M.Phil. Physics

Programme outcomes of M.Phil (Science)

- Critically analyze issues related to the areas of specialization and develop innovative methodologies to tackle identified issues.
- Acquire knowledge and skills required for teaching in Higher Education Institutions
- Review literature, identify research problems, check the scientific content and develop social competency to work with self-confidence globally.

Programme Specific outcomes

No	Upon completion of the programme, the students will be able to	PSO NO
1	Do scientific research for the benefit of the society	PSO-1
2	Develop specialized skills through knowledge applicable to their own area of research.	PSO-2
3	Acquire in-depth knowledge of the process of developing new materials as well as expert knowledge of well defined area of research in physics.	PSO-3
4	Carry out independent research in trust areas of physics (Nanophysics, crystal physics, thin films, theoretical physics)	PSO-4
5	Develop innovative methodologies' to tackle issues identified and contribute to the development of technological knowledge and intellectual property	PSO-5
6	Evolve as excellent professionals in the public sector units BARC/ISRO/DRDO/CSIR laboratories and contribute towards the scientific growth of the country	PSO-6

Semester I

C1: Professional Skills for Teaching – Learning

Sub Code: MPE181

No. of hours per week			Credit	Total no. of hours	Marks
T	P	Library	3 + 1	75	100
3	2	2			

Course Outcomes

Co No.	Upon completion of this course, scholars will be able to
CO-1	Communicate competently in groups and organizations
CO-2	Construct effective written messages in various formats and styles to a variety of audiences
CO-3	Asses the various theories of learning and their association in the development of learning process in children and adults

Teaching Plan

Total Contact hours : 75 (Lectures, Assignments, Teaching practice and tests)

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ evaluation
I	**Soft Skills**					
	1	Introduction to soft skills, Soft skills vs Hard Skills, Types of soft skills	1	Distinguish between soft skills and hard skills	Brain storming, Lecture with PPT	Formative Assessment I
	2	Communication skills: Basics in communication, structure of written and oral sentences, verbal, non verbal, body language, interpersonal and intra personal communication	3	To communicate competently in groups and organisations	Lecture with PPT, Conversation session, Inquiry based activity , Role play	
	3	Behavioural skills: Leadership skills, time management, Creativity and Lateral Thinking	3	To comprehend the leadership skills and to perform effectively as a leader	Lecture ,Group Discussion, Role Play	
	4	Interview skills: Resume writing, different types of interviews, Etiquettes in interviews, mock interviews	3	To apply the principles and techniques in resume writing and in interviews	Lecture, Demonstration, Mock interview	
	5	Team building and group discussion: progressive stages of team building, parameters of GD	3	To apply the procedures of GD in real life situation during formal interviews	Lecture, video clippings, mock group discussion	
	6	Language skills: Strategies to acquire LSRW skills	2	To comprehend listening texts/ speeches by the native speakers. To read effectively with considerable speed and comprehend the texts. To speak and write on simple known topics.	Session in the Language lab for acquiring LSRW skills	
II	**Techniques and dynamics of teaching-learning**					
	1	Emerging trends in	2	To understand the	Brain	

		educational psychology: meaning, scope and methods		significance of various methods of educational psychology	storming, Lecture with PPT	Formative Assessment I
	2	Learning: Theories of learning, Approaches to learning (Classical conditioning –Ivan Pavlov and Operant conditioning-B.F.Skinner), kinds of learning, factors that affect learning	5	To review the various theories of learning and their association in the development of learning process in children and adults	Video clippings, Lecture with PPT	Formative Assessment II
	3	Motivation: Intrinsic and extrinsic, development of memory and intelligence	3	To apply the effect of motivation in the development of memory and intelligence	Lecture with PPT, Video clippings and Lecture	Formative Assessment II
III	**Incorporating Teaching and learning via Modern Gadgets**					
	1	MS Word-2007, MS Excel-2007,MS Power point-2007, Concepts in e-resources: making use of web resources	6	To develop an understanding of the various e-resources	Lecture, Preparation of documents in word, excel and Power point (Practical session)	Formative Assessment II
	2	ICT for Research: On-line journals, e-books, courseware, Tutorials, Technical reports, Theses and dissertation	6	To acquire skills to use the e-resources in teaching, learning and research work	Lecture, tutorial based on e-content, methods of preparation of dissertation	Formative Assessment II
IV	**Instructional Technology**					
	1	Definition, objectives and types of instruction technology, difference between teaching and instruction	2	To understand the difference between teaching and instruction	Lecture	Presentations by the learner using creative methods
	2	Lecture technique: steps, planning and delivery of lecture, lecture with PPT, LCD Projector, AV aids, Smart Class room	3	To classify the various methods of lecturing using ICT tools. To apply the various techniques in the class room techniques.	Lecture with PPT and demonstration on how to use LCD projector, Smart class rooms and AV aids	Presentation by the learner using creative methods

