



Ph D Program in Physics
School of Physical Sciences
Doon University

Pre-PhD Course Work Syllabus

COURSE CODES, TITLES AND CREDITS

| Course Code | Title | Credits | Remark |
|--------------------|---------------------------------------|----------------|----------------------------------|
| PHC-701 | Research Methodology | 4 | Compulsory Course |
| PHC-702 | Research and Publication Ethics (RPR) | 2 | Compulsory Course |
| PHE-701 | Advanced Solid-State Physics | 4 | Elective Compulsory Course (ECC) |
| PHE-702 | Advanced Computational Physics | 4 | Elective Compulsory Course (ECC) |
| PHE-703 | Characterization of materials | 4 | Elective Compulsory Course (ECC) |
| PHE-704 | Advanced Mathematical Physics | 4 | Elective Compulsory Course (ECC) |
| PHE-705 | Atomistic Modelling and Simulations | 4 | Elective Compulsory Course (ECC) |
| PHE-706 | Nanotechnology | 4 | Elective Compulsory Course (ECC) |
| PHE-707 | Research Review | 4 | Elective Compulsory Course (ECC) |
| PHE-708 | Advanced Electrodynamics | 4 | Elective Compulsory Course (ECC) |

- The pre Ph D course will be of 14 credits and the duration of the course work is of 6 months.
- All the candidates admitted to Ph D program are required to take two compulsory courses (Research Methodology and Research and Publication Ethics) of 4 and 2 credits, respectively.
- All the candidates admitted to Ph D program have the liberty to opt any of the two courses from elective compulsory courses of 4 credits each.

Program Objectives:

The objectives of the program are as follows:

1. To inculcate the concepts of research and encourage the students for research and development in the advanced areas of research.
2. the capacity to devise, design and conduct research that has real academic weight, is targeted and shows integrity.
3. To understand the importance of experimental research and theoretical simulation.
4. The ability to make original and significant contributions to scientific knowledge base in their area of research.
5. The capacity to develop further the progress made in technological and social terms within an academic and professional context.
6. Satisfying standards associated with national and international peer-reviewed publications.
7. To emphasize the importance of Physics as the most important discipline for sustaining the existing industries and establishing new ones to create job opportunities at all levels of employment.
8. To develop human resource with a solid foundation in theoretical and experimental aspects as a preparation for career in academia and industry.

Program Learning Outcomes:

The Ph D in Physics should

1. have a coherent understanding and knowledge of basic and advanced concepts in core physics, maths, chemistry and current physics research topics.
2. have the knowledge of the concepts, techniques, and literature associated with the student's specific research subfield (e.g., theoretical condensed matter physics, etc.).
3. Development of experimental skills by working on advanced systems and an ability to design and conduct original experiments along with theoretical and mathematical approaches to describe the physical world.
4. An ability to work collaboratively with their group and able to teach and mentor others effectively.
5. be capable of demonstrating ability to think and analyze rationally with modern and scientific outlook and identify ethical issues related to one's work, avoid unethical behavior such as fabrication, falsification or misrepresentation of data or committing plagiarism.
6. Develop communication skills and writing skills involving the ability to listen carefully, to read texts and research papers analytically and to present complex information in a concise manner to different groups.
7. Developing an ability to involve in a productive research and academic career, including publications, proposal submission and conference presentations.
8. be able to develop a national as well as international perspective for their career in the chosen field of the academic and research activities.

9. An ability to identify important scientific problems and to use modern experimental, and computational techniques to solve scientifically and societally relevant problems.

DETAILED SYLLABUS:

PHC-701: RESEARCH METHODOLOGY

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Objective:

1. To apprise students of basics methods, ethics, tools and practices in research.
2. To enable the students to choose right problem and methodology.
3. To explain the students about conducting research work and formulating research synopsis and report.
4. To familiarize participants national and international journals.
5. To impart knowledge about scientific writing and various data packages and software's.

