Central University of Punjab

Ph.D. in Computational Physics

Batch 2024

Department of Computational Sciences

School of Basic Sciences

Programme Outcome

The above-mentioned program will enrich students with the advanced knowledge of theoretical/computational physics in the field of basic as well as applied research. On successful completion of the Ph.D. program the students will able to:

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

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

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

4. Construct themselves as Industrious research personnel

5. 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.702	Research and Publication Ethics	CC	2	0	0	2
3	CCS.703	Review Writing and Presentation	CC	2	0	0	2
4	UNI.753	Curriculum, Pedagogy and Evaluation	CC	1	0	0	1
5	CCS.752	Teaching Assistantship	CC	0	0	2	1
Student has to opt any two of the following courses:							
4	CCS.704	Electronic Structure Theory	DE	3	0	0	3
5	CCS.708	Scientific Programming	DE	3	0	0	3
6	CCS.709	Scientific Programming Lab (Practical)	SBE	0	0	6	3
7	PCP.710	Condensed Matter Physics	DE	3	0	0	3
8	PCP.711	Computational Solid State Physics Laboratory	SBE	0	0	6	3
9	CCS.712	Numerical Methods	DE	3	0	0	3
10	CCS.713	Numerical Methods Lab (Practical)	SBE	0	0	6	3
11	PCP.714	Integrating AI and DFT for Materials Modelling	DE	3	0	0	3
12	PCP.715	Computational tools for Materials Characterization	DE	3	0	0	3
13	CCS.717	Atomic and Molecular Spectroscopy	DE	3	0	0	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 Course
Code: CCS.701
Course Type: CC Total
Hours: 30

L	T	P	Cr
2	0	0	2

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

CLO1: Perform Literature survey, critically analyze 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:** Peer discussion, real world application, brain storming.	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:** Peer discussion, real world application, brain storming.	CLO2
III 5 Hours	**Library:** Classification systems, e-Library, web-based literature search engines **Learning Activities:** Peer discussion, real world application, 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 limited, partnership, sole proprietorship) employment, self-employment and entrepreneurship, financial management-importance and techniques, financial statements- importance and its	CLO4

	interpretation, and Intellectual Property Rights (IPRs). **Learning Activities**: Peer discussion, real world application, brain storming	

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: Research and Publication Ethics
Course Code: CCS.702
Course Type: CC Total
Hours: 30

L	T	P	Cr
2	0	0	2

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

CLO1: Describe with 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**: Peer discussion, real world application and brain storming.	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 Plagisrism (FFP) 4. Redundant publications: duplicate and overlapping publications, salami slicing 5. Selective reporting and misrepresentation of database. **Learning Activities**: Peer discussion, real world application and brain storming.	CLO2
III 5 Hours	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	CLO3

	5. Violation of publication ethics, authorship and contributorship 6. Identification of publication misconduct complaints and appeals 7. Predatory publishers and journals **Learning Activities**: Peer discussion, real world application and brain storming.	
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**: Peer discussion, real world application and brain storming.	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**: Peer discussion, real world application and brain storming.	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**: Peer discussion, real world application and brain storming.	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). Available at: elsevier.com/editors/perk/plagiarism-complaints. Accessed on June 17, 2017.

Course Title: Review Writing and Presentation Course
Code: CCS.703
Course Type: CC Total
Hours: 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 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:
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 **Learning Activities:** Peer discussion, real world application, brain storming.	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. **Learning Activities:** Peer discussion, real world application, brain storming.	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 **Learning Activities:** Peer discussion, real world application, brain storming	CLO3
IV	**Learners' Assessment:** Assessment Preparation: Concept, purpose, and principles of	CLO4

4 Hours	preparing objective and subjective 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. **Learning Activities**: Peer discussion, real world application, brain storming	

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

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	Credit
0	0	2	1

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

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: identify and define basic terms and concepts, which are needed for this specialized corse.
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 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. **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
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. **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
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 **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3

