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-IV 2022 PATTERN

Academic Year 2022-2025

Anekant Education Society's

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M.Sc. II Course Structure

Semester-IV

Course		Course Name		Credit
Number				
7	PSPH 241	Nuclear & Particle Physics		4
8	PSPH 242	Material Science		4
9	PSPH 243	Experimental Techniques in Physics-II		4
10	PSPH 244	CB Group –II		4
		A) NANO-TECHNOLOGY-II	OR	
		B) ENERGY STUDIES- II	OR	
		C) BIOPHYSICS-II	OR	
		D) PHYSICS OF THIN FILMS-II	OR	
		E) ELECTRONIC INSTRUMENTATION-II	OR	
		F) DFT-II		
11	PSPH 245	Special Lab-III		4
12	PSPH 246	Project		4
		Total Credit		24

Programme Outcomes (POs)

PO1	Disciplinary Knowledge: 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	Critical Thinking and Problem solving: 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	Social competence: 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	Research-related skills and Scientific temper : 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	Trans-disciplinary knowledge: Create new conceptual, theoretical and
	methodological understanding that integrates and transcends beyond discipline-
	specific approaches to address a common problem.
PO6	Personal and professional competence: 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	Effective Citizenship and Ethics: 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	Environment and Sustainability: Understand the impact of the scientific
	solutions in societal and environmental contexts and demonstrate the knowledge
	of and need for sustainable development.
PO9	Self-directed and Life-long learning: 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) M. Sc-II (Physics) Semester-IV PSPH 241: NUCLEAR PHYSICS

Credit: 04

Total No. of Lectures: 60

Course Objectives:

- 1. Describe the structure of the atom.
- 2. Describe the constituents of the nucleus, and different types of radiation.
- 3. Give definitions of basic nuclear physics terms and units of measure.
- 4. Use a periodic table and chart of the nuclides to identify specific isotopes and elements and their properties.
- 5. Explain the interactions of radiation with matter and the physics of nuclear fission.
- 6. Complete simple calculations using energy and mass relationships, atomic density, and radioactive decay.
- 7. Use the basic laws in determination of particle properties and properties of processes in the subatomic world.
- 8. Describe the particle interactions with matter and basic models of the atomic nucleus.
- 9. Learn the concepts of the radiation detectors and accelerators.
- 10. Describe the Nuclear Physics applications.

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

CO1: Can express the basic concepts of nuclear physics.

CO2: Can tell a chronology of some of the major events in nuclear physics.

CO3: Can express the radioactive decays.

CO4: Can state some quantities characterizing the decay such as half-life, decay constant.

- CO5: Can list the types of decay.
- CO6: Can express the alpha decay.
- CO7: Can express reaction equation and Q values and Energy of alpha particles.
- CO8: Can explain the alpha process by using quantum theory.
- CO9: Can calculate the half-times based on quantum theory.

UNIT 1: General Properties and Concepts of Nuclei

Introduction, Basic properties of nucleus: Composition, charge, size, density of nucleus, Nuclear Angular momentum, Nuclear magnetic dipole moment, Electric quadrupole moment, parity and symmetry, Mass defect and Binding energy, packing fraction, classification of nuclei, stability of nuclei, Problems.

Radioactivity: law of radioactive decay-half life, mean life, Unit of Radioactivity, Alpha Decay: range of Alpha Particles and Geiger-Nuttall law, Range-Energy Relationship, Geiger-Nuttal Law, Beta Decay: Conditions for Spontaneous Emission of β -& β +, Applications of radioactivity, Selection Rules, Origin of Beta Spectrum-Neutrino Hypothesis, Gamma Decay. Problems

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UNIT 2: Nuclear Models, Nuclear Accelerators and Nuclear Detectors

Introduction, Shell model-assumptions and limitations of shell model, liquid drop model, Semiempirical mass formula, Detectors: Gas filled detectors, Ionisation chamber, Geiger-Mueller counter, Scintillation counter, Bubble Chamber, Cloud Chamber, Spark Chamber, Linear Accelerator, Collective Model, problems.

UNIT 3: Reaction Dynamics and Accelerators

Introduction, Reaction Dynamics: Types of Nuclear Reactions, Conservation Laws in Nuclear Reactions, Q value of Nuclear Reaction, Compound Nucleus Hypothesis, Fission and Fusion Reactions, Four Factor Formula General Properties and Concepts of Nuclear Reactors, Reactor Materials, Types of Reactors, List of Different Types of Reactors, Accelerators: Van de Graff, Microtron, Electron & Proton Synchrotron, Pelletron, Cyclotron, Problems.

UNIT 4: Elementary Particle Physics

Classification of Elementary Particles and their Quantum Numbers (Charge, Spin, Parity, Iso Spin, Strangeness, Baryon number, Hypercharge etc.), conservation laws, Classification of Quarks, Their masses and spins, Quark contents of particles, Parity non conservation in weak interactions, Gell-Mann-Nishijima formula.

Reference Books:

- 1. K.S. Krane, Introductory Nuclear Physics, Wiley, India, 1988
- 2. B.L. Cohen, Concepts of Nuclear Physics, Tata McGraw Hill
- 3. I. Kaplan, Nuclear Physics, 2nd Edition, Narosa, New Delhi, 1989
- 4. S.N. Ghoshal, Atomic and Nuclear Physics, S. Chand
- 5. S.B. Patel Nuclear Physics: An Introduction, New Age International, 1991
- 6. D.C. Tayal, Nuclear Physics, Himalaya Publishing House
- 7. R.D. Evans, The Atomic Nucleus, Tata McGraw Hill
- 8. G.F. Knoll, Radiation Detection and Measurement, 3rd Edition, Wiley India
- 9. S.S. Kapoor and V.S. Ramamurthy, Nuclear Radiation Detectors, Wiley Eastern Limited
- 10. R.R. Roy, B.P. Nigam, Nuclear Physics-Theory and Experiment, Wiley Eastern Limited
- 11. Blatt and Weisskopf, Theoretical Nuclear Physics, New York, Wiley
- 12. S. Sharma, Atomic and Nuclear Physics, Pearson Education 2008

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

Justification

PO1: Disciplinary Knowledge

CO1: Can express the basic concepts of nuclear physics. Weightage: 3

This CO directly aligns with the objective of developing disciplinary knowledge in nuclear physics.

PO2: Critical Thinking and Problem Solving

CO2: Can tell a chronology of some of the major events in nuclear physics. Weightage: 2

Understanding the chronological sequence in nuclear physics requires critical thinking skills to analyze and interpret historical events.