Course Content:

Introduction: Philosophy of research, Introduction to research methods, Relevance and ambiguity in applied research, Ethics in research, Scientific explanation and understanding in science, characteristics of scientific research and logic of scientific enquiry, Introduction to different perspectives and types of research.

Designing Research: Meaning, Elements and Need of research design, Features of a good design, Different types of research design, Developing a research plan, Defining the research problem and hypothesis, Selecting a problem, Necessity of defining the problem, Techniques involved in defining a problem; Hypothesis – Types of hypothesis, Differences between hypothesis and research problem.

Priority Setting in Research: Introduction to setting research priorities - Process – Links with planning, participation, time and information, Steps – choosing the right problem, Defining objectives and Options, Choosing and evaluating, Preparing for implementation, Type of research, Choosing a Methodology, Methods of setting research priorities.

18 Lectures

Review of Published Research: *Print:* Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and Wiki-Databases, Academic databases and search engines: Science Direct, SciFinder, Scopus, Web of knowledge. Finding and citing published information.

12 Lectures

Designing Research Projects: Project Cycle Management (PCM) – Six stages, Introduction, Preparation, Appraisal, Proposal preparation, Approval, Financing, Implementation, Monitoring, Evaluation; Logical Framework Analysis (LFA) – What is LFA? History, when should be used? Analyzing the situation – Problem analysis, Stakeholder analysis, Objective analysis, Assumptions and risks, Indicators, Means of verification, Selection of a preferred implementable strategy, Costing and Schedule, Implementation, Strengths and weaknesses of LFA

8 Lectures

Methods of Scientific Writing: Reporting practical and project work, Writing literature surveys and reviews, Organizing a poster display, Giving an oral presentation, Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics, Avoiding plagiarism. Introduction to LaTeX.

5 Lectures

Computer Applications in Research: Data storage, Data Analysis: *The Investigative Approach:* Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments; *Analysis and Presentation of Data:* Descriptive statistics. Choosing and using statistical tests. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis; Scientific simulation, Instrumentation control and automation, Softwares for data interpretation and analyses. Plotting: Introduction to GNU PLOT/MATLAB Plotting/Origin/XMGRACE/SIGMAPLOT. Introduction to VIM/EMACS: basic commands. Basics of LINUX/UNIX commands.

10 Lectures

Communicating Results for Application: Identifying users and their needs, Channels of communication with users, Type of research – user linkages, Management options for strengthening researcher-user communication; Communicating Scientific Results: Importance of research communication in science, Overview of research communication process in science, Role of scientific journals – quality of journals, citation index, Other options for communicating results.

7 Lectures

Reference Books:

- Research Methodology in Chemical Sciences: Experimental and Theoretical Approach Tanmoy Chakraborty, Lalita Ledwani, CRC Publishers
- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) Practical skills in chemistry. 2nd Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) Data analysis for chemistry. Oxford University Press.
- Topping, J. (1984) Errors of observation and their treatment. Fourth Ed., Chapman Hall, London.
- Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ. Press (2001) 487 pages.
- Date, C. J. An Introduction to Database System, Addison Wesley, U.K (1986).
- Caulcutt R, R Boddy, Statistics for Analytical Chemists, First Ed. 1983, By, Chapman & Hall.
- Medhi, J. Statistical Methods. Wiley Eastern, New Delhi (1992).
- Barnett, V. Environmental Statistics: Methods and Applications, John Wiley and Sons, New Delhi (2006).
- Chapin Paul G., Research Projects and Research Proposals: A Guide for Scientists Seeking Funding, Cambridge University Press.
- OSU safety manual 1.01.
- Latex: A Document Preparation System: User's Guide and Reference Manual.
- Learning the vi and Vim Editors: Text Processing at Maximum Speed and Power: Andy Oram.
- Gnuplot in Action; Philipp K. Janert.