IV 10 Hours	**DFT and Force Field methods:** Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO4 CLO5

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*, OUP 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: Scientific Programming
Paper Code: CCS.708
Total Hours: 45

L	T	P	Cr
3	0	0	3

Couse Learning Outcomes (CLO): 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 CLO
I 10 Hours	**Introduction to Computers and Fortran language**: 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**: Brain storming and problem solving.	CLO1 CLO2
II 10 Hours	Constants and variables, assignment statements and arithmetic calculations, Expression writing, intrinsic functions, Program design and branching structures, loop and character manipulation. **Learning Activities**: Brain storming and problem solving.	CLO2
III 15 hours	Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable arrays in procedures, derived data types. Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object-oriented programming in Fortran. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO2 CLO3

IV 10 Hours	What is parallel programming, why use parallel programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO2 CLO3

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

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. 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

Couse Learning Outcomes (CLO): At the end of this course, students will be able to:
CLO1: Identify/characterize/define a computational problem CLO2:
Design a fortran program to solve the problem
CLO3: Create pseudo executable code CLO4:
Read most of the basic fortran code

Units/Hours	Contents	Mapping with CLO
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.	CLO1
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 arrays in procedures, derived data types.	CLO2
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.	CLO3
IV 20 Hours	What is parallel programming, why use parallel programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting	CLO4

Transactional Modes: Laboratory based practical; 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: Condensed Matter Physics
Paper Code: PCP.710
Total Lecture: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Learn the various types of crystal structure, and symmetries,
CLO2: Appreciate and apply the theories for calculation of energy band structure.
CLO3: Understand the fundamentals of magnetism corresponding theories,
CLO4: Better understanding about superconductivity

Units/Hours	Contents	Mapping with CLO
I 10 Hours	**Symmetry and Structures:** Building blocks of crystals: Bravais lattices, crystal structure, different symmetry elements in the crystals, point and space groups, analysis and interpretation of space group symbols and notations, Wyckoff positions. Representing simple and complex crystals by space group notation. Reciprocal lattice, Brillouin zones, different zone schemes, Brillouin zone folding., liquids and liquid crystals, Incommensurate structures, magnetic order, Fourier transforms. **Learning Activities**: Brain-storming, Problem Solving, Group discussion, Flip classroom	CLO1
II 12 Hours	**Electronic properties and band theory:** Electronic structure of solids. Fundamentals of band structure and significance on materials properties. Band theory, tight-binding model, Wigner-Seitz cell and method, augmented plane wave (APW) method, orthogonal plane wave (OPW) method. Overview of Linearized Augmented Plane Wave (LAPW) method. Brillouin zones and zone folding, Fundamentals of Fermi surfaces and their significance. 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. **Learning Activities**: Brain-storming, Problem Solving, Group discussion and Flip classroom	CLO2
III 12 Hours	**Magnetic properties of Materials:** Behavior of substances in a magnetic field, effect of temperature: origin of magnetic moment, Overview of Langevin theories of para and diamagnetism. Curie and Curie-Weiss law, ferromagnetic, antiferromagnetic and ferromagnetic ordering, role of exchange interaction in magnetism, Stoner and Heisenberg models for magnetism. Super exchange, magnetic domains, hysteresis, domain-wall theory. **Optical properties of solids:** Maxwell's equations, Polarization, Macroscopic and local electric field, Lorentz field, dipole contribution, Dielectric constant and ionic and electronic polarizability, Clausius-	CLO3

	Mossotti relation, Ferroelectricy, piezoelectricity. Multiferroic crystals. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	
IV 11 Hours	**Crystal defects:** 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 T_C superconductors and their applications. High pressure superconductors, superconducting hydrides, topological superconductors. Learning Activities: Brain-storming, Problem Solving, Group discussion, Flip classroom	CLO4

