COURSE STRUCTURE AND SYLLABUS

APPROVED BY THE

BOARD OF STUDIES OF CENTRE FOR COMPUTATIONAL SCIENCES

FOR

MSc Physics (Computational Physics)

FOR
BATCHES STARTING FROM 2016
Central University of Punjab
Bathinda-151001

Declaration

The syllabus of MSc Physics (Computational Chemistry) has been designed
(i) to ensure maximal overlap with the CSIR-NET syllabus.
(ii) in alignment with the Choice Based Credit System (CBCS) of UGC.
The percentage of foundation, core and elective courses for this programme are given below:

Course Type	Percentage of course type in the Programme	Percentage of course type required under CBCS
Foundation courses	14.5%	10-15%
Core Courses	60.4%	50-65%
Elective Courses	25.0%	25-35%

Eligibility Criteria for M. Sc. Physics (Computational Chemistry):

Same as the eligibility criteria prescribed for the M. Sc. Physics course of Centre for Physical Sciences of CUPB.

M. Sc. Physics (Computational Physics) programme Objective:

The objective of M. Sc. Physics (Computational Physics) Programme is that a student graduating after successful completion of the Programme shall be proficient in understanding the intricacies of relationship and interplay between Physics and Computational Sciences. In order to ensure this, wherever possible, computer programming exercises will be given to students based on Chemistry related problems in the courses taught to students in different semesters. This course is expected to enable the students to attain a Master's level understanding of Physics in general and Computational Physics in particular. In addition, based on the research training provided in this course, the students should be enabled to understand concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology and carry out further research in higher degrees. Further, extensive stress on logic based discipline would ensure development of scientific temperament among the students. Therefore graduated students of MSc Physics (Computational Physics) would be a valuable asset for the nation by virtue of their scientific abilities. The student can expect successful career / employment in academic / research / industry by undertaking this course. A special effort has been made to enable the student clear national level tests for teaching ability and research fellowships especially, CSIR-NET.

CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001

Centre for Computational Sciences

M. Sc. Physics (Computational Physics) Course Structure

Course Structure and Syllabus as per Choice Based Credit System (CBCS)

Semester I

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	% Weightage				e
								a	b	c	d	
1	**CSP.451**	**Introduction to Computational Sciences**	F	2	-	-	2	25	25	25	25	50
2	**PHY.501**	**Mathematical Physics**	C	4	-	-	4	25	25	25	25	100
3	**PHY.502**	**Classical mechanics**	C	4	-	-	4	25	25	25	25	100
4	**PHY.503**	**Quantum Mechanics**	C	4	-	-	4	25	25	25	25	100
5	**PHY.504**	**Electronic Circuit Theory**	C	4	-	-	4	25	25	25	25	100
6	**PHY.505**	**Electronic Circuit Laboratory**	C	-	-	8	4	-	-	-	-	100
7		**Interdisciplinary Elective**	E	2	-	-	2	25	25	25	25	50
		Total		20	0	8	24	-	-	-	-	600

Semester II

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	% Weightage				
								a	b	c	d	
1	**PHY.404**	**Computational Methods**	F	2	-	-	2	25	25	25	25	
2	**PHY.405**	**Computational Methods Laboratory**	F	-	-	4	2	25	25	25	25	
3	**PHY.506**	**Statistical Mechanics**	C	4	-	-	4	25	25	25	25	
4	**PHY.507**	**Electromagnetic Theory**	C	4	-	-	4	-	-	-	-	
5	**PHY.508**	**Digital Electronics**	C	4	-	-	4	-	-	-	-	
6	**PHY.509**	**Digital Electronics Laboratory**	E	2	-	-	2	25	25	25	25	
8	**PHY.510**	**Modern Physics Laboratory**	E	-	-	8	4	25	25	25	25	
9		**Humanities for Science Students**	E	2	-		2	25	25	25	25	
		Total		24	0	12	24	-	-	-	-	

Semester III

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage				e
								a	b	c	d	
1	**PHY.601**	**Solid State Physics**	C	4	-	-	4	25	25	25	25	100
2	**PHY.602**	**Nuclear and Particle Physics**	C	4	-	-	4	25	25	25	25	100
3	**PHY.603**	**Atomic and Molecular Physics**	C	4	-	-	4	25	25	25	25	100
5	**CSP.551**	**Research Methodology**	F	2	-	-	2	25	25	25	25	50
6	**CSP.552**	**Scientific Programming**	F	2	-	-	2	25	25	25	25	50
7	**CSP.553**	**Introduction to Scripting**	F	2	-	-	2	25	25	25	25	100
8	**CSP.554**	**Programming and Scripting Lab**	E	-	-	4	2	-	-	-	-	50
	CSP.604/ CSP.605	**Elective Course-I**	E	4	-	-	4	25	25	25	25	100
Choose any one of these courses:												
8	**CSP.604**	**Density Functional Theory**	E	4	-	-	4	25	25	25	25	100
9	**CSP.605**	**Quantum Dynamics**	E	4	-	-	4	25	25	25	25	100
		Total		22	-	4	24					600

Semester IV

S. No.	Paper	Course Title		L	T	P	Cr	Weightage	

	Code							a	b	c	d	e
1	**CSP.606**	**Molecular Mechanics and Simulation Methods**	C	4	-	-	4	25	25	25	25	400
2	**CSP.607**	**Molecular Mechanics and Simulation Methods Lab**	C	-	-	4	2	-	-	-	-	100
3	**CSP.599**	**Seminar**	F	-	-	4	2	-	-	-	-	50
4	**CSP.608**	**Dissertation Research**	C	-	-	16	8	25	25	25	25	100
Choose any two of the following courses:												
4	**CSP.609**	**Computer Modeling in Material Sciences**	E	4	-	-	4	25	25	25	25	100
5	**CSP.610**	**Computational Modeling Lab**	E	4	-	-	4	25	25	25	25	100
6	**CSP.611**	**Introduction to Biophysics**	E	4	-	-	4	25	25	25	25	100
7	**CSP.612**	**Computational Fluid Dynamics**	E	4	-	-	4	25	25	25	25	100
		Total										

a: **Continuous Assessment:** Subjective by enlarge
b: **Mid-Term Test-1:** Based on Objective Type & Subjective Type Test
c: **Mid-Term Test-2:** Based on Objective Type & Subjective Type Test
d: **End-Term Exam (Final):** Based on Objective Type Tests
e: Total Marks
L: Lectures **T:** Tutorial **P:** Practical **Cr:** Credits
F: Foundation Course **C:** Core Course **E:** Elective course

SEMESTER- I

Objective and Expected Learning Outcomes: The course structure of semester I of this Programme is designed to ensure complete overlap with courses taught to students of M. Sc. Physics, and is designed to provide breadth of knowledge in the discipline of Physics. The breadth knowledge gained in this semester will help students better understand the interdisciplinary area of Computational Physics. The list of courses to be taught in this semester is provided below, and is adapted from the Course structure of M. Sc. Physics programme currently running in the Centre for Physical Sciences of CUPB.