Course Learning Outcome:

1. Acquaint the students about the Principles and types of researches.
2. Examine the various methods of data collection, research tools and techniques of research.
3. Develop understanding on various kinds of research, objectives of doing research, research process, research designs and sampling.
4. Make the students aware about the theory construction Impart knowledge about programme evaluation and use of computer in research and evaluation.
5. Ability to define problems and select the journals for publishing research work.

Evaluation: On Continuous Basis

| | |
|--------------------------|---------------------|
| Mid Semester Examination | 30 Marks (2 hours), |
|--------------------------|---------------------|

| | |
|--------------------------|--|
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation) |

PHC-702: RESEARCH AND PUBLICATION ETHICS

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 2 | 0 | 0 | 2 | 30 |

Course Objective:

This course is focused to facilitate student to understand

1. the basics of philosophy of science and ethics.
2. research integrity and publication ethics.
3. research misconduct and predatory publications.
4. research metrics and plagiarism tools

Course Content:

Unit 1: Philosophy and Ethics

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

4 Lectures

Unit 2: 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 data

6 Lectures

Unit 3: Publication Ethics

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

3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behaviour 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

6 Lectures

Unit 4: Open Access Publishing

1. Open access publications 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 Suggestor, etc.

4 Lectures

Unit 5: 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

5 Lectures

Unit 6: Database 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

5 Lectures

Reference Books:

- Bird, A. Philosophy of Science. Routledge.
- MacIntyre Alasdair (1967) A short History of Ethics. London
- P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865
- National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). On Being a Scientist: A guide to responsible conduct in Research: Third edition. National Academies Press.

- Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019), ISBN:978-81-939482-1-7.
http://www.insaindia.res.in/pdf/Ethics_Book.pdf
- Resnik, D.B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from
<https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm>
- Beall, J.(2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179-179.
<http://doi.org/10.1038/489179a>

Course Learning Outcome

1. Understand the research and publication ethics and their importance.
2. Use of plagiarism tools while analysis of data, writing research papers, research proposals and presentation of research data.
3. Understanding research metrics (h-index, i-index)

Evaluation: On Continuous Basis

| | |
|--------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours), |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-701: ADVANCED SOLID STATE PHYSICS

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Objective:

1. To make students learn more about the theoretical models for studying condensed matter.
2. To enable the students to develop an understanding of relation between band structure and the electrical/optical properties of a material.
3. To study some of the basic properties of the condensed phase of matter especially solids.

Course Content:

Semiconductors: Intrinsic and extrinsic semiconductors. carrier concentration and Fermi levels of intrinsic and extrinsic semi-conductors. Bandgap. Direct and indirect gap semiconductors. Hydrogenic model of impurity levels.

10 Lectures

Band Theory (Advanced form Solid State Physics I): Tight Binding, Pseudo potential methods, De Haas von Alfen Effect, AC conductivity and optical properties, plasma oscillations.

Defects in Crystals: Vacancy formation, Mechanism of Plastic deformation in solids, Stress Imperfections in crystals: Lattice defects & configurational entropy, vacancies, Schottky & Frankel pairs, Edge & screw dislocations (qualitative ideas), Frank-Read Sources, Dislocations in FCC, BCC and HCP structures Experimental methods of detecting defects.

15 Lectures

Magnetism: Magnetic properties of solids. Diamagnetism, Langevin equation. Quantum theory of paramagnetism. Curie law. Hund's rules. Paramagnetism in rare earth and iron group ions. Elementary idea of crystal field effects. Ferromagnetism. Curie-Weiss law. Heisenberg exchange interaction. Mean field theory. Antiferromagnetism. Neel point. Other kinds of magnetic order. Nuclear magnetic resonance, Hall effects, Elementary ideas of Quantum Hall effect, Cyclotron resonance and magnetoresistance

20 Lectures

Superconductivity: Survey of important experimental results. Critical temperature. Meissner effect. Type I and type II superconductors. Thermodynamics of superconducting transition. London equation. London penetration depth. Basic ideas of BCS theory. High- T_c superconductors, Josephson junctions.