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

Suggested Readings

1. J. Ziman, (2011) *Principles of the Theory of Solids,* Cambridge University Press, Cambridge, U.K..
2. C. Kittel, (2007) *Introduction to Solid State Physics,* Wiley India (P) Ltd., New Delhi, India.
3. R.J. Singh, (2011) *Solid State Physics,* Pearson, New Delhi, India.
4. A.J. Dekker, (2012) *Solid State Physics,* Macmillan, London, U.K..
5. N. W. Ashcroft and N. D. Mermin, (2003) *Solid State Physics,*
    a. Thomson Press,.
6. A.R. Verma and O.N. Srivatava, (2012) *Crystallography Applied to Solid state physics,* New Age International,
7. Lilia Boeri (2018) "*Understanding Novel Superconductors with Ab Initio Calculations*" W. Andreoni, S. Yip (eds.), *Handbook of Materials Modeling*, Springer International Publishing https://doi.org/10.1007/978-3-319-50257-1_21-1
8. Boeri Lilia et al (2022) "*The 2021 room-temperature superconductivity roadmap*" J. Phys.: Condens. Matter 34 183002

Course Title: Computational Solid State Physics Laboratory
Paper Code: CCS.711
Total Hours: 90

L	T	P	Cr
0	0	6	3

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

- learn the computational methods for CSCl crystal structure determination
- carry out the geometry optimization of molecular crystals
- measure the Infrared spectra of crystals, and Raman spectra
- interpret the dispersion relation and cut-off frequency for the mono-atomic lattice

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

1. Creating the crystal structure, calculating bond length and X-ray diffraction pattern for various crystals using VESTA software (NaCl, Diamond, CsCl, ZnS, Perovskite structures).
2. Determine the crystal structure of CsCl using Gaussian package.
3. Geometry optimization of crystals using Gaussian package.
4. Determination of Infrared spectra of crystals using Gaussian package.
5. X-ray diffraction refinement using ICSD data.
6. Determination of Raman spectra using Gaussian package.
7. To compute lattice parameters of different cubic (SC, FCC, BCC) crystals using ELK package.
8. To compute the electronic band structure and density of states (DOS) for simple crystals (Al, Cu, Si, Diamond, NaCl, GaAs) using ELK package.
9. To compute magnetic moment and spin resolved band structure and DOS for BCC iron and FCC Ni.
10. To compute the band structure for antiferromagnetic and ferrimagnetic crystals using ELK.
11. To compute the phonon dispersions and obtain various thermal properties using ELK code.
12. To compute superconducting transition temperature of any material (Nb) within McMillan formula using ELK package.

Transactional Modes: Computation work, Experimentation and Viva-voce.

Suggested Readings

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

Course Title: Numerical Methods
Paper Code: CCS.712
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: 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 CLO**
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. **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
II 10 Hours	**Matrix and Determinants:** Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method. **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
III 15 hours	**Interpolations:** Concept of linear interpolation-Finite differences- Newton's and Lagrange's interpolation formulae- principles and Algorithms	CLO3

	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. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	
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. **Learning Activities**: Brain storming 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: 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 optimization
- 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: Atomic and Molecular Spectroscopy
Paper Code: CCS.717
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Learn the various types of atomic spectra and their corresponding features,
CLO2: Learn the various types of Molecular spectra and their corresponding features
CLO3: Gain knowledge about various molecular spectroscopic techniques,
CLO4: Apply the theories of molecular spectroscopy

Units/Hours	Contents	Mapping with CLO
I 12 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. **Learning Activities**: Brain storming and problem solving.	CLO1
II 11 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 **Learning Activities**: Brain storming and problem solving.	CLO2
III 11 Hours	**Advanced Spectroscopy:** Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO_2), FT-IR instrumentation **Learning Activities**: Brain storming and problem solving.	CLO3
IV 11 Hours	**Spectroscopy of Special Materials**: Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines, Vibrational spectroscopy of diatomic molecules, Franck-Condon factor, rotational fine structure. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO4

