Central University of Punjab

Ph.D. in Theoretical and Computational Chemistry

Session 2025

Department of Computational Sciences
School of Basic Sciences

Graduate Attributes

Students graduating from the Ph.D. in Theoretical and Computational Chemistry will contribute to the teaching and research needs in Theoretical and Computational Chemistry in academia, industry and research institutions at local, regional, national and international levels. They will be part of the scientific workforce that will transform material and catalysis, pharmaceutical, and scientific software sectors employing higher order thinking skills and capabilities. On successful completion of this programme the students will able to:

- Design independent research problems and choose suitable methodologies in Theoretical and Computational Chemistry
- Examine real-life chemistry problems with the help of computational tools
- Execute research in this new spectrum of multidisciplinary area of science at the national and international platform
- Construct themselves as an Industrious research personnel
- Continue life-long learning as an autonomous learner and apply and nurture critical and creative thinking.

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
3	CCS.703	Review Writing and Presentation	CC	0	0	4	2
4	UNI.753	Curriculum, Pedagogy and Evaluation	CC	1	0	0	1
5	CCS.752	Teaching Assistantship	CC	0	0	2	1
Opt any two of the following courses:							
4	CCS.704	Electronic Structure Theory	DE	3	0	0	3
5	CCS.725	Structural Bioinformatics	DE	3	0	0	3
6	CCS.724	Protein Engineering and Design	DE	3	0	0	3
7	CCS.706	Advanced Statistical Mechanics	DE	3	0	0	3
8	CCS.708	Scientific Programming	DE	3	0	0	3
9	CCS.709	Scientific Programming Lab (Practical)	SBE	0	0	6	3
10	CCS.712	Numerical Methods	DE	3	0	0	3
11	CCS.713	Numerical Methods Lab (Practical)	SBE	0	0	6	3
12	CCS.714	Introduction to Quantum Dynamics	DE	3	0	0	3
13	CCS.715	Molecular Dynamics	DE	3	0	0	3
14	CCS.716	Molecular Dynamics Lab (Practical)	SBE	0	0	6	3
15	CCS.717	Advanced Biomolecular Modeling	DE	3	0	0	3
	Total			14 Credits			

Mode of Transaction
Lecture, Laboratory-based practical, seminar, group discussion, team teaching, self-learning, and online tools.

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

SEMESTER I

Course Title: Research Methodology Course

L	T	P	Cr
2	0	0	2

Code: CCS.701
Course Type: CC Total
Hours: 30

Course Learning Outcomes (CLO):

On completion of this course, students will be able to:

CLO1: Perform Literature survey, critically analyse the scientific problem and develop a research plan
CLO 2: Write a good to technical report, manuscripts and scientific proposals CLO 3: Use reference management systems and perform literature reviews using online resources
CLO4: Describe the importance of IPR and develops interest in entrepreneurship

Units/ Hours	**Contents**	**Mapping with CLO**
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. **Learning Activities**: Perform literature survey, Research paper presentation, Peer discussion,	CLO1
II 10 Hours	**Technical writing:** Scientific writing that includes the way of writing Synopsis, research paper, poster preparation and presentation, and dissertation. **Learning Activities**: Writing and Evaluation of research proposals, technical presentation, group discussion	CLO2
III 5 Hours	**Library:** Classification systems, e-Library, web-based literature search engines **Learning Activities**: Perform literature survey, Peer discussion, brain storming	CLO3
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	CLO4

	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). **Learning Activities**: Concept built with real examples, case studies, Student presentation and group discission.	

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.
5. Gould, J. R. (2020). Directions in Technical Writing and Communication. Routledge.
6. Denisova-Schmidt, E. (2021). Book Review: A Roadmap to the Future of Academic Integrity Research. Academy of Management Learning & Education.

Course Title: Research and Publication Ethics

L	T	P	Cr
2	0	0	2

Course Code:
CCS.702 Course
Type: CC Total
Hours: 30

Course Learning Outcomes (CLO):

On completion of this course, students will be able to:

CLO1: Describe the ethics of research.
CLO2: Outline the good practices to be followed in research and publication.
CLO3: Describe various aspects of Publication ethics
CLO4: Appreciate the importance of Open access publication
CLO5: Identify the misconduct, fraud and plagiarism in research.
CLO6: Utilize various online resources and software to analyse their research output.

