc. Physics (Computational Physics)

Session: 2020-22

Department of Computational Sciences

Programme Outcomes (MSc Physics (Computational Physics))

The Master program in Computational Physical Science i.e. M.Sc. computational Physics will enable to;

- analyze the knowledge, general competence, and analytical skills as well as computational aspect on an advanced level, needed in industry, consultancy, education, research, or public administration.
- Evaluate the contributions of basic knowledge of science background and experience to successfully carry out advanced tasks and projects, both independently and in collaboration with others and the role of computational sciences in society and the background to consider ethical problems.

Course Structure of the Programme

SEMESTER – I							
Sr. No	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	CCC.524	Statistical Mechanics	CC	4	0	0	4
2	PCP.506	Mathematics for Computational Sciences	CF	4	0	0	4
3	PCP.507	Classical Mechanics	CF	4	0	0	4
4	CCC.508	Scientific Programming	CF	4	0	0	4
5	CCC.515	Scientific Programming (Practical)	SBC	0	0	8	4
6	XXX	Interdisciplinary Course	IDC	2	0	0	2
Interdisciplinary course offered for other departments							
	CCC.516	Chemistry without test tube	IDC	2	0	0	2
Total				**18**	**0**	**8**	**22**

SEMESTER – II							
Sr. No	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	PCP.525	Solid State Physics	CC	4	0	0	4
2	PCP.526	Computational Solid State Physics Laboratory	SBC	0	0	6	3
3	PCP.527	Quantum Mechanics	CC	4	0	0	4
4	CCC.525	Computational Methods	CC	4	0	0	4
5	CCC.528	Computational Methods Lab (Practical)	SBC	0	0	8	4
6	PCP.542	Seminar	SBE	0	0	0	1
7	XXX	Interdisciplinary Course	IDC	2	0	0	2
Interdisciplinary course offered for other departments							
	CCC.516	Chemistry without test tube	IDC	2	0	0	2
Choose any one of these courses/MOOC							
8	CCC.529	Density Functional Theory	DE	4	0	0	4
9	CCC.530	Introduction to Quantum Dynamics	DE	4	0	0	4
10	PHY.523	Quantum, Atomic and Molecular Physics	DE	4	0	0	4
11	PHY.524	Electromagnetic Theory	DE	4	0	0	4
Total				**18**	**0**	**14**	**26**

SEMESTER – III							
Sr. No	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
Choose any two of these courses							
1	CCC.556	Electronic Structure Theory	DE	4	0	0	4
2	PCP.557	Atomic and Molecular Spectroscopy	DE	4	0	0	4
3	PHY.554	Advanced Solid State Physics	DE	4	0	0	4
4	PHY.557	Functional Materials and Devices	DE	4	0	0	4
5	PHY.555	Nuclear Techniques	DE	4	0	0	4
Choose any one (theory and related lab) of these courses							
6	CCC.554	Fundamentals of Molecular Simulations	DE	4	0	0	4
7	CCC.555	Molecular Simulations Lab (Practical)	SBE	0	0	8	4
8	PHY.552	Nuclear and Particle Physics	DE	4	0	0	4
9	PHY.553	Nuclear Physics Laboratory	SBE	0	0	8	4
10	PCP.599	M.Sc. Project-I	SBE	0	0	0	6
11	CCC.559	Introduction to Molecular Docking	VAC	1	0	0	1
Total				**13**	**0**	**8**	**23**

SEMESTER – IV							
Sr. No	**Course Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**
1	PCP.573	Electronics	CC	4	0	0	4
2	PCP.572	Enrich Physics Course - I	DEC	2	0	0	2
3	PCP.579	Enrich Physics Course - II	DEC	2	0	0	2
Choose any one of these courses							
4	CCC.574	Advanced Statistical Mechanics and Molecular Reaction Dynamics	DE	4	0	0	4
5	PHY.571	Research Methodology	DE	4	0	0	4
6	PHY.574	Introduction to Mesoscopic	DE	4	0	0	4

		Physics					
7	PHY.578	Particle Physics	DE	4	0	0	4
8	PHY.576	Nanostructured Materials	DE	4	0	0	4
9	PHY.577	Materials Characterization	DE	4	0	0	4
10	PCP.599	M. Sc. Project Work - II	SBE	0	0	0	6
Choose any one of these courses							
11	CCC.573	Electronic Structure Theory Lab (Practical)	DE	0	0	8	4
12	CCC.575	Advanced Molecular Simulation Lab (Practical)	DE	0	0	8	4
13	CCC.577	Practicals in Biomolecular Structure Modeling	DE	0	0	8	4
14	LBI.574	Bioinformatics for Transcriptomics and Metabolomics	VAC	1	0	0	1
Total				**13**	**0**	**8**	**23**
Grand Total			**94 Credits**				

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

Evaluation Criteria for Theory Courses

A. Continuous Assessment: [25 Marks]
- i. Surprise Test (minimum three) - Based on Objective Type Tests (10 Marks)
- ii. Term paper (10 Marks)
- iii. Assignment(s) (5 Marks)

B. Mid Semester Test-1: Based on Subjective Type Test [25 Marks]
C. End Semester Test-2: Based on Subjective Type Test [25 Marks]
D. End-Term Exam: Based on Objective Type Tests [25 Marks]

*Every student has to take up 2 ID courses of 2 credits each (Total 04 credits) from other disciplines in any two semesters of the program.
CF: Compulsory Foundation, CC: Core Course, DE: Discipline Elective, IDE: Inter-Disciplinary Elective, SBC: Skill-based Core, SBE: Skill-based Elective, VAC: Value Added Courses
L: Lecture, T: Tutorial, P: Practical

SEMESTER-I

Paper Code: CCC.524
Course Title: Statistical Mechanics
Total Lectures: 60

L	T	P	Credits	
4	0	0	4	

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 **16 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 **16 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 **14 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 **14 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.

Suggested Readings

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

Course Code: PCP.506
Course Title: Mathematics for Computational Sciences
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: 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 **15 hours**

Matrices & Vector Calculus: matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors, curvilinear coordinates. (Vector calculus: properties of Gradient, divergence and Curl, spherical and cylindrical coordinates)
Differential calculus: Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials with their applications to thermodynamic properties.

Unit-II **15 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 **15 hours**

Delta, Gamma, and Beta Functions: Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions.
Special Functions: Legendre, Bessel, Hermite and Laguerre functions, recurrence relations, Orthogonality and special properties. Associated Legendre functions: recurrence relations, Parity and orthogonality, functions, Green's function,

Unit-IV **15 hours**

Differential Equations Solutions of Hermite, Legendre, Bessel and Laugerre Differential equations, basics properties of their polynomials, and associated Legendre polynomials, Partial differential equations (Laplace, wave and heat equation in two and three dimensions), Boundary value problems and Euler equation.

