Central University of Punjab, Bathinda

Ph.D. in Bioinformatics/
Ph.D. in Computational Chemistry/
Ph.D. in Computational Physics

Session 2020

Department of Computational Sciences

Programme Outcomes:

- On successful completion of the Ph.D. programme, the students will able to:
- Design independent research problems in the field of Theoretical / Computational Sciences
- Explore real-life problems with the help of computational tools
- Pursue research in this multidisciplinary area of science

SEMESTER I							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCS.701	Research Methodology	CC	2	0	0	2
2	CCS.751	Research and Publication Ethics	CC	2	0	0	2
Opt any two of the following courses:							
3	CCS.704	Computational Chemistry	DE	4	0	0	4
4	CCS.705	Sequence and Structural Bioinformatics	DE	4	0	0	4
5	CCS.706	Statistical Mechanics	DE	4	0	0	4
6	CCS.707	Mathematics for Computational Sciences	DE	4	0	0	4
7	CCS.708	Scientific Programming	DE	4	0	0	4
8	CCS.709	Scientific Programming Lab (Practical)	SBE	0	0	8	4
9	CCS.710	Solid State Physics	DE	4	0	0	4
10	CCS.711	Computational Solid State Physics Laboratory	SBE	0	0	8	4
11	CCS.712	Computational Methods	DE	4	0	0	4
12	CCS.713	Computational Methods Lab	SBE	0	0	8	4
13	CCS.714	Introduction to Quantum Dynamics	DE	4	0	0	4
14	CCS.715	Molecular Dynamics	DE	4	0	0	4
15	CCS.716	Molecular Dynamics Lab	SBE	0	0	8	4
16	CCS.717	Atomic and Molecular Spectroscopy	DE	4	0	0	4
17	CCS.718	Biomolecular Structure Modelling and Drug Design	DE	4	0	0	4
	Total			**12 Credits**			

Mode of Transaction

Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning.

Evaluation Criteria

As per UGC guidelines on adoption of CBCS. CC: Core Course, DE: Discipline Elective, SBE: Skill Based Elective

SEMESTER- I

Course Title: Research Methodology
Paper Code: CCS.701
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:

- prepare a research plan, reading and gain knowledge from scientific papers
- develop skills for scientific writing, research proposal writing, ethics, plagiarism, and lab safety issues

Unit 1 **15 Hours**

General principles of research: Meaning and importance of research, critical thinking, formulating hypothesis and development of research plan, review of literature, interpretation of results and discussion.

Unit 2 **15 Hours**

Technical writing: Scientific writing that includes the way of writing Synopsis, research paper, poster preparation and presentation, and dissertation.

Unit 3 **15 Hours**

Library: Classification systems, e-Library, web-based literature search engines

Unit 4 **15 Hours**

Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, characteristics of entrepreneurs, developing entrepreneurial competencies, types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship) employment, self-employment and entrepreneurship, financial management-importance and techniques, financial statements- importance and its interpretation, and Intellectual Property Rights (IPRs).

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

Recommended Readings

1. Kothari, C. R. (2014). Research methodology (s). New Age International (p) Limited. New Delhi.

2. Sahay, Vinaya and Pradumna Singh (2009). Encyclopedia of Research Methodology in life sciences. Anmol Publications. New delhi
3. Kauda J. (2012). Research Methodology: A Project Guide for University Students. Samfunds literature Publications.
4. Dharmapalan B. (2012). Scientific Research Methodology. Narosa Publishing House ISBN: 978-81-8487-180-7.

Course Title: Research and Publication Ethics
Paper Code: CCS.751
Total Lectures: 30

L	T	P	Cr
2	0	0	2

Learning Outcomes: After completion of this course, students will be able to:

- gain a deep knowledge about research misconduct and predatory publications
- learn indexing and citation databases, open access publications, research metrics
- execute various plagiarism tools for plagiarism check

Unit 1 **5 Hours**

Philosophy and Ethics

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

Unit 2 **5 Hours**

Scientific Conduct

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagisrism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of database

Unit 3 **5 Hours**

Publication Ethics

1. Publication ethics: definition, introduction and importance
2. Best practices/standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest

4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct complaints and appeals
7. Predatory publishers and journals

Practice:

Unit 4 **5 Hours**

Open Access Publishing

1. Open access publication and initiatives
2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester etc.

Unit 5 **5 Hours**

Publication Misconduct:

A. Group Discussion:

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software Tools:

Use of plagiarism software like Turnitin, Urkund and other open source software tools

Unit 6 **5 Hours**

Databases and Research Metrics

A. Databases

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g-index, i10 index, altmetrics

Transactional Modes: Class room teaching. guest lecture, group discussion, and practical sessions.