Course Title: Introduction to Computational Sciences
Paper Code: CSP.451
Total Lectures: 36

L	T	P	Credits	Marks
2	0	0	2	50

Course Objective and Learning Outcomes: This course has been designed to provide an introductory understanding of the broad filed of Computational Sciences. The course covers various aspects of the field and attempts to provide a bird’s eye view of the scientific potential of this growing field.

Unit-I[1,5] **(09)**

Introduction: Overview of Computational Sciences and its applications to Natural Sciences, Nobel Prize winners in Computational Natural Sciences and their contributions to the field, Modelling process and its types, Computational Toolbox- errors and their types, rate of change, fundamental concepts of integral calculus, Importance of Learning Computer Programming in Computational Natural Sciences.

Unit-II[2,5]

Applications of Computational Sciences in Chemistry (09)

Computational Quantum Chemistry and its applications, Prediction of Molecular Properties using Computational Chemistry, Overview of Quantum Chemistry Theories and their level of accuracy and hierarchy of computational requirements, Overview of Computer aided drug design and QSAR, Promises of Computational Chemistry

Unit-III[3,5] (09)

Applications of Computational Sciences in Physics

Computational Sciences in Molecular Physics, Computational Modeling of materials and prediction of material properties, Overview of Computational Fluid Dynamics and Computational Biophysics, Modeling force and motion, Overview of Cellular Automata Simulations, promises of Computational Physics

Unit IV[4,5]

Applications of Computational Sciences in Life Sciences
(09)

Overview of Computational Biology and bioinformatics, Structural Bioinformatics, Genomic data and its interpretation, Molecular Dynamics Simulations on Biological Systems, Hybrid Computational Methods for Studying Structure, Dynamics and Functions of Large Biological Systems, Promises of Computational Biology.

Recommended Books and References:

1. A. B. Shiflet and G. W. Shiflet. Introduction to Computational Sciences (Overseas Press (India) Pvt. Ltd., New Delhi, India), 2011.
2. F. Jensen. Introduction to Computational Chemistry (Second Edition, Wiley), 2007.
3. J. Hasbun, P. Devries. A First Course in Computational Physics. (Viva Books Pvt. Ltd., New Delhi), 2011.
4. D. W. Mount. Bioinformatics (2nd Edition, Cold Spring harbour Press, New Jersey), 2004.
5. Some examples will be taken from Selected Articles from Standard /Reputed Journals.

Course Title: Mathematical Physics
Paper Code: PHY.501

L	T	P	Credits	Marks
4	0	0	4	100

Total Lectures: 60

Course Objective and 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.

Unit-I (15)

Vector Algebra and Matrices: Dimensional analysis, Vector algebra and vector calculus, Linear algebra, matrices, Caley-Hamilton theorem, Eigen values and Eigen vectors, curvelinear coordinates.

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

Unit-II **(15)**

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, Tensors, Introductory group theory:SU(2), O3.

Unit-III **(15)**

Complex Variable: Elements of complex analysis, Analytical functions, Cauchy-Riemann equations, Cauchy theorem, Properties of analytical functions, Contours in complex plane, Integration in complex plane, Deformation of contours, Cauchy integral representation, Taylor and Laurent series, Isolated and essential singular points, Poles, Residues and evaluation of integerals, Cauchy residue theorem and applications of the residue theorem.

Unit-IV **(15)**

Fourier and Laplace Transforms: Fourier series, Dirichlet condition, General properties of Fourier series, Fourier transforms, Their properties and applications, Laplace transforms, Properties of Laplace transform, Inverse Laplace transform and application.

Differential Equations: Linear ordinary differential equations of first and second order, Partial differential equations (Laplace, wave and heat equation in two and three dimensions), Boundary value problems and Euler equation.

Recommended Books:

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) Limited, New Delhi) 2000

Course Title: Classical Mechanics
Paper Code: PHY.502
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and 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. Student will gain 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.

Unit-I **(18)**

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 **(10)**

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 **(17)**

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)**

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, Two and three coupled pendulums, 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, Hamiltonian and Electrodynamics.

Recommended books:

1. S.T. Thornton and J.B. Marion, *Classical Dynamics of Particles and Systems* (Cengage Learning, Boston/Massachusetts, United State), 5^{th} edition, 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.

Course Title: Quantum Mechanics
Paper Code: PHY.503
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes:
The objective of this course is to develop familiarity with the physical concepts of quantum mechanics and its mathematical formulation. Student will learn basics of the subject and make them understand the concept of operators, observables, Schrodinger equation and applies it to simple physical systems, angular momentum, scattering and perturbation theories with emphasis on the physical structure of the theory.

Unit-I **(14)**

Limitations of Classical Physics and Basics of Quantum Mechanics: Black body radiation, Photoelectric effect, Compton Effect, Electron diffraction, Wave particle duality and Heisenberg uncertainty principle, Review of linear algebra and Hilbert space, Dirac notation, Matrix mechanics.

Wave Mechanics: Schrödinger wave equation (Time dependent and time independent), Postulates of quantum mechanics, Probability current density and conservation of probability, Wave-function in coordinate and momentum representations, Free particle wave function, Observables, Hermitian operators, Expectation values, Ehrenfest's theorem, Stationary states, Superposition principle, Commutation relations.

Unit-II **(16)**

Applications of Schrödinger Wave Equation: Eigen value problems; Particle in one dimensional box, Potential step, Square well, Tunneling through barrier, Linear harmonic oscillator, Spherically symmetric potential, Hydrogen atom.

Angular momentum: Motion in central potential: orbital angular momentum, Angular momentum algebra, Commutators, Concept of spin, Stern-Gerlach experiment, Linear harmonic oscillator problem using commutation relations, Matrix representation of angular momentum operators, Addition of angular momenta (C.G. coefficients).

Unit-III **(14)**

Scattering Theory: Elementary Scattering theory, Central force problem, Partial wave analysis, Phase shifts, Optical theorem, Bound states and resonances, Scattering cross section, Green's functions, Born approximation, Scattering for different kinds of potentials, Applications.

WKB Approximation and its Applications: WKB approximation, Development and validity of WKB approximation, Application of WKB technique to barrier penetration, Cold emission of electrons from metals, Alpha-decay of nuclei, Relativistic quantum mechanics: Klein-Gordon and Dirac equations.