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

Suggested Readings:

1. G. Arfken, H. Weber and F. Harris, *Mathematical Methods for Physicists* (Elsevier Academic Press, Massachusetts, USA) 2012.
2. E. Kreyszig, *Advanced Engineering Mathematics* (Wiley India Pvt. Ltd., New Delhi, India) 2011.
3. L. A. Pipes, *Applied Mathematics for Engineers and Physicist* (McGraw-Hill, Noida, India) 1985.
4. D. G. Zill, *Advanced Engineering Mathematics* (Jones & Barlett Learning, Massachusetts, USA) 2012.
5. P. K. Chattopadhyay, *Mathematical Physics* (New Age International (P) Ltd., New Delhi) 2000
6. Mathematical Physics, B.S. Rajput, Pragati Prakashan

Course Code: PCP.507
Course Title: Classical Mechanics
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: 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 **16 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, Lagrangian for a charged particle moving in an electromagnetic field, Cyclic-coordinates, Symmetry, Conservations laws (Invariance and Noether's theorem).

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, Dynamical systems, Phase space dynamics and stability analysis.

Unit-II **14 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 **15 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: Central force motions, Reduction to the equivalent one-body problem, Differential equation for the orbit, Condition for closed orbits (Bertrand's theorem), Virial theorem, Kepler's laws and their derivations, Classification of orbits, Two body collisions, Scattering in laboratory and centre-of-mass frames.

Unit-IV **15 hours**

Theory of Small Oscillations: Periodic motion, Types of equilibria, General formulation of the problem, Lagrange's equations of motion for small oscillations, Normal modes, Applications to linear triatomic molecule, Double pendulum and N-Coupled oscillators.

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.

Suggested Readings

1. S.T. Thornton and J.B. Marion, *Classical Dynamics of Particles and Systems* (Cengage Learning, Boston/Massachusetts, United State), 2013.

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

Paper Code: CCC.508
Course Title: Scientific Programming
Total Lectures: 60

L	T	P	Credits	
4	-	0	4	

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.
- 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 **15 hours**
Introduction to Computers and Fortran language: History and evolution of Fortran language, Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program.

Unit-II **15 hours**
Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit-III **15 hours**
Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and 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.

Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran.

Unit-IV **15 hours**

What is parallel programming, Why use parallel programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting.

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

Suggested Readings

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

Paper Code: CCC.515
Course Title: Scientific Programming (Practical)
Total Lectures: 120

L	T	P	Credits	Marks
-	-	8	4	

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

1. Structure of a Fortran Program, compiling, linking and executing the Fortran programs. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.
2. Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and 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.

3. Pointers and dynamic data structures-using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran. Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination.
4. Parallel Program Design, Shared Memory & Message Passing, Algorithms.

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

Suggested Readings

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

SEMESTER-II

Paper Code: PCP.525
Course Title: Solid State Physics
Total Lecture: 60

L	T	P	Credits	
4	0	0	4	

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 **16 hours**

Crystal Structure: Bravais lattices, Crystal structures, Reciprocal lattices, Ewald sphere, X-ray diffraction, Lattice parameter determination, Atomic and

crystal structure factors, Bonding of solids, kinds of liquid crystalline order, Quasi crystals.
X-ray diffraction: X-ray diffraction, Bragg law, Laue equations, atomic form factor and structure factor. Concept of reciprocal lattice and Ewald's construction. Experimental diffraction methods: Laue rotating crystal method and powder method.

Unit-II **15 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; superconductors, Meissner effects, basic concepts of BCH theory.

Unit-III **14 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 **15 hours**
Defects in solids: Point defects: Schottky and Frenkel defects and their equilibrium concentrations. Line defects: dislocations, multiplication of dislocations (Frank – Read mechanism). Plane defects grain boundary and stacking faults.
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.

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

Paper Code: PCP.526
Course Title: Computational Solid State Physics Laboratory
Total Hours: 120

L	T	P	Credits	
0	0	6	3	

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

Course Code: PCP.527
Course Title: Quantum Mechanics
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: 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 **16 hours**

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian, theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor, angular momentum, eigenvalues of angular momentum operator, Particle on a Ring, Hydrogen Atom, Spin angular momentum: Pauli matrices and their properties.

Unit-II **16 hours**

Approximation methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples, WKB method, time-dependent perturbation theory, radiative transitions, Einstein coefficients.

Unit-III **16 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 **14 hours**

Scattering Theory: Scattering Theory: Quantum Scattering theory, Scattering cross-section and scattering amplitude, Born scattering formula, Central force problem, Partial wave analysis, Phase shifts, Optical theorem, Low energy s-wave and p-wave scatterings, Bound states and resonances

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

Suggested Readings:

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

Paper Code: CCC.525
Course Title: Computational Methods

L	T	P	Credits	
4	0	0	4	

Total Hours: 60
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 optimization, 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 **15 hours**
Linear and Non –Linear equations: Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basic principles-Formulae-algorithms.
Simultaneous equations: Solutions of simultaneous linear equations-Guass

elimination and Gauss Seidel iterative methods-Basic principles- Formulae-Algorithms, Pivotal Condensation.

Unit-II **15 hours**

Matrix and Determinants: Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

Unit-III **16 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 **14 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, Computer Oriented Numerical Methods, PHI, 1993.
2. E. Balaguruswamy, Numerical Methods, Tata McGraw Hill, 2017.
3. F.Acton, Numerical Methods that Work, Harper and Row, 1997.
4. S. D. Conte and C.D.Boor, Elementary Numerical Analysis, McGraw Hill, 2005.
5. S. S. Shastri, Introductory Methods of Numerical Analysis, PHI, 2012.

Paper Code: CCC.528
Course Title: Computational Methods lab (Practical)
Total Hours: 120

L	T	P	Credits	
0	0	8	4	

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

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

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

Course Content

Jacobi Method of Matrix Diagonalization, Solution of transcendental or polynomial equations by the Newton Raphson method, Linear curve fitting and calculation of linear correlation coefficient, Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination, Finding Eigen values and eigenvectors, Matrix factorizations Curve Fitting – Polynomial curve fitting on the fly, Least squares curve fitting, General nonlinear fits, Lagrange interpolation based on given input data, Numerical integration using the Simpson's method, Numerical integrationg using the Gaussian quadrature method, Solution of first order differential equations using the Rung-Kutta method, Numerical first order differentiation of a given function, Fast Fourier Transform, Monte Carlo integration.