1. Superfluidity. Ordered phases of matter: translational and orientational order, kinds of liquid crystalline order. Quasi crystals.
2. Transport properties in solids: Boltzmann transport equation, resistivity of metals and semiconductors, thermoelectric phenomena, Onsager coefficients.

15 Lectures

Course Learning Outcome:

Students shall be able

1. To grow their understanding about the quantitative hypotheses of energy levels, band gap computation based upon different approaches,
2. Understand the defects in crystals, magnetic properties, superconductivity and superfluidity.
3. Explain the concept of energy bands and effect of the same on electrical properties.

Reference Books:

- John Singleton: Band theory and Electronic properties of Solids (Oxford University Press; Oxford Master Series in Condensed Matter Physics).
- Ibach & Luth: Solid State Physics
- Elementary Dislocation Theory: Weertman and Weertman
- M. Ali Omar: Elementary solid state physics (Addison-wesley)
- C. Kittel: Solid-state physics (Wiley eastern) (5th edition)
- Solid State Physics, A.J.Dekker, Macmillan India Ltd
- Material Science & Engineering, V.Raghavan, Prentice –Hall of India, New Delhi (2001)

Evaluation: On Continuous Basis

| | |
|--------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours), |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-702: ADVANCED COMPUTATIONAL PHYSICS

| | | | |
|---|---|---|----|
| L | T | P | Cr |
| 2 | 0 | 2 | 4 |

Course Objective:

1. To enable students, learn the essentials of essential and practical computational methods and techniques used to solve physics problems numerically.
2. To enable the students to understand the programming languages such as FORTRAN, C and C++.

Course Contents:

Overview of computer organization: Hardware, software, scientific programming in FORTRAN and/or C, C++.

10 Lectures

Numerical Techniques: Sorting, interpolation, extrapolation, regression, numerical integration, quadrature, random number generation, linear algebra and matrix manipulations, inversion, diagonalization, eigenvectors and eigenvalues, integration of initial-value problems, Euler, Runge-Kutta, and Verlet schemes, root searching, optimization, fast Fourier transforms.

18 Lectures

Simulation Techniques: Monte Carlo methods, molecular dynamics, simulation methods for the Ising model and atomic fluids, simulation methods for quantum-mechanical problems, time-dependent Schrödinger equation, discussion of selected problems in percolation, cellular automata, nonlinear dynamics, traffic problems, diffusion-limited aggregation, celestial mechanics, etc.

18 Lectures

Parallel Computation: Introduction to parallel computation.

4 Lectures

Reference Books:

- V. Rajaraman, Computer Programming in Fortran 77.
- W.H. Press, B.P. Flannery, S.A. Teukolsky and W.T. Vetterling, Numerical Recipes in FORTRAN 77: The Art of Scientific Computing. (Similar volumes in C, C++.)
- H.M. Antia, Numerical Methods for Scientists and Engineers.
- D.W. Heermann, Computer Simulation Methods in Theoretical Physics.

- H. Gould and J. Tobochnik, An Introduction to Computer Simulation Methods.
- J.M. Thijssen, Computational Physics.
- Selim G. Akl, Parallel computation.
- Roman Trobec, Parallel computing: Numerics, Applications and Trends.
- D. J. Evans, Parallel computing: Methods, Algorithms and Applications.

Course Learning Outcome:

1. Students shall be able to learn a computer programming language and basics of computational methods in interpolation, root finding, differentiation, integration, eigen value determination, FFT, solution of differential equation etc.
2. They will apply the computational methods in more applied computing case studies such as Monte Carlo methods, molecular dynamics, Ising model etc.
3. An introduction to the parallel computation is covered in this course.

