Central University of Punjab

Ph.D. in Theoretical and Computational Chemistry

Session 2021--

Department of Computational Sciences

School of Basic Sciences

Programme Outcome

The above mentioned programmes will enrich students with the fundamental knowledge of theoretical/computational sciences in the field of basic as well as applied research. On successful completion of the Ph.D. programme the students will able to:

1. Design independent research problems in the field of Theoretical / Computational Sciences

2. Examine real-life problems with the help of computational tools

3. Execute research in this new spectrum of multidisciplinary area of science at the national and international platform.

4. Construct themselves as an Industrious research personnel

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.703	Review Writing and Presentation	CC	2	0	0	2
3	CCS.751	Research and Publication Ethics		2	0	0	2
4	CCS.752	Teaching Assistantship		0	0	2	1
5	UNI.753	Curriculum, Pedagogy and Evaluation		1	0	0	1
Opt any two of the following courses:							
4	CCS.704	Electronic Structure Theory	DE	3	0	0	3
5	CCS.706	Statistical Mechanics	DE	3	0	0	3

6	CCS.708	Scientific Programming	DE	3	0	0	3
7	CCS.709	Scientific Programming Lab (Practical)	SBE	0	0	6	3
8	CCS.712	Computational Methods	DE	3	0	0	3
9	CCS.713	Computational Methods Lab (Practical)	SBE	0	0	6	3
10	CCS.714	Introduction to Quantum Dynamics	DE	3	0	0	3
11	CCS.715	Molecular Dynamics	DE	3	0	0	3
12	CCS.716	Molecular Dynamics Lab (Practical)	SBE	0	0	6	3
	Total			14 Credits			

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

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: 30

L	T	P	Cr
2	0	0	2

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 I **5 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 II **10 Hours**
Technical writing: Scientific writing that includes the way of writing

Synopsis, research paper, poster preparation and presentation, and dissertation.

Unit III **5 Hours**
Library: Classification systems, e-Library, web-based literature search engines

Unit IV **10 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.

Suggested 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: Review Writing and Presentation
Paper Code: CCS.703
Total Lectures: 60

L	T	P	Cr
0	0	4	2

Course Objectives and Learning Outcomes: The objective of this course would be to ensure that the student learns the aspects of the Review writing and seminar presentation. Herein the student shall have to write a 5000 words review of existing scientific literature with simultaneous identification of knowledge gaps that can be addressed through future work.

The evaluation criteria for “Review Writing and Presentaion” shall be as follows:

Maximum Marks: 100

S.No.	Criteria	Marks
1.	Review of literature	25
2.	Identification of gaps in knowledge	15
3.	References	10
4.	Content of presentation	15
5.	Presentation Skills	20

6.	Handling of queries	15
	Total	100

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

Course Code: CCS.751

Course Title: Research and Publication Ethics

L	T	P	Credits
2	0	0	2

Total Hours: 30

Unit I Philosophy and Ethics **3 hours**

- Introduction to Philosophy : definition, nature and scope, content, branches
- Ethics : definition, moral philosophy, nature of moral judgements and reactions

Unit II Scientific Conduct **5 hours**

- Ethics with respect to science and research
- Intellectual honesty and research integrity
- Scientific misconducts : Falsification, Fabrication, and Plagiarism (FFP)
- Redundant publications : duplicate and overlapping publications, salami slicing
- Selective reporting and misrepresentation of data

Unit III: Publication Ethics **7 hours**

- Publication ethics : definition, introduction and importance
- Best practices/ standards setting initiatives and guidelines: COPE, WAME, etc.
- Conflicts of interest
- Publication misconduct : definition, concept, problems that lead to unethical behaviour and vice versa, types
- Violation of publication ethics, authorship and contributor ship
- Identification of publication misconduct, complaints and appeals
- Predatory publishers and journals

Unit IV Open Access publishing **4 hours**

- Open access publications and initiatives

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

Unit V Publication Misconduct **4 hours**

- Group Discussions: Subject specific ethical issues, FFP, authorship; conflicts of interest; complaints and appeals: examples and fraud from India and abroad
- Software tools: Use of plagiarism software like Turnitin, Urkund and other open source software tools

Unit IV Databases and Research Metrics **7 hours**

- Databases: Indexing databases; Citation database: Web of Science, Scopus etc.
- Research Metrics: Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics : h-index, g-index, i10 index, almetrics

Course Code: CCS.752

Course Title: TEACHING ASSISTANTSHIP

L	T	P	Credit
0	0	2	1

Total Hours: 30

Learning Outcome:

At the end of this skill development course, the scholars shall be able to

1. familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system
2. manage large and small classes using appropriate pedagogical techniques for different types of content

Activities and Evaluation:

- The scholars shall attend Master degree classes of his/her supervisor to observe the various transaction modes that the supervisor follows in the class room delivery or transaction process one period per week.