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

Suggested Readings:

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

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

L	T	P	Credits	
4	0	0	4	

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 **14 hours**

Many-body Approximations: Schrodinger equation and its solution for one electron and two electron systems, Hamiltonian of many particles system, Born-Oppenheimer approximation, Hartree theory, Idea of self consistency, Exchange energy and interpretation, Identical particles and spin, Hartree-Fock theory, Antisymmetric wavefunctions and Slater determinant, Koopmans' theorem, Failures of Hartree-Fock in solid state, Correlation energy, Variational principle, Connection between Quantum Mechanics,Variational Principle and Classical Mechanics.

Unit-II **15 hours**

From Wave Functions to Density Functional: 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. Self-interaction corrections (SIC).

Unit-III **16 hours**

Practical Implementation of Density Functional Theory (DFT): Kohn-Sham formulation: Plane waves and pseudopotentials, Janak's theorem, Ionization potential theorem, Self consistent field (SCF) methods, Understanding why LDA works, Consequence of discontinuous change in chemical potential for exchange-correlation, Strengths and weaknesses of DFT.

Unit-IV **15 hours**

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

Paper Code: CCC.530
Course Title: Introduction to Quantum Dynamics
Total Lecture: 60

L	T	P	Credits	
4	0	0	4	

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

- learn systematic theoretical validations of the separation of electronic and nuclear motions
- gain the knowledge about the basic aspects of time dependent quantum wavepacket dynamics
- understand various numerical methods for solving the TDSE

Course Content

Unit-I **15 hours**

Separation of electronic and nuclear motions: adiabatic representation, Born-Oppenheimer approximation, Hellmann-Feynman theory, diabatic representation, transformation between two representations, crossing of adiabatic potentials.
TDSE: separation of variables and reconstitution of the wavepacket, expectation values, free-particle wavepacket: centre and dispersion of the wavepacket.

Unit-II **16 hours**

Gaussian wavepacket: Gaussian free particle, general properties of Gaussian wavepackets, Gaussian in a quadratic potential. Correspondence between Classical and Quantum Dynamics: Ehrenfest's Theorem, Bohmian Mechanics and the Classical limit.

Unit-III **14 hours**

Spectra as Fourier transforms of wavepacket correlation functions. 1D barrier scattering: wavepacket formulation of reflection and transmission coefficients, cross-correlation function and S-matrix.

Unit-IV **15 hours**

Numerical methods for solving the TDSE: spectral projection and collocation, pseudospectral basis, gaussian quadrature, represntation of the hamiltonian in the reduced space, discrete variable representation, Fourier method, time propagation.

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

Suggested Readings:

1. D. J. Tannor, *Introduction to Quantum Mechanics: A Time-dependent Perspective*, University Science Books, 2006.

2. Edited by R E Wyatt and J Z H Zhang, *Dynamics of Molecules and Chemical Reactions*, CRC Press, 1996.
3. K. C. Kulander, *Time-dependent Methods for Quantum Dynamics*, Elsevier Science, 1991.
4. J. Z. H. Zhang, *Theory and application of Quantum Molecualr Dynamics*, World Scientific Publishing Company, 1998.
5. Edited by M Brouard and C Vallance, *Tutorials in Molecular Reaction Dynamics,* Royal Society of Chemistry, 2010.
6. Edited by D. A. Micha, I. Burghardt, *Quantum Dynamics of Complex Molecular Systems*, Springer-Verlag, 2006.

Course Title: Seminar
Paper Code: PCP.542

L	T	P	Cr
0	0	0	1

Learning objective: The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:

Continious Evaluation:

S.No.	Criteria	Marks
1.	Knowledge of Subject: In depth coverage, ability to interpret science	25
2.	Questions: Understanding of questions, ability to reply with logic	25
End Term:		
1.	(a) Presentation: Voice, Ability to command attention, (b) Handling of queries	50
	Total	**100**

SEMESTER-III

Paper Code: CCC.556
Course Title: Electronic Structure Theory
Total Hours: 60

L	T	P	Credits	
4	0	-	4	

Learning Outcomes: This is an advanced course for students who specialize in Computational Chemistry. The objective of this course is that students learn the techniques of molecular quantum chemistry (eg. Hartree-Fock SCF and

Roothaan-Hartree-Fock method, CI Interaction, CCSD, CCSD(T), Kohn-Sham equations) and apply them to study chemical and biochemical problems.

Course Content

Unit-I **16 hours**
Review of molecular structure calculations, Hartree-Fock SCF method for molecules

Unit-II **15 hours**
Roothaan-Hartree-Fock method, selection of basis sets.

Unit-III **14 hours**
Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method.

Unit-IV **15 hours**
Energy as a functional of charge density, Kohn-Sham equations, different functionals.

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

Suggested Readings:
1. Introduction to Computational Chemistry, F. Jensen, Wiley-Blackwell (2006).
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, OUP, Oxford (1997).
3. Quantum Chemistry, H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
4. Quantum Chemistry, I.N. Levine, (2000), Pearson Educ., Inc., New Delhi.
5. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

Paper Code: PCP.557
Course Title: Atomic and Molecular Spectroscopy
Total Lectures: 60

L	T	P	Credits	
4	0	0	4	

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 **14 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 **16 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 **16 hours**

Molecular Spectroscopy: Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO2), FT-IR instrumentation, Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines. Vibronic spectroscopy of diatomic molecules, Franck-Condon factor, rotational fine structure.

Unit-IV **14 hours**

Elementary particles: Classification of fundamental forces. Elementary particles and their quantum numbers (charge, spin, parity, isospin, strangeness, etc.). Gellmann-Nishijima formula. Quark model, baryons and mesons. C, P, and T invariance. Application of symmetry arguments to particle reactions. Parity non-conservation in weak interaction. Relativistic kinematics.

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

Suggested Readings

1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons, Ltd. (2004).
2. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill (1962).
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, Tata McGraw Hill, New Delhi (1994).
4. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, Springer.
5. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, Chapman and Hall, London (1979).
6. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, Addison Wesley, Longman Ltd, London (1986).
7. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, (Tata, McGraw Hill Publishing Company Limited).

8. C.J. Foot, Atomic Physics (Oxford University Press, Oxford, U. K.) 2005.

Course Code: PHY.554
Course Title: Advanced Solid State Physics
Total Hours: 60

L	T	P	Cr
4	0	0	4

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 **15 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 **15 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 **15 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 **15 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, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, U.K.) 2011.
2. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007.
3. R.J. Singh, *Solid State Physics* (Pearson, New Delhi, India) 2011.
4. A.J. Dekker, *Solid State Physics* (Macmillan, London, U.K.) 2012.
5. N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Thomson Press), 2003.

Course Code: PHY.557
Course Title: Functional Materials and Devices
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: Physicists and Chemists are now playing an important role in the growing field of materials research. The aim of this course is to introduce students to this area of modern materials. The students after the completion of this course will have solid understanding of the fundamental principles of various advanced functional materials and Devices.