Units/ Hours	Contents	Mapping with CLO
I 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 **Learning Activities**: Case studies, Student presentation and group discission.	CLO1
II 5 Hours	**Scientific Conduct** 1. Ethics with respect to science and research 2. Intellectual honesty and research integrity 3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP) 4. Redundant publications: duplicate and overlapping publications, salami slicing 5. Selective reporting and misrepresentation of database **Learning Activities**: Case studies, Problem based learning, Student presentation and group discission.	CLO2
III 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	CLO3

	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 **Learning Activities**: Case studies, Problem based learning, Student presentation and group discission	
IV 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. **Learning Activities**: Case studies, Problem based learning, Student presentation and group discission.	CLO4
V 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 **Learning Activities**: Case studies, Problem based learning, Student presentation and group discission.	CLO5
VI 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 **Learning Activities**: Concept mapping, Problem based learning, Student presentation and group discission.	CLO6

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). (2017) Available at: elsevier.com/editors/perk/plagiarism-complaints.

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 Presentation" 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 Title: CURRICULUM, PEDAGOGY AND EVALUATION
Course Code: **UNI.753**
Course Type: CC Total
Hours: 15

L	T	P	Cr
1	0	0	1

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Analyze the principles and bases of curriculum design and development
CLO2: Examine the processes involved in curriculum development
CLO3: Develop the skills of adopting innovative pedagogies and conducting students' assessment
CLO4: Develop curriculum of a specific course/programme

Units/ Hours	Contents	Mapping with CLO
I 4 Hours	**Bases and Principles of Curriculum** • Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development. • 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.	CLO1
II 4 Hours	**Curriculum Development** Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process. Comparison among Interdisciplinary, multidisciplinary and trans-disciplinary approaches to curriculum.	CLO2
III 3 Hours	**Curriculum and Pedagogy** Conceptual understanding of Pedagogy. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning. Three e- techniques: Moodle, Edmodo, Google Classroom	CLO3
	Learners' Assessment Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective	

IV 4 Hours	questions. Conducting Assessment: Modes of conducting assessment – offline and online; use of ICT in conducting assessments. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria.	CLO4

Course Content

Transaction Mode

Lecture, dialogue, peer group discussion, workshop

Evaluation criteria

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

Suggested Readings

1. Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). *Curriculum Planning and Development*. Boston: Allyn & Bacon.
2. Brady, L. (1995). *Curriculum Development*. Prentice Hall: Delhi. National Council of Educational Research and Training.
3. Deng, Z. (2007). Knowing the subject matter of science curriculum, *Journal of Curriculum Studies*, 39(5), 503-535. https://doi.org/10.1080/00220270701305362
4. Gronlund, N. E. & Linn, R. L. (2003). *Measurement and Assessment in teaching*. Singapore: Pearson Education
5. McNeil, J. D. (1990). *Curriculum: A Comprehensive Introduction*, London: Scott, Foreman/Little
6. Nehru, R. S. S. (2015). *Principles of Curriculum*. New Delhi: APH Publishing Corporation.
7. Oliva, P. F. (2001). *Developing the curriculum* (Fifth Ed.). New York, NY: Longman
8. 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-learning-excellence/Pages/Principles-of-a-Flipped-Classroom.aspx
- http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621- Article-The-Basic-Principles-of-Dialogue-by-Renate-van-der-Veen-and- Olga-Plokhooij.pdf

Course Title: TEACHING ASSISTANTSHIP
Course Code: CCS.752
Course Type: CC Total
Hours: 30

L	T	P	Cr
1	0	0	1

Course Learning Outcomes:

On completion of this course, students will be able to:

CLO1: Familiarize themselves with the pedagogical practices of effective classroom delivery and knowledge evaluation system

CLO2: Manage large and small classes using appropriate pedagogical techniques for different types of content

Activities and Evaluation:

- The scholars shall attend master's 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's degree students adopting appropriate teaching strategy(s).
- The scholars shall be involved in the examination and evaluation system of the master's 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's 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 Title: Electronic Structure Theory Paper
Code: CCS.704
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of this course, students will be able to
CLO1: identify and define basic terms and concepts which are needed for this specialized course.
CLO2: describe the HF SCF method.
CLO3: select the basis sets.
CLO4: compare post-HF methods.
CLO5: develop how to apply quantum chemistry to study chemical and biochemical problems.