CO3: Can express the radioactive decays. Weightage: 3

Expressing radioactive decays involves critical thinking and problem-solving skills related to understanding complex processes.

CO4: Can state some quantities characterizing the decay, such as half-life, decay constant.

Weightage: 3

Calculating quantities like half-life and decay constant involves critical thinking and problemsolving skills.

PO4: Research-related Skills and Scientific Temper

CO5: Can list the types of decay. Weightage: 2

Listing types of decay requires knowledge of research findings and contributes to scientific temper.

CO7: Can express reaction equation and Q values and Energy of alpha particles. Weightage: 3

Expressing reaction equations and understanding Q values involve research-related skills and scientific temper.

PO6: Personal and Professional Competence

CO3: Can express the radioactive decays. Weightage: 2

Expressing radioactive decays contributes to personal and professional competence by building a foundational understanding of nuclear physics.

PO9: Self-directed and Life-long Learning

All COs can be related to this PO to some extent, as they contribute to building a foundation for continuous learning. Weightage: 2

Each CO requires a level of self-directed learning, and the knowledge gained contributes to lifelong learning.

SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023) M. Sc-II (Physics) Semester-IV PSPH 242: MATERIAL SCIENCE

Credit: 04

Total No. of Lectures: 60

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

CO1: Qualitatively describe the bonding scheme and its general physical properties, as well as possible applications.

CO2: Describe physical origin of defects and its effects on various mechanical, electrical, thermal and other properties of the materials.

CO3: Describe resultant elastic properties in terms of its 1D and 2D defects.

CO4: Understand diffusion mechanisms and solve problems related to diffusion processes.

CO5: Understand alloy systems, families of engineering alloys.

CO6: Understand thermodynamic origin of phase diagrams, draw phase diagrams.

CO7: Understand phase diagrams and apply their knowledge of phase diagrams for various applications.

Unit 1: Properties of Materials and Defects in Solids (15L)

Structure, property-processing relationship, Mechanical, electrical, magnetic, thermal, and structural properties.

Point defects - Vacancies, interstitials, non-stoichiometry, substitution, Schottky and Frenkel defects with proofs.

Line defects - Edge and screw dislocations, properties of dislocations – force on dislocation, energy of dislocation, pinned dislocation (These properties with derivation), dislocation density, interaction between dislocations, motion of a dislocation (cross-slip and climb), dislocation generator (Frank Read source).

Surface defects – grain boundaries with explanation of high angle, low angle, tilt and twist boundaries, stacking fault.

Volume defect- twin boundary

Solid Solution - Types of solid solutions (Substitutional and Interstitial), Factors governing solid solubility (Hume - Rothery rule), Atomic size and size factor in solid solutions, Vegard's law.

Unit 2: Diffusion in Solids

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Introduction, types of diffusion, Diffusion mechanism, Fick's first and second laws of diffusion, solution to Fick's second law (without proof, introduction of error function), Factors governing

diffusion, Factors affecting diffusion coefficient (D), Experimental determination of D, Diffusion in oxides and ionic crystals, Applications of diffusion: Corrosion resistance of duralumin, Decarburization of steel, Doping of semiconductors.

Unit 3: Metallurgical Thermodynamics

Revision of laws of thermodynamics, Auxiliary thermodynamic functions, measurement of changes in enthalpy and entropy, Richard's rule, Trouton's rule, Chemical reaction equilibrium, Thermodynamic properties of solutions (mixing processes – Rault's law, activity coefficient; regular solution behaviour – Henry's law), Gibb's phase rule: proof, explanation, and application to single component (H₂O) and binary phase diagram

Unit 4: Phase diagrams and Phase transformations

Phase diagrams: Thermodynamic origin of phase diagrams, Lever rule, Type I (Cu-Ni) phase diagram, Type II (explanation only) phase diagram, Type III (Pb-Sn) phase diagram, Maxima and minima in two-phase regions, Miscibility gaps, Topology of binary phase diagrams (Explanation in short of eutectic, peritectic, Monotectic, eutectoid, peritectoid, syntactic reaction, extension rule), Applications of phase diagrams.

Phase transformation: Introduction, Mechanism of Phase Transformation, kinetics of Solid-state reaction, Nucleation and Growth, Applications of phase transformations.

Reference books:

Elements of Materials Science and Engineering (5th edition) - Lawrence H. Van Vlack, Addison

 Wesley Publishing Co.

2. Materials Science and Engineering - V. Raghvan

3. Physical Metallurgy (Part I) R. W. Cahn and P. Hassen, North Holland Physics Publishing, New York

4. Introduction to Materials Science for Engineers (6th edition) - J.F. Shaekelford and M. K. Murlidhara - Pearson Education

5. Materials Science - Kodgire and Kodgire

6. Materials Science - S L Kakani and Amit Kakani

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Course				Progra	mme Ou	tcomes						
Outcomes	PO 1	PO 1 PO 2 PO 3 PO 4 PO 5 PO 6 PO 7 PO8 I										
CO 1	3											
CO 2		3										
CO 3				2								
CO 4				2								
CO 5					2							
CO 6					2							
CO7						2						

Justification

PO1: Disciplinary Knowledge

CO1: Qualitatively describe the bonding scheme and its general physical properties, as well as possible applications. Weightage: 3

This directly aligns with acquiring disciplinary knowledge in materials science and bonding schemes.

PO2: Critical Thinking and Problem Solving

CO2: Describe the physical origin of defects and its effects on various mechanical, electrical, thermal, and other properties of materials. Weightage: 3

Critical thinking is required to understand the complex relationship between defects and material properties.

PO4: Research-related Skills and Scientific Temper

CO3: Describe resultant elastic properties in terms of its 1D and 2D defects.

CO4: Understand diffusion mechanisms and solve problems related to diffusion processes.

Weightage: 2

Justification: While these outcomes involve research-related skills, they might not directly align with the entire spectrum of scientific temper.

PO5: Trans-disciplinary Knowledge

CO5: Derive various metallurgical thermodynamics equations and functions.

CO6: Understand and apply Gibb's phase rule to various systems of materials.

Weightage: 2

These outcomes involve knowledge that spans multiple disciplines within materials science.

PO6: Personal and Professional Competence

CO7: Understand alloy systems, families of engineering alloys.

Weightage: 2

Understanding alloy systems contributes to professional competence in materials engineering.

SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023) M. Sc-II (Physics) Semester-IV PSPH 243: EXPERIMENTAL TECHNIQUES IN PHYSICS-II

Credit: 04

Total No. of Lectures: 60

Course Objectives:

- 1. The course is to provide a broad overview about different techniques available for structural characterization of various materials systems.
- 2. It is an amalgamation of the science behind these characterization techniques and their application in material systems.
- 3. Students gain knowledge about the principles of various techniques.
- 4. Student acquires knowledge of the different existing experimental techniques for the microstructural and physicochemical characterizations of materials.

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: Radiation Sources and Detectors

Electromagnetic spectrum, Sources of Electromagnetic Radiations: Different types of radiations (γ - rays, X-rays, UV-VIS, IR, microwaves) and their sources, Detectors: γ -rays, X-rays, UV-VIS, IR, microwaves

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Unit-2: Structural Characterization and Thermal Analysis

X-ray Diffraction – Production of X-rays, Types (continuous and characteristics), Bragg's diffraction condition, principle, instrumentation (with filters) and working, Techniques used for XRD – Powder method, Derivation of Scherrer formula for size determination, Neutron Diffraction: Principle, Instrumentation and Working, Thermal analysis: Principle, Instrumentation and Working: Thermo-gravimetric (TGA), Differential Thermal Analysis (DTA), Numericals

Unit-3: Morphological and Magnetic Characterization

Optical Microscopy: Principle, Instrumentation and Working of optical microscope, Electron Microscopy: Principle, Instrumentation and Working of Scanning Electron Microscope (SEM), Field Emission Scanning Electron Microscope (FESEM) –Advantages over SEM, Transmission Electron Microscope (TEM), Selected Area Electron Diffraction (SAED), Probe Microscopy : Principle, Instrumentation and Working of Scanning Tunnelling Microscope (STM) and Atomic Force Microscope (AFM), Magnetic Characterization: Principle, Instrumentation and Working of Vibrating Sample Magnetometer (VSM), Analysis of Hysteresis loop, SQUID Technique : Principle only, Numericals

Unit 4: Spectroscopic Analysis

Spectroscopic characterization (principle, instrumentation and working): Infra-Red (IR), Fourier Transform Infra-Red (FTIR), Ultraviolet-Visible (UV-VIS), Diffused Reflectance Spectroscopy (DRS), X-ray Absorption (XPS), Electron Spin Resonance (ESR), Nuclear Magnetic Resonance (NMR), Raman Spectroscopy, Numericals

References:

1. Nuclear Radiation Detectors, S.S. Kapoor, V. S. Ramamurthy, (Wiley-Eastern Limited, Bombay)

2. Instrumentation: Devices and Systems, C.S. Rangan, G.R. Sarma and V.S.V. Mani, Tata Mc Graw Hill Publishing Co. Ltd.

3. Characterization of Materials, John B. Wachtman and Zwi. H. Kalman, Pub. Butterworth Heinemann (1992)

4. Instrumental Methods of Chemical analysis, G. Chatwal and S. Anand, Himalaya Publishing House

5. Elements of X-ray Diffraction, B. D. Cullity, S. R. Stock, (Printice Hall)

6. Instrumental Methods of Analysis, H. H. Willard, l. L. Merritt, J. A. Dean, CBS Publishers

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Course												
Outcomes	PO 1	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				2								
CO 5				2								
CO 6						3						
CO7						3						

Justification

PO1: Disciplinary Knowledge

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

Weightage: 3

This directly aligns with acquiring disciplinary knowledge in materials science and involves applying techniques for microstructure examination.

PO2: Critical Thinking and Problem Solving

CO2: Choose an appropriate electron microscopy technique to investigate the microstructure of materials at high resolution.

CO3: Determine the crystal structure of a specimen and estimate its crystallite size and stress. Weightage: 3

These outcomes involve critical thinking to choose the right techniques and solve problems related to microstructure and crystallography.

PO4: Research-related Skills and Scientific Temper

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

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

Weightage: 2

These outcomes involve research-related skills and align with a scientific temper, though the connection might not be as direct.

PO6: Personal and Professional Competence

CO6: Demonstrate conceptual understanding of fundamental physics principles.

CO7: Solve physics problems using qualitative and quantitative reasoning, including sophisticated mathematical techniques.

Weightage: 3

These outcomes contribute to personal and professional competence by requiring a deep understanding of physics principles and problem-solving skills.

SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023) M. Sc-II (Physics) Semester-IV PSPH 244 (A): NANOTECHNOLOGY-II

Credit: 04

Total No. of Lectures: 60

Course Objectives:

The course main objective is to enhance critical, creative, and innovative thinking. The course encourages multicultural group work, constructing international 'thinking tanks' for the creation of new ideas. Throughout the course, you will be asked to reflect upon your learning, think "out of the box", and suggest creative ideas. The course is set to encourage the understanding of:

- 1. The importance of nanoscale materials for sensing applications.
- 2. Approaches used for characterizing sensors-based nanomaterials.
- 3. Approaches used for tailoring nanomaterials for a specific sensing application.
- 4. Metallic and semiconductor nanoparticles.
- 5. Organic and inorganic nanotubes and nanowires.
- 6. Optical, mechanical, and chemical sensors based on nanomaterials.
- 7. Hybrid nanomaterial-based sensors.

Course Outcomes:

At the end of the course, the student will be able to

- CO1: To learn basic material science with special, emphasize on nanomaterials.
- CO2: To know about processes in handling polymers and nanostructured materials.
- CO3: To understand various forms of nanomaterials and polymers for special applications.
- CO4: Understand Metal/Ceramic Powder synthesis methods for composite.
- CO5: Understand the environmental impact of nanostructured materials.
- 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: Nano sensors

Introduction to sensors. Characteristics and terminology - static and dynamic characteristics. Micro and nano-sensors, Fundamentals of sensors, biosensor, micro fluids, Packaging and characterization of sensors, Sensors for aerospace and defence. Organic and inorganic nano sensors.

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Unit 2. Nanotechnology enabled devices

Nanomaterials and nanostructured films, Nanoscale electronic and ionic transport. Sensor for biomedical applications. Bioelectronics, Nanoparticle biomaterial hybrid systems for sensing applications. Gas sensor.

Unit 3: Biosensors:

Principles, DNA and nucleotide-based biosensors, Protein-based biosensors, Materials for biosensor applications, Fabrication of biosensor devices, Detection in Biosensors – fluorescence, absorption, electrochemical methods, Techniques used for microfabrication, Future direction in biosensor research.

References:

- 1. Chemical Sensors and Biosensors; Brian, R Eggins; Wiley; New York, Chichester, 2002.
- 2. Biosensors: A Practical Approach, J. Cooper & C. Tass, Oxford University Press, 2004.
- 3. Nanomaterials for Biosensors, Cs. Kumar, Wiley VCH, 2007. 4. Smart Biosensor Technology,

G.K. Knoff, A.S. Bassi, CRC Press, 2006.