Unit-IV **(16)**

Time-independent Perturbation Theory and its Applications: Stationary perturbation theory: Degenerate case, Variational methods, Polarizability of hydrogen, Non-degenerate perturbation theory, Harmonic oscillator subject to perturbing potential, Degenerate perturbation theory, Stark effect, spin orbit coupling, Fine structure of hydrogen, Zeeman effect.

Time-dependent Perturbation Theory: Time development of states and transition probability, Constant perturbation, Fermi golden rule, Adiabatic approximation, Semi-classical theory of radiations: Interaction of one-electron atom with electromagnetic field, Harmonic perturbation theory, Spontaneous emission: Einstein A and B coefficients, Selection rules for electric dipole transitions, Lifetime and line-width, Identical particles, Pauli exclusion principle, spin-statistics connection.

Recommended books:

1. E. Merzbacher, *Quantum Mechanics* (Wiley India Pvt. Ltd., New Delhi, India) 2011.
2. L.I. Schiff, *Quantum Mechanics* (Tata McGraw-Hill Education, Noida, India) 2010.
3. N. Zettili, *Quantum Mechanics-Concepts and Applications* (John Wiley & Sons Ltd., Sussex, U.K.) 2009.
4. K. Venkatesan, P.M. Mathews, *A Textbook of Quantum Mechanics* (Tata McGraw - Hill Education, Noida, India) 2010.

Course Title: Electronic Circuits Theory
Paper Code: PHY.504
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

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

Unit-I **(10)**

Network Theorems: Superposition theorem, Thevenin's and Norton's theorems, A. C. equivalent circuits of networks with active devices.

Power Supplies: Fourier transforms, Half-wave, Full-wave and bridge rectifiers with capacitive input, Inductance input, T and π filters, Regulated power supplies: Shunt regulated power supplies using Zener diodes.

Unit-II **(20)**

Transistor Amplifiers: Theory of semiconductors, Semiconductor devices: diode, homo and hectojunction devices, Transistor, Device structure and characteristics, Amplifiers, Frequency dependence and applications, Impedance matching, H and R parameters and their use in small signal amplifiers, Conversion formulae for the h-parameters of the different transistor configurations, Analysis of a transistor CE amplifier at low frequencies using h-parameters, CE amplifier with unbypassed emitter resistor, Emitter follower at low frequencies, Emitter-coupled differential amplifier and its characteristics, Cascaded amplifiers, Transistor biasing, Self-bias and thermal stability, Noise reduction, Low frequency power amplifiers, High frequency devices.

Unit-III **(12)**

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-IV **(18)**

Feedback: The gain of an amplifier with feedback, General characteristics of negative feedback/instrumentation amplifiers, Stability of feedback amplifiers, Barkhaussen criteria, Grain and phase margins, Compensation, Sinusoidal oscillators: RC oscillators: Phase shift and the Wien's bridge oscillators, LC oscillators, Frequency stability and the crystal oscillators, lockin detector , Box Car integrator and modulation techniques.

Operational Amplifier and Their Applications: Characteristics of an ideal operational amplifier, Amplification, Applications of operational amplifiers: Inverting and non-inverting amplifiers, Summing circuits, Integration and differentiation, Waveform generators signal conditioning and recovery.

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.

Course Title: Electronic Circuit Laboratory
Paper Code: PHY.505
Total Hours: 120

L	T	P	Credits	Marks
0	0	8	4	100

Course Objective and Learning Outcomes: The laboratory exercises have been so designed that the students can verify some of the concepts learnt in the electronic circuit theory classes. During these laboratory they will get sufficient training to carrying out precise measurements and handling sensitive equipment.

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

1. Power supplies: Bridge rectifiers with capacitive input filters.
2. Power supplies: Shunt Voltage regulator using Zener diode.
3. Clipping and Clamping along with CRO.
4. Common Emitter Amplifier with and without feedback.
5. Determination of h-parameters in the CE configuration using the measured input and output characteristics of a BJT.
6. Common Source and Common Drain Amplifiers using JFET.
7. RC Oscillators: Phase shift oscillator using RC ladder network as the phase shifting Network.
8. Wien's Bridge Oscillator.
9. Colpitts Oscillators.
10. Hartley Oscillators.
11. Emitter Coupled Differential Amplifier using BJT's.

12. Multivibrators – Bistable, Monostable and Free Running multivibrators
13. Op-Amp characteristics: V_{io}, I_b, V_{ol}, CMRR, Slew Rate. Applications of Op-amps: inverting Amplifier, Unity Gain Buffer, Summing Amplifier.
14. 555 IC timers. Free Running and Monostable Multivibrators, Sawtooth wave generator.

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 India, 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.

Course Title: Humanities for Science Students

Paper Code: XXX.4XX

Total Hours: 30

L	T	P	Credits	Marks
2	0	0	2	50

Semester II

Objective and Expected Learning Outcomes: The course structure of semester II of this Programme is designed to ensure complete overlap with courses taught to students of M. Sc. Physics. The breadth knowledge in Physics gained in this semester will help students better understand the interdisciplinary area of Computational Physics. The list of courses to be taught in this semester is provided below, some of which are adapted from the Course structure of M. Sc. Physics programme currently running in the Centre for Physical Sciences of CUPB.

Course Title: Computational Methods
Paper Code: PHY.404
Total Lectures: 30

L	T	P	Credits	Marks
2	0	0	2	50

Course Objective and Learning Outcomes: The course on Computational Methods has been framed to equip the students of M.Sc. Physics with knowledge of programming in C, roots of equation, interpolation, curve fitting, numerical differentiation, numerical integration, solution of ordinary differential equations and probability.

Unit-I **(07)**

Programming with C: Introduction to the concept of object oriented programming, Advantages of C over conventional programming languages, Introduction to classes, objects, C programming syntax for Input/Output, Operators, Loops, Decisions, Simple and inline functions, Arrays, Strings, Pointers.

Unit-II **(07)**

Roots of Algebraic and Transcendental Equations: Element of computational techniques: roots of functions, Interpolation, Extrapolation, One point and two-point iterative methods such as bisection method and Newton Raphson methods.

Unit-III **(08)**

Integration and Differential: Integration by Trapezoidal and Simpson's rule, Solution of first order differential equation using Runge-Kutta methods, Finite difference methods.

Data Interpretation and Error analysis: Dimensional analysis, Precision and accuracy, error analysis, Propagation and errors.

Unit-IV **(08)**

Least square fitting: Least square fitting, Linear and nonlinear curve fitting, Chi square test.

Random numbers: Introduction to random numbers, Monte Carlo method for random number generation.

Probability Theory: Elementary probability theory, Random variables, Binomial, poisson and normal distributions, Central limit theorem.

