

**Anekant Education Society's**

**TULJARAM CHATURCHAND COLLEGE OF ARTS, SCIENCE AND COMMERCE,**

**BARAMATI**

**(Autonomous Status)**

**(Affiliated to Savitribai Phule Pune University, Pune)**

Faculty of Science

## **Department of Physics**

Syllabus

**M.Sc. in Physics**

**Semester-III**

**2022 PATTERN**

**Academic Year 2022-2025**

# Anekant Education Society's

TULJARAM CHATURCHAND COLLEGE OF ARTS, SCIENCE AND COMMERCE, BARAMATI

## (Autonomous Status)

(Affiliated to Savitribai Phule Pune University, Pune)

### M.Sc. II Course Structure

#### Semester-III

Course Number	Course Code	Course Name	Credit
1	PSPH 231	STATISTICAL PHYSICS	4
2	PSPH 232	SOLID STATE PHYSICS	4
3	PSPH 233	EXPERIMENTAL TECHNIQUES IN PHYSICS- I	4
4	PSPH 234	<b>CBCS Group I</b> A) NANO TECHNOLOGY I OR B) ENERGY STUDIES-I OR C) BIOPHYSICS-I OR D) PHYSICS OF THIN FILMS-I OR E) ELECTRONIC INSTRUMENTATION-I OR F) DFT -I	4
5	PSPH 235	SPECIAL LAB- I	4
6	PSPH 236	SPECIAL LAB- II PYTHON PROGRAMMING IN PHYSICS	4
<b>Total Credit</b>			<b>24</b>

## Programme Outcomes (POs)

PO1	<b>Disciplinary Knowledge:</b> Demonstrate comprehensive knowledge of the discipline that forms a part of a postgraduate Programme. Execute strong theoretical and practical understanding generated from the specific Programme in the area of work.
PO2	<b>Critical Thinking and Problem solving:</b> Exhibit the skill of critical thinking and understand scientific texts and place scientific statements and themes in contexts and also evaluate them in terms of generic conventions. Identify the problem by observing the situation closely, take actions and apply lateral thinking and analytical skills to design the solutions.
PO3	<b>Social competence:</b> Exhibit thoughts and ideas effectively in writing and orally; communicate with others using appropriate media, build effective interactive and presenting skills to meet global competencies. Elicit views of others, present complex information in a clear and concise way and help reach conclusions in group settings.
PO4	<b>Research-related skills and Scientific temper :</b> Infer scientific literature, build a sense of enquiry and able to formulate, test, Analyse, interpret and establish hypothesis and research questions; and to identify and consult relevant sources to find answers. Plan and write a research paper/project while emphasizing on academics and research ethics, scientific conduct and creating awareness about intellectual property rights and issues of plagiarism.
PO5	<b>Trans-disciplinary knowledge:</b> Create new conceptual, theoretical and methodological understanding that integrates and transcends beyond discipline-specific approaches to address a common problem.
PO6	<b>Personal and professional competence:</b> Perform independently and also collaboratively as a part of a team to meet defined objectives and carry out work across interdisciplinary fields. Execute interpersonal relationships, self-motivation and adaptability skills and commit to professional ethics.
PO7	<b>Effective Citizenship and Ethics:</b> Demonstrate empathetic social concern and equity centered national development, and ability to act with an informed awareness of moral and ethical issues and commit to professional ethics and responsibility.
PO8	<b>Environment and Sustainability:</b> Understand the impact of the scientific solutions in societal and environmental contexts and demonstrate the knowledge of and need for sustainable development.
PO9	<b>Self-directed and Life-long learning:</b> Acquire the ability to engage in independent and life-long learning in the broadest context of socio-technological changes.

# **SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023)**

**Academic Year 2023-2024**

**M. Sc-II (Physics) Semester-III**

## **PSPH 231: STATISTICAL PHYSICS**

**Credit: 04**

**Total No. of Lectures: 60**

### **Course Objectives:**

1. To do the calculation of macroscopic (bulk) properties of pure substances and mixtures from the microscopic properties of the molecules and their interactions.
2. to derive the classical thermodynamics of materials in terms of the properties of their constituent particles and the interactions between them.
3. To provide the information on the nature of statistical errors and variations of thermodynamic parameters.
4. To evaluate the laws of classical thermodynamics for macroscopic systems using the properties of its atomic particles.

### **Course Outcomes:**

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

CO1: Understand the relevant quantities used to describe macroscopic systems, thermodynamic potentials, and ensembles.

CO2: Understand the concepts of statistical errors, partition functions by considering the different types of ensembles.

CO3: Describe the consequences in classical and quantum statistics.

CO4: Understand fermions, bosons and differentiate between FD statistics and BE statistics.

CO5: Show an analytic ability to solve the statistical mechanics problems.

CO6: Explore fluctuations and correlations in statistical systems.

CO7: Understand the connection between classical and quantum statistical mechanics.

### **Unit 1: Statistical Description and Thermodynamics of Particles (1 Credit)**

Specification of the state of the system, Macroscopic and Microscopic states, Phase space, Statistical ensemble, Postulate of equal a priori probability, Probability calculations, Behaviour of density of states, Liouville's theorem(Classical)and constraints, Equilibrium conditions and constraints, Distribution of energy between systems in equilibrium, Approach to thermal equilibrium, Temperature, Heat reservoir, Sharpness of the probability distribution, Dependence of the density of states on the external parameters, Equilibrium between interacting systems, Problems.

**Unit 2: Classical Statistical Mechanics: (1 Credit)**

Ensembles, Micro-canonical ensemble, System in contact with heat reservoir, Canonical ensemble, Applications of canonical ensembles ( Paramagnetism, Molecule in an ideal gas, Law of atmosphere), System with specified mean energy, Calculation of mean values and fluctuations in a canonical ensemble, Grand-canonical ensemble, Physical interpretation of  $\alpha$ , Chemical potential in the equilibrium state, Mean values and fluctuations in grand canonical ensemble, Thermodynamic functions in terms of the Grand partition function, Problems.

**Unit 3: Applications of Statistical Mechanics and Quantum Distribution (1 Credit)**

Calculations of thermodynamic quantities, Ideal monoatomic gas, Gibbs paradox, Equipartition theorem and its Simple applications. i) Mean kinetic energy of a molecule in a gas ii) Brownian motion iii) Harmonic Oscillator iv) Specific heat of solid, Maxwell velocity distribution, Related distributions and mean values Symmetry of wave functions, Quantum distribution functions, Boltzmann limit of Boson and Fermions gases, Maxwell Boltzmann statistics, B-E statistics, F-D statistics, comparison of M-B statistics, F-D statistics, and B-E statistics, Evaluation of the partition function, Partition function for diatomic molecules, Equation of state for an ideal gas, quantum mechanical paramagnetic susceptibility, Problems.