List of Practical's:

- 1. Temperature measurement
- 2. Ph measurement
- 3. Humidity Measurement
- 4. Blood pressure measurement
- 5. Blood sugar Measurement
- 6. UV- Vis Absorption, reflection and transmittance
- 7. Gas sensor.
- 8. Water flow meter

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Course Outcomes				Progra	mme Ou	itcomes			
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				2					
CO 5								2	
CO 6						3			
CO7				2					

Justification

PO1: Disciplinary Knowledge

CO1: To learn basic material science with special emphasis on nanomaterials.

Weightage: 3

This aligns directly with acquiring disciplinary knowledge in material science, with a focus on nanomaterials.

PO2: Critical Thinking and Problem Solving

CO2: To know about processes in handling polymers and nanostructured materials.

CO3: To understand various forms of nanomaterials and polymers for special applications.

Weightage: 3

These outcomes require critical thinking in understanding the processes and applications of polymers and nanostructured materials.

PO4: Research-related Skills and Scientific Temper

CO4: Understand Metal/Ceramic Powder synthesis methods for composites.

CO7: To introduce advanced ideas and techniques required in the emergent area of nanotechnology. Weightage: 2

These outcomes involve research-related skills and introduce advanced ideas, contributing to a scientific temper.

PO6: Personal and Professional Competence

CO6: Apply principles of basic science concepts in understanding, analysis, and prediction of matter at the Nano scale.

Weightage: 3

Applying basic science concepts at the Nano scale contributes to personal and professional competence.

PO8: Environment and Sustainability

CO5: Understand the environmental impact of nanostructured materials.

Weightage: 2

Understanding the environmental impact aligns with the broader concepts of environment and sustainability.

SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023) M. Sc-II (Physics) Semester-IV PSPH 244 (B): ENERGY STUDIES-II

Credit: 04

Total No. of Lectures: 60

Learning Objectives:

1. To develop capability to understand the fundamentals of science and energy technology for analysing the engineering problems with futuristic approach.

2. To foster a confident and competent post graduate capable to solve real life practical engineering problems fulfilling the obligation towards society.

3. To nurture and nourish effective communication and interpersonal skill to work in a team with a sense of ethics and moral responsibility for achieving goal.

Course Objectives:

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

CO1: The course providing a basic understanding of theory and practice of various photovoltaic technologies and design concepts.

CO2: To understand the physical principles of the photovoltaic (PV) solar cell.

CO3: Discuss the positive and negative aspects of solar energy in relation to natural and human aspects of the environment.

CO4: Gain knowledge about working principle of various solar energy systems.

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: Photovoltaic converters

Interaction of solar radiations with semiconductors, photovoltaic effect, types of solar cell, equivalent circuit diagram of a solar cell, determination of series resistance (Rs) and shunt resistance (Rsh), ideal properties of semiconductor for use its solar cell, carrier generation and recombination, dark and illuminated characteristics of solar cell, solar cell output parameters: RL, Voc, Isc, Pm, FF, efficiency, performance dependence of a solar cell on band gap energy, diffusion length and carrier life time, Types of heterojunction, construction of energy band diagram of heterojunctions, origin of capacitance in a heterojunction, expression for junction capacitance, Mott – Schottky relation, problems.

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Unit-2: Materials and Solar cell Technology

Fabrication technology of solar cell, Single, poly – and amorphous silicon, GaAs, CdS, Cu2S, CuInSe2, CdTe etc. technologies for fabrication of single and polycrystalline silicon solar cells, amorphous silicon solar cells and tandem cells, solar cell modules, photovoltaic systems, space quality solar cells, dye synthesized solar cell, perovskite solar cell, Different materials used in solar cells, problems.

Unit-3: Photochemical Converters

Semiconductor – electrolyte interface, Helmholtz double layer, Gouy-Chapman model, Stern model, Principle of photoelectrochemical solar cells, conversion efficiency in relation to different material properties, photo electrolysis cell, driving force of photo electrolysis, alkaline fuel cell, semiconductor- septum storage cell, concept of photocatalysis and photo electrocatalysis process, problems.

Unit 4: Thermoelectric Converters

Thermoelectric effects, solid state description of thermoelectric effect, Kelvin's thermodynamic relations, analysis of thermoelectric generators, basic assumptions, temperature distribution and thermal energy transfer for generator, co-efficient of performance for thermoelectric cooling, problems.

References:

- 1. Solar energy conversion: The solar cell, by Richard C. Neville.
- 2. Photoelectrochemical solar cells Suresh Chandra
- 3. Solar energy conversion A. E. Dixon and J. D. Leslie.
- 4. Solar cells Martin A. Green
- 5. Heterojunction and metal semiconductor junctions A.G. Milnes and D. L.Feucht.
- 6. Solid state electronic devices B.G. Streetman.
- 7. Principles of solar engineering Frank Kreith and Janf Kreider.
- 8. Direct energy conversion (4th edition) Stanley W Angrist

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- 1. Recording the amount of sunlight receives throughout a day using Sunshine Recorder
- 2. Bio-gas Production from Kitchen waste.
- 3. Energy Content in Wind.
- 4. Utilizing the latent heat released by the condensing water steam using Solar Still
- 5. Performance evaluation of box type and concentrating type solar cooker
- 6. Find out the kinetics of photocatalytic reaction
- 7. Measure the solar radiation flux density using Pyrometer
- 8. Determining efficiency of lighting system/loads

Course				Progra	mme Ou	itcomes			
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			2					3	
CO 4		3							
CO 5				3					
CO 6				3					
CO7						2			

Justification

PO1: Disciplinary Knowledge

CO1: The course provides a basic understanding of the theory and practice of various photovoltaic technologies and design concepts.

Weightage: 3

This aligns directly with acquiring disciplinary knowledge in photovoltaic technologies and design concepts.

PO2: Critical Thinking and Problem Solving

CO2: To understand the physical principles of the photovoltaic (PV) solar cell.

CO4: Gain knowledge about the working principle of various solar energy systems.

Weightage: 3

Understanding the physical principles and working mechanisms involves critical thinking and problem-solving skills.

PO3: Social Competence

CO3: Discuss the positive and negative aspects of solar energy in relation to natural and human aspects of the environment.

Weightage: 2

Considering the environmental aspects involves an understanding of social and natural contexts, contributing to social competence.

PO4: Research-related Skills and Scientific Temper

CO5: Understand the materials used for energy appliances.