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

Suggested Readings

1. J. M. Hollas, (2004) Modern Spectroscopy, John Wiley & Sons, Ltd. .
2. G. M. Barrow, (1962) Introduction to Molecular Spectroscopy, McGraw- Hill .
3. C. N. Banwell and E.M. Mc Cash, (1994) Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, New Delhi .
4. L. R. Lakowicz, (2006) Principle of Fluorescence Spectroscopy 3rd Edition, Springer.
5. A. Carrington and A. D. Mc Lachlan, (1979) Introduction to Magnetic Resonance Chapman and Hall, London.
6. R. K. Harris, (1986) Nuclear Magnetic Resonance Spectroscopy, Addison Wesley, Longman Ltd, London.
7. C.J. Foot, (2005) Atomic Physics (Oxford University Press, Oxford, U. K.)

L	T	P	Cr
3	0	0	3

Course Title: Integrating Machine Learning and DFT for Materials Modelling
Paper Code: PCP.714
Total Lectures: 45

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Fundamentals of density functional theory.
CLO2: Fundamentals of Machine Learning.
CLO3: Basics of python required for machine learning.
CLO4: Applications of machine learning and DFT for study of materials

Units/ Hours	**Contents**	Mapping with CLO
I 12 Hours	**Fundamentals of Density functional theory:** Many particle Hamiltonian and quantum mechanics of materials. Electronic band structure, density of states for free electron gas and beyond. Models for incorporating electron-nuclei interaction: Planewaves, augmented planewaves, pseudopotentials. Electron-electron interaction, Hartree, Hartree-Fock approximation. Density functionals for kinetic energy, electron-electron coulomb, exchange and correlation energy. Kohn- Sham Hamiltonian. Local density approximation (LDA) and generalized gradient approximation (GGA). **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
II 8 Hours	**Fundamentals of Machine Learning:** Machine learning process: Data collection, data processing, feature engineering, training model, model evaluation. Basic statistics and principles for machine learning. K nearest neighbors (KNN), K means clustering. Linear regression and supervised learning. Sampling, Unsupervised machine learning, deep learning, ensemble learning, Reinforced learning, Bayesian learning. Image processing in machine learning. **Learning Activities**: Brain storming and problem solving.	CLO1 CLO2
III 12 hours	**Python for Scientific computing:** Basics of python, Python datatypes, Python operators, Condition statements in python, loops, functions in python: built-in and user defined functions, Modules in python, Math module, Basics of NUMPY, PANDAS, RANDOM, MATPLOTLIB module. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO3

IV 13 Hours	**DFT and Machine learning integration:** Supervised learning: Predict structure-property relationship, develop model Hamiltonians, predict and classify crystal structures Unsupervised learning: Analyze composition spreads from combinatorial experiments, analyze micrographs and identify descriptors. Generative models, Data driven materials discovery, Process optimization, High throughput screening. Database of materials science for machine learning, important feature vectors for describing materials properties. Some case studies for prediction of materials properties using machine learning. **Learning Activities**: Brain storming and problem solving, modelling and scaffolding.	CLO4 CLO5

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

Suggested Readings

1. *Density Functional Theory: A Practical Introduction*, (2009) David S. Sholl, Janice A. Steckel, John Wiley & Sons, Inc.
2. *Pattern Recognition and Machine Learning* by Christopher M. Bishop
3. A. Szabo and N. S. Ostlund, (1982). *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure*, Dover, New York.
4. *Machine Learning with Python* Abhishek Vijayvargia BPB Publications (2018)
5. *Chapter 04* "*Machine Learning in Materials Science: Recent Progress and Emerging Applications*" Tim Muller, Aaron G. Kusne, Rampi Ramprasad https://doi.org/10.1002/9781119148739.ch4 (2016)
6. *A Strategic Approach to Machine Learning for Material Science: How to Tackle Real-World Challenges and Avoid Pitfalls* Piyush Karande et al. Chem. Mater. 34 (2022) 7650−7665
7. *Scope of machine learning in materials research-A review* M. H. Mobarak et al. Applied Surface Science Advances 18 (2023) 100523
8. *Recent advances and applications of machine learning in solid state materials science* J. Schmidt et al. npj Computational Materials (2019) 5:83 https://doi.org/10.1038/s41524-019-0221-0
9. *Explainable machine learning in materials science* X. Zhong et al. npj Computational Materials (2022) 8:204 https://doi.org/10.1038/s41524-022-00884-7