**Unit 4: Ideal Bose and Fermi Systems: (1 Credit)**

Photon gas – i) Radiation pressure ii) Radiation density iii) Emissivity iv) Equilibrium number of photons in the cavity. Einstein derivation of plank's law, Bose-Einstein Condensation, Specific heat, Photon gas – Einstein and Debye's model of solids. Mean energy of fermions at absolute zero, Fermi energy as a function of temperature, Problems.

**Reference books:**

1. Fundamentals of Statistical and Thermal Physics, - F. Reif,
2. Fundamentals of Statistical Mechanics, B.B. Laud, New Age International Publication
3. Statistical Mechanics, R.K. Pathria, Bufferworgh Heinemann (2nd Edition)
4. Statistical Mechanics, K. Huang, John Willey and Sons (2nd Edition)
5. Statistical Mechanics, Satya Prakash and Kedar Nath Ram, Nath Publication (2008)
6. Statistical Mechanics by Loknathan and Gambhir

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3								
CO 2	3								
CO 3	3								
CO 4	3								
CO 5	3	3							
CO 6	3					2			
CO7	3								

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: Understand the relevant quantities used to describe macroscopic systems, thermodynamic potentials, and ensembles.

CO2: Understand the concepts of statistical errors, partition functions by considering the different types of ensembles.

CO3: Describe the consequences in classical and quantum statistics.

CO4: Understand fermions, bosons and differentiate between FD statistics and BE statistics.

CO5: Show an analytic ability to solve the statistical mechanics problems.

CO6: Converse with correct concepts of thermodynamics and statistical mechanics.

CO7: Understand statistics of particles and statistics of fields.

Weightage: 3

All the specified course outcomes directly contribute to acquiring disciplinary knowledge in statistical mechanics.

#### **PO2: Critical Thinking and Problem Solving**

CO5: Show an analytic ability to solve the statistical mechanics problems.

Weightage: 3

The analytic ability to solve problems is a key aspect of critical thinking and problem-solving skills.

#### **PO6: Personal and Professional Competence**

CO6: Converse with correct concepts of thermodynamics and statistical mechanics.

Weightage: 2

Conveying correct concepts in these areas contributes to personal and professional competence.

**M. Sc-II (Physics) Semester-III**  
**PSPH 232: SOLID STATE PHYSICS**

**Credit: 04**

**Total No. of Lectures: 60**

**Course objectives:**

The course gives an introduction to solid state physics and will enable the student to employ classical and quantum mechanical theories needed to understand the physical properties of solids.

**Course outcomes:**

After successful completing this course, the student will be able to

CO1: Explain mechanical, electrical, and magnetic properties of solid matter, and connect these to bond type.

CO2: Explain simple theories for conduction of heat and electrical current in metals.

CO3: Know the basic physics behind dia, para and ferromagnetism.

CO4: Critically evaluate the approximations needed to build models to understand the solid state.

CO5: Explore the behaviour of magnetic materials, including ferromagnetism, antiferromagnetism, and Paramagnetism.

CO6: Study the phenomenon of superconductivity and the properties of superconducting materials.

CO7: Understand the BCS theory and the Meissner effect.

**Unit 1: Band Theory of Solids**

**(1 Credit)**

Introduction, Nearly free electron model, DC and AC electrical conductivity of metals, Bloch theorem (with proof), Kronig-Penney model, Motion of electron in 1-D according to band theory, Distinction between metals, insulators and intrinsic semiconductors, Reduced, periodic & extended zone schemes, Cyclotron resonance, Quantization of electronic orbit in a magnetic field.

The electrical conductivity at low temperature, The thermal conductivity of metals, Dielectric Properties of insulators. Macroscopic electrostatic Maxwell equations, Theory of Local Field, Theory of polarizability, Clausius- Mossotti relation, Long- wavelength optical modes in Ionic crystals.

**Unit 2: Diamagnetism and Paramagnetism**

**(1 Credit)**

Introduction, Classical theory of diamagnetism, Langevin theory of Paramagnetism, Quantum theory of Paramagnetism, Paramagnetic susceptibility of conduction electron, Magnetic properties of rare earth ions & iron group ions with graphical representation, Crystal field splitting, Quenching of orbital angular momentum.

**Unit 3: Ferromagnetism, Antiferromagnetism and Ferrimagnetism (1 Credit)**

Introduction, Ferromagnetism: Weiss theory, Curie point, Exchange integral, saturation magnetization and its temperature dependence, Saturation magnetization at absolute zero, ferromagnetic domains, Anisotropy energy, Bloch wall, Quantum theory of ferromagnetism  
Magnetic resonance, Nuclear magnetic resonance (NMR), The resonance condition, Anti ferromagnetism: Neel temperature, Ferrimagnetism: Curie temperature, susceptibility of ferrimagnets.

**Unit 4: Carbon and its oxides (1 Credit)**

**Occurrence of carbon, Allotropes of carbon:** Crystalline, Amorphous

**Bonding in Carbon: Carbon nanostructure:** Fullerenes, Carbon Nanotube (CNTs), Carbon Nanofiber (CNFs), Graphene

**Graphene:** Applications

**Reference Books:**

1. Introduction to solid states Physics - Charles, Kittel 7th Edition
2. Introductory Solid States Physics – H. P. Myers
3. Solid States Physics - S.O. Pillai (latest edition)
4. Elementary Solid States Physics- M. Ali Omar
5. Problem in Solid State Physics – S.O. Pillai
6. Solid States Physics – A.J. Dekkar
7. Solid states Physics – Wahab
8. Solid State Physics: Neil W. Ashcroft, N. David Mermin
9. Solid States Physics – Ibach & Luth
10. Solid States Physics – C. M. Kacchawa
11. Wet Chemical Synthesis of Graphene for Battery Applications - Ida Johansen



## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3								
CO 2		3							
CO 3		3							
CO 4		3							
CO 5		3							
CO 6						2			
CO7									

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: After successfully completing this course, the student will be able to...

Weightage: 3

The course completion objectives directly contribute to acquiring disciplinary knowledge in the field.

#### **PO2: Critical Thinking and Problem Solving**

CO2: Explain mechanical, electrical and magnetic properties of solid matter, and connect these to bond type.

CO3: Explain simple theories for conduction of heat and electrical current in metals.

CO4: Know the basic physics behind dia, para and ferromagnetism.

CO5: Critically evaluate the approximations needed to build models to understand the solid state.

Weightage: 3

All these outcomes involve critical thinking and problem-solving skills in understanding various properties and theories related to solid matter.

#### **PO6: Personal and Professional Competence**

CO6: Defines Bonds in crystals, Inert gas crystals, Van der Waals-London interaction, Repulsive interaction and Binding energy.

Weightage: 2 (Moderate or partial relation)

Justification: Defining various bonds contributes to personal and professional competence, albeit not as directly as other outcomes.