CO6: Apply the concepts of materials required for energy storage and energy generation. To impart knowledge about the concepts of Photovoltaic system.

Weightage: 3

These outcomes involve research-related skills and align with a scientific temper in understanding materials for energy systems.

PO6: Personal and Professional Competence

CO7: Understand the material used for energy appliances. Weightage: 2 Understanding materials for energy appliances contributes to personal and professional competence.

PO8: Environment and Sustainability

CO3: Discuss the positive and negative aspects of solar energy in relation to natural and human aspects of the environment.

Weightage: 3

Understanding the environmental aspects directly aligns with the concepts of environment and sustainability.

SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023) M. Sc-II (Physics) Semester-IV PSPH 244 (C): BIOPHYSICS-II

Credit: 04

Total No. of Lectures: 60

Course Objectives:

This course aims to introduce Biophysics:

- 1. To study the basic concepts regarding Cellular and Molecular Biology
- 2. To impart knowledge about Biophysical Techniques
- 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: Basics of Biophysics

Introduction to Biophysics, General organization of prokaryotic and eukaryotic organisms' basic concepts and their detailed structure and functions, Cell, Animal and Plant Cell, Types of Cell and its composition, Prokaryotic cell wall, Eukaryotic cell wall, their functions, ribosomes, Physical and biological properties of protoplasm. Cytoskeleton – basic components, properties, and functions in prokaryotic and eukaryotic cells.

Unit 2: Properties of Lipid Membrane

Cell surface charge, Resting membrane potential, Action potential, properties of action potential, Nernst-Plank equation, Hodgkin- Huxely equation, Hodking-Kartz experiment, Voltage clamp, Na+, K+ conductance, Membrane impedance and capacitance, Transmembrane potential, Zeta, stern and total electrochemical potential, Chemical synapse, post synaptic potential, Historical perspective of lipid model systems lipid monolayer. Liposomes: small and large unilamellar and multilamellar vesicles, planner lipid bilayer, Application of liposomes in biology and medicine.

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(15 L)

Unit 3: Molecular Biophysics

Types of Protein structure (Primary, secondary and Tertiary), polypeptide chains, potential energy, hydrogen bonding, hydrophobic interactions, disulfide bonds & ways of pairing, Protein stability, chemical & surface denaturation, primary structure sequencing of polypeptide, α and β -helix, Ramchandran plot, protein folding & misfolding, Types of DNA, properties of DNA & RNA, Nucleotide structure, Base pairing, Genetic code symmetry, Structure& function of water and carbohydrates

Unit 4: Neuro-biophysics

(15 L)

Neuron –structure and function, excitable membrane, Ion channels, Resting membrane potential, Depolarization, Hyper-polarization, Nernst equation, Goldman equation, Passive electrical prop. of neuron, Nerve conduction, Cell equivalent circuits, Synaptic Integration & transmission, Voltage clamp technique, coding of sensory information, MRI Technique, PET (Positron Emission Tomography) Technique, CT (Computed Tomography).

Reference Books:

- 1. Biophysics by G. R. Chatwal, Himalaya Publishing House, Mumbai, (2011)
- 2. Principles of neural science by E. R. Kandel& J. H. Schwatz, Elsevier, North Holland, (1982)
- 3. Neuron to Brain by S. W. Kuffler and J. G. Nichols, SinacuerAsso. Inc., (1995)
- 4. Biophysics by Mohan P. Arora, Himalaya Publishing House, (2012)
- 5. Biophysics An Introduction by Rodney Cotterill, Wiley, (2014)
- 6. Essentials of Biophysics by P. Narayanan, New Age International Publication, (2005)

Mapping of H	Program (Outcomes	with	Course	Outcomes
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Course				Progra	mme Ou	itcomes			
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									
CO 5					2				
CO 6						3			
CO7				3					

Justification

PO1: Disciplinary Knowledge

CO1: Understand Basic Structure of Cell.

Weightage: 3

Acquiring knowledge about the basic structure of a cell is a fundamental aspect of disciplinary knowledge in biology.

PO2: Critical Thinking and Problem Solving

CO2: Identify Biophysical Techniques.

Weightage: 3

Identifying and selecting appropriate biophysical techniques require critical thinking and problemsolving skills.

PO4: Research-related Skills and Scientific Temper

CO3: Properties and their significance.

CO7: Find out structural & molecular properties of different biomolecules.

Weightage: 3

Understanding properties and molecular structures involves research-related skills and aligns with a scientific temper.

PO5: Trans-disciplinary Knowledge

CO5: Apply the knowledge of Physics in Living things.

Weightage: 2

Applying physics knowledge to living things suggests a connection between different disciplines, though it may not be as strong as within the biology domain.

PO6: Personal and Professional Competence

CO6: Understand the basic concept of atomic and molecular structure.

Weightage: 3

Understanding atomic and molecular structures is crucial for personal and professional competence in the field of biology.

SYLLABUS (CBCS) FOR M.Sc. PHYSICS (W.E.F. June 2023) M. Sc-II (Physics) Semester-IV PSPH 244 (D): PHYSICS OF THIN FILMS-II

Credit: 04

Total No. of Lectures: 60

Course Objectives

1.To make the students to understand about the difference between bulk and thin film, the optical, electrical, dielectric, and magnetic properties of thin film, the theories explaining the formation of thin film and the fabrication and advantages of thin film devices.

2.Learn the fundamental atomistic mechanisms

3. Know thin film deposition techniques

4. Acquire knowledge on thin film device

5.Acquaint with thin film

6. Appreciate applications of thin films

7.Narrate various thin film deposition techniques

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: Thin Film Characterization Methods

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Monitoring and Analytical Technique, Deposition Rate and Thickness Measurement, X-ray diffraction, Microstructural Analysis- SEM, TEM, AFM & Composition Analysis

Unit 2: Thin Films In Optics

Optics of Thin Films, Antireflection Coatings, Single-Layer AR Coatings, Double-Layer AR Coatings, Multilayer and Inhomogeneous AR Coatings, Reflection Coatings- Metal Reflectors, All-Dielectric Reflectors, Interference Filters- Edge Filters, Band-Pass Filters,

Thin Film Polarizers, Beam Splitters- Polarizing Beam Splitter, Dichroic Beam Splitter, Integrated Optics- Waveguides, Thin Film Optical Components, Passive Devices: Couplers Active Devices

Unit 3: Optoelectronic Applications

Introduction Photon Detectors- Photoconductive Detectors, Photoemissive Detectors