L	T	P	Cr
1	0	2	3

Course Title: Computational tools for Materials Characterization

Code: PCP.715
Total Lectures: 45

Course Learning Outcomes (CLO):
On completion of this course, students will be able to:
CLO1: Learn various visualization techniques for crystals in real and reciprocal space.
CLO2: Learn and calculate materials properties using Quantum Espresso package. Role of convergences in computational modelling.
CLO3: Explore the SIESTA code and its applications for study of bulk and nanostructures.
CLO4: Explore the full-potential LAPW ELK code for study of various properties of materials.

Units/Hours	Contents	Mapping with CLO
I 10 Hours	**Structure Visualization (VESTA & XCRYSDEN):** Visualization of crystal morphologies, visualization of electron/nuclear densities, structural models, volumetric data, and crystal faces, Visualization of isosurfaces with multiple levels, electron and nuclear densities from structure parameters, X-ray diffraction data, neutron diffraction data, Visualization of crystal structures, Brillouin zones and high symmetry paths using XCRYSDEN. **Learning Activities**: Brainstorming and problem solving.	CLO1
II 12 Hours	**Characterization techniques (QE):** Overview of density functional theory and self consistent field (SCF). Lattice constant calculation for cubic and non-cubic crystals using energy versus lattice parameters and stress minimization. Bulk modulus and other elastic constants. Electronic band structure and density of states. Charge density contours and Wannier functions. Lattice dynamics: phonon dispersions and density of states, lattice specific heat using phonon dispersions. Pseudopotentials, exchange correlation approximations: LDA, GGA, hybrid functionals. **Learning Activities**: Brainstorming and problem solving.	CLO2
III 12 Hours	**Characterization techniques (SIESTA):** Atomic scale materials modelling, electronic structure calculations, bond length and vibrational frequencies. Layered materials and their electronic structure. Nanostructures and their electronic structure. Ab-initio molecular dynamics (AIMD) band structure calculation. **Learning Activities**: Brainstorming and problem solving.	CLO3

IV 11 Hours	**FP-LAPW ELK code:** Basics of planewaves and augmented planewaves (APW). Linearization of APW. Muffin-tin potential and full potential version. Computing structural, electronic, optical and magnetic properties using ELK code. Ferromagnetic, anti-ferromagnetic and ferrimagnetic structures using ELK code. Fermi surfaces using ELK code. Virtual crystal approximation and crystal doping. **Learning Activities (ELK)**: Brainstorming and problem solving, modelling and scaffolding.	CLO4

Transactional Modes: Lecture; Tutorial; Lab sessions; Self-learning.

Suggested Readings

1. June Gunn Lee *Computational Materials Science: An Introduction* CRC Press (2011).
2. David S. Sholl and Janice A Steckel, *Density functional theory: A Practical Introduction*, John Wiley and Sons (2009)
3. N. T. Hung Ahmad R. T. Nugraha and R. Saito *Quantum Espresso course for Solid State Physics*, Jenney Standford Publishing Pte. Ltd. (2023)
4. K. Momma and F. Izumi, "*VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data*," J. Appl. Crystallogr., 44, 1272-1276 (2011).
5. M., Wentzcovitch. "*QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*" Journal of Physics: Condensed Matter, 21 (2009)
6. http://www.xcrysden.org/XCrySDen.html
7. https://elk.sourceforge.io/
8. https://siesta-project.org/siesta/About/overview.html