## M. Sc-II (Physics) Semester-III

### PSPH 233: EXPERIMENTAL TECHNIQUES IN PHYSICS- I

**Credit: 04**

**Total No. of Lectures: 60**

#### **Course Objectives:**

1. Mastered the assessment of reasonable experimental uncertainty in a variety of different measurements and understood how to minimize that uncertainty.
2. Rigorously analysed experimental data using accepted error analysis methodologies to verify theoretical predictions.

**Course Outcomes:** On successful completion of this course students will be able to do the following:

CO1: Apply appropriate characterization techniques for microstructure examination at different magnification level and use them to understand the microstructure of various materials.

CO2: Choose and appropriate electron microscopy techniques to investigate microstructure of materials at high resolution.

CO3: Determine crystal structure of specimen and estimate its crystallite size and stress.

CO4: Use appropriate spectroscopic technique to measure vibrational / electronic transitions to estimate parameters like energy band gap, elemental concentration, etc.

CO5: Apply thermal analysis techniques to determine thermal stability of and thermodynamic transitions of the specimen.

CO6: Gain experience in working with high vacuum systems.

CO7: Understand the principles of vacuum technology and its applications in experimental physics.

#### **Unit 1: Vacuum Physics**

**(1 Credit)**

Important and fields applications of vacuum, kinetic theory of gases, impingement rate of molecules on a surface, average velocity of gas and mean free path, gas transport properties (thermal conductivity, viscosity and diffusion), various ranges of vacuum, gas conductance of a vacuum line, gas impedance of a vacuum line, pumping speed, flow of gases through apertures, elbows, tubes etc. for viscous and molecular flow regimes, pump down time, Numericals

#### **Unit 2: Pumps for High Vacuum (HV) and Ultra High Vacuum (UHV)**

**(1 Credit)**

Principles of pumping concept, Types of vacuum pumps: Rotary, Molecular drag, Diffusion, Cryogenic, Getter, Titanium sublimation, Sputter ion, Orbitron

### **Unit 3: Vacuum Measurements and Low Temperature Technique (1 Credit)**

Vacuum Gauges: McLeod, Thermocouple (Pirani), Penning, Hot cathode ionization (triode type), Bayard-Alpert leak detection: simple methods of LD, palladium barrier and halogen leak detectors.

Production of low temperatures: Adiabatic cooling, the Joule-Kelvin expansion, adiabatic demagnetization, <sup>3</sup>He cryostat, the dilution refrigerator, principle of Pomeranchuk cooling, principle of nuclear demagnetization; measurement of low temperatures. (Throttling process)

### **Unit 4: Atomic Absorption Spectrometry (1 Credit)**

Fundamentals: principle, basic equipment, operation, monochromator action, modulation; apparatus: double beam instrument, radiation sources, aspiration and atomization; interferences, control of AAS parameters, reciprocal sensitivity and detection limit techniques of measurement : routine procedure, matrix matching method

#### **References:**

1. Instrumentation: Devices and Systems, C.S. Rangan, G.R. Sarma and V.S.V. Mani, Tata Mc Graw Hill Publishing Co. Ltd.
2. Hand Book of Thin Film Technology, Maissel and Glange
3. Vacuum Physics and Techniques, T. A. Delchar, Chapman and Hall
4. Vacuum Technology, A. Roth, (North Holland, Elsevier Science B.V. 1990)
5. High Vacuum Techniques, J. Yarwood, (Chapman and Hall, Londong, 1967)
6. Experimental Principles and Methods below 1K, O. U. Lounasmaa, (Academic Press, Londonand, New York, 1974)
7. Thermometry at Ultra Low Temperatures, W. Weyhmann 10. Methods of Experimental Physics, Vol. II (R. V. Coleman, Academic Press, New York and London, 1974)
8. Cryophysics, K. Mendelssohn, Interscience (London, 1960)
9. Optical trapping and manipulation of neutral particles usinglasers, by Arthur Ashkin, Proceeding of National Academy of Sciences May 13, (1997) (4 (10) 4853-4860.
10. Atomic absorption spectroscopy - B.Welz (Verlag Chemie, New York) 1976.
11. Atomic absorption spectroscopy- R.J. Reynolds,K.Aldous & K.C. Thompson (CharlesGriffin and company Ltd. London) 1970.

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3								
CO 2		3							
CO 3		3							
CO 4		3							
CO 5				2					
CO 6				2					
CO7									

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: Learn to operate and implement tools and techniques used by experimental physicists in their research.

Weightage: 3

Learning to operate experimental tools and techniques is a fundamental aspect of acquiring disciplinary knowledge in experimental physics.

#### **PO2: Critical Thinking and Problem Solving**

CO2: Put the scientific process into practice by forming hypotheses, designing experiments, taking and analysing data relevant to the experiment, and using this data to form concrete, well-supported conclusions.

CO3: Mastered the assessment of reasonable experimental uncertainty in a variety of different measurements and understood how to minimize that uncertainty.

CO4: Rigorously analysed experimental data using accepted error analysis methodologies to verify theoretical predictions.

Weightage: 3

All these outcomes involve critical thinking and problem-solving skills in the context of experimental design, data analysis, and error assessment.

#### **PO4: Research-related Skills and Scientific Temper**

CO5: Developed scientific presentation skills.

CO6: Learned to efficiently search the scientific literature and critically assess the scientific merit of what they read.

Weightage: 2

Developing presentation skills and efficiently searching and critically assessing scientific literature contribute to research-related skills and scientific temper.

**M. Sc-II (Physics) Semester-III**  
**PSPH 234 (A): NANO TECHNOLOGY I**

**Credit: 04**

**Total No. of Lectures: 60**

**Course objectives:**

After completing this course students will be able to:

1. Learn about the background on Nanoscience
2. Understand the synthesis of nanomaterials and their application and the impact of nanomaterials on environment
3. Apply their learned knowledge to develop Nanomaterial's.

**Course outcomes:**

After successful completing this course, the student will able to

CO1: To understand the nature and properties of nanomaterials.

CO2: To provide scientific understanding of application of nanomaterials and nanotechnology in agriculture, health and environmental conservation.

CO3: To foundational knowledge of the Nanoscience and related fields.

CO4: To make the students acquire an understanding the Nanoscience and Applications

CO5: To help them understand in broad outline of Nanoscience and Nanotechnology

CO6: Build models to understand the physical properties of different nano materials

CO7: Critically evaluate the approximations needed to build models to understand the solid state.

**Unit 1: Science at Nano scale**

**(1 Credit)**

**Nano and Nature:** Nanoscopic colours (Butterfly wings), Bioluminescence (fireflies), Tribology (Gecko's Sticky Feet, Nasturtium Leaf-Lotus effect etc) in nature.