Recommended Books:

1. P.R. Bevington and D. K. Robinson, *Data Reduction and Error analysis for Physical Sciences* (McGraw Hill, Noida, India) 2003.
2. Y. Kanetkar, *Let Us C* (BPB Publications, New Delhi, India) 2012.
3. E. Balaguruswamy, *Numerical Methods* (Tata McGraw Hill, Noida, India) 2009.
4. S. S. Sastry, *Introductory Methods of Numerical Analysis* (PHI Learning Pvt. Ltd., New Delhi, India) 2012.

Course Title: Computational Methods Laboratory
Paper Code: PHY.405
Total Hours: 60

L	T	P	Credits	Marks
0	0	4	2	50

Course Objective and Learning Outcomes: The laboratory exercises have been so designed that the students learn to verify some of the mathematical concepts. They are trained in carrying out numerical problems using C language.

Student has to perform at least eight experiments out of the following list of experiments.

1. Data handling: find standard deviation, mean, variance, moments etc. of at least 25 entries.
2. Choose a set of 10 values and find the least squared fitted curve.
3. To find the roots of quadratic equations.
4. Perform numerical integration on 1-D function using Simpson rules.
5. Perform numerical integration on 1-D function using Trapezoid rule.
6. To generate random numbers between (i) 1 and 0, (ii) 1 and 100.
7. To find the value of π using Monte Carlo simulation.
8. To find the solution of differential equation using Runge-Kutta method.
9. To find the solution of differential equation using Euler's method.
10. To find the value of y for given value of x using Newton's interpolation method.

Recommended Books:

1. P.R. Bevington and D. K. Robinson, *Data Reduction and Error analysis for Physical Sciences* (McGraw Hill, Noida, India) 2003.
2. Y. Kanetkar, *Let Us C* (BPB Publications, New Delhi, India) 2012.
3. E. Balaguruswamy, *Numerical Methods* (Tata McGraw Hill, Noida, India) 2009.
4. S. S. Sastry, *Introductory Methods of Numerical Analysis* (PHI Learning Pvt. Ltd., New Delhi, India) 2012.

Course Title: Statistical Mechanics
Paper Code: PHY.506
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: This course is designed to provide basic concept of thermodynamics and statistical mechanics to M.Sc. Physics students. The course has been framed to teach the techniques of ensemble theory to understand the macroscopic properties of the matter in bulk in terms of its microscopic constituents.

Unit-I **(12)**

Introduction: Laws of thermodynamics and their consequences, Thermodynamic potentials and Maxwell relations, Micro- and macro- states, Ergodic hypothesis, Postulate of equal a priori probability, Boltzmann's postulate of entropy, Phase space, Phase equilibria, Entropy of ideal gas, Gibbs' paradox, Liouville's theorem.

Unit-II **(12)**

Canonical Ensemble: System in contact with a heat reservoir, Expression of entropy, Partition function, Free energy and its connection with thermodynamics quantities, Fluctuation of internal energy, Micro-canonical, Canonical and grand-canonical ensembles, System in contact with a particle reservoir, Chemical potential, Grand canonical partition function and grand potential, Fluctuation of particle number, Chemical potential of ideal gas.

Unit-III **(18)**

Classical and Quantum Statistics: Black body radiation and Plank's distribution law, Quantum Liouville theorem, Identical particles in B-E and F-D distributions, Quantum mechanical ensemble theory, Super-fluidity in liquid He II, First and second order phase transitions, Low temperature behaviour of Bose and Fermi gases, Ising model, Mean-field theory in zeroth and first approximations, Exact solution in one dimension.

Unit-IV **(18)**

Ideal Bose and Fermi Gas: Ideal gas in different quantum mechanical ensembles, Equation of state, Bose-Einstein condensation, Equation of state of ideal Fermi gas, Fermi gas at finite temperature. Thermodynamics, Pauli paramagnetism, Landau diamagnetism, Ferromagnetism, de Hass van Alphen effect, Principle of detailed balance.

Diffusion: Diffusion equation, Random walk and Brownian motion, Introduction to nonequilibrium processes.

Recommended books:

1. R.H. Swendsen, *An Introduction to Statistical Mechanics and Thermodynamics* (Oxford University Press, Oxford, U.K.) 2012.

2. M.V. Sadovskii, *Statistical Physics* (Walter de Gruyter GmbH and Co. KG, Berlin/Boston, USA) 2012.
3. R.K. Patharia and Paul D. Beale, *Statistical Mechanics* (Elsevier, USA) 2011.
4. B.B. Laud, *Fundamentals of Statistical Mechanics* (New Age International, New Delhi, India) 2012.
5. K. Huang, *Statistical Mechanics* (Wiley India Pvt. Ltd., New Delhi, India) 1987.

Course Title: Electromagnetic Theory
Paper Code: PHY.507
Total Lecture: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: The Electromagnetic Theory is a course that covers electrostatics, magnetostatics, dielectrics, and Maxwell equations. The course has also been framed to solve the boundary value problems. The course contains the propagation of electromagnetic waves in dielectrics, metals and plasma. The course also covers the motion of relativistic and non- relativistic charged particles in electrostatic and magnetic fields.

Unit-I **(18)**

Electrostatics: Gauss's law and its applications, Work and energy in electrostatics, Electrostatic potential energy, Poisson and Laplace equations, Uniqueness theorem I & II, Energy density and capacitance.

Boundary Value Problems: General methods for the solution of boundary value problems, Solutions of the Laplace equation in rectangular cartesian, spherical polar and cylindrical coordinates, Various boundary value problems.

Multipoles and Dielectrics: Multipole expansion, Multipole expansion of the energy of a charge distribution in an external field, Dielectrics and conductors, Gauss's law in the presence of dielectric, Boundary value problems with dielectrics, Molar polarizability and electrical susceptibility, Electrostatic energy in dielectric media.

Unit-II **(12)**

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

Magnetic Fields in Matter: Magnetization, Dia, para and ferro-magnetic materials, Field of a magnetized object, Magnetic susceptibility and permeability.

Unit-III **(16)**

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

Time Varying Fields and Conservation Laws: Scalar and vector potentials, Gauge invariance, Lorentz gauge and Coulomb gauge, Poynting theorem and conservations of energy and momentum for a system of charged particles, EM fields.

Plane Electromagnetic Waves and Wave Equations: EM wave in free space, Dispersion characteristics of dielectrics, Waves in a conducting and dissipative media, Reflection and refraction, Polarization, Fresnel's law, Interference, Coherence and diffraction, Dispersion relation in plasma, Skin effect, Transmission lines and wave guides.