Units/ Hours	Contents	Mapping with CLO
I 13 Hours	Review of molecular structure calculations and Hückel Molecular Orbital Theory, Hartree products and Hartree-Fock Approximation. One and Two-Electron Integrals, General Rules, Coulomb and Exchange Integrals, **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 Hours	Second-Quantized Operators and Matrix Elements. The Fock Operator, HF Equations, Roothaan Equations, SCF Procedure. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
III 10 hours	Polyatomic Basis sets, Minimal, Double zeta, triple zeta and Polarized basis sets. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO3
IV 11 Hours	Configuration Interaction, Multi-Configuration Self-Consistent Field, Multireference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4 CLO5

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

Suggested Readings

1. F. Jensen, (2006) Introduction to Computational Chemistry, Wiley- Blackwell.
2. P. W. Atkins and R. S. Friedman, (1997) Molecular Quantum Mechanics, OUP, Oxford.
3. H. Eyring, J. Walter and G.E. Kimball, (1944) Quantum Chemistry, John Wiley, New York (1944).
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 (1982).

Course Title: Structural Bioinformatics
Course Code: CCS.725
Course type: CF
Total Hours: 45

L	T	P	Cr
2	0	2	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:

CLO1: Describe the macromolecular structures and the experimental methods to determine it
CLO2: Apply various structure analysis tools to assign protein fold, biological function and analyse the intramolecular interactions.
CLO3: Predict the protein tertiary structures from its amino acid sequence.
CLO4: Identify the membrane bound regions, stabilizing interactions and biological function using computational tools
CLO5: Analyse various forces, which stabilize macromolecular structure and biological assembles.
CLO6: Describe the role of structural genomics in explaining life process and drug discovery

Units/ Hours	Contents	Mapping with CLO
I 12 Hours	**Macromolecular Structures** Introduction to biological macromolecules, Structural organization of proteins, Forces Stabilizing Proteins, Structure determination methods - X-ray crystallography, NMR, Cryo-electron microscopy, small angle X-ray scattering and Neutron scattering. Introduction to PDB Data-file formats, visualizing Structures, reading coordinate files, potential challenges. Structure validation- Ramachandran plot. Software for quality check. **Learning Activities**: Peer discussion, visualization and analysing of protein structures, training on various structural databases and validation, Visit and demonstration of X-ray, NMR and EM facilities.	CLO1
II 10 Hours	**Structure comparison and alignment** Impact of protein structure comparison and alignment, sequence-structure relationship, general approaches, statistical analysis Structure comparison, multiple structure alignment, software/tools for structure comparison and alignment **Structure-function relationship** Secondary structure assignment methods, Structural classification of proteins, Structural domains, Relationship between structure and function, assigning function from structure.	CLO2

	Learning Activities: Problem based learning, Students Teams, hands-on training on structure comparison and derive structure-function relationships, Case studies, research paper discussion	
III 12 Hours	Secondary structure prediction methods, Protein tertiary structure prediction- Comparative modeling, Threading, Ab initio modeling, introduction to artificial intelligence, Deep- learning algorithms in protein structure prediction, CASP experiments. Membrane Protein Structure Prediction, Transmembrane region prediction, difficulty in solving membrane protein structures; structural genomics of membrane proteins; tools and databases for identification of membrane proteins and the prediction of their structures. **Learning Activities**: Hands-on training on structure prediction, membrane structure prediction, Peer group discussion on structural genomics findings, Student seminars on recent developments	CLO3 CLO4
IV 11 Hours	Protein-Protein Interaction, evolutionary features related to structure and function, prediction of interacting regions and interaction partners. Structural analysis on protein– DNA interactions, protein–DNA binding specificity, Inter- and intramolecular interactions in protein–DNA recognition-prediction of DNA-binding sites, databases and tools for protein–DNA interactions. Introduction to RNA Structural Bioinformatics **Structural Genomics** Structural annotation of genomes and structural genomics, structural genomics initiatives, impact of structural genomics on drug discovery, structural genome annotation resources. **Learning Activities**: Peer discussion, Visualizing Protein-protein/DNA interactions Exploring the outcomes of various Structural genomics initiatives, Case studies on the role of structural genomics in drug discovery.	CLO5 CLO6