**Classification of nano materials:** 0D,1D,2D and 3D and types of nano materials (QDs, QW, CNT's, Bucky Balls, Nano composites etc)

**Nano science:** Quantum mechanics, Brownian motion, surface forces, surface to volume ratio

**Making of nanostructures:** Top down Overview of top down nano fabrication processes. Mechanical grinding (ball milling)

**Making of nano structures:** Bottom up, overview of bottom up nanofabrication processes Solid state phase synthesis

## **Unit 2: Physical Properties of Nano materials**

**(1 Credit)**

### **Surface Properties:**

Surface energy – chemical potential as a function of surface curvature-Electrostatic stabilization- surface charge density-electric potential at the proximity of solid surface-Van der Waals attraction potential

### **Mechanical properties**

Melting point and lattice constants, Electrical conductivity (Surface scattering, Change of electronic structure, quantum transport).

### **Magnetic properties of Nano materials**

Origin of magnetism in materials, Classification into Dia-, Para- and Ferro-magnetic materials, Hysteresis in ferromagnetic materials, domains, soft and hard magnetic materials, Coercivity vs particle size

## **Unit 3: Nano structured materials**

**(1 Credit)**

### **Nano ceramics:**

Dielectrics, ferroelectrics and magneto ceramics, Magnetic properties

### **Nano polymers:**

Preparation and characterization of di block Copolymer based Nano composites, Nanoparticles polymer ensembles; Applications of Nano polymers

### **Nano composites:**

Metal-Metal nano composites, Polymer-Metal nano composites, Ceramic nano composites

### **Special Nano materials:**

Graphene, Carbon nano tubes and Types (CNT), Fullerenes, Aerogels, Core Shell Nanostructures.

## **Unit 4: Synthesis techniques of Nano materials**

**(1 Credit)**

### **Physical methods:**

Vacuum Techniques (i) Thermal evaporation methods: Resistive heating, Electron Beam Evaporation, (ii) Sputtering system: Glow discharge, DC sputtering, Radio frequency sputtering, Magnetron sputtering, Ion beam sputtering.

### **Chemical Methods:**

Chemical bath deposition: Ionic and solubility products, Preparation of binary semiconductors, Electrochemical deposition: Deposition mechanism and Preparation of compound thin films, Spray pyrolysis: Deposition mechanism and preparation of compound thin films.

## Reference books:

- 1 Nanotechnology principle and practices by Sulabha K. Kulkarni (2007).
- 2 Klabunde, K.J. (Ed.), "Nanoscale Materials in Chemistry", John Wiley & Sons Inc. 2001
- 3 Nalwa, H.S. (Ed.), "Encyclopedia of Nanoscience and Nanotechnology" 2004
- 4 Sergeev, G.B. Nanochemistry, Elsevier, B.V. 2010
- 5 Schmid, G. (Ed.), "Nanoparticles", Wiley-VCH Verlag GmbH & Co. KgaA.2004
- 6 Rao, C.N.R., Müller, A. and Cheentham, A.K. (Eds.), "Chemistry of Nanomaterials",  
Wiley – VCH. 2005
- 7 Carbon Nanotubes: Properties and Applications- Michael J. O'Connell.
- 8 Carbon Nanotechnology- Liming Dai.
- 9 Nanotubes and Nanowires- CNR Rao and A Govindaraj RCS Publishing.

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3								
CO 2					2				
CO 3	3								
CO 4	3								
CO 5	3								
CO 6		3							
CO7		3							

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: To understand the nature and properties of nanomaterials.

CO3: To foundational knowledge of Nanoscience and related fields.

CO4: To make the students acquire an understanding of Nanoscience and Applications.

CO5: To help them understand the broad outline of Nanoscience and Nanotechnology.

Weightage: 3

All these course outcomes directly contribute to acquiring disciplinary knowledge in the field of Nanoscience.

#### **PO2: Critical Thinking and Problem Solving**

CO6: Build models to understand the physical properties of different nanomaterials.

CO7: Critically evaluate the approximations needed to build models to understand the solid state.

Weightage: 3

Building models and critically evaluating approximations involve critical thinking and problem-solving skills, especially in the context of nanomaterials and solid-state physics.

#### **PO5: Trans-disciplinary Knowledge**

CO2: To provide a scientific understanding of the application of nanomaterials and nanotechnology in agriculture, health, and environmental conservation.

Weightage: 2

Understanding the application of nanomaterials in diverse fields contributes to trans-disciplinary knowledge.



**M.Sc. II (Physics) Semester III**

**PSPH 234 (B): ENERGY STUDIES-I**

**Credit: 04**

**Total No. of lectures: 60**

**Course Objectives:**

1. To create awareness about use of renewable energy sources.
2. To develop the technologies have low cost.
3. To create surrounding without pollution.
4. To use the hydrogen as clean source of energy.
5. To use storage devices like batteries and super capacitors.
6. To foster scientific attitude, provide in-depth knowledge of scientific and technological concepts of Physics.
7. To familiarize with recent scientific and technological developments.
8. To create foundation for research and development in Physics.
9. To help students to build-up a progressive and successful career in Physics.

**Course Outcomes:**

After completion of the course, the student should be able to:

CO1: Describe environmental impacts of renewable sources of energy.

CO2: Describe hydrogen as clean sources of energy.

CO3: Understand the concept of superconductors and fuel cell energy resources.

CO4: Understand the batteries and super capacitors.

CO5: Understand the challenges and solutions for integrating renewable energy sources into existing energy grids.

CO6: Explore the role of energy storage and grid management in facilitating renewable energy integration.

CO7: Explore methods for promoting energy literacy and awareness.

**Unit 1: Environmental Impacts of Renewable Energy Sources**

**(1 Credit)**

Energy flow diagram to the earth, Carbon cycle, Ecological Niche, Green house effect. Energy Consumption in India, Environmental degradation due to conventional energy production and utilization: Asian Brown Cloud Effect, Environmental impacts of Biomass energy, solar energy systems, wind energy and ocean thermal energy. Power co-generation.

**Unit 2: Hydrogen as clean source of Energy****(1 Credit)**

Sources of hydrogen, Thermodynamics of water splitting, Hydrogen production methods, Photo electrolysis of water, Direct decomposition of water, Thermochemical production of hydrogen; Hydrogen storage methods: Conventional, Liquid Hydrogen storage, Metal Hydrides, and Cryo-adsorbing storage.

**Unit 3: Superconductors and Fuel Cell Technology****(1 Credit)**

Cuprates and  $MgB_2$  superconductors and their properties, superconducting wires, Role of superconductor in Electric generator, Magnetic energy storage devices and power transmission. Working principle of fuel cell, Components of fuel cell, EMF of fuel cell and polarization in fuel cells, Types of fuel cells, Advantages and disadvantages of fuel cell, Power generation with fuel cells.

**Unit 4: Batteries and Supercapacitors****(1 Credit)**

Energy storage systems, Faradaic and non-Faradaic processes, Types of capacitors and batteries, Comparison of capacitor and battery, Charge discharge cycles, experimental evaluation using Cyclic voltammetry and other techniques, Energy and entropy stored by capacitor, Electrochemical behaviour of  $RuO_2$ ,  $IrO_2$  and mixed oxides, Energy density and power density, Applications for electric vehicle drive systems.