Course Content

Unit-I **15 hours**

Advanced Ceramic and Smart Materials: Ceramic Materials: Classification, Preparation and Properties, Composites, Smart Materials exhibiting: Ferroelectric, Dielectrics, Piezoelectric, Thermoelectric, Luminescence, Photocromics, Thermocromics and Electrocromic Materials, Phase Change Material, Shape Memory Alloys, Smart Structure and Robotics.

Unit-II **15 hours**

Magnetic and Multiferroics Materials: Ferrites, Gaint magnetoresistance (GMR), Magnetic materials for recording and computers., Spin Polarization, Colossal Magnetoresistance (CMR), La and Bi-based Perovskite, Spin-Glass, Spintronics: Magnetic tunnel junction, Spin transfer torque, Applications, Multiferroics: Types and Mechanism, $BiFeO_3$ and $BaTiO_3$ Multiferroics.

Unit-III **15 hours**

Polymers and Composites: Basic Concepts on Polymers, Polymers (Insulating, electronic and functionalized), Polymer Configuration (Tacticity), Polymer Conformation (Trans, Staggered, Gauche, Eclipsed), Polymer processing: Hot molding, Film blowing, Melt spinning etc Composites: Varieties, Role of Matrix Materials, Mixing Rules, Polymer composites and nanocomposites (PNCs), PNCs for Li-ion battery, Supercapacitor, fuel cell, LED's and solar cell, synthesis and engineering of PNCs.

Unit-IV **15 hours**

Devices: Photovoltaic, Solar Energy, Nanogenerators, LED, Electrochromic displays (n & p-type materials, electrolytes, device fabrication and property measurements), Resistive switching, Supercapacitor and Li-ion batteries (Types and Properties: Crystallinity, Free ions and ion pair's contribution, Ionic radii of migrating species, Ionic Conductivity, Transport parameters, Transference Number, Thermal Stability, Porosity and Electrolyte Uptake/Leakage, Thermal Shrinkage, Glass transition temperature, Electrochemical Stability, Mechanical Stability) Advantages and Disadvantages, Ragone plot, Nyquist plot, Charging-discharging.
Fuel Cell (Alkaline Fuel Cell, Polymer Electrolyte Membrane Fuel Cell, Direct Methanol Fuel Cell, Solid Oxide Fuel Cell,).

Transaction Mode: Lecture and PPT, Problem Solving through Assignments.

Suggested Readings

1. Mel Schwartz, Smart Materials, CRC Press, Boca Raton, 2009
2. Handbook of Inorganic Electrochromic Materials, by C.G. Granqvist; Elsevier Science, 1995.
3. Lithium Batteries: Advanced Technologies and Applications, by Bruno Scrosati, K. M. Abraham, Walter Van Schalkwijk, and Jusef Hassoun; John Wiley & Sons, Inc, 2013.
4. Advanced functional materials: a perspective from theory and experiment. Edited by Biplab Sanyal, and Olle Eriksson
5. S.B. Ogale, T.V. Venkatesan, M. Blamire, *Functional Metal Oxides* (Wiley-VCH Verlag GmbH, Germany) 2013.
6. S. Banerjee and A.K. Tyagi, *Functional Materials: Preparation, Processing and Applications* (Elsevier, Insights, Massachusetts, USA) 2011.
7. D.D.L. Chung, *Composite Materials: Functional Materials for Modern Technologies* (Springer, New York, USA) 2003.
8. Deborah D. L. Chung, *Functional Materials: Electrical, Dielectric, Electromagnetic, Optical and Magnetic Applications* (World Scientific Publishing Company, Singapore) 2010.
9. B.D. Cuility and C.D. graham, *Introduction to Magnetic Materials* (Willey, New Jersey) 2009.
10. K.C. Kao, *Dielectric Phenomena in Solids* (Elsevier, Academic Press, London, U. K.) 2004.
11. S. O. Kasap, *Principles of Electronic Materials and Devices* (McGraw Hill Publications)
12. B E Conway Brian E Conway Conway, *Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications* (Springer) 1999.

Course Code: PHY.555
Course Title: Nuclear Techniques
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: This course will introduce the students with different techniques used to study nuclear physics, starting from design of different radiation source, detection, interaction and its applications.

Course Content

Unit: 1 **15 hours**

Accelerators: Motion of charged particles in electric and magnetic fields, Axial and radial magnetic field distributions in dipole, quadrupole and hexapole arrangement, Equipotential lines in different electrodes arrangement, Particle trajectory in electric and magnetic field, Electron sources, ion sources, Van de Graaf generator, DC linear accelerator, RF linear accelerator, Cyclotron, Microtone, introduction to advance accelerator (LHC)

Unit: II **15 hours**

Detectors: Relation detectors Gaseous ionization, ionization and transport phenomena in gases, proportional counters, organic and inorganic scintillators, detection efficiency for various types of radiation, photomultiplier gain, semiconductor detectors, surface barrier detector, Si(Li), Gel(Li) and HPGe detectors.

Interaction of radiation with matter: General description of interaction processes, photoelectric effect, Compton Effect, pair production, interactions of directly ionizing radiation, stopping power, linear energy transfer, range of particles, interaction of indirectly ionizing radiation attenuation coefficient.

Unit: III **15 hours**

Reactors and artificial radioisotopes: Neutron sources, neutron detectors, measurement of cross-sections for nuclear reaction, thermal and fast reactors, Q values, Fission, Fusion, production of radioisotopes, Reactor operation, thermal neutrons, neutron scattering and applications.

Unit: IV **15 hours**

Analysis Nuclear reaction: Elemental analysis by neutron activation analysis, proton induced X-ray emission, Rutherford backscattering, Resonance nuclear reaction, Elastic RDA, ion scattering and Neutron Depth Profile.

Transaction Mode: Lecture, demonstration, PPT

Suggested Readings:

1. Nuclear radiation detectors, S. S. Kappor and V. S. Rmanurthy. (Wiley Eastern Limited, New Delhi,) 1986.
2. Introduction to radiation protection dosimetry, J. Sabol and P. S. Weng, (World Scientific), 1995.
3. Techniques for nuclear and particle physics, W. R. Len (Springer), 1955.
4. Nuclear radiation detection, W. J. Price, (McGraw-Hill, New York), 1964.

5. Alphas, beta and gamma-ray spectroscopy, K. Siegbahn, (North Holland, Amsterdam), 1965.
6. Introduction to experimental nuclear physics, R. M. Singru, (John Wiley and Sons), 1974.

Paper Code: CCC.554
Course Title: Fundamentals of Molecular Simulations
Total Lecture: 60

L	T	P	Credits	Marks
4	0	0	4	

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 **15 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 **15 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 **15 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 (c) Statistical Mechanics of Fluids.