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

Suggested Readings

1. Branden, C. and Tooze, J. (1999). Introduction to Protein Structure, Garland Publishing Inc., 2e

2. Pal, S. (2020). Fundamentals of Molecular Structural Biology. Academic Press. ISBN: 9780128148556.
3. Gu, J. and Bourne, P. E. (2009) Structural Bioinformatics, John Wiley & Sons, 2e,
4. Liljas, A and L. Liljas, J. Piskur, G. Lindblom, P. Nissen and M. Kjeldgaard. (2016) Textbook of Structural Biology. World Scientific Publishing Co.
5. Timir Tripathi, Vikash Dubey, (2022) Advances in Protein Molecular and Structural Biology Methods, Academic Press, 1e.
6. Rupp, B. (2009) Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology. Garland Science.
7. Gromiha, M.M., (2010) Protein Bioinformatics, From Sequence to Function, Academic Press, USA, 1e.
8. Zhou, Y., Kloczkowski, A., Faraggi, E., and Yang, Y. (2017). Prediction of protein secondary structure. Humana Press. ISBN: 9781493964048, 9781493964048.
9. Anderson, W. F. (2014). Structural genomics and drug discovery. Methods and Protocols, 1. Humana Press. ISBN: 9781493903535, 9781493903535.

Web resources:

NPTL http://nptel.ac.in/syllabus/syllabus.php?subjectId=104102016

MIT OpenCourseWare
http://ocw.mit.edu/courses/biological-engineering/20-442-molecular-structure-of-biological-materials-be-442-fall-2005/

Course Title: Protein Engineering and Design Course
Code: CCS.724
Course type: DE Total
Hours: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:

CLO1: Describe the protein folding process, mechanism and its importance.
CLO2: Choose a suitable experimental technique to introduce desired amino acid modifications to wild type proteins
CLO3: Design and modify sequence for a protein with a desired structure and/or property
CLO4: Design the protein molecules with the desired bonded and non-bonded interactions using computational methods
CLO5: Describe the importance of protein designing for various applications.

Units/ Hours	Contents	Mapping with CLO
I 10 Hours	**Protein Folding and Engineering Methods:** Protein structural features, Protein Folding: Theory and Experiment- Protein Renaturation, Determinants of Protein Folding, Folding Pathways, Folding Accessory Proteins. Introduction to Conformational Diseases. Protein stabilising factors, Protein Denaturation, Explaining the Stability of Thermostable Proteins **Protein Engineering Methods** Protein expression systems (*E. coli* and *S. cerevisiae*), optimization of protein production and purification. In vitro mutagenesis- chemical mutagenesis – oligonucleotide - based mutagenesis - cassette mutagenesis – PCR based mutagenesis - saturation mutagenesis favouring the mutants. Protein engineering using non-canonical amino acids - methodologies; applications-side chain packing - backbone mutations- dissecting collagen mutations **Learning Activities**: Peer discussion, demonstration using physical and computer models on folding process, Student seminars	CLO1 CLO2
II 13 Hours	**Strategies for Protein Design:** Protein design; strategies for the design of structure - self-assembly - ligand-induced assembly - assembly via covalent cross-linking - assembly of peptides on	CLO3

	a synthetic template. Strategies for the design of	

	function-novel functions by retrofitting natural proteins - incorporation of binding sites into *de novo* proteins - design of catalytically active proteins - membrane proteins and ion channels - design of new materials. **Learning Activities**: Peer discussion, Case studies, research paper discussion, Problem based learning	
III 10 Hours	**Computational Protein Design:** Methods of Computational Protein Design, core and full repacking, predicting native protein core sequences; altering protein folds. Geometry and stereochemistry-based design, Case studies on Computationally Designed Proteins. **Learning Activities**: Problem based learning, demonstration using and computer models and experimental evidences, Classroom presentation	CLO4
IV 12 Hours	Tools and applications of Protein Engineering, Food and detergent industry applications, Environmental applications, Medical and nanobiotechnology applications. Modulating protein interactions by rational approach. Future challenged of computational protein design. Case studies on recent research articles. **Learning Activities**: Peer discussion, Case studies, research paper discussion, Problem based learning	CLO5