Photovoltaic Devices-Thin Film Solar Cells, Applications in Imaging, Electrophotography (Xerography and Electro fax), Thin Film Displays- Electroluminescent (EL) Displays, Electrochromic Displays

Unit 4: Microelectronic Applications

Introduction, Thin Film Passive Components, Electrical Behaviour of Metal Films, Dielectric Behaviour of Insulator Films- Resistors, Capacitors, Inductors, Conductors (Interconnections and Contacts), Thin Film Active Components- Thin Film Transistor (TFT), Thin Film Diodes Thin Film Integrated Circuits, Microwave Integrated Circuits (MICs), Charge-Coupled Devices (CCDs): Introduction, Principle, Applications- Thin Film Strain Gauges, Gas Sensors **Reference books:**

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

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List of practical:

- 1. Thickness measurement of thin film.
- 2. Study of optical absorption of thin film (UV-visible spectroscopy) and determination of band gap of semiconductor thin film
- 3. Determination of particle size of thin film from X-ray diffraction.
- 4. Determination of grain size and microstructure description of thin film from SEM
- 5. Resistivity measurement of thin film by two probe method
- 6. Crystal structure of thin film

Course				Progra	mme Ou	tcomes			
Outcomes	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO8	PO9
CO 1	3			2					
CO 2				2					
CO 3									
CO 4				2		2			
CO 5		2				2	2		
CO 6		2							
CO7			2						
CO8					2				
CO9					2				

Justification

PO1: Disciplinary Knowledge

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

alignment ensures that students not only understand the theoretical aspects of thin film deposition but also possess the knowledge and skills necessary to make informed decisions in practical engineering applications.

PO2: Critical Thinking and Problem Solving

CO5: Problem solving ability.

ensures that students not only develop problem-solving abilities but also cultivate a broader set of critical thinking skills that can be applied across various disciplines and context.

CO6: Critical analysis

ensures that students not only develop problem-solving abilities but also cultivate the specific skill of critically analysing problems, components, and potential solutions in a systematic and informed manner.

PO3: Social Competence

CO7: Discuss the differences and similarities between different vacuum-baseddeposition Techniques.

enhancing communication skills, promoting collaboration and knowledge sharing, facilitating peer learning and support, understanding diverse perspectives, developing professional interaction skills, enhancing presentation skills, encouraging constructive dialogue, and building conflict resolution skills.

PO4: Research-related Skills and Scientific Temper

CO1: To understand the principle, differences and similarities, advantages, and disadvantages of different thin film deposition Techniques emphasis on promoting research inquiry, experimental understanding, literature review and synthesis, analytical skills, critical evaluation, scientific methodology, problem-solving, and research ethics. This alignment ensures that students not only grasp the theoretical aspects of thin film deposition but also develop the practical research skills and scientific temper necessary for conducting meaningful and ethical research in the field.

CO2: To understand and evaluate and use models for understanding nucleation and growth of thin films. Students not only grasp theoretical models but also develop the practical skills and scientific temper necessary for effective and ethical engagement in research related to thin film processes.

CO4: To improve problems solving skills related to evaluation of different properties of thin films. Not only gain theoretical knowledge but also develop practical problem-solving abilities essential for conducting meaningful and effective research in the evaluation of thin film properties.

PO5: Trans-disciplinary Knowledge

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

the nucleating and growth of thin films is justified by its emphasis on promoting trans-disciplinary understanding, facilitating the synthesis of theoretical frameworks, cultivating interdisciplinary problem-solving skills, promoting cross-domain application of concepts, fostering systems thinking, encouraging a holistic approach to research, enhancing communication skills across disciplines, and emphasizing ethical conduct in trans-disciplinary research.

CO9: Asses the relation between deposition technique, film structure, and film properties. students gain a comprehensive understanding of the intricate relationships in material science and are equipped with the skills necessary for trans-disciplinary analysis in this field.

PO6: Personal and Professional Competence

CO4: To improve problems solving skills related to evaluation of different properties of thin films. Emphasis on fostering critical thinking, analytical skills, the application of theoretical knowledge, practical competencies, decision-making skills, interpersonal competence, adaptability, resilience, communication skills, and overall professional competence.

CO5: Problem solving ability.

Students not only acquire problem-solving skills but also develop a comprehensive set of personal and professional competencies necessary for success in various contexts.

PO7: Effective Citizenship and Ethics

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

Students learn to appreciate cultural differences, recognizing that ethical considerations may vary

in different regions, contributing to their cultural sensitivity as responsible citizens.

PSPH 244 (E): ELECTRONIC INSTRUMENTATION-II

Credit: 04

Total No. of Lectures: 60

Learning Objectives: The specific learning objectives of this paper are as follows:

- 1. To understand the fundamental principles and techniques involved in measurement and instrumentation.
- 2. To learn about various types of sensors and transducers used for measuring physical quantities.
- 3. To understand the fundamentals of process control and its significance in industrial and engineering applications.
- 4. Explore the components of control systems, including controllers, actuators, and control valves.
- 5. To understand the process of signal conditioning to improve the quality of measured signals.
- 6. To understand various control modes, such as on-off control, PI, PD, PID control.
- 7. To demonstrate the use of PLCs in process control and automation.
- 8. To motivate students to work on projects based on process control instrumentation techniques.

Learning Outcomes: On successful completion of this course the students will be able to do the

following:

- CO1: Understand the basic ideas and techniques applied in instrumentation and measurement.
- CO2: The students will be able to identify and explain the key components of control systems.
- CO3: Design and implement circuits for signal conditioning for quality control.
- CO4: The students will be able to measure and control a variety of process variables,
- CO5: Students will understand and apply various control modes and techniques.
- CO6: To demonstrate abilities in designing and using data acquisition systems.
- CO7: Process and analyze measurement data and present results effectively.

TOPICS/CONTENTS:

Unit 1: Introduction to Process Control

Introduction, Control systems, Process control block diagram, Control system Evaluation and Control system Objective, Evaluation Criteria- Damped response, Cyclic response, Process Control Drawing and symbols with their meaning, Discrete Process Control: Introduction, definitions of discrete state process control, Characteristics of the systems, relay, controllers, and ladder diagrams PLC's, interfacing with LAN, SCADA systems. Problems.