Unit-IV **(14)**

Radiation from Moving Point Charges and Dipoles: Retarded potentials, Lienard-Wiechert potentials, Radiation from a moving point charge and oscillating electric and magnetic dipoles, Dipole radiation, Multipole expansion for radiation fields. **Relativistic Electrodynamics:** Lorentz transformation law for the electromagnetic fields and the fields due to a point charge in uniform motion, Field invariants, Covariance of Lorentz force equation and dynamics of a charged particle in static and uniform electromagnetic fields, Lorentz invariance of Maxwell equations, Energy-momentum tensor and the conservation laws for the electromagnetic field.

Recommended books:

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

Course Title: Digital Electronics
Paper Code: PHY.508
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: The course on Digital Electronics is introduced to familiarize the students with the idea of logic in designing of electronic devices, circuits, operations, data signal processing and applications.

Unit-I **(14)**

Digital Circuits: Logic gates and their realization using diodes and transistors, Boolean algebra, Boolean equation of logic circuits, De-Morgan theorem, Method of realization a circuit for given truth table, Sum of product (SOP) and product of sum (POS) representation, Karnaugh map and their applications, Half adder and full adder circuits, Half substractor and full sbubstractor.

Unit-II **(14)**

Combinational Circuits: Design procedure, Adders-subtractors, Carry look ahead adder, BCD adder, Magnitude comparator, Multiplexer/demultiplexer, Encoder/decoder, Comparator, Parity checker, Code converters, Implementation of combinational logic.

Unit-III **(17)**

Sequential Circuit: SR, JK, D and T flip flop, Master slave flip flops, Triggering mechanism of flip flop, Realization of one flip flop using other flip flops, Asynchronous/ripple counters, Synchronous counters, Shift counters, Shift registers, Universal shift register and similar circuits, MSI and LSI based design, MSI and LSI implementation on sequential circuit.

Unit-IV **(15)**

Memory Devices: Classification of memories, RAM write operation and read operation, Static RAM cell and Bipolar RAM cell, Programmable logic device (PLD), Programmable logic array (PLA), Implementation of ROM and PLA.

Data Converters: Analog to digital (A/D) data converters, Digital to analog (D/A) data converters, Logic families, Microprocessors and micro controller basics.

Recommended books:

1. G. Saha, A.P. Malvino and D.P. Leach, *Digital Principles and Applications* (Tata McGraw - Hill Education, Noida, India) 2011.
2. P. Malvino and J.A. Brown, *Digital Computer Electronics* (Tata McGraw - Hill Education, Noida, India) 2011.
3. C. Hawkins and J. Segura, *Introduction to Modern Digital Electronics* (Scitech Publishing, New York, USA) 2010.

Course Title: Digital Electronics Laboratory
Paper Code: PHY.509
Total Hours: 60

L	T	P	Credits	Marks
0	0	4	2	50

Course Objective and Learning Outcomes: The laboratory exercises have been so designed that the students can verify some of the concepts learnt in the Digital Electronics classes. During these laboratory they will get sufficient training to carrying out precise measurements and handling sensitive equipment.

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

1. Realization of universal logic gates.
2. Implementation of the given Boolean function using logic gates in both SOP and POS form.
3. Verification of logic state tables of RS and JK flip-flops using NAND & NOR gates.
4. Verification of logic state tables of T and D flip-flops using NAND & NOR gates.
5. Verification of logic state tables of master slave flip flop using NAND & NOR gates.
6. Triggering mechanism of flip flop.
7. Realization of Half adder and full adder.
8. Realization of Half substractor and full substractor.
9. Decoders and code converters.
10. Up/Down Counters.
11. Shift Resistor.

Recommended books:

1. G. Saha, A.P. Malvino and D.P. Leach, *Digital Principles and Applications* (Tata McGraw - Hill Education, Noida, India) 2011.
2. P. Malvino and J.A. Brown, *Digital Computer Electronics* (Tata McGraw - Hill Education, Noida, India) 2011.
3. C. Hawkins and J. Segura, *Introduction to Modern Digital Electronics* (Scitech Publishing, New York, USA) 2010.

Course Tile: Modern Physics Laboratory
Paper Code: PHY.510
Total Hours: 120

L	T	P	Credits	Marks
0	0	8	4	100

Course Objective and Learning Outcomes: The laboratory exercises have been so designed that the students can verify some of the concepts learnt in the Atomic Molecular and Laser Physics theory classes. During this laboratory they will get sufficient training to carrying out precise measurements and handling sensitive equipment.

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

1. Ionization potential by Franck Hertz experiment.
2. Photo electric effect.
3. Band gap of a semiconductor by Four Probe method.
4. Wavelength measurement of laser using diffraction grating.
5. Michelson interferometer.
6. Dual nature of electron experiment.
7. Millikan's oil drop experiment.
8. Stefan's law
9. Zeeman effect experiment

Recommended books:

1. R.A. Serway, C.J. Moses and C.A. Moyer, *Modern physics* (Brooks Cole, Massachusetts, USA) 2012.
2. S.T. Thornton, *A. Rex Modern Physics for Scientists and Engineers* (Thomson Brooks/Cole, Massachusetts, USA) 2012.
3. K.S. Krane, *Modern Physics* (Wiley India (P) Ltd., New Delhi, India) 2012.
4. A. Beiser, *Concepts of Modern Physics* (Tata McGraw - Hill Education, Noida, India) 2007.

Semester-III

Objective and Expected Learning Outcomes: The course structure of semester III of this Programme is designed to provide students with courses that build their depth in the field of Computational Physics. In addition to a few courses in core areas of Physics, this semester includes advanced courses in Computational Physics and foundation courses in computer programming. The list of courses to be taught in this semester is provided below.

Course Title: Solid State Physics
Paper Code: PHY.601
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes:
The objectives of this physics course are to provide the student with a clear and logical presentation of the basic and advanced concepts and principles of solid state physics. The contents of the course are designed so as to expose the students to the topics like crystal

structure, lattice vibrations, band theory of solids, magnetic properties of solids, defects, superconductivity so that they are able to use these techniques in investigating the aspects of the matter in condensed phase.

Unit-I **(15)**

Crystal Structure and its determination: Bravais lattices, Crystal structures, Reciprocal lattices, Ewald sphere, X-ray diffraction, Lattice parameter determination, Atomic and crystal structure factors, Intensity of diffraction maxima, Electron and neutron diffraction, Bonding of solids.

Lattice Dynamics: Elastic properties of solids, Vibrations of linear monatomic and diatomic lattices, Acoustical and optical modes, Long wavelength limits, Optical properties of ionic crystal in the infrared region, Normal modes and phonons, Inelastic scattering of neutron by phonon, Lattice heat capacity, models of Debye and Einstein, Comparison with electronic heat capacity, Thermal expansion, Thermal conductivity.