**Reference Books :**

- 1) Biological paths to self reliance- Russell E. Anderson.
- 2) Encyclopedia of Environmental Energy Resources- G.R. Chhatwal Vol. 1 & 2.
- 3) Renewable Energy Sources and their Environmental Impacts- S.A. Abbasi & N. Abbasi.
- 4) Electrochemical supercapacitors by B. E. Conway, Kluwer Academic Press.
- 5) Hydrogen as an Energy Carrier- T. Carl-Jochen Winter, Joachim Nitsch (eds.)
- 6) Advances in Renewable Energy Technologies- S.H. Pawar, and L. A. Ekal (eds.)
- 7) Handbook of Batteries and Fuel Cells- David Linden.

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3								
CO 2	3								
CO 3	3								
CO 4	3								
CO 5		3							
CO 6		3							
CO7	3								

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: Describe environmental impacts of renewable sources of energy.

CO2: Describe hydrogen as clean sources of energy.

CO3: Understand the concept of superconductors and fuel cell energy resources.

CO4: Understand the batteries and supercapacitors.

CO7: Explain the field applications of solar energy.

Weightage: 3

All these course outcomes directly contribute to acquiring disciplinary knowledge in the field of renewable energy.

#### **PO2: Critical Thinking and Problem Solving**

CO5: Perform an initial design of a renewable energy system.

CO6: Use laboratories and emulators of renewable energy systems to analyze relevant issues.

Weightage: 3

Performing a design and analysing issues related to renewable energy systems involve critical thinking and problem-solving skills.

#### **PO8: Environment and Sustainability**

CO1: Describe environmental impacts of renewable sources of energy.

Weightage: 2

Describing environmental impacts aligns with the environmental and sustainability aspect of PO8.

**M. Sc-II (Physics) Semester-III**  
**PSPH 234 (C): BIOPHYSICS-I**

**Credit: 04**

**Total No. of Lectures: 60**

**Course Objectives:**

The main aim of biophysics is to understand biological systems, while the aim of bioengineering is to make practical devices.

1. The perspective that biological processes can be understood from the interactions between and within the constituent molecules.
2. Students demonstrate the ability to analyze scientific problems, generate logical hypotheses, evaluate evidence, and tolerate ambiguity.
3. Students demonstrate the ability to apply knowledge of biophysics in one area to make appropriate intellectual connections and solve problems in other areas of biophysics or other fields.

**Course Outcomes:** Upon completion of the course, the student will be able to,

CO1: Understand Basic Structure of Cell

CO2: Identify Biophysical Techniques

CO3: Properties and their significance

CO4: Working of Nervous System

CO5: Apply the knowledge of Physics in Living things.

CO6: Understand the principles of electrical signalling in biological systems, including nerve impulses and action potentials.

CO7: Understand the role of biophysics in the study of sensory receptors and signal transduction.

**UNIT 1: Introduction of Biophysics**

**(1 Credit)**

History of Biophysics, Concept of Biophysics and Physical properties applied to biology- Surface tension, Viscosity, adsorption, diffusion, osmosis, Definition for Biostatistics and Biometry, Cell: Animal and plant cell, types of cell, Functional aspects of cell membrane, cytoplasm, nucleus, mitochondria and chloroplast, Protein structure (Primary and Secondary), amino acid structure, Genetic code- symmetry, DNA structure, Photosynthesis process:- electron transport, Gibbs's free energy, Redox couple, Redox potential, Oxidation and reduction, Examples of redox potential in biological system.

**UNIT 2: Bio-potentials****(1 Credit)**

Bioelectric signals: structure of neuron, resting potential, action Potential, Nernst equation, Bioelectrodes- Half-cell potential, polarizable and non-polarizable electrodes, Microelectrode- metal and glass electrode, Study of Cardiovascular system, Compound action potential of human body-ECG (Electrocardiography), Electrodes for ECG

**UNIT 3: Bio-instruments****(1 Credit)**

Basic principle, Construction and working of colorimeter, spectrophotometer, PH meter and Centrifuge measurement. Electron Microscope: SEM, TEM.

**UNIT 4: Radiation Biophysics****(1 Credit)**

Definition, Units of Radioactivity and radiation doses, Types of radiation (Ionizing and non-ionizing), radio immunoassays. Applications: PET (Positron Emission Tomography), NMR (Nuclear Magnetic Resonance), MRI (Magnetic Resonance Imaging Techniques), Ultrasonography, CT (Computed Tomography) Scan.

**Reference books:**

1. Introduction to Biophysics - by P. Narayanan .New Age P.
2. Medical Instrumentation - by Khandpur, TMH
3. Laboratory Manuals of Biophysics Instruments - by P.B. Vidyasagar
4. Biophysics -by Vatsala Piramal, Dominant Publisher and Distributors, New Delhi-110002
5. Textbook of Biophysics - by R.N. Roy
6. Photosynthesis - by Hall and Rao.
7. Introduction to Biomedical Equipment Technology (Fourth Edition) by-Joseph J.Carr
8. Text Book of Bio-medical Electronics-by S.S. Agrawal

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3								
CO 2				2					
CO 3		3							
CO 4		3							
CO 5	3								
CO 6									
CO7	3								

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: Foundations: Examine biophysical scenarios using both a conceptual understanding of the core concepts of biology, chemistry, and physics, and calculations using the appropriate methods of mathematical, theoretical, and computational physics.

CO5: The studies also include awareness of various radiation disasters across the world.

CO7: This course is included to discuss the principles of radioactivity and different sources of radiation.

Weightage: 3

All these course outcomes contribute significantly to acquiring disciplinary knowledge in biophysics and radiation physics.

#### **PO2: Critical Thinking and Problem Solving**

CO3: Experimental Methods: Devise, implement, and refine an experiment to assess biophysics questions using appropriate statistical and computational methods to interpret the data and draw valid scientific conclusions.

CO4: Applications: Apply their physics and biophysics experience and knowledge to analyze new biophysical situations and to develop and refine experimental methods for new biophysical applications.

Weightage: 3

These outcomes involve critical thinking and problem-solving skills in the context of experimental design, data analysis, and application of biophysics knowledge.

#### **PO4: Research-related Skills and Scientific Temper**

CO2: Scientific Communication: Effectively communicate biophysics content through both written reports and oral presentation.

Weightage: 2

Effective scientific communication contributes to research-related skills and scientific temper.

**M. Sc-II (Physics) Semester-III**  
**PSPH 234 (D): PHYSICS OF THIN FILMS**

**Credit: 04**

**No. of Lectures: 60**

**Course objectives:**

1. This course introduces students to thin film growth methodologies, to the chemical and physical mechanisms that control thin film deposition and to the applications of thin film growth for the engineering of multilayer thin film structures.
2. Evaluate and use models for nucleating and growth of thin films.