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

Suggested Readings

1. Zhao,H. (2021) Protein Engineering: Tools and Applications, Wiley-VCH Verlag GmbH & Co
2. Park, S.J., and Cochran, J.R. (2010). Protein Engineering and Design, 1/e, Taylor and Francis Inc., CRC Press, USA.
3. Carey, P.R. (1996) Protein Engineering and Design, 1/e, Academic Press Inc, USA.
4. Samish,I. (2017). Computational Protein Design, 1/e, Humana Press, New York.
5. Branden, C. I., & Tooze, J. (1999)., Introduction to Protein Structure, 2/e, Garland Science, USA.
6. Stefan, L. and Uwe, T.B. (Eds), (2012) Protein Engineering Handbook: Volume 3, 1/e, Wiley-VCH Verlag GmbH & Co.

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

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:

On completion of this course, students will be able to:

CLO1: learn the postulates of statistical mechanics, Liouville's Theorem and statistical interpretation of thermodynamics, the microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function.
CLO2: learn the Ising Model, Lattice Gas, Broken Symmetry, and Mean Field Theory
CLO3: learn the methods of statistical mechanics and their use to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases
CLO4: learn the theorem of non-equilibrium statistical mechanics and the advanced topics related to the range of modern day research based problems.

Units/ Hours	Contents	Mapping with CLO
I 12 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. **Learning Activities**: Brain-storming and Problem Solving	CLO1
II 11 Hours	**Phases & Phase Transitions:** The Ising Model: Stability of Thermodynamics Phases, First-order Phase transitions, Interfaces, The Ising Model, Lattice Gas, Broken Symmetry, Mean Field Theory.	CLO2

	A brief introduction to Liquid Theory: Averages, Distribution Functions, Reversible Work Theorem, Radial distribution function, Molecular liquids **Learning Activities**: Peer discussion, and Problem Solving	
III 11 Hours	**Bose-Einstein distribution:** Einstein condensation. Thermodynamic properties of ideal BE gas. **Fermi-Dirac distribution:** Degenerate Fermi gas. Electrons in metals. Magnetic susceptibility. **Learning Activities**: Problem based learning sessions, Class quiz.	CLO3
IV 11 Hours	**Non-equilibrium systems:** Fluctuation-Dissipation Theorem, Onsager's Regression Hypothesis Brownian Motion, Friction and the Langevin Equation, Transport, Time Correlation Functions. **Special topics:** Free energy perturbation, The Jarzynski Equality, Electron transfer--quantum rare events--golden rule--Marcus theory, Monte Carlo and Biased Monte Carlo methods. **Learning Activities**: Peer Discussion, and Research paper presentation.	CLO4

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

Suggested Readings

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

Course Title: Scientific Programming Paper Code: CCS.708
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of this course, students will be able to:
CLO1: identify and describe the basic art of scientific programming related to Fortran 95/2003.
CLO2: demonstrate concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
CLO3: develop skills to write programs related to standard problems and as well as to chemistry/physics.

Units/ Hours	Contents	Mapping with Course Learning Outcome
I 10 Hours	Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program. Constants and variables, assignment statements and arithmetic calculations **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 Hours	Intrinsic functions, Program design and branching structures, loop and character manipulation. Basic I/O concepts, Formatted READ and WRITE statements, **Learning Activities**: Peer discussion, Problem based learning.	CLO2
III 13 hours	Introduction to File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable arrays in procedures, derived data types. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO2 CLO3
IV 10 Hours	What is parallel programming, Why use parallel programming, Parallel Architecture,	CLO2 CLO3

	Open MP & MPI, Models of Parallel Computation, **Learning Activities**: Peer discussion on various parallel algorithms, problem solving.	