Suggested Readings

1. Lillie, W. (1967). An Introduction to Ethics. Allied Publishers Pvt. Ltd.; 1 edition.
2. MacKenzie, J.S. (2005). A Manual of Ethics. Cosimo Classics.
3. Committee on Publication Ethics (COPE). How to handle authorship disputes: a guide for new researchers. 2003. Available at: publicationethics.org/files/2003pdf12.pdf. Accessed on June 17, 2017.
4. Elsevier. Publishing Ethics Resource Kit (PERK). Available at: elsevier.com/editors/perk/plagiarism-complaints. Accessed on June 17, 2017.

L	T	P	Cr
4	0	0	4

Course Title: Computational Chemistry

Paper Code: CCS.704

Total Lectures: 60

Course Objectives and Learning Outcomes: The objective of this subject is to ensure that a student learns basis of computational chemistry to ensure that they understand the intricacies of applying computational chemistry methods in their research work.

Unit 1 **15 Hours**

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important 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.

Unit 2 **15 Hours**

Many Electron atoms: Angular momentum, eigenvalues of angular momentum operator, Particle in a Ring, Hydrogen Atom. Electron correlation, addition of angular momentum, Clebesch-Gordan series, total angular momentum and spin-orbit interaction.

Unit 3 **15 Hours**

Ab Initio Methods: Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, selection of basis sets.

Electron Correlation and Basis Sets: Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster, Basis sets.

Unit 4 **15 Hours**

DFT and Force Field methods: Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

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, Oxford University Press, 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.

Course Title: Sequence and Structural Bioinformatics
Paper Code: CCS.705
Total Lectures: 60

L	T	P	Cr
4	0	0	4

Course Objectives and Learning Outcomes: The objective of this subject is to ensure that a student learns advanced concepts in Bioinformatics.

Unit 1 **15 Hours**

Biological data Types of biological data (various omics)
Biological Databases Nucleic acid and protein sequence and protein structure databases Overview of available Bioinformatics resources on the web

Unit-2 **15 Hours**

DNA sequence analysis

Sequence annotation and sequence analysis - Phylogeny of gene (blast, fasta, HMMer) and residue conservation. Primer design and Tm Calculation, DNA Restriction pattern analysis.Condon bias and its effect on the protein expression with reference to various expression system.

Unit 3 **15 Hours**

Bioinfo tools

Protein sequence and structure insights (PSSI) X-ray, NMR, Comparative modeling, ab initio, threading methods. Structure refining techniques Energy minimization approaches (Steepest descent, Conjugate gradient etc), Basis of Molecular dynamics simulations and its application.

Unit 4 **15 Hours**

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.

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

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. A.D. Baxevanis *et. al.*, Current Protocols in Bioinformatics, (2005) Wiley Publishers
3. David W.Mount Bioinformatics (2001) Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
4. Computational Molecular Biology by P. A. Pevzner, Prentice Hall of India Ltd, (2004) ISBN81-203-2550-8
5. D.E.Krane and M.L.Raymer Fundamental concepts of Bioinformatics (2003) Pearson Education ISBN 81-297-0044-1
6. N.Gautham Bioinformatics Narosa publications. (2006) ISBN-13: 9781842653005
7. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
8. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
9. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Course Title: Statistical Mechanics
Paper Code: CCS.707
Total Hours: 60

L	T	P	Cr
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.

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 Title: Mathematics for Computational Sciences

Paper Code: CCS.708

Total Lectures: 60

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

1. identify and describe the basic mathematical techniques that are commonly used by chemist.
2. develop skills in vectors, matrices, differential calculus, integral calculus and probability.
3. apply the principles to a number of simple problems that have analytical solutions.
4. design different methods to problems related to chemistry.