**Course Outcomes:**

CO1: To understand the principle, differences and similarities, advantages, and disadvantages of different thin film deposition Techniques.

CO2: To understand and evaluate and use models for understanding nucleation and growth of thin films.

CO3: To understand about different instrumentation techniques and to analyze thin film properties to apply for various applications.

CO4: To improve problems solving skills related to evaluation of different properties of thin films.

CO5: Problem solving ability

CO6: Critical analysis

CO7: Discuss the differences and similarities between different vacuum based deposition techniques

CO8: Evaluate and use models for nucleating and growth of thin films

CO9: Asses the relation between deposition technique, film structure, and film properties

**Unit 1: Introduction to thin films**

**(1 Credit)**

Overview of vacuum techniques, Comparison of thin and thick films, Theory of growth of thin films: Nucleation, condensation, Frank-Van der Merwe model, Volmer-Weber model, Stranski-Krastanov model, Capillarity model, Atomistic model, comparison of models, various stages of film growth.

**Unit 2: Deposition Techniques and Measurement of thickness**

**(1 Credit)**

Physical methods: Vacuum Techniques (i) Thermal evaporation methods: Resistive heating, Electron Beam Evaporation, (ii) Sputtering system: Glow discharge, DC sputtering, Radio frequency sputtering, Magnetron sputtering, Ion beam sputtering. Chemical Methods: Chemical vapor deposition system (CVD), Chemical bath deposition: Ionic and solubility products,

Preparation of binary semiconductors, Electrochemical deposition: Deposition mechanism and Preparation of compound thin films, Spray pyrolysis: Deposition mechanism and preparation of compound thin films. Doctor blade technique, Dip coating and Spin coating, Photolithography, Electron–beam deposition, Pulsed Laser Ablation, Tolansky technique, Talystep (styles) method, Quartz crystal microbalance, Stress measurement by optical method, Gravimetric method.

### **Unit 3: Properties of thin films**

**(1 Credit)**

Electrical Properties: Source of Resistivity in Metallic conductors, Influence of thickness on the resistivity of thin films, Hall Effect & Magnetoresistance in thin films, Fuch-Sondhemir theory, TCR and its effects. Mechanical properties: Adhesion & its measurement with mechanical and nucleation methods, stress measurement by using optical method. Optical properties: Absorption and transmission.

### **Unit 4: Applications of Thin Films**

**(1 Credit)**

Resistors, capacitors, Junction devices (Metal semiconductor junction) Solar cells, ICs, Optical coating, Thin film sensors (gas and humidity), Thin films for information storage, electro acoustics and telecommunication.

### **Reference books:**

1. Hand book of Thin Film Technology: Maissel and Glang, (Mc Graw Hill)
2. Thin Film Phenomena: K. L. Chopra, (Mc Graw Hill)
3. Material Science of Thin Films: M. Ohring, (Academic Press)
4. Thin Film Process: J. L. Vossen and Kern, (Academic Press)
5. Vacuum Technology (2 nd revised edition), A. Roth, (North Hollad)



## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9
CO 1	3			2					
CO 2	3					2			
CO 3	3					2	3	2	
CO 4									
CO 5		2							
CO 6									
CO7			2		2				
CO8		3		2					2
CO9		3							

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: To understand the principle, differences and similarities, advantages, and disadvantages of different thin film deposition Techniques. Weightage: 3

Acquiring technical skills in a laboratory setting is fundamental to building disciplinary knowledge.

CO2: To understand and evaluate and use models for understanding nucleation and growth of thin films. CO3: To understand about different instrumentation techniques and to analyze thin film properties to apply for various applications. Weightage: 3

Creating experimental models for better understanding involves disciplinary knowledge and direct application, indicating a strong relationship. Weightage: 3

Visualizing and experiencing abstract concepts directly contribute to disciplinary knowledge.

#### **PO2: Critical Thinking and Problem Solving**

CO8: Evaluate and use models for nucleating and growth of thin films: 3

CO9: Asses the relation between deposition technique, film structure, and film properties.

Weightage3

Critical thinking is essential in use models for nucleating and growth of thin films and interpreting Assess the relation between deposition technique, film structure, and film properties

CO4: To improve problems solving skills related to evaluation of different properties of thin films.

CO5: Problem solving ability Weightage: 2

Applying knowledge in project work involves problem-solving skills, but the link may not be as direct as in other cases.

#### **PO3: Social Competence**

CO7: Discuss the differences and similarities between different vacuum based deposition techniques. Weightage: 3

Collaborative learning and teamwork in a laboratory setting directly contribute to social competence.

**PO4: Research-related Skills and Scientific Temper**

CO1: To understand the principle, differences and similarities, advantages, and disadvantages of different thin film deposition Techniques. Weightage: 2

Acquiring technical skills can be part of research-related skills, but the link may not be as direct.

CO8: Evaluate and use models for nucleating and growth of thin films. Weightage: 2

Evaluate and use models can be part of developing a scientific temper, but the link may not be as strong.

**PO5: Trans-disciplinary Knowledge**

CO7: Discuss the differences and similarities between different vacuum based deposition techniques. Weightage: 2

Collaborative learning and teamwork contribute to trans-disciplinary knowledge, but the link may not be as strong.

**PO6: Personal and Professional Competence**

CO2: To understand and evaluate and use models for understanding nucleation and growth of thin film Weightage: 2

Collaborative learning and teamwork contribute to personal and professional competence, though the link may not be as direct.

CO3: To understand about different instrumentation techniques and to analyze thin film properties to apply for various applications.

Collaborative learning and teamwork contribute to personal and professional competence, though the link may not be as direct.

**PO7: Effective Citizenship and Ethics**

CO2: To understand and evaluate and use models for understanding nucleation and growth of thin films. Weightage: 3

Understanding laboratory procedures, especially safety and scientific methods, directly contributes to effective citizenship and ethics.

**PO8: Environment and Sustainability**

CO3: To understand about different instrumentation techniques and to analyze thin film properties to apply for various applications. Weightage: 2

Adhering to laboratory safety procedures can indirectly contribute to considerations of environment and sustainability.

**PO9: Self-directed and Life-long Learning**

CO8: Evaluate and use models for nucleating and growth of thin film. Weightage: 2

Applying knowledge in project work is relevant to self-directed and life-long learning, though the link may not be as direct.

## M. Sc-II (Physics) Semester-III

### PSPH 234 (E): ELECTRONIC INSTRUMENTATION-I

**Credit: 04**

**Total No. of Lectures: 60**

**Course Outcomes:** After successful completion of this course the students will be able to-

CO1: Understand the principles and functions of different instruments.

CO2: Use different instruments for measurement of various parameters.

CO3: Design experiments using sensors.

CO4: Recognize the importance of instrumentation in various engineering and scientific applications.

CO5: Study various types of sensors and transducers.