					(Language lab)	
	3	Teaching learning techniques: Team teaching, group discussion, seminar, workshop, symposium and panel discussion	4	To differentiate the learning techniques and the strategies to be followed by adopting various methods	Lecture with PPT	Presentations by the learner using creative methods
	4	Modes of teaching: CAI, CMI and WBI	2	To develop the methods of teaching using technology. To apply computer assisted technology for automatic grading.	Lecture with PPT	Presentations by the learner using creative methods
V	**Learning, teaching and Evaluation Practice**					
	1	Teacher assisted class room teaching	5	To develop teaching skills	Lecture	Teacher evaluation and suggestions
	2	Teacher assisted laboratory practice	3-5 sessions	To improve instructional practices	Demonstration	Teacher evaluation and suggestions

Name &Signature of the Instructor: Mr. Arun, 'Vantage', Nagercoil
Ms. P. Sathya, Dr. Brisca Renuga and Dr. Sheeba Daniel -Guest Lecturers

Name &Signature of the coordinator: Dr. Sr. Gerardin Jayam, M.Phil. Coordinator

Semester - I
C2: Research Methodology
Subject Code: MPP182

No of hours per week		**No of credits**	**Total no of hours**	**Marks**
Contact	Library	4	75	100
5	3			

Objectives: 1. To understand the essential knowledge and skills needed for Physics research.
2.To apply their skills to develop new materials and devices.

Course outcomes

CO No	Upon completion of this course, students will be able to	**PSOs addressed**	**CL**
CO-1	Understand the basic concepts of research and its methodologies of scholarly writing.	PSO-1	U

CO-2	Solve partial differential equations and special function of mathematical physics (gamma function, Green's functions, Legendre functions, Bessel functions, Hermite and Laguerre functions and Dirac Delta function).	PSO-5	Ap
CO-3	Evaluate of the basic features and concepts of the Sun and other stars(expanding Universe using concepts of the Big Bang, sunspots, Van Allen Belts , Ionization potentials)	PSO-5	Ap
CO-4	Examine the fundamentals principles ,theories and applications of photonics cystals.	PSO-2	An
CO-5	Explain the characterization of thin film in terms of its optical, electrical, magnetic and mechanical properties.	PSO-4	E

Teaching Plan

Total Hours: 90 (Including Seminar & Test)

Unit	Module	Topics	Lecture hours	Learning outcome	Pedagogy	Assessment/ Evaluation
I	**Research methodology**					
	1	Research and its importance, Research methods and research methodology, Types of research, Identification of a research problem, Literature survey, Reference collection, Internet browsing.	4	To understand the basic concepts of research	Illustration, Descriptive lecture	Class Test Quiz Seminar short questions Formative assessment (I CIA)
	2	Mode of approach : research design , Possible approaches; Actual Investigations; Results and Conclusion	4	To acquire knowledge on the mode of approach for the pre-doctoral research work.	Illustration, Descriptive lecture PPT	
	3	Presenting a scientific seminar-oral report; Art of writing a research paper and thesis-outline, lay out; Writing a research paper for publication in a journal	4	To understand the art of writing and presenting research papers in seminars and writing the thesis	Illustration, Descriptive lecture	
II	**Mathematical Physics**					