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

L	T	P	Cr
4	0	0	4

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: **14 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,

L	T	P	Cr
4	0	0	4

Unit IV: **16 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. E. Kreyszig, *Advanced Engineering Mathematics* (Wiley India Pvt. Ltd., New Delhi, India) 2011.
2. L. A. Pipes, *Applied Mathematics for Engineers and Physicist* (McGraw-Hill, Noida, India) 1985.
3. D. G. Zill, *Advanced Engineering Mathematics* (Jones & Barlett Learning, Massachusetts, USA) 2012.
4. P. K. Chattopadhyay, *Mathematical Physics* (New Age International (P) Ltd., New Delhi) 2000
5. The chemistry Mathematics Book, E.Steiner, Oxford University Press (2008).
6. Mathematical for Physical Chemistry : F. Daniels, Mc. Graw Hill (1959).
7. Chemical Mathematics D.M. Hirst, Longman (1979).
8. Basic Mathematics for Chemists, Tebbutt, Wiley (1994).
9. G. Arfken, H. Weber and F. Harris, *Mathematical Methods for Physicists* (Elsevier Academic Press, Massachusetts, USA) 2012.

Course Title: Scientific Programming
Paper Code: CCS.708
Total Hours: 60

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

- identify and describe the basic art of scientific programming related to Fortran 95/2003.

- demonstrate concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
- develop skills to write programs related to standard problems and as well as to chemistry.

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 attays 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 paralle 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 Wngineers, 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).

Course Title: Scientific Programming Lab (Practical)
Paper Code: CCS.709
Total Hours: 120

L	T	P	Cr
0	0	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 and C 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

Unit I **15 Hours**

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.

Unit II **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 attays in procedures, derived data types.

Unit III **15 Hours**

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.

Unit IV **15 Hours**

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

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

Suggested Readings:

1. Chapman, Fortran 95/2003 for Scientists and Wngineers, 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.

L	T	P	Cr
4	0	0	4

Course Title: Solid State Physics

Paper Code: CCS.710

Total Lecture: 60

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.

Unit I **18 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 **14 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 **14 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. Srivatava, *Crystallography Applied to Solid state physics* (New Age International), 2012

Course Title: Computational Solid State Physics Laboratory

L	T	P	Cr
4	0	0	4

Paper Code: CCS.711

Total Hours: 120

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

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:

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

Delhi, India) 2014.

Course Title: Computational Methods
Paper Code: CCS.712
Total Hours: 60

L	T	P	Cr
4	0	0	4

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

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

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

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.

L	T	P	Cr
0	0	8	4

Course Title: Computational Methods lab

Paper Code: CCS.713

Total Hours: 120

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.

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).

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

L	T	P	Cr
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

Unit I **12 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 **11 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 **11 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 **11 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: Molecular Dynamics
Paper Code: CCS.715
Total Lecture: 60

L	T	P	Cr
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.

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.

Course Title: Molecular Dynamics Lab (Practical)
Paper Code: CCS.716
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:

- 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

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 Title: Atomic and Molecular Spectroscopy
Paper Code: CCS.717
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:

- 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

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 (CO_2), 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 Title: Biomolecular Structure Modeling and Drug Design

L	T	P	Cr
4	0	0	4

Paper Code: CCS.718
Total Lectures: 60

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

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

Unit 1 **15 Hours**

Introduction to Molecular Geometry, Coordinate Space for Optimization of Algorithm of Molecular Geometry, Z-Matrix, Molecular Vibrations, Electrostatic Charges, Electrostatic Charges, Multipole Moments,

Unit 2 **15 Hours**

Modelling and structure: From protein sequence to structure, theoretical and practical aspects of protein sequence alignments, secondary, tertiary structure prediction, comparative modeling, Docking, protein-protein and protein-ligand docking.

Unit 3 **15 Hours**

Computational drug designing: Structure-based drug design, virtual screening, quantitative structure activity relations, Cheminformatics, Historical Perspective and Viewpoint of Pharmacophore, Functional Groups Considered as Pharmacophores, Ehrlich's "Magic Bullet", Fischer's "Lock and Key", Two-dimensional Pharmacophores, Three-dimensional Approach of Pharmacophores, Criteria for Pharmacophore Model,

Unit 4 **15 Hours**

Pharmacophore Model Generation Software Tools, Molecular Alignments, Handling Flexibility, Alignment Techniques, Scoring and Optimization, Pharmacophores, Validation and Usage, Automated Pharmacophore Generation Methods, GRID-based Pharmacophore Models, Pharmacophores for Hit Identification, Pharmacophores for Human ADME/Tox-related Proteins.

Transactional Modes: Lecture; Tutorial; 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
3. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
4. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
5. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.
6. Molecular and Structural Database, Protein Data Bank, Bioactivity Databases, Gene and Protein Sequence Databases,Cambridge Crystallographic Database, Compound Storage and Management.