CO6: Understand the working principles and characteristics of different sensor.

CO7: Learn techniques for conditioning and processing electrical signals from sensors.

#### **Unit 1: General Background and Measurements**

**(1 Credit)**

General configuration and functional description of measuring instruments with examples of instruments and their functional description. (Ref.1: #2.1 to 2.4).

Input output configuration of measuring instruments, and methods of correction of unwanted inputs. (Ref.1: #2.5) Qualities of measurements (Ref.9 Ch# 1) I] Static characteristics II] Dynamic characteristics: Generalized mathematical model of measurement System, III] Order of instruments: zero, first and second order. (Ref.1: #3.3 94 to 115 & 123 to131) Errors in measurement, Types of errors, sources of errors (Ref.9)

**References: 1, 3, 8**

#### **Unit 2: Transducers**

**(1 Credit)**

Displacement Measurement: a) Resistive Transducers (variable resistance, Strain gauges, Electrical strain gauges), b) Inductive transducers (LVDT, variable reluctance ), c) Capacitive transducers

Pressure Measurement: a) Non-Elastic pressure transducers (Barometer, Manometer) b) Elastic pressure transducers (Diaphragm, Bellows, Bourdon gauge), c) Electrical pressure transducers (Piezoelectric transducer)

Temperature Measurement: a) Electrical Method (RTD, Platinum resistance thermometer, Thermistor), b) Thermocouple EMF measuring Circuit, c) Non-contact Type (Semiconductor temperature sensors, Radiation pyrometers)

**References: 8**

#### **Unit 3: Signal Conditioners, Data acquisition and conversion**

**(1 Credit)**

Signal conditioners: Op-amps, instrument amplifier, bridge, phase sensitive detector

Data Acquisition System (DAS): DAS, hardware, Single channel DAS, Multi channel DAS

Data Converters: D to A and A to D converters, Data loggers,

**References: 8**

**Unit 4: Indicators, Display system and Oscilloscope****(1 Credit)**

Digital display system and Indicators, Classification of Displays, Light Emitting Diodes (LED) Liquid Crystal Display (LCD), Printers: principle of Laser printers, Cathode Ray Oscilloscope (CRO)

**References: 8****Reference Books:**

1. Measurement systems- applications and design. 4th E. O. Doebelin.
2. Measurement system – applications and design by E.O. Doblin and Manik .
3. Instrumentation, measurement and systems. Nakra and Chaudhary.
4. Electronic Instrumentation and measurement techniques by A. D. Helfrick and W. D. Cooper. (Pearson.)
5. Instrumentation, devices and systems. Rangan, Mani and Sarma Prentice Hall of India.
6. Process controlled instrumentation by C. D. Johnson.
7. Sensors and transducers. Patrabis.
8. Electronics Instrumentation. Kalsi (Tata McGraw-Hill)

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9
CO 1	3								
CO 2	3								
CO 3		3	2						
CO 4	3			3					
CO 5				3					
CO 6		3		3					
CO7	3								

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: Understand the principles and functions of different instruments.

CO2: Use different instruments for measurement of various parameters.

CO4: Develop the knowledge of theoretical and mathematical principles of electrical measuring instruments.

CO7: Develop the knowledge of theoretical and mathematical principles of electrical measuring instruments.

Weightage: 3

These outcomes directly contribute to acquiring disciplinary knowledge in the field of instrumentation and electrical measurements.

#### **PO2: Critical Thinking and Problem Solving**

CO3: Design experiments using sensors.

CO6: Set up testing strategies to evaluate performance characteristics of different types of sensors and transducers and develop professional skills in acquiring and applying the knowledge outside the classroom through the design of a real-life instrumentation system.

Weightage: 3

Designing experiments and setting up testing strategies involve critical thinking and problem-solving skills in the context of instrumentation and sensor applications.

#### **PO3: Social Competence**

CO3: Design experiments using sensors.

Weightage: 2 (moderate or partial relation)

Justification: While CO3 primarily focuses on the technical aspect of designing experiments using sensors, it indirectly contributes to social competence by fostering collaborative and communicative skills when working in a team setting.

**PO4: Research-related Skills and Scientific Temper**

CO4: Recognize the importance of instrumentation in various engineering and scientific applications.

CO5: Study various types of sensors and transducers.

CO6: Understand the working principles and characteristics of different sensors.

Weightage: 3 (strong or direct relation)

Justification: CO4 emphasizes the recognition of instrumentation's significance in scientific applications, while CO5 and CO6 delve into research-related skills by studying various types of sensors and understanding their working principles.

**M.Sc. II (Physics) Sem-III**  
**PSPH 234 (F): Density Functional Theory -I**

**Credit: 04**

**Total no. of Lectures: 60**

**Learning Objectives:**

The students will be expected to: explain key concepts in density-functional theory, perform derivations involving density functional,

**Learning Outcomes:**

CO1: The course is designed for materials scientists, chemists, physicists, and applied mathematicians, who are seeking to know both the basic concept and certain advanced topics in density functional theory.

CO2: Density functional theory (DFT) is widely used nowadays in both industry and academia to simulate various properties of materials and molecules, such as electronic properties, crystal structures, and chemical reactions.

CO3: In this course, Students will learn both the theoretical and numerical aspects of DFT.

CO4: We will also learn how to perform DFT calculations on simple.

CO5: Students should gain a solid understanding of the fundamental principles of quantum mechanics, as DFT is based on quantum mechanical principles.

CO6: Practical experience in implementing DFT calculations using computational software packages.

CO7: Ability to review the relevant literature in the field of DFT.

**Unit 1: Basics Of Solids State Physics** **(1 Credit)**

Bravais lattice, reciprocal space, Bloch theorem, and Brillouin zone, Pseudopotentials: norm-conserving pseudopotential, nonlinear core correction, and project-augmented wave technique, Numerical aspects of Kohn-Sham DFT: smearing, k-point sampling, Gaussian basis set, and plane-wave basis set, Geometry optimization: Hellmann-Feynman force, Pulay force, and stress, Ab initio molecular dynamics, Physical meaning of Kohn-Sham eigenvalues, and fractional number of electrons.

**Unit 2: Basic concepts in Density Functional Theory** **(1 Credit)**

Hohenberg-Kohn theorem, Levy-Lieb constrained-search formulation of DFT, Kohn-Sham equation, and spin-polarized DFT.

**Unit 3: Properties of exchange and correlation function** **(1 Credit)**

Exchange correlation functionals: local density approximation, hybrid exchange-correlation functional, self-interaction correction, Orbital-dependent exchange correlation functionals: optimized effective potential, exact exchange, and random phase approximation.