Evaluation: On Continuous Basis

| | |
|----------------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours) |
| End Semester Examination | 30 Marks (3 hours) |
| Laboratory/Practical Examination | 20 Marks |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-703: CHARACTERIZATION OF MATERIALS

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Objective:

1. To impart the knowledge about the essential characterization techniques in materials science.
2. To enable the students to understand about X-ray diffraction and electron diffraction for structural and microstructural analysis, respectively.
3. To acquaint about advanced characterization techniques such as scanning electron microscopy, transmission electron microscopy, atomic force microscopy, etc.

Course Contents:

1. Crystallography, X-ray Diffraction Methods, Reitveld Refinement, Neutron Diffraction, X-ray absorption, X-ray Fluorescence spectroscopy, Electron Diffraction-diffraction pattern in specific modes **20 Lectures**
2. LEED and RHEED, Electron optics, Electron Microscopy-Scanning and Transmission electron microscopy, **15 Lectures**
3. Atomic Force microscopy, Scanning Tunneling Microscopy, Compositional analysis employing AES, ESCA and Electron Probe Microanalysis **15 Lectures**
4. Raman spectroscopy, UV-Vis spectroscopy **10 Lectures**

Compulsory Project related to characterization of materials.

Reference Books:

- Elements of X-ray Diffraction by B.D. Cullity
- X-Ray Diffraction - A Practical Approach by C. Suryanarayana
- Electron Diffraction and Crystallography by Fultz
- Scanning Electron Microscopy and X-ray Microanalysis: by Joseph Goldstein
- Introductory Raman Spectroscopy (Second Edition) by John R. Ferraro, Kazuo Nakamoto and Chris W. Brown

Course Learning Outcome:

1. They will be given a project to learn one or more of such techniques in more details.
2. The students will learn the theoretical principles of ERD, Neutron Diffraction, X-ray absorption, Electron diffraction, AFM, STM AES, ESCA, Raman spectroscopy UV-viz etc.
3. The students will be able to relate the learned techniques in their Ph D work.

Evaluation: On Continuous Basis

| | |
|--------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours) |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-704: ADVANCED MATHEMATICAL PHYSICS

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Objective:

1. To enable students, learn more involved mathematical tools for study of most recent advances of physics.
2. To Understand about partial differential equations and their applications.
3. To impart the knowledge about group theory and tensors.
4. To Learn the basic concept about statistics and various tests.

Course Content:

Partial differential equations: Important partial differential equations: The wave equation, The diffusion equation, Laplace's equation, Poisson's equation, Schrodinger equation, General and Particular solutions. Characteristics and the existence of the solutions. Uniqueness of the solutions. Separation of variables method, Superposition of separated solutions, Separation of variable in Polar coordinates. Integral Transform method.

10 Lectures

Introduction to Group Theory: Groups, Finite Groups, Non-Abelian Groups, Permutation Groups, Subgroups, translation and rotation groups, $O(N)$ and $U(N)$ groups. Basics of Representation theory. **15 Lectures**

Basics of Tensors: Notations, Higher order Cartesian tensors, The algebra of tensors, The quotient law, Isotropic tensors, Improper rotations and pseudotensors, Dual tensors, The metric tensor, Relative tensors, Christoffels symbols, Vector Operators and absolute derivatives along curves. **15 Lectures**

Statistics: Experiments, samples and population; Estimators and sampling distribution, Maximum likelihood method, The method of least squares, Hypothesis testing. **10 Lectures**

Integral Equations: Obtaining an integral equation from a differential equation, Types of integral equations, Operator notation and the existence of solutions, Closed form solutions, Neumann series, Fredholm theory, Schmidt-Hilbert theory. **10 Lectures**

Reference Books:

- G.B. Arfken, Mathematical Methods for Physicists.
- P. Dennery and A. Krzywicki, Mathematics for Physicists.
- P.K. Chattopadhyay, Mathematical Physics.
- A.W. Joshi, Matrices and Tensors in Physics.
- R.V. Churchill and J.W. Brown, Complex Variables and Applications.
- P.M. Morse and H. Feshbach, Methods of Theoretical Physics (Volume I & II).
- M.R. Spiegel, Complex Variables.
- Riley, Mathematical Methods for Physics and Engineering.