Unit-IV **15 hours**

Simulation Methods: Monte Carlo: (a) MC integration and Markov chains, (b) The Metropolis method, (c) Biased MC

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, Nose-Hoover Dynamics, (f) Pressure Control: Andersen's Method, Nose-Hoover Method, Rahman-Perrinilo Method, (g) Calculating properties from MD trajectories, (h) Hybrid MC,
Free Energy: (a) Perturbation Methods, (b) TI (Thermodynamic Integration)
Brownian dynamics and the Langevin Equation.

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

Suggested Readings

1. Computer Simulation of Liquids, by M.P. Allen and D.J. Tildesley, (QC 145.2.A43 1992)
2. Understanding molecular simulation, by Daan Frenkel and Berend Smit, (QD 461 .F86 1996)
3. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.

Paper Code: CCC.555
Course Title: Molecular Simulations Lab (Practical)
Total Lecture: 120

L	T	P	Credits	
0	0	8	4	

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 liquid structure and dynamics
    b. Simulation of Ionic Solutions
    c. Simulation of Protein in Water
    d. Simulation of Membrane Proteins
    e. Simulations of DNA
8. Review of Molecular Dynamics Principles

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

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

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

L	T	P	Cr
4	0	0	4

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 **15 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.

Two Nucleon Problems: Nature of nuclear forces, Deuteron problem, Spin dependence of nuclear forces, Form of nucleon-nucleon potentials, Electromagnetic moment and magnetic dipole moment of deuteron, General form of nuclear force. Experimental n-p scattering data, Partial wave analysis and phase shifts, Scattering length, Magnitude of scattering length and strength of scattering, Charge independence, Charge symmetry and iso-spin invariance of nuclear forces.

Unit-II **15 hours**

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.

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.

Unit-III **15 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,

Neutron Physics: Neutron Sources, absorption and moderation of neutrons, Introduction to nuclear fission and fusion.

Unit-IV **15 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, *Nuclear & Particle Physics* an Introduction: (John Wiley & Sons, Inc., New Jersey, USA) 2011.
2. K.S. Krane, *Introductory Nuclear Physics* (John Wiley & Sons, Inc., New Jersey, USA) 2008.
3. C.A. Bertulani, *Nuclear Physics in a Nutshell* (Princeton University Press, Princeton, USA) 2007.

4. S.S.M. Wong, *Introductory Nuclear Physics* (John Wiley & Sons, Inc., New Jersey, USA) 2008.
5. K. Heyde, *Basic Ideas and Concepts in Nuclear Physics* An Introductory approach : (CRC Press, London, U. K.) 2004.
6. B. Povh, K. Rith, C. Scholz, *Particles and Nuclei: An Introduction to the Physical Concepts* (Springer, New York, USA) 2012.
7. D.H. Perkin, *Introduction to High Energy Physics* (Cambridge University Press, Cambridge, U.K.) 2000.
8. I.S. Hughes, *Elementary Particles* (Cambridge University Press, Cambridge, U.K.) 1991.
9. W.R. Leo, *Techniques for Nuclear and Particle Physics Experiments* (Springer, New York, USA) 2009.
10. T. Stefan, *Experimental Techniques in Nuclear and Particle Physics* (Springer, New York, USA) 2010.
11. D.J. Griffiths, *Introduction to Elementary Particles* (Wiley-VCH Verlag GmbH, Germany) 2008.

Course Code: PHY.553
Course Title: Nuclear Physics Laboratory
Total Hours: 120

L	T	P	Cr
0	0	8	4

Learning Outcomes: At the end of the course the students will be able to perform and explain the various experiments related with G.M counter and gamma ray spectrometer.

Course Content

Student has to perform ten experiments out of the following list of experiments.

1. Study of the characteristics of a GM tube and determination of its operating voltage, plateau length / slope etc.
2. Verification of inverse square law for gamma rays.
3. Study of nuclear counting statistics.
4. Estimation of efficiency of the G.M. detector for beta and gamma sources.
5. To study beta particle, range and maximum energy (Feather Analysis).
6. Backscattering of beta particles.
7. Production and attenuation of bremsstrahlung.
8. Measurement of short half-life
9. Demonstration of nucleonic level gauge principle using G.M counting system and detector.
10. Beam interruption detection system to check packs for content level, or counting of individual items.
11. Scintillation detector: energy calibration, resolution and determination of gamma ray energy.
12. Alpha spectroscopy using surface barrier detectors.

13. Study of energy resolution characteristics of a scintillation spectrometer as a function of applied high voltage and to determine the best operating voltage
14. Measurement of resolution for a given scintillation detector using Cs-137 source.
15. Finding the resolution of detector in terms of energy of Co-60 system.
16. Energy calibration of gamma ray spectrometer (Study of linearity).
17. Spectrum analysis of Cs-137 and Co-60 and to explain some of the features of Compton edge and backscatter peak.
18. Unknown energy of a radioactive isotope.
19. Variation of energy resolution with gamma energy.
20. Activity of a gamma source (Relative and absolute methods).
21. Measurement of half value thickness and evaluation of mass absorption coefficient.
22. Back scattering of gamma Rays.

Transaction Mode: Demonstration, experimentation

Suggested Readings:

1. G.F. Knoll, *Radiation Detection and Measurement* (John Wiley & Sons, Sussex, U.K.) 2010.
2. W.R. Leo, *Techniques for Nuclear and Particle Physics Experiments: a how-to approach* (Springer, New York, USA) 2012.
3. K. Beach, S. Harbison, A. Martin, *An Introduction to Radiation Protection* (CRC Press, London, U.K.) 2012.
4. N. Tsoulfanidis, S. Landsberger, *Measurement and Detection of Radiation* (CRC Press, London , U.K.) 2010.
5. H. Nikjoo, S. Uehara, D. Emfietzoglou, *Interaction of Radiation with Matter* (CRC Press, London, U.K.) 2012.

Paper Code: CCC.559
Course Title: Introduction to Molecular Docking
Total Hours: 15

L	T	P	Credits	
1	0	0	1	

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

- demonstrate various force field for biomolecular modeling
- execute various molecular docking methods
- identify the dynamics of strcutural transitions
- which will help them to devlop the molecular docking techniques in their further potential careers in academia and industry.

Course Content

Unit 1 **3 Hours**

Biomoleuclar structure and molecular recognition,

Unit 2 **4 Hours**
3D structure determination and molecular modeling,
Unit 3 **4 Hours**
Protein structure prediction, force fields for molecular dynamics simulation,
Unit 4 **4 Hours**
Different molecular docking methods, software's used in molecular docking.

Transactional Modes: Lectures; Problem solving; Self-learning.