## Unit 4. Applications

(1 Credit)

Installation of quantum espresso, Input file generation of simple material, Input file for k path finder, SCf calculation, NSCf calculation, Band calculations, Dos calculations, PDOS calculation

### References:

1. "Density-Functional Theory of Atoms and Molecules" by Parr and Yang.
2. "The ABC of DFT", by Kieron Burke, <http://dft.uci.edu/doc/g1.pdf>
3. "Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory", Szabo and Ostlund.
4. "A bird's-eye view of density-functional theory" by K Capelle, Brazilian Journal of Physics 36, pp 1318 (2006).
5. "Challenges for Density Functional Theory", Cohen et al., Chemical Review 112, pp 289 (2012).
6. "Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients", Payne et al., Review of Modern Physics 64, pp 1045 (1992).
7. "Orbital-dependent density functionals: theory and applications" Kümmel and Kronik, Review of Modern Physics, 80, pp 3 (2008)
8. "Random-phase approximation and its applications in computational chemistry and materials science", Ren et al., Journal of Materials Science 47, pp 7447 (2012).



## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9
CO 1	3								
CO 2	3								
CO 3	3								
CO 4				2					
CO 5						2			
CO 6		3							
CO7						2			

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: The course is designed for materials scientists, chemists, physicists, and applied mathematicians, who are seeking to know both the basic concept and certain advanced topics in density functional theory.

CO2: Density functional theory (DFT) is widely used nowadays in both industry and academia to simulate various properties of materials and molecules, such as electronic properties, crystal structures, and chemical reactions.

CO3: In this course, students will learn both the theoretical and numerical aspects of DFT.

Weightage: 3

These outcomes directly contribute to acquiring disciplinary knowledge in the field of density functional theory.

#### **PO2: Critical Thinking and Problem Solving**

CO6: Students can solve physics, chemistry, and material science problems with DFT.

Weightage: 3

Solving problems in physics, chemistry, and material science using DFT involves critical thinking and problem-solving skills.

#### **PO4: Research-related Skills and Scientific Temper**

CO4: We will also learn how to perform DFT calculations on simple systems.

Weightage: 2

Performing DFT calculations on simple systems contributes to research-related skills and developing a scientific temper.

#### **PO6: Personal and Professional Competence**

CO5: Students can use DFT software in a high-performance computing environment.

CO7: Students can learn different programs related to DFT.

Weightage: 2

Using DFT software in a high-performance computing environment and learning different programs related to DFT contribute to personal and professional competence.

## M. Sc-II (Physics) Semester-III

### PSPH 236: SPECIAL LAB– II PYTHON PROGRAMMING IN PHYSICS

**Credit: 04**

**No of Practicals: 10**

#### Course Objectives:

1. To understand the object-oriented concepts using Python in problem solving.
2. To understand the fundamentals of Python programming concepts and its applications.
3. To elucidate solving Physics problems using Python programming language
4. To train the students in solving computational physics problems

#### Course Outcomes:

CO1: Apply the knowledge of Physical science to solve complex real-life Physics problems.

CO2: Identify, formulate, review research literature, and analyze complex Physics problems and reaching substantiated conclusions.

CO3: Use research-based knowledge and research methods, including design of experiments, analysis and interpretation of data and synthesis of the information to provide valid conclusion.

CO4: Demonstrate knowledge and understanding of the Physics and Python programming principles and apply these to one's own project work.

CO5: Develop a solid understanding of the Python programming language.

CO6: Apply Python programming to solve physics problems numerically.

CO7: Gain hands-on experience in implementing Monte Carlo simulations using Python.

#### List of Experiments:

1	Write a program of Bisection method of finding a root
2	Write a program of Newton's method of finding a root
3	Write a program that uses the trapezoid method to return the integral of a function over a given range
4	Write a program of Simpson's Method
5	Plot sine and cosine over the range $\{-\pi, \pi\}$
6	Write a program of Runge-Kutta Methods
7	Write a program to find prime number

8	Write simple Python program using operators: a) Arithmetic Operators b) Logical Operators
9	Write a Python program to print out the first N numbers in the Fibonacci sequence
10	A ball is thrown upwards with initial velocity $v_0 = 5\text{m/s}$ and an initial height $y_0 = 3\text{ m}$ . Write a Python program to plot $y(t)$ from $t = 0$ until the ball hits the ground.
11	Program to plot the motion of a mass and spring on a horizontal surface with friction .
12	The number of radioactive atoms that decay in a given time period is proportional to the number of atoms in the sample. Write a program that uses Euler's method to plot $N(t)$ . Have your program also plot the exact solution, $N(t) = N_0 e^{-\lambda t}$ , for comparison.
13	Program to plot the motion of a simple pendulum
14	Program to plot the motion of a spring pendulum
15	Use of Monte Carlo method
16	Program to plot the wave motion

**Additional Activity (Any one Activity equivalent to two experiments)**

Students must perform at least one additional activity out of two activities in addition to eight experiments mentioned above. Total Laboratory work with additional activities should be equivalent to ten experiments.

1. **Simulation/Demonstration/Mini Project**
2. **Industrial Visit / Study Tour / Field visit**

## Mapping of Program Outcomes with Course Outcomes

Course Outcomes	Programme Outcomes								
	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9
CO 1	3								
CO 2		3							
CO 3				3					
CO 4						2			
CO 5					2				
CO 6									3
CO7									3

### Justification

#### **PO1: Disciplinary Knowledge**

CO1: Apply the knowledge of Physical science to solve complex real-life Physics problems.

Weightage: 3

Justification: CO1 directly aligns with the core objective of PO1, which is about applying disciplinary knowledge to solve real-life problems in Physics.

#### **PO2: Critical Thinking and Problem Solving**

CO2: Identify, formulate, review research literature, and analyze complex Physics problems and reaching substantiated conclusions.

Weightage: 3

Justification: CO2 involves critical thinking, problem formulation, and analysis, which directly aligns with the focus of PO2.

#### **PO4: Research-related Skills and Scientific Temper**

CO3: Use research-based knowledge and research methods, including design of experiments, analysis and interpretation of data and synthesis of the information to provide valid conclusion.

Weightage: 3

Justification: CO3 is directly related to research-related skills and the scientific temper emphasized in PO4.

#### **PO5: Trans-disciplinary Knowledge**

CO5: Develop a solid understanding of the Python programming language.

Weightage: 2

Justification: While not directly trans-disciplinary, CO5 introduces a cross-cutting skill (programming) that is applicable in various disciplines.

**PO6: Personal and Professional Competence**

CO4: Demonstrate knowledge and understanding of the Physics and Python programming principles and apply these to one's own project work.

Weightage: 2

Justification: CO4 relates to personal and professional competence by integrating physics and programming skills in project work.

**PO9: Self-directed and Life-long Learning**

CO6: Apply Python programming to solve physics problems numerically.

CO7: Gain hands-on experience in implementing Monte Carlo simulations using Python.

Weightage: 3 for both CO6 and CO7

Justification: CO6 and CO7 contribute to developing skills in self-directed and life-long learning, as they involve applying programming techniques to solve physics problems, fostering continuous learning.