Course Learning Outcome:

1. The students will learn more details of partial differential equation, Group theory applied in crystallography and high energy physics, basics of tensors, basic statistics tools and Integral equations.

Evaluation: On Continuous Basis

| | |
|--------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours), |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-705: ATOMISTIC MODELLING AND SIMULATIONS

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Objective:

1. To develop the theoretical understanding towards materials modeling through atomistic simulations.
2. To develop an understanding about *ab initio* methods and density functional theory.

Course Content:

Useful concepts of Molecular modeling: Mathematical concepts and review of related basics.

10 Lectures

Empirical Force Field Models: Molecular Mechanics force fields, bond stretching, angle bending, Van der Waals interactions, pair potentials, Common and popular force field potentials. An Introduction to the Computational Mechanics: One electron atom.

15 Lectures

Advanced *ab initio* methods, Density Functional Theory: Open shell systems, Electron correlation, Valence bond theories, The Hartree-Fock equations, semi-empirical methods.

15 Lectures

Energy minimization and related methods: Non-derivate minimization methods, Second derivative methods, Quasi Newton methods.

5 Lectures

Simulations and molecular dynamics methods: Calculating thermodynamic properties, Truncation of potentials, Long range potentials, Constraint dynamics, Time dependant properties. Monte Carlo simulations: Theoretical background of the Metropolis method, Implication of Monte Carlo simulations.

15 Lectures

Reference Books:

- R. Leach, Molecular Dynamics.
- R. M. Martin, Electronic Structure: Basic theory and practical methods.
- J. Kohnoff, Electronic structure calculations for solids and molecules.
- D. Frenkel, Understanding Molecular Dynamics.
- J. M. Haile, Molecular Dynamics Simulations.
- M. P Allen, Computer Simulations of Liquids.

Course Learning Outcome:

1. The students will learn the basics of molecular modeling, density functional theory and Monte Carlo methods.

Evaluation: On Continuous Basis

| | |
|--------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours), |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-706: NANOTECHNOLOGY

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Objective:

1. To enable students, have overview of theory and challenges of nanotechnology.
2. To understand the concepts of 1D, 2D and 3D confinement along with the density of states.
3. To acquaint the students with nanoscale systems, 1D, 2D and 3D systems.
4. To understand about the growth and synthesis of nanostructure materials by various deposition processes along with the growth mechanism models.

Course Content:

Physics of low-dimensional materials, 1D, 2D and 3D confinement, Density of states, Excitons, Coulomb blockade **10 Lectures**

Surface plasmon, Size and surface dependence of physical, electronic, optical, luminescence, thermo-dynamical, magnetic, catalysis, gas sensing and mechanical properties. **15 Lectures**

Physical and chemical techniques for nanomaterial synthesis, Physical Vapor Deposition, Glow Discharge and Plasma, Sputtering–mechanisms and yield, Chemical Vapor Deposition, Chemical Techniques - Spray Pyrolysis, Electrodeposition, Sol Gel **20 Lectures**

Nucleation & Growth: capillarity theory, atomistic and kinetic models of nucleation, basic modes of nanostructure growth, Growth mechanisms, Epitaxy Assembling and self organization of nanostructures, Nanoscale manipulation, Nanotube and wire formation, Importance of size distribution control, size measurement and size selection **15 Lectures**

Reference Books:

- The Physics of Low Dimensional Semiconductors: An Introduction by John H. Davies.
- Materials Science of Thin Films by Milton Ohring.
- Nanotechnology: Gregory L.Timp.
- Thin Film Phenomena by K.L. Chopra .
- F. C. Phillips: An introduction to crystallography (wiley)(3rd edition)
- Introduction of Solids: L.V. Azaroff.
- Solid State Physics-Structure and Properties of Materials: M.A. Wahab.
- Solid State Physics: N.W. Ashcroft and N.D. Mermin.
- C. Kittel: Solid-state physics (Wiley eastern) (5th edition).