- The scholars shall be assigned one period per week under the direct supervision of his/her supervisor to teach the Master degree students adopting appropriate teaching strategy(s).
- The scholars shall be involved in examination and evaluation system of the Master degree students such as preparation of questions, conduct of examination and preparation of results under the direction of the supervisor.
- At the end of the semester, the supervisor shall conduct an examination of teaching skills learned by the scholar as per the following evaluation criteria:
- The scholars shall be given a topic relevant to the Master degree course of the current semester as his/her specialization to prepare lessons and deliver in the class room before the master degree students for one hour (45 minutes teaching + 15 minutes interaction).
- The scholars shall be evaluated for a total of 50 marks comprising content knowledge (10 marks), explanation and demonstration skills (10 marks), communication skills (10 marks), teaching techniques employed (10 marks), and classroom interactions (10).

Course Code: UNI.753

Course Title: CURRICULUM, PEDAGOGY AND EVALUATION

L	T	P	Credit
1	0	0	1

Learning outcomes: **Total Hours: 15**

After completion of the course, scholars shall be able to:

- analyze the principles and bases of curriculum design and development
- examine the processes involved in curriculum development
- develop the skills of adopting innovative pedagogies and conducting students' assessment
- develop curriculum of a specific course/programme

Course Content

Unit I Bases and Principles of Curriculum **4 hours**

1. Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development.

2. Types of Curriculum Designs- Subject centered, learner centered, experience centered and core curriculum. Designing local, national, regional and global specific curriculum. Choice Based Credit System and its implementation.

Unit II Curriculum Development **4 hours**

1. Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process.
2. Comparison among Interdisciplinary, multidisciplinary and trans-disciplinary approaches to curriculum.

Unit III Curriculum and Pedagogy **3 hours**

1. Conceptual understanding of Pedagogy.
2. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning
3. Three e- techniques: Moodle, Edmodo, Google classroom

Unit IV Learners' Assessment **4 hours**

1. Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions.
2. Conducting Assessment: Modes of conducting assessment – offline and online; use of ICT in conducting assessments.
3. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria.

Transaction Mode

Lecture, dialogue, peer group discussion, workshop

Evaluation criteria

There shall be an end term evaluation of the course for 50 marks for duration of 2 hours. The course coordinator shall conduct the evaluation.

Suggested Readings

- Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). Curriculum Planning and Development. Boston: Allyn & Bacon.
- Brady, L. (1995). Curriculum Development. Prentice Hall: Delhi. National Council of Educational Research and Training.
- Deng, Z. (2007). Knowing the subject matter of science curriculum, Journal of Curriculum Studies, 39(5), 503-535. https://doi.org/10.1080/00220270701305362
- Gronlund, N. E. & Linn, R. L. (2003). Measurement and Assessment in teaching.
- Singapore: Pearson Education

- McNeil, J. D. (1990). Curriculum: A Comprehensive Introduction, London: Scott,
- Foreman/Little
- Nehru, R. S. S. (2015). Principles of Curriculum. New Delhi: APH Publishing Corporation.
- Oliva, P. F. (2001). Developing the curriculum (Fifth Ed.). New York, NY: Longman
- Stein, J. and Graham, C. (2014). Essentials for Blended Learning: A Standards-Based Guide. New York, NY: Routledge.

Web Resources

- https://www.westernsydney.edu.au/__data/assets/pdf_file/0004/467095/Fundamentals_of_Blended_Learning.pdf
- https://www.uhd.edu/academics/university-college/centers-offices/teaching-learningexcellence/Pages/Principles-of-a-Flipped-Classroom.aspx
- http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621-Article-The-BasicPrinciples-of-Dialogue-by-Renate-van-der-Veen-and-Olga-Plokhooij.pdf

Course Title: Electronic Structure Theory
Paper Code: CCS.704
Total Lectures: 45

L	T	P	Cr
3	0	0	3

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 I **10 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 II **10 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 III **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 IV **10 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. F. Jensen, (2006). Introduction to Computational Chemistry, Wiley-Blackwell .
2. P. W. Atkins and R. S. Friedman, (1997). Molecular Quantum Mechanics, Oxford University Press, Oxford .
3. H. Eyring, J. Walter and G.E. Kimball, (1944) Quantum Chemistry, John Wiley, New York.
4. I.N. Levine, (2000), Quantum Chemistry, Pearson Educ., Inc., New Delhi.
5. A. Szabo and N. S. Ostlund, (1982), Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, Dover, New York.