Unit-II **(15)**

Band Theory of Solids: Free electron theory, Density of states, Boltzmann transport equation, Drude model of electrical and thermal conductivity and Sommerfield theory, Hall effect and quantum Hall effect, Electrons motion in periodic potentials, Bloch theorem, Kronig Penny model, Nearly free electron theory, Band gap, Number of states in a band, Tight binding method, Effective mass of an electron in a band, Classification of metal, Semiconductor and insulator, Thermoelectric power, Response and relaxation phenomena.

Unit-III **(15)**

Magnetic Properties of Solids: Classical and quantum theory of diamagnetism and paramagnetism, Pauli paramagnetism, Landau diamagnetism, Cooling by adiabatic demagnetization, Weiss theory of ferromagnetism, Curie-Weiss law, Heisenberg's model and molecular field theory, Domain structure and Bloch wall, Neel model of antiferromagnetism and ferrimagnetism, Spin waves, Bloch $T^{3/2}$ law, ESR, NMR and chemical shifts.

Unit-IV **(15)**

Defects and Dislocations: Point defects (Frenkel and Schottky), Line defects (slip, plastic deformation, Edge dislocation, Screw dislocation, Burger's vector, Concentration of line defects, Estimation of dislocation density, Frank-Reid mechanism of dislocation multiplication (dislocation reaction), Surface (Planar) defects, Grain boundaries and stacking faults.

Superconductivity: Meissner effect, Type-I and type-II superconductors; Heat capacity, energy gap and isotope effect, BCS theory, London equation, Flux quantization, Coherence, AC and DC Josephson effect, Superfluity, High T_C superconductors (information only).

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.

Course Title: Nuclear and Particle Physics
Paper Code: PHY.602
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: The objective of the course on Nuclear and Particle Physics is to teach the students the basic of nuclear properties, nuclear interactions, nuclear decay, nuclear models, detectors, nuclear reactions and elementary particles.

Unit-I **(12)**

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, RMS radius, Spin dependence of nuclear forces, Form of nucleon-nucleon potentials, Electromagnetic moment and magnetic dipole moment of deuteron, General form of nuclear force and the necessity of tensor forces. 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 **(16)**

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, Fermi-Curie plot, Selection rules for Fermi and Gamow-Teller transitions, Parity non-conservation and Wu's experiment.

Nuclear Models: Evidence of shell structure, Single particle shell model, Its validity and limitations, Rotational spectra, Shell model, Liquid drop model, Semi empirical mass formula.

Unit-III **(18)**

Detectors: Properties of radiation detectors, Gas detectors: GM counter, Proportional counters, Ionization chambers, Scintillation detectors: NaI(Tl), CsI(Tl), Photomultiplier tubes, Semiconductor diode detectors, Different kinds of silicon detectors, HPGe detectors, Slow and fast neutron detection methods.

Nuclear Reactions: Different types of nuclear reactions, Conservation laws, Reaction cross section, Reaction mechanism, Compound nuclei and direct reactions, Fusion-evaporation and fusion-fission reactions, Optical model; Super-heavy nuclei.

Unit-IV **(14)**

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, Relativistic kinematics, K-3π decay, τ-θ puzzle.

Recommended books:

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 Title: Atomic and Molecular Physics
Paper Code: PHY.603
Total Lectures: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: The main objective of the course on Atomic and Molecular Physics for the students of M.Sc. Physics is to teach the knowledge of atomic, molecular, electronic, rotational, vibrational, and Raman spectra. The course also covers the basic concepts and applications of lasers.

Unit-I **(18)**

One and Two Electrons Systems: Quantum state of an electron in an atom, Spectrum of hydrogen, helium and alkali atoms, Electron spin, Spin - orbit coupling, Mass correction term, Two electron system, Pauli's exclusion principle, Level scheme for two electron atoms- LS and JJ coupling – multiplet splitting – Lande's 'g' factor, Lande's interval rule, Fine structure, Relativistic correction for energy level of hydrogen atom, Selection rules, Lamb shift, Zeeman effect. Paschen-Back effect, Stark effect, Hyperfine structure and isotopic shift, Width of spectral lines.

Unit-II **(10)**

Many Electron Atom: Independent particle model, Central field approximation for many electron atom, Slater determinant, Equivalent and nonequivalent electrons, Energy levels and spectra, Spectroscopic terms, Hund's rule.

Unit-III **(18)**

Molecular Structure: Molecular potential, Separation of electronic and nuclear wave functions, Born-Oppenheimer approximation, Molecular orbital and electronic configuration of diatomic molecules: H_2, and NO, LCAO approach, States for hydrogen molecular ion, Coulomb, Exchange and overlap integral, Shapes of molecular orbital, Sigma and pi bond.

Unit-IV **(14)**

Molecular Spectra: Electronic, Vibrational and rotational spectrum of diatomic molecules, Frank-Condon principle, Raman transitions and Raman spectra, Normal vibrations of CO_2 and H_2O molecules.

Recommended Books:

1. C.J. Foot, *Atomic Physics* (Oxford University Press, Oxford, U. K.) 2005.
2. W. Demtroder, *Molecular Physics* (Springer, New York, USA) 2008.
3. J.M. Hollas, *Basic Atomic and Molecular Spectroscopy* (Royal Society of Chemistry, London, U.K.) 2002.
4. G. Herzberg, *Atomic Spectra and Atomic Structure* (Dover Publications, New York, USA) 2010.

Course Title: Research Methodology
Paper Code: CSP.551
Total Lectures: 36

L	T	P	Credits	Marks
2	0	0	2	50

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

Unit-I[1-5]
(09)

Introduction: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Hypothesis formulation and development of research plan, Art of reading and understanding scientific papers, Literature survey, Interpretation of results and discussion.

Unit-II[1-5] **(09)**

Library: Classification systems, e-Library, Reference management, Web-based literature search engines, Intellectual property rights (IPRs).

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

Unit-III[1-5] **(09)**

Scientific and Technical Writing: Role and importance of communication, Effective oral and written communication, Scientific writing, Research paper writing, Technical report writing, Making R and D proposals, Dissertation/Thesis writing, Letter writing and official correspondence, Oral and poster presentation in meetings, Seminars, Group discussions, Use of modern aids; Making technical presentations.

Unit-IV[1-5]
(09)

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

Recommended Books:

1. R. Kumar, *Research Methodology* (SAGE Publications India Pvt. Ltd., New Delhi, India), 2012.

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

Course Title: Scientific Programming
Paper Code: CSP.552
Total Lectures: 36

L	T	P	Credits	Marks
2	0	0	2	50

Course Objective and Learning Outcomes: The objective of this course is to introduce students to the art of scientific programming. The theory part practical aspects of scientific programming languages Fortran and C will be taught to students in this course.