References: 1

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Unit 2: Controller Principles

Introduction of controller, Process Characteristics- Process Load, Transient, Process Lag Control System Parameters, Error, Variable Range, Control Parameter Range, Control Lag, Dead Time, Cycling, Controller Modes, reverse and direct action, discontinuous controller modes, two position, Neutral Zone, Applications, Multi position controller floating control mode- Continuous controller modes, Proportional Control Mode, Integral Control Mode, Derivative Control Mode, Composite Control, PI Control, PD Control Mode, Three Mode Controller (PID), Problems References: 1

Unit 3: Types of Controllers

Analog Controllers: Electronic controller with design considerations: Proportional (P), Integral (I), Derivatives (D), PI, PD and PID, Digital Control: Introduction two position controls and multivariable alarms.

References: 1

Unit 4: Modelling, Simulation and Programming

Introduction to modelling and simulation: Mathematical model, equivalent circuit model, Empirical Model, methodology, concept and need of simulation and its applications. Introduction to MATLAB/ SciLab.

References: 2 and 3

References Books:

- 1. Process Control Instrumentation Technology, Curtis D. Johnson, 7th Edition, Prentice Hall India Pvt. Ltd.
- 2. Computer based industrial controls K. Kant PHI publications.
- 3. MATLAB an introduction and applications", by Amos Gilat, Wiley Students Edition
- 4. Instrumentation, measurement, and systems. Nakra and Chaudhary.
- Electronic Instrumentation and measurement techniques by A. D. Helfrick and W. D. Cooper.
- 6. Instrumentation, devices, and systems. Rangan, Mani and Sarma Prentice Hall of India.
- 7. Electronics Instrumentation. Kalsi (Tata McGraw-Hill)
- 8. Measurement system applications and design by E.O. Doblin and Manik .

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Course Outcomes				Progra	mme Ou	itcomes			
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: Understand the basic ideas and techniques applied in instrumentation and measurement. Weightage: 3

Justification: Acquiring knowledge about instrumentation and measurement techniques directly aligns with disciplinary knowledge in the field.

PO2: Critical Thinking and Problem Solving

CO2: The students will be able to identify and explain the key components of control systems.

CO3: Design and implement circuits for signal conditioning for quality control.

CO5: Students will understand and apply various control modes and techniques.

Weightage: 3

Identifying components, designing circuits, and applying control modes involve critical thinking and problem-solving skills.

PO4: Research-related Skills and Scientific Temper

CO4: The students will be able to measure and control a variety of process variables.

CO6: To demonstrate abilities in designing and using data acquisition systems.

CO7: Process and analyze measurement data and present results effectively.

Weightage: 3

These outcomes involve research-related skills and align with a scientific temper in the context of measurement and control.

PSPH 244 (F): DENSITY FUNCTION THEORY-II

Credit: 04

Total No. of Lectures: 60

Course Objectives:

- 1. 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.
- 2. 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.
- 3. In this course, you will learn both the theoretical and numerical aspects of DFT.
- 4. We will also learn how to perform DFT calculations on simple molecules and solids using DFT programs such as NWChem and ABINIT.

. Course Outcomes:

- CO1: Learn theoretical concepts of different computational techniques in materials science. CO2: Simulate and compute material properties using density functional theory, molecular dynamics and Monte Carlo methods.
- CO3: Understand SCF and convergence test.
- CO4: Ability to understand interpretation of data for physical properties of materials.
- CO5: Ability to understand interpretation of data for magnetic properties of materials.
- CO6: Ability to understand interpretation of data for optical properties of materials.
- CO7: Practical experience in implementing DFT calculations using computational software packages.

Unit 1: Basic concepts in DFT

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

Unit 2: Exchange correlation functionals

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

Unit 3: Basics of solids state physics

Bravais lattice, reciprocal space, Bloch theorem, and Brillouin zone. Pseudopotentials: normconserving pseudopotential, nonlinear core correction, and project augmented wave technique.

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Unit 4: 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 5: Applications

Vibrational frequencies, enthalpy, and Gibbs free energy of molecules. Bulk modulus, shear modulus, phase transition pressure, reaction barrier, vacancy formation energy, surface adsorption energy, surface energies, and charge analysis.

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. Supplementary References "Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory", Szabo and Ostlund.
- "A bird's-eye view of density-functional theory" by K Capelle, Brazilian Journal of Physics 36, pp 1318 (2006).
- "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).
- "Orbital-dependent density functionals: theory and applications" K"ummel 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). Grading Policy

List of Practical's:

- 1. Self-Consistent calculation
- 2. Convergence Test
- 3. Structure Optimisation
- 4. DOS Calculations
- 5. Band structure
- 6. P dos calculations

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Course				Progra	mme Ou	tcomes			
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				2					

Justification

PO1: Disciplinary Knowledge

CO1: Learn theoretical concepts of different computational techniques in materials science. Weightage: 3

Acquiring knowledge of theoretical concepts in computational techniques aligns directly with disciplinary knowledge in the field of materials science.

PO2: Critical Thinking and Problem Solving

CO2: Simulate and compute material properties using density functional theory, molecular dynamics, and Monte Carlo methods.

CO3: Understand SCF and convergence test.

CO4: Ability to understand interpretation of data for physical properties of materials.

CO5: Ability to understand interpretation of data for magnetic properties of materials.

CO6: Ability to understand interpretation of data for optical properties of materials.

Weightage: 3

Simulation, computation, and understanding of data interpretation involve critical thinking and problem-solving skills.

PO4: Research-related Skills and Scientific Temper

CO7: Can use DFT software in a high-performance computing environment.

Weightage: 2

Using DFT software in a high-performance computing environment contributes to research-related skills and aligns with a scientific temper.

PSPH 235: SPECIAL LAB- I / PSPH 245: SPECIAL LAB- III

Credit: 04

No of Practicals: 10

List of Experiments:

(Students must perform Any 8 Experiments)

(CB Group –I: PSPH 234 (A): NANO TECHNOLOGY-I &

CB Group –II: PSPH 244 (A): NANO TECHNOLOGY-II):

1	Synthesis of Fe ₂ O ₃ by sol-gel method
2	Preparation of Mn ₃ O ₄ thin film by SILAR method
3	Synthesis of metal oxides by spray pyrolysis method
4	Synthesis of metal nanoparticles using green route
5	Band gap energy Measurement of thin films by UV-Visible spectrophotometer
6	Use of FT-IR for functional group identification (in CNT, graphene etc.)
7	Data plotting using Origin 8 software
8	Photoluminescence study of nano materials
9	Thickness measurement of thin film by weight difference method
10	Electro-deposition of Cu nano particle
11	Deposition of thin films by CBD method
12	Synthesis of ferrites by Co-precipitation method
13	Preparation of film by Doctor Blade method
14	Resistivity measurement of thin film by two probe method
15	Contact angle measurement of thin films
16	Structural properties of nano materials by XRD
17	Analysis of surface morphology by TEM
18	Morphological study by SEM

PSPH 235: SPECIAL LAB- I / PSPH 245: SPECIAL LAB- III

Credit: 04

No of Practicals: 10

Learning objectives:

1) Understand the principle in measuring the thickness of thin films and to find a suitable method for measuring the thickness of thin films.