Course Title: Statistical Mechanics
Paper Code: CCS.706
Total Hours: 45

L	T	P	Cr
3	0	0	3

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

- apply the classical laws of thermodynamics and their application, mathematical review of classical mechanics
- learn the postulates of statistical mechanics, Liouville's Theorem, and statistical interpretation of thermodynamics
- identify the microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function, elementary probability theory, distributions and fluctuations
- learn the methods of statistical mechanics and their use to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases

After, completion of this course will help the students to apply the principles and techniques from statistical mechanics to a range of modern day research based problems.

Unit I **15 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 **10 Hours**
Elementary Probability Theory
Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem
Distributions & Fluctuations: Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable

Unit III **10 Hours**
Basic Thermodynamics: Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function

Unit IV **10 Hours**
Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas.
Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

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

Suggested Readings

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

Course Title: Scientific Programming

L	T	P	Cr
3	0	0	3

Paper Code: CCS.708
Total Hours: 45

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 **10 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 **10 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 **10 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, (2006) Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York .
2. V. Rajaraman, (1997) Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi .
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996) Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press .
4. M J Quinn (2003) Parallel Programming in C with MPI and OpenMP.
5. IAnanth Grama, George Karypis, Vipin Kumar, and Anshul Gupta (2003) ntroduction to Parallel Computing.

Course Title: Scientific Programming Lab (Practical)

L	T	P	Cr
0	0	6	3

Paper Code: CCS.709
Total Hours: 90

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 **30 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 **20 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 **20 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 **20 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, (2006) Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York .
2. V. Rajaraman, (1997) Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi .
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, (1996) Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press .

4. M J Quinn (2003) Parallel Programming in C with MPI and OpenMP.
5. Ananth Grama, George Karypis, Vipin Kumar, and Anshul Gupta (2003) ntroduction to Parallel Computing.

Course Title: Computational Methods
Paper Code: CCS.712
Total Hours: 45

L	T	P	Cr
3	0	0	3

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 **10 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 **10 Hours**
Matrix and Determinants:
Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

Unit III **15 Hours**
Interpolations:
Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms
Numerical differentiation and integration:
Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor's series, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration.
Curve Fit:

least square, straight line and polynomial fits.

Unit IV **10 Hours**

Numerical Solution of Differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

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

Suggested Readings

1. V. Rajaraman, (1993) Computer Oriented Numerical Methods, PHI.
2. E. Balaguruswamy, (2017) Numerical Methods, Tata McGraw Hill.
3. F.Acton, (1997) Numerical Methods that Work, Harper and Row.
4. S. D. Conte and C.D.Boor, (2005) Elementary Numerical Analysis, McGraw Hill.
5. S. S. Shastri, (2012) Introductory Methods of Numerical Analysis, PHI.

Course Title: Computational Methods Lab (Practical)
Paper Code: CCS.713
Total Hours: 90

L	T	P	Cr
0	0	6	3

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

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

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

Course Content

To write and execute computer programs in Fortran/Python language for the following problems:

1. Solution of transcendental or polynomial equations by the Newton Raphson method.
2. Matrix summation, subtraction and multiplication.
3. Matrix inversion using Gauss-Jordan's Matrix-Inversion Method.
4. Solution of Simultaneous Linear Equations: Gaussian Elimination, Gauss Seidel Iteration Method.
5. Finding Eigen values and Eigenvectors.

6. Newton/Lagrange interpolation based on given input data.
7. Numerical first order differentiation of a given function.
8. Numerical integration using Trapezoidal, Simpson's 1/3, Gaussian Quadrature methods.
9. Solution of first order differential equations using the Rung-Kutta method,
10. Monte Carlo integration.

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

Suggested Readings

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

Course Title: Introduction to Quantum Dynamics
Paper Code: CCS.714
Total Lecture: 45

L	T	P	Cr
3	0	0	3

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 **10 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 **10 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 **10 Hours**

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

Unit IV **15 Hours**

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

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

Suggested Readings

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

Course Title: Molecular Dynamics
Paper Code: CCS.715
Total Lecture: 45

L	T	P	Cr
3	0	0	3

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

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

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

Unit I **10 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 **10 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 **10 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. M.P. Allen and D.J. Tildesley, (2017) Computer Simulation of Liquids 2nd Edition, Oxford University Press.
2. D. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.
3. A. R. Leach, (2001) Molecular Modelling Principles and Applications 2nd Edition. Pearson.
4. S. Alavi, (2020) Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.

Course Title: Molecular Dynamics Lab (Practical)
Paper Code: CCS.716
Total Hours: 90

L	T	P	Cr
0	0	6	3

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. M.P. Allen and D.J. Tildesley, (2017) Computer Simulation of Liquids 2nd Edition, Oxford University Press.
2. D. Frenkel and B. Smit, (2001) Understanding Molecular Simulation 2nd Edition, Academic Press.
3. A. R. Leach, (2001) Molecular Modelling Principles and Applications 2nd Edition. Pearson.
4. S. Alavi, (2020) Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.