Suggested Readings

1. Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo Molecular design : concepts and applications Weinheim: Wiley-VCH, c2008
2. Andrew R.Leach Molecular Modelling Principles and applications, (2001) Prentice Hall.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. http://autodock.scripps.edu/faqs-help/manual/autodock-4-2-user-guide/AutoDock4.2_UserGuide.pdf

Paper Code: LBI.560
Course Title: Bioinformatics for Transcriptomics and Metabolomics
Total Hours: 15

L	T	P	Credits	
1	0	0	1	

Learning Outcomes: The course covers advanced technology and in depth study for exploring the possible coding region of genome in various conditions. Further the metabolomics study opens up new pathways which could interconnect with expression data analysis. On completion of the course the student should be able to:

- identify to process the raw read file generated by illumina sequencing.
- carry out the reference base expression estimation analysis
- learn alignment QC, visualization and differential expression studies

Course Content

Unit I **4 Hours**
Introduction to NGS techniques: Illumina (Solexa) sequencing, Roche 454 sequencing,

Unit II **4 Hours**
Ion torrent: Proton/PGM sequencing, SOLiD sequencing; sequence formats and quality.

Unit III **4 Hours**
Alignment of Next-Gen sequences to reference sequences, RNA-Seq analysis-Transcriptome mapping and differential expression: tools and pipeline.

Unit IV **3 Hours**

Introduction to metabolomics.

Transactional Modes: Lectures; Problem solving; Self-learning.

Suggested Readings

1. Shawn E. Levy and Richard M. Myers, "Advancements in Next-Generation Sequencing". Annu. Rev. Genom. Hum. Genet. 2016. 17:16.1–16.21
2. Beginner's Handbook of Next Generation Sequencing, Genohub
3. Next Generation Sequencing Methods and Protocols. Head, Steven R., Ordoukhanian, Phillip, Salomon, Daniel R.

Course Title: M.Sc. Project I
Paper Code: PCP.599
Invested Hours: 180

L	T	P	Cr
0	0	0	6

Course Objective and Learning Outcomes: The objective of project part I would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
Continuous Assessment		
1.	Review of literature and Bibliography	10
2.	Identification of gaps in knowledge	10
3.	Objective formulation	15
4.	Methodology	15
5.	Continuous evaluation of student by guide	30
Research Presentation		
6.	Presentation	20
	Total	100*

The final presentation shall be evaluated by a three membered committee consisting of

a. HOD/OHOD of the department
b. VC nominee
c. Supervisor (and Co-supervisor if applicable)

***Evaluation Criteria:**
S or Satisfactory: >= 60
U or Unsatisfactory: < 60

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

SEMESTER-IV

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

L	T	P	Credits	
4	0	0	4	

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 **15 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 **15 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 **15 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 **15 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.

Recommended books

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

Course Title: Advanced Statistical Mechanics and Molecular Reaction Dynamics

Paper Code: CCC.574

Total Lectures: 60

L	T	P	Cr
4	0	0	4

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

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

Course Content

Unit I **16 Hours**

Review of Statistical Mechanical concepts, Phases & Phase Transitions: The Ising Model: Stability of Thermodynamics Phases, First-order Phase transitions, Interfaces, The Ising Model, Lattice Gas, Broken Symmetry, Mean Field Theory.

A brief introduction to Liquid Theory: Averages, Distribution Functions, Reversible Work Theorem, Radial distribution function, Molecular liquids

Atomic and continuum models of liquids: The Lennard-Jones Fluid, Molecular dynamics simulation, Correlation functions and measurements, elements of linear response theory, Linear models (a) Langevin equations (diffusion, friction and memory). (b) Gaussian fields (Debye-Huckel and beyond), The hard sphere model, WCA theory, Chemical equilibrium and relaxation.

Unit II **14 Hours**

Non-equilibrium systems: Fluctuation-Dissipation Theorem, Onsager's Regression Hypothesis

Brownian Motion, Friction and the Langevin Equation, Transport, Time Correlation Functions.

Special topics: Free energy perturbation, The Jarzynski Equality, Electron transfer--quantum rare events--golden rule--Marcus theory, Path integrals, Tunneling—instantons, Ising model / Quantum correspondence, Monte Carlo and Biased Monte Carlo methods.

Unit III **14 Hours**

Potential Energy Surfaces: Long-range Potentials, Empirical Intermolecular Potentials, Molecular Bonding Potentials, Internal Coordinates and Normal Modes of Vibration, Ab Initio Calculation of Potential Energy Surfaces, Analytic Potential Energy Functions, Details of the Reaction Path.Dynamics of Bimolecular Collisions: Simple Collision Models, Two-Body Classical Scattering, Complex Scattering Process.

Unit IV **16 Hours**

Transition State Theory: Basic Postulates and Derivation of Transition State Theory, Dynamical Derivation of Transition State Theory, Quantum Mechanical Effects in Transition State Theory, Thermodynamic Formulation of Transition State Theory, Applications of Transition State Theory.Unimolecular Reaction Dynamics: The Lindmann-Hinshelwood Mechanism, Statistical Energy-dependent Rate Constant, RRKM Theory, Applications of RRKM Theory to Thermal Activation.

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

Suggested Readings

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

L	T	P	Cr
4	0	0	4

Course Code: PHY.571
Course Title: Research Methodology
Total Hours: 60

Learning Outcomes: The course Research Methodology will introduce the students of M. Sc. Physics to basic concepts of research methods. The students will learn about the preparation of research plan, reading and understanding of scientific papers, scientific writing, research proposal writing, ethics, plagiarism, laboratory safety issues and intellectual property rights etc.

Course Content

Unit-I **15 hours**

General principles of research: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Formulating hypothesis and development of research plan, Review of literature, Interpretation of results and discussion.

Bibliographic index and research quality parameters- citation index, impact factor, *h*-index, i10 index, etc. Research engines such as google scholar, Scopus, web of science, Scifinder etc.

Unit-II **15 hours**

Technical & scientific writing- theses, technical papers, reviews, electronic communication, research papers, etc., Poster preparation and presentation, and project. Making R and D proposals, Reference management using various softwares such as Endnote, reference manager, Refworks, etc. Communication skills–defining communication; type of communication; techniques of communication, etc.

Data Analysis: Graph plot, Error analysis, Curve fitting: linear and nonlinear.

Unit-III **15 hours**

Library: Classification systems, e-Library, Reference management, Web-based literature search engines.

Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials, Radiation safety.

Entrepreneurship and Business Development: Importance of entrepreneurship and its relevance in career growth, Types of enterprises and ownership.

Unit-IV **15 hours**

Plagiarism: Plagiarism, definition, Search engines, regulations, policies and documents/thesis/manuscripts checking through softwares, Knowing and Avoiding Plagiarism during documents/thesis/manuscripts/ scientific writing.