2) Understand, analyze and treating the Structural defects in thin films.

3) Understanding the mechanical behaviour of thin films.

Learning Outcomes:

1) Students will have acquired necessary skills for working in research institutes.

2) Students will have acquired necessary skills and expertise to work in industry related to materials processing and quality control

List of Experiments:

(CB Group –I: PSPH 234 (B): ENERGY STUDIES-I &

CB Group –II: PSPH 244 (B): ENERGY STUDIES-II):

1	Recording the amount of sunlight receives throughout a day using Sunshine Recorder
2	Bio-gas Production from Kitchen waste.
3	Energy Content in Wind.
4	Utilizing the latent heat released by the condensing water steam using Solar Still
5	Performance evaluation of box type and concentrating type solar cooker
6	Find out the kinetics of photocatalytic reaction
7	Measure the solar radiation flux density using Pyrometer
8	Determining efficiency of lighting system/loads

PSPH 235: SPECIAL LAB- I / PSPH 245: SPECIAL LAB- III

Credit: 04

No of Practicals: 10

Learning objectives:

1) Understand the principle in measuring the thickness of thin films and to find a suitable method for measuring the thickness of thin films.

2) Understand, analyze and treating the Structural defects in thin films.

3) Understanding the mechanical behavior of thin films.

Learning Outcomes:

1) Students will have acquired necessary skills for working in research institutes.

2) Students will have acquired necessary skills and expertise to work in industry related to materials processing and quality control

List of Experiments:

(CB Group –I: PSPH 234 (C): BIOPHYSICS-I &

CB Group –II: PSPH 244 (C): BIOPHYSICS -II):

1	Light microscopy: Observing live cells and tissues.
2	UV-Visible spectroscopy: Determining absorption spectra of biomolecules.
3	Fluorescence spectroscopy: Studying molecular interactions and conformational changes.
4	Circular dichroism spectroscopy: Analysing the secondary structure of proteins.
5	Electromyography (EMG): Recording electrical activity in muscles.
6	Tensile strength tests: Assessing the mechanical properties of biological tissues.
7	Molecular dynamics simulations: Modelling the behaviour of biomolecules over time.
8	Laser tweezers: Manipulating and studying individual cells or particles with laser beams.
9	Photochemical reactions: Investigating the effects of light on biological systems.
10	Studying the mobility of ions in gases for the analysis of biomolecules.

PSPH 235: SPECIAL LAB- I / PSPH 245: SPECIAL LAB- III

Credit: 04

No of Practicals: 10

Learning objectives:

1) Understand the principle in measuring the thickness of thin films and to find a suitable method for measuring the thickness of thin films.

2) Understand, analyze and treating the Structural defects in thin films.

3) Understanding the mechanical behavior of thin films.

Learning Outcomes:

1) Students will have acquired necessary skills for working in research institutes.

2) Students will have acquired necessary skills and expertise to work in industry related to materials processing and quality control

List of Experiments:

(CB Group –I: PSPH 234 (D): PHYSICS OF THIN FILM-I &

CB Group –II: PSPH 244 (D): PHYSICS OF THIN FILM-II):

1	Deposition of metallic thin films by vacuum evaporation method
2	Deposition of thin films by spray pyrolysis method and thickness measurement by gravimetric method
3	Thin film formation by Electro-chemical deposition technique.
4	Deposition of thin films by spin coating method and resistance measurement.
5	Deposition of thin film by Dip Coating method and thickness measurement.
6	Thickness measurement of thin film by Tolansky method.
7	Study of optical absorption of thin film (UV-visible spectroscopy) and determination of particle size
8	Determination of particle size of thin film from X-ray diffraction.
9	Determination of grain size of thin film from SEM
10	Resistivity measurement of thin film by two probe method
11	Band gap energy of thin film
12	Crystal structure of thin film
13	Electron Spin Resonance (ESR)
14	Development of microstructures by photolithography.

PSPH 235: SPECIAL LAB- I / PSPH 245: SPECIAL LAB- III

Credit: 04

No of Practicals: 10

Learning Objectives:

- 1. To develop analytical abilities toward real life problems
- 2. To familiarize with recent scientific and technological developments
- 3. To enrich knowledge through problem-solving, hands-on training, study visits, projects etc

Learning Outcomes:

After successfully completing this laboratory course, the students will be able to do the following:

- 1. Demonstrate an ability to collect data through observation and/or experimentation and interpreting data.
- 2. Demonstrate a deeper understanding of abstract concepts and theories gained by experiencing and visualizing them as authentic phenomena.
- 3. Acquire the complementary skills of collaborative learning and teamwork in laboratory settings.

(CB Group –II: PSPH 234 (E): ELECTRONIC INSTRUMENTATION-I&

CB Group –IV: PSPH 244 (E): ELECTRONIC INSTRUMENTATION-II):

1	Application of ultrasonic pressure transducer.
2	Temperature Characteristic of Thermistor
3	D to A converter circuit (R-2R & binary weighted).
4	V to F, converter as basic concept of ADC.
5	Op-amp as Instrumentation amplifier.
6	Characteristics and applications of photoelectric devices, LED, Photodiode
7	Study of Sample and Hold Circuits
8	F to V Converter using OP-AMP
9	Study of Data Acquisition System
	Measurement of temperature by thermocouple
11	Measurement of displacement using LVDT
12	Temperature Characteristic of strain gauges and its application
13	Logarithmic amplifier using op-amp 741

14	Measurement of load using strain gauge-based load cell
15	Measurement of temperature by RTD
16	Study of storage oscilloscope and determination of transient response of RLC Circuit
17	Determination of characteristics of a Fiber-optic sensor
18	Study of data acquisition system using "lab view" software and test all signal points
19	Measurement of water level using strain gauge-based water level transducer
20	Study of P, PI and PID controllers

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

PSPH 235: SPECIAL LAB- I / PSPH 245: SPECIAL LAB- III

Credit: 04

No of Practicals: 10

(CB Group –II: PSPH 234 (F): DENSITY FUNCTION THEORY-I &

CB Group –**IV:** PSPH 244 (F): DENSITY FUNCTION THEORY-**II**):

1	Self-Consistent calculation
2	Convergence Test
3	Structure Optimisation
4	DOS Calculations
5	Band structure
6	P dos calculations