Unit I **(09)**
Introduction to Computers and Fortran and C languages: History and evolution of Fortran and C languages, Basic elements of Fortran and C: Character sets, structure of statements, Structure of a Fortran and C Program, compiling, linking and executing the Fortran and C programs.

Unit II **(09)**
Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit III **(09)**
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 attays in procedures, derived data types.

Unit IV **(09)**
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 and C.

Book Recommended:

1. Chapman, Fortran 95/2003 for Scientists and Beginners, 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. R. L. Schwartz, T. Christiansen, L. Wall, Learning Perl Second Edition, O'Reilly Media (1997).
5. Foy, Mastering Perl First Edition, O'Reilly Media (2007).

Course Title: Introduction to Scripting
Paper Code: CSP.553

L	T	P	Credits	Marks
2	1	0	2	50

Total Hours: 72

Objective and Learning Outcomes: The objective of this course is that students learn the basics of computer scripting language perl and python and apply them to study chemical and biochemical problems.

Unit I **(9)**

Introduction to computer scripting and perl language, Basic elements of perl, perl syntax, executing the perl programs, arrays, lists.

Unit II **(9)**

Hashes regular expressions, loops and decisions, files and data, running and debugging perl, advanced concepts in perl

Unit III **(9)**

Introduction to python language, basic elements of python, python syntax, executing the python programs, numbers and operators, variables, using names for data, using built-in types.

Unit IV **(9)**

Python language and the standard library: M aking decisions, functions, classes and objects, files and directories, text processing.

References:

1. Learning Perl, R. L. Schwartz, B. D. Foy and T. Phoenix, O' Reilly 6th Edition (2011).
2. Beginning Python, J. Payne, Wiley India Edition (2010).
3. Perl Basic Practices, D. Conway, O' Reilly 1st Edition (2005).
4. Learning Python, M. Lutz, O' Reilly, Tenth Edition (2012).

Course Title: Programming and Scripting Lab
Paper Code: CSP.554

L	T	P	Credits	Marks
0	1	4	2	50

Total Hours: 72

Course Objective: This course will provide practical experience to the students through applications of Fortran, C, perl and python programming and scripting languages to problems of chemical interest. Thus, this lab course will strongly align with the theory courses CSC.501 (Scientific Programming) and CSC.551 (Introduction to Scripting) to provide practical programming experience to students.

Course Title: Density Functional Theory
Paper Code: CSP.604

L	T	P	Credits	Marks
4	0	0	4	100

Total Lecture: 72

Objective and Learning Outcomes: This is a specialization course for students of Computational Chemistry. The objective of this course is to make the students understand the basics of Density Functional Theory (DFT), which is a popular electronic structure method. With the increasing power of computers, DFT-based calculations are emerging as a useful tool to characterize the properties of molecules and materials. This course will review the various theories/approximations necessary to understand most popular framework of modern DFT.

Unit-I **(18)**

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 **(18)**

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 **(18)**

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 **(18)**

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.

Recommended Books:

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

Course Title: Quantum Dynamics

Paper Code: CSP.605

L	T	P	Credits	Marks
4	1	0	4	100

Total Lecture: 72

Course Objective and Learning Outcomes: This course will introduce the basic aspects of time dependent quantum wavepacket dynamics to Masters students.

Unit I[1-6] **18 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[1-6] **18 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[1-4] **18 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[1-6] **18 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.

Books

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: Molecular Mechanics and Simulation Methods
Paper Code: CSP.606
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning outcomes: The objective of this subject is to ensure that a student learns modelling of molecular structures and understanding 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.

Unit I **(18)**

Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example. Techniques for Conformational Sampling- Monte Carlo, global optimization, etc.

Unit II **(18)**

Molecular Mechanics: general features, bond stretching, angle bending, improper torsions, out of plane bending, cross terms, non-bonded interactions, Ramachandran diagram point charges, calculation of atomic charges, polarization, van der waals interactions, hydrogen bond interactions, Water models, Force field, all atoms force field and united atom force field.

Unit III **(18)**

Energy minimization: Steepest descent, conjugate gradient – Derivatives, First order steepest decent and conjugate gradients. Second order derivatives Newton-Raphson, Minima, maxima saddle points and convergence criteria.-non derivatives minimization methods, the simplex, sequential univariative, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, Solvent access, Equilibration, cut-offs.

Unit IV **(18)**

Simulation methods : algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods. Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics, simulation softwares. Various methods of MD, Monte Carlo, systematic and random search methods.

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 Title: Molecular Mechanics and Simulation Methods Lab
Paper Code: CSP.607
Total Lecture: 36

L	T	P	Credits	Marks
0	0	4	2	100

Course Objective and Learning outcomes: The objective of this subject is to ensure that a student gains practical in-hand experience of various modeling and classical simulation tools, including, but not limited those that are used in macromolecular modeling. The course will help the students learn the use the techniques of molecular simulations, which will enhance their employability in their further potential carrers in academia and industry.

1. Advanced Visualization Software and 3D representations with VMD and Rasmol.
2. Coordinate generations and inter-conversions.
3. Secondary Structure Prediction.
4. Fold Recognition, *ab initio method.*
5. Homology based comparative protein modeling.
6. Energy minimizations and optimization.
7. Validation of models.
    a. WHATIF
    b. PROSA
    c. PROCHECK
    d. VERIFY 3D
8. Protein Structure Alignment.
9. Modeller
10. Structure based Drug Design

a. Molecular Docking
b. De Novo Ligand Design
c. Virtual Screening

11. Ligand based Drug Design
    a. Pharmacophore Identification
    b. QSAR
12. Molecular Dynamics with Gromacs
13. Binding Site Identification

Suggested Reading

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 Title: Seminar
Paper Code: CSP.599

L	T	P	Credits	Marks
0	0	4	2	50

Objective: The objective of this course would be that students gain in depth knowledge of a chosen topic/research paper, and gain practical presentation skills.
The evaluation criteria for this course shall be as follows:

Maximum Marks: 50

S.No.	Criteria	Marks
1.	Content of presentation	15
2.	Presentation Skills	15
3.	Handling of queries	20
Total		50

Course Title: Dissertation Research
Paper Code: CSP.608

L	T	P	Credits	Marks
0	0	16	8	200

Objective: The objective of this course would be to ensure that the student carries research in the topic chosen. The evaluation criteria for this course shall be as follows:

Maximum Marks: 200

S.No.	Criteria	Marks
1.	Continuous assessment by the supervisor	50

2. First mid-semester presentation (synopsis) 50
3. Second mid-semester presentation (presubmission) 50
4. External review and final presentation 50

Total 200

Course Title: Computer Modeling in Material Sciences
Paper Code: CSP.609
Total Lecture: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objectives: This course will introduce the modelling of materials through modern computational tools to analyze materials at nanoscale. It is an initiative to make students familiar with the power of first principles electronic structure theory techniques in condensed matter and materials physics.