Intellectual Property Rights: Intellectual Property, intellectual property protection (IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), Nuts and Bolts of Patenting, Technology Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

1. S. Gupta, *Research Methodology and Statistical techniques* (Deep and Deep Publications (P) Ltd. New Delhi, India) 2005.
2. R. Kothari, *Research Methodology* (New Age International, New Delhi, India) 2008.
3. **Web resources:** www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.
4. **Web resources:** www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

Course Code: PHY.574
Course Title: Introduction to Mesoscopic Physics
Total Hours: 60

L	T	P	Cr
4	0	0	4

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 ohmic regime 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 **15 hours**
Introduction, Why Electrons Flow, Conductance Formula, Ballistic Conductance, Diffusive Conductance, Connecting Ballistic to Diffusive, Dispersion Relation, Drude Formula.

Unit II **15 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 **15 hours**
Boltzmann Equation, Semiclassical Model,Quantum Model, Landauer Formulas, NEGF Equations, Self-Energy, Surface Green's Function, Current Operator, Scattering Theory, Transmission, Golden Rule, Quantum Master Equations.

Unit IV **15 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. Quantum Transport Atom to Transistor by Supriyo Datta (CAMBRIDGE)
2. Lessons from Nanoelectronics: A New Perspective on Transport: Volume 1 & 2 by Supriyo Datta (World Scientific)
3. Theory of Quantum Transport at Nanoscale: An Introduction by Dmitry A Ryndyk (Springer)
4. Quantum Transport: Introduction to Nanoscience by Yuli V. Nazarov and Yaroslav M. Blanter (CAMBRIDGE)

Course Code: PHY.578
Course Title: Particle Physics
Total Hours: 60

L	T	P	Cr
4	0	0	4

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 **15 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 **15 hours**

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

Symmetries and Conservation Laws: Space- time symmetries, Invariance Principles, Parity, Intrinsic parity, Parity constraints on the S- Matrix for Hadronic Reactions, Time – Reversal Invariance, conservation of Quantum Numbers, Isospin, Charge Conjugation, G- parity, CP and CPT Invariance (statement and consequences only).

Unit-III **15 hours**

Internal symmetries:, Isospin, strangeness, charm quantum numbers, unitary groups, Isospin and SU (2), SU(3), Octet and decuplet irreducible representations of SU(3), SU(3) classification of mesons and baryons,

Applications of Flavor SU(3), Gell- Mann Okubo Mass Formula, omega-phi mixing, Isospin relations for Pion-nucleon strong interaction.
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 **15 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, *Techniques for Nuclear and Particle Physics Experiments* (Springer, New York, USA) 2009.
2. D.H. Perkin, *Introduction to High Energy Physics* (Cambridge Univ. Press, U.K.) 2000.
3. D.J. Griffiths, *Introduction to Elementary Particles* (Wiley-VCH GmbH, Germany) 2008.
4. I.S. Hughes, *Elementary Particles* (Cambridge University Press, Cambridge, U.K.) 1991.
5. M.P. Khanna, Particle Physics, Prentics Hall. Pub., N. Delhi.
6. M.P. Khanna, Quantum Mechanics, Har Anand Pub. N. Delhi. (1999)
7. T. Stefan, *Experimental Techniques in Nuclear and Particle Physics* (Springer, New York, USA) 2010.
8. V.K. Mittal, R.C. Verma & S.C. Gupta, Nuclear & Particle Physics, Prentics Hall Pub. N. Delhi, 3rd edition, (2015)
9. V.K. Thankappan, Quantum Mechanics, New Age Pub. N. Delhi.
10. W.E. Burcham and M. Jobes, Nuclear Physics, (Indian edition) Addison Wesley. Pub.

Course Code: PHY.576
Course Title: Nanostructured Materials
Total Hours: 60

L	T	P	Cr
4	0	0	4

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 **15 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 **15 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 **15 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 **15 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. Functional Metal Oxides: New Science and Novel Applications by S. B. Ogale, T. V. Venkatesan, and M. G. Blamire, Wiley-VCH (2013)
2. Physical Metallurgy, Vol. 1 and Vol. 2 by R. W. Chan and P. Hassen North Holland Publishing Company, New York, (1983).
3. Modern Physical Metallurgy and Materials Engineering 6th Edition by R. E. Smallman, Butterworth-Heinemann, (1999)
4. Atomic Force Microscopy: Understanding Basic Modes and Advanced Applications by Greg Haugstad (John Wiley & Sons, 2012).

5. Textbook of Nanoscience and Nanotechnology by B.S Murty, P.Shankar, B. Raj, B. B. Rath, and J. Murday (Springer, 2013).
6. Handbook of Nanophysics by Klaus D. Sattler (CRC press, 2010).
7. Nanostructured Materials and Nanotechnology by Claudia Gutirrez-Wing, Jos Luis Rodrguez-Lpez, Olivia A. Graeve, and Milton Muoz-Navia (Cambridge University Press, 2013).

Course Code: PHY.577
Course Title: Materials Characterizations
Total Hours: 60

L	T	P	Cr
4	0	0	4

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 **15 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 **15 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 **15 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 **15 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. Materials Characterization: Introduction to Microscopic and Spectroscopic Methods, 2nd Edition, by Yang Leng, WILEY (2013).
2. Atomic Force Microscopy: Understanding Basic Modes and Advanced Applications, by Greg Haugstad, WILEY (2012)
3. Introduction to Scanning Tunneling Microscopy, by C. Julian Chen, Oxford Unive. Press (1993)
4. An Introduction to Surface Analysis by XPS and AES, by John F. Watts, and John Wolstenholme, WILEY (2003)

Paper Code: CCC.573
Course Title: Electronic Structure Theory Lab (Practical)
Total Hours: 120

L	T	P	Credits	
0	0	8	4	

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

Course Content

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, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
2.http://departments.icmab.es/leem/siesta/Documentation/Manuals/manuals.html
3.http://blogs.cimav.edu.mx/daniel.glossman/data/files/Libros/Exploring%20Chemistry%20With%20Electronic%20Structure%20Methods.pdf
4. http://ambermd.org/tutorials/

Paper Code: CCC.575
Course Title: Advanced Molecular Simulation Lab
Total Lectures: 120

L	T	P	Credits	
0	0	8	4	

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

- learn various tools for protein structure prediction
- learn the homology and comparative modeling techniques
- understand the effect of sequence on the molecular model building
- learn the structure based drug designing
- gain the knowledge about various advanced molecular modeling techniques

Course Content

1. Introduction to protein structure prediction
2. Homology or comparative modeling using MODELLER
3. Effect of sequence on model accuracy (eg. FABP)
   a. Select template structures
   b. How to validate protein structure
   c. Validate homology model and compare with x-ray structure
4. Homology Modeling and MD Refinement
5. Molecular Recognition
   a. Prediction of Protein-ligand interaction sites
   b. Prediction of Protein-nucleic acid interaction sites
   c. Prediction of Protein-protein interaction sites
6. Structure based Drug Designing
   a. Molecular Docking
   b. De Novo Ligand Design
   c. Virtual Screening