Course Learning Outcome:

After the successful completion of the course, the student will learn the following:

1. Concept of Quantum confinement, 1D, 2D, and 3D nanosystems with examples.
2. The students will be able to learn the properties of low-dimensional materials, the theoretical concepts involved and various physiochemical properties as depending upon the dimensionality.
3. Different synthesis techniques including PVD and CVD systems along with the growth models.
4. Characterization of nanostructured materials using X-ray diffraction, electron microscopy, Atomic Force Microscopy and Scanning Tunneling Microscopy.
5. Physical, electronic, magnetic and optical properties of nanostructured materials.

Evaluation: On Continuous Basis

| | |
|--------------------------|--|
| Mid Semester Examination | 30 Marks (2 hours) |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |

PHE-707: RESEARCH REVIEW

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 0 | 4 | 4 | 4 | 60 |

Course Objective:

This course is focused to facilitate student to gain skills of collecting, interpreting and presenting information of interest through seminar and report presentation.

Research Review of the work related to Ph D, presentation, writing review

Course Learning Outcome

1. Identify and understand assumptions and arguments that exist in the national and international literature in the identified area of work/topic.
2. Evaluate and synthesize evidence in order to draw conclusions based on research gaps.
3. Ask meaningful questions and originate plausible research and technical gaps and the implications of the expected outcomes.

Evaluation: On Continuous Basis

| | |
|-------------------------------|-------------------------------------|
| Mid Semester Examination | 30 Marks (Presentation and Viva) |
| End Semester Examination | 40 Marks (Presentation and Viva) |
| Submission of Research Review | 30 Marks |

PHE-708: APPLIED ELECTRODYNAMICS

| L | T | P | Cr | Hours |
|---|---|---|----|-------|
| 4 | 0 | 0 | 4 | 60 |

Course Content:

1. To review the basics of electrodynamics studied in previous classes.
2. To learn various concepts related with electromagnetic waves, their propagation characteristics in various medium including waveguides.
3. To understand basic concepts of Plasma, its properties and wave propagation

Course Content:

Review of basics electrodynamics:

Electrostatics, conductors, dielectrics, magnetostatics, boundary value problems, time dependent fields, vector and scalar potentials, gauge symmetry, Coulomb and Lorentz gauges, electromagnetic energy and momentum, conservation laws), inhomogeneous wave equation and Green's function solution, waves in a medium, relativistic formulation of Maxwell's equations, Conservation laws, radiation from accelerating charges, scattering of electromagnetic waves.

20 Lectures

Electromagnetic Waves:

Plane waves in a dielectric medium, reflection and refraction at dielectric interfaces, frequency dispersion in dielectrics and metals, dielectric constant and anomalous dispersion, wave propagation in one dimension, group velocity, metallic wave guides, boundary conditions at metallic surfaces, propagation modes in wave guides

20 Lectures

Basics of Plasma Physics: Introduction to plasma, Debye shielding, Single particle motion in E and B fields, Mirror confinement, Plasma oscillations, Waves in unmagnetized plasmas, Solitons, Two stream instability, Rayleigh Taylor instability, Vlasov equation and Landau damping, Waves in magnetized plasmas (A-H Equation), Applications to astrophysics and astronomy.

20 Lectures

Course Learning Outcome

Should be able to explain

1. Various conservation laws in electrodynamics, concepts of Maxwell's equations and electromagnetic waves.
2. Explain wave propagation in bounded medium, wave dispersion, group and phase velocity.
3. Explain the concept of plasma and wave propagation in the magnetized and non-magnetized plasma.

Evaluation: On Continuous Basis

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| Mid Semester Examination | 30 Marks (2 hours) |
| End Semester Examination | 50 Marks (3 hours) |
| Internal Assessment | 20 Marks (Tutorials, Assignments, Quizzes, Presentation and discussion), |