Unit-I **(16)**

Materials Modelling through VASP and SIESTA: Basis Sets: plane waves versus numerical atomic orbitals basis sets, Pseudopotentials: ultrasoft versus norm conserving pseudopotentials. Numerical solutions of Kohn-Sham equations, Diagnolization procedure, SCF cycles and mixing scheme, Smearing: Gaussian, Fermi and Methfessel-Paxton smearing.

SIESTA and VASP package to perform: electronic structure calculations, relaxation of atomic positions and unit cell parameters. Structural properties: equilibrium lattice constant, cohesive energy, bulk modulus.

Unit-II **(14)**

DFT Calculations for Simple Solids: Crystal structure, Reciprocal lattice, Bonding in crystal, Supercells, Face centered cubic materials, Hexagonal closed packed materials, Crystal structure prediction, Phase transformations, Reciprocal space and k-points**,** Choosing k-points in Brillouin zone, Energy Cutoff, DFT total energies and its relation to various properties, Geometry optimization. Electronic density of states, local density of states and atomic charges, Magnetism.

Unit-III **(16)**

DFT Calculations for Surfaces: Periodic boundary conditions and slab model, Calculations of surface energies, Symmetric and asymmetric slab model, Surface relaxation, Surface reconstruction, Adsorbate on surface, Surface Coverage, modelling of one-dimensional systems such as nanotubes, nanoribbons and nanowires, modelling of fullerene-like cages.

DFT Calculations of Vibrational Frequencies: Lattice vibrations and phonons, Isolated Molecules, Vibrations of a collection of atoms, Molecules on surface, Zero-point energies, Phonons and delocalization modes.

Unit-IV **(14)**

Calculations beyond Standard DFT: Accuracy of DFT calculations: energy, geometry, vibrational frequencies, Crystal structures and cohesive energies, adsorption energies and bond lengths. DFT+U and DFT+D method for the treatment of electron correlation, Spin-orbit coupling, GW approximation, Excited states properties: dielectric functions and absorption spectra.

Recommended Readings:

1. David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).

2. June Gunn Lee, *Computational Materials Science: An Introduction*, (CRC Press 2011)
3. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007
4. www.vasp.at/index.php/documentation
5. http://departments.icmab.es/leem/siesta/Documentation/Manuals/manuals.html

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Course Title: Computational Modeling Lab
Paper Code: CSP.610

L	T	P	Credits	Marks
0	0	8	4	100

Following experiments will be carried out in the lab.
1. Introduction to Gaussian calculations.
2. Carrying of conformational analysis of small molecules using G09.
3. Vibrational spectra, NMR spectra and TDDFT calculations using G09.
4. Modeling chemical reactions including transition state calculations.
5. 2D potential energy suface generation for two torsion angles.
6. Pseudopotential generation and testing of Si atom.
7. Functional and basis set dependent lattice constant and bulk modulus of Fe solid.
8. Total energy versus cell size and binding energy of H_2 and H_2O molecules.
9. Density of states and electronic band structure of bulk Si.
10. To study the structural and electronic properties of graphene and its nanoribbon.
11. Building macromolecules, extracting crystal structure/NMR coordinates and generating models for MD simulations. RESP charge calculation.
12. Energy minimization during MD simulations- Steepest descent and conjugate gradient methods.
13. Gas phase MD simulations.
14. MD simulations in implicit solvent.
15. MD simulations in Explicit solvents.

References:

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/

Course Title: Introduction to Biophysics
Paper Code: CSP.601
Total Lecture: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objectives: This course will introduce the fundamental aspects of Biophysics to students.

Unit I **(15)**

Biophysics and fundamental principles of Biology: Biological structures, morphology of cells, biological membranes, cell evolution.

Physical Principles and Methods in biology: The electronic structure of atoms, Structure of molecules and molecular complexes, absorption and emission spectroscopy, infrared and Raman spectroscopy, magnetic resonances, size and shapes of biomolecules, X-ray crystal structure analysis.

Unit II: (15)

Structure and Functions of proteins and Nucleic Acids: The structure of proteins, enzymes, Recognition Proteins, Genetic system, its regulation and control, recombinant DNA

Biological Energy Conversion: Biological Energy Flow, ATP, Fermentation and glycolysis, citric acid cycle, respiration.

Unit III: (15)

Photosynthesis: Photosynthetic structures, transfer and trapping of excitation energy, electron transport in higher plants, reaction centres, carbon fixation.

Biological transport processes: Passive and active transport, osmotic equilibrium, ionic equilibrium, flow across membranes, transport mechanisms.

Unit IV: (15)

Introduction to Biophysics of nerves, contractility and sensory systems.

Theoretical biology: Physical Concepts in biology, Nonequilibrium thermodynamics, modelling, cybernetics, Generalizations in Biology.

References:

1. Biophysics- An Introduction. Christiaan Sybesma.

Course Title: Computational Fluid Dynamics
Paper Code: CSP.612
Total Lecture: 60

L	T	P	Credits	Marks
4	0	0	4	100

Course Objectives: This course will introduce the fundamental aspects of Computational Fluid to students.

Unit I (15)

The basic equations of Fluid Dynamics: Vector analysis, The total derivative and the transport theorem, conservation of mass, momentum and energy, Bernoulli's theorem, Kelvin's circulation theorem and potential flow, Euler equations, convention-diffusion equation, conditions for incompressible flow, turbulence, stratified flow and free convection, moving frame of reference, shallow water equations.

Unit II (15)

Finite volume and finite difference discretization on nonuniform grids: Elliptic equation, vertex centered discretization, cell-centered discretization, upwind discretization, nonuniform grids in one dimension.

The stationary convection-diffusion equation: Finite volume discretization, numerical experiments, schemes of positive type, upwind discretization, defect correction.

Unit III: (15)

The nonstationary convection-diffusion equation: Examples of instability, stability definitions, discrete maximum principle, derivation of von Neumann stability conditions. The Incompressible Navier-Stokes equations.

Unit IV: (15)

Discretization in General Domains: Introduction, types og grids, boundary fitted grids, geometric properties of grid cells, Introduction to tensor analysis.

The Euler Equations in one space dimension: Analytic aspects, Osher scheme, Flux splitting scheme, Jameson-Schmidt-Turkel scheme, Higher order schemes.

References:

1. Principles of Computational Fluid Dynamics. Pieter Wesseling, Springer-Verlag Berlin Heidelberg, 2001, softcover printing 2009.