   Ligand based Drug Design

a. Pharmacophore Identification
b. QSAR

7. Special Topic: (a) Umbrella Sampling
(b) Free Energy Calculations
(c) Multicomponent Systems

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

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications, (2009) II ed . Pearson Education.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Paper Code: CCC.577
Course Title: Practicals in Biomolecular Structure Modelling
Total Hours: 120

L	T	P	Cr	
0	0	8	4	

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

- identify different types of protein–ligand interactions and characterise binding pockets
- apply different search methods to find compounds with specific properties in large compound databases
- evaluate different virtual screening methods using large datasets
- devise and set up molecular dynamics simulations and free energy calculations

Course Content

The following experiments should be conducted by the students:

A. Molecular Recognition
1. Prediction of Protein-ligand interaction sites
2. Prediction of Protein-protein interaction sites
3. Prediction of Protein-membrane interaction sites
4. Prediction of Protein-nucleic acid interaction sites

B. Docking
1. Protein Ligand Docking using
(i) Autodock

(ii) Vina
(iii) Dock
2. Protein-protein docking by HADDOCK or other similar methods
C. Modelling macromolecular structure
1. Homology modeling
2. *ab-initio* structure modeling

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

Suggested Readings

1. *Grant, Guy H.; Richards, W. Graham* Computational chemistry Oxford: Oxford Univ. Press, 1995
2. *Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo* Molecular design : concepts and applications. Weinheim: Wiley-VCH, c2008

Paper Code: LBI. 574
Course Title: Bioinformatics for Transcriptomics and Metabolomics
Total Hours: 15

L	T	P	Credits	
1	0	0	1	

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

1. Identify to process the raw read file generated by illumina sequencing.
2. carry out the reference base expression estimation analysis
3. learn alignment QC, visualization and differential expression studies

Course Content

Unit I **4 Hours**
Introduction to NGS techniques: Illumina (Solexa) sequencing, Roche 454 sequencing,

Unit II **4 Hours**
Ion torrent: Proton/PGM sequencing, SOLiD sequencing; sequence formats and quality.

Unit III **4 Hours**
Alignment of Next-Gen sequences to reference sequences, RNA-Seq analysis-Transcriptome mapping and differential expression: tools and pipeline.

Unit IV **3 Hours**
Introduction to metabolomics.

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

Suggested Readings

1. Shawn E. Levy and Richard M. Myers, "Advancements in Next-Generation Sequencing". Annu. Rev. Genom. Hum. Genet. 2016. 17:16.1–16.21
2. Beginner's Handbook of Next Generation Sequencing, Genohub
3. Next Generation Sequencing Methods and Protocols. Head, Steven R., Ordoukhanian, Phillip, Salomon, Daniel R

L	T	P	Cr
0	0	0	6

Course Title: M.Sc. Project-II
Paper Code: PCP.599
Total Hours: 180

Course Objective and Learning Outcomes: The objective of project part II would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
Continuous Assessment		
1.	Research work and Report writing	40
2.	Continuous evaluation of student by guide	30
Research Presentation		
3.	Presentation and defense of research work	30
	Total	100*

The final presentation shall be evaluated by a three membered committee consisting of

a. HOD/OHOD of the department
b. VC nominee
c. Supervisor (and Co-supervisor if applicable)

***Evaluation Criteria:**
S or Satisfactory: >= 60
U or Unsatisfactory: < 60

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

Course Code: CPC.572
Course Title: Enrich Physics Course - I
Total Lectures: 30

L	T	P	Credits	
2	0	0	2	

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

- understand, how transducers work for different media, measurement and control of electronic signals
- learn the impedance and amplification of signals with various instruments.
- Identify and apply the advanced mathematics for electronic signals with the help of Fourier transform.

Course Content

Unit-I **8 hours**

Transducers (temperature, pressure/vacuum, magnetic fields, vibration, optical, and particle detectors). Linear and nonlinear curve fitting, chi-square test

Unit-II **8 hours**

Measurement and control. Signal conditioning and recovery. Microprocessor and microcontroller basics.

Unit-III **7 hours**

Impedance matching, amplification (Op-amp based, instrumentation amp, feedback), filtering and noise reduction, shielding and grounding.

Unit-IV **7 hours**

Fourier transforms, lock-in detector, box-car integrator, modulation techniques. High frequency devices (including generators and detectors).

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

Suggested Readings

1. B. L. Theraja, *Basic Electronics: Solid State* (S. Chand & Company Ltd., New Delhi, India) 2010.
2. D. Chattopadhyay and P. C. Rakshit, *Electronics: Fundamentals and Applications* (New Age International, New Delhi, India) 2008.
3. G. Saha, A.P. Malvino and D.P. Leach, *Digital Principles and Applications* (Tata McGraw - Hill Education, Noida, India) 2011.
4. P. Malvino and J.A. Brown, *Digital Computer Electronics* (Tata McGraw - Hill Education, Noida, India) 2011.

Course Code: CPC.579
Course Title: Enrich Physics Course - II
Total Lectures: 30

L	T	P	Credits	
2	0	0	2	

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

- Gain deep knowledge on elastic properties of condensed matter physics, thermal conductivity, band theory of solids and lattice specific heat.
- Learn the various types of Maxwell's equations in different media, propagation of electromagnetic waves, transmission lines and wave guides.

Course Content

Unit-I **8 hours**

Elastic properties, phonons, lattice specific heat. Free electron theory and electronic specific heat. Response and relaxation phenomena.

Unit-II **7 hours**

Drude model of electrical and thermal conductivity. Hall effect and thermoelectric power. Electron motion in a periodic potential, band theory of solids: metals, insulators and semiconductors.

Unit-III **8 hours**

Electromagnetic induction. Maxwell's equations in free space and linear isotropic media; boundary conditions on the fields at interfaces. Scalar and vector potentials, gauge invariance. Electromagnetic waves in free space. Dielectrics and conductors.

Unit-IV **7 hours**

Dispersion relations in plasma. Lorentz invariance of Maxwell's equation. Transmission lines and wave guides. Radiation- from moving charges and dipoles and retarded potentials.

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

Suggested Readings

1. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007.
2. A.R. Verma and O.N. Srivatava, *Crystallography Applied to Solid state physics* (New Age International), 2012
3. David J. Griffiths, *Introduction to Electrodynamics , 4th Edition, (Addison-Wesley), 2012*
4. Sadiku, Matthew Olanipekun, Elements of Electromagnetics (4th ed.), Oxford University Press, 2006.