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

Suggested Readings

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

Course Title: Scientific Programming Lab (Practical) Paper
Code: CCS.709
Total Hours: 90

L	T	P	Cr
0	0	6	3

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

1. identify/characterize/define a computational problem
2. design a Fortran program to solve the problem
3. create pseudo executable code
4. read most of the basic Fortran code

Course Content

1. Compiling, linking and executing the Fortran programs.
2. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions,
3. Program design and branching structures, loop and character manipulation.
4. Basic I/O concepts, Formatted READ and WRITE statements,
5. Read/write of a Files.
6. Introduction to Arrays and procedures, Additional features of arrays and procedures.
7. Pointers and dynamic data structures using pointers in assignment statements.
8. Matrix summation, subtraction and multiplication, Matrix inversion.

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

Suggested Readings

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

Course Title: Numerical Methods

Paper Code: CCS.712 Total Hours: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:

On completion of this course, students will be able to:

CLO1: the large scale systems of linear, non-linear and simultaneous equations
CLO2: the matrix and determinants, interpolations, polynomial and spline interpolation
CLO3: the numerical differentiation and integration
CLO4: complex curve fitting methods, explicit schemes to solve differential equations
CLO5: apply numerical methods to obtain approximate solutions of complex mathematical problems.

Units/ Hours	**Contents**	**Mapping with Course Learning Outcome**
I 13 Hours	**Introduction:** Errors, Successive Approximation, Taylor's Series, Polynomial Evaluation **Matrix and Determinants:** Pivotal Condensation Method, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method. **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
II 12 Hours	**System of Linear Algebraic Equations:** System of Linear Equations, Gauss Elimination Method, Importance of Diagonal Dominance, Gauss Seidel Iteration Method, Matrix Inversion Method: Gauss-Jordan's Matrix-Inversion Method **Learning Activities**: Brainstorming and problem solving.	CLO1 CLO2
III 10 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	CLO3

	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. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	
IV 11 Hours	**Numerical Solution of Differential Equations:** Picard's Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method. **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	CLO4 CLO5

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: Numerical Methods Lab (Practical) Paper
Code: CCS.713
Total Hours: 60

L	T	P	Cr
0	0	6	3

Learning Outcomes:

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

- demonstrate computer code for the large scale systems of transcendental and polynomial equations
- execute numerical strategies to write a computer code for the solution of matrix and determinants, interpolations, polynomial and spline interpolation
- construct 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 Eigenvalues 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 Runge-Kutta method,
10. Monte Carlo integration.

Transactional Modes: Laboratory based practical; 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: Molecular Dynamics Paper Code: CCS.715
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes:
On completion of this course, students will be able to:
CLO1: learn the modelling of small to large molecular environments
CLO2: understand various force field for biomolecular simulation in details,
CLO3: learn different methods for simulating large systems,
CLO4: gain the knowledge about different molecular simulation techniques,
CLO5: understand the dynamics of the structural transitions

Units/Hours	Contents	Mapping with CLO
I 13 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. **Learning Activities**: Brain-storming and Problem Solving	CLO1 CLO2
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 **Learning Activities**: Brain-storming and Problem Solving	CLO3
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,	CLO4

	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 **Learning Activities**: Brainstorming and problem solving, modelling and scaffolding.	
IV 12 Hours	**Simulation Methods:** **Monte Carlo:** The Metropolis method **Molecular Dynamics:** (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method (f) Pressure Control: Andersen’s Method **Learning Activities**: Brain-storming and Problem Solving	CLO5

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: 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 wave packet, expectation values, free-particle wave packet: centre and dispersion of the wave packet.

Unit II **10 Hours**

Gaussian wave packet: 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 wave packet 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, representation 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 Molecular 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 Simulations 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:
- discuss the basics of Linux environment
- use the remote computing as a tool for high performance computation
- solve different energy minimization techniques
- design molecular model from scratch, and high definition images using various graphics tools
- execute the practical in-hand experience of various modeling and classical simulation tools
- construct the use of different in silico techniques for biomolecular simulations

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

Course Content

1. Linux basics and remote computing
2. Coordinate generations and interconversions of small molecules
3. Energy minimizations and optimization
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
6. Protein Structure Prediction using AlphaFold
7. Molecular Dynamics
    a. Water structure and dynamics
    b. Binary Mixtures
    c. HP36 in Water
    d. Serotonin 1A in Membrane Bilayers
    e. Hydration Free Energy of Methane
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.