	1	Special functions, Laguerre, Generating function, orthogonality, recurrence relations, Green's function, Green's function for one dimensional case, Green's function for Poisson's equation	4	To understand the concept of recurrence relations, Green's function	PPT Illustration, Descriptive lecture	Evaluation through: quiz,
	2	Quantum mechanical scattering problem, Interpolation, Finite differences : Newton's forward and backward interpolations, Newton's backward interpolations, Divided differences	4	To solve the Newton's forward and backward interpolations problems	Problem solving techniques Assignment	Problem solving Class test
	3	Curve fitting, linear least square fit, Non-linear fit; parabola, Solving Eigen value equation, Jacobi method	4	To acquire knowledge on curve fitting and Eigen value equation	Descriptive lecture Problem solving	Formative assessment (I&II CIA)
III	**Photonics**					
	1	Postulates of ray optics and wave optics, Transmission through optical components, Optical Fourier transform, Holography, Principles of electro optics	4	To understand the basic postulates of ray optics	Illustration, Descriptive lecture	Evaluation through: quiz,
	2	Electro optics in anisotropic and liquid crystals, Photonic Crystals - Basics concepts, Features of photonic crystals, Methods of fabrication	5	To acquire knowledge on photonic crystals and methods of fabrication	Descriptive lecture, PPT Videos	Assignments, Seminar Descriptive answers
	3	Nonlinear photonic crystals, Photonic crystal fibers, Photonic crystals and optical communications, Photonic crystal sensors.	4	To be able to understand the concept of Photonic crystal sensors.	Descriptive lecture, PPT, Videos	Formative assessment (II CIA)
IV	**Astrophysics**					
	1	Spectral classification of stars, Boltzmann's formula, Saha 's equation of thermal ionization, Harvard system of spectral	4	To understand the spectral classification	PPT Illustration, Descriptive lecture.	Evaluation through quiz Descriptive

		classification				answers
	2	Theory of sunspots, Solar flares, Stellar temperatures, Classification of variable stars, Erupting and exploding stars, Distribution of novae in our galaxy, Cosmology , red shift and the expansion of universe	4	To acquire knowledge on Erupting and exploding stars	Descriptive lecture, PPT Videos	Class Test Assignment Formative assessment(II &III)
		Big bang, Dark matter and dark energy, Elementary particles and their interactions, Van Allen Belt , Evolution of stars	3	To know the concept of elementary particles and their interactions	Descriptive lecture, PPT,Videos	
V	**Recent Trends in Thin Film Technology**					
	1	Thin Film optics, Optical constants of thin films, Filters, Antireflection coatings, Four vector form of Lorentz equations, Thin film solar cells: Role and progress, Production of thin film solar cells	5	To acquire knowledge on thin film optics, thin film solar cells	PPT Illustration, Descriptive lecture	quiz Assignments Seminars
	2	Photovoltaic parameters, Thin film silicon (Polycrystalline) solar cells, Current status of bulk silicon solar cells	4	To understand the concept of photovoltaic parameters	Descriptive lecture,PPT Videos	Descriptive answers
	3	Fabrication technology photovoltaic performance, Emerging solar cells: GaAs and CuInSe	4	To be able to know the fabrication and photovoltaic performance of solar cells	Descriptive lecture PPT Videos	Class Test Formative assessment (III CIA)

Course Instructor: Dr. S.Sonia Head of the Department: Dr.S.Mary Delphine

Semester - I

C3: Advanced Physics

Subject code: MPP183

No of hours per week		**No of credits**	**Total no of hours**	**Marks**
Contact	Library			
5	3	5	75	100

Objectives: 1.To highlight the topics such as solid state theory, high temperature Superconductivity, crystal growth studies.

2.To analyze the material properties and various sensing mechanisms.

Course Outcomes

CO	Upon completion of this course the students will be able to :	PSO addressed	CL
CO- 1	Discuss the Fermi surfaces and band structure of materials	PSO-2	C
CO- 2	Explain the High Temperature superconductors and its applications in microwave technology	PSO-2	U
CO- 3	Apply different methods used to grow crystals and determination of growth parameters	PSO-3	Ap
CO -4	Explain the different types of sensors and sensing mechanisms involved.	PSO-4	U
CO- 5	Utilize different characterization methods to estimate structural, surface and thermal properties of materials	PSO-5	An

Teaching Plan

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Solid State Theory**					
	1	Fermi surfaces, Construction of Fermi surfaces, Electrons in an uniform magnetic field, Anomalous skin effect.	4	To understand the basic concepts of Fermi surfaces and magnetic field	Lecture with PPT Illustration	Class Test Quiz short questions Formative assessment (I CIA)
	2	Cyclotron resonance, Closed orbits and open orbits, De HAAS, van ALPHEN effect	3	To understand the cyclotron resonance ,De HAAS and van ALPHEN effect	Lecture cum Discussion	
	3	Nearly Free electron approximation, The density of states in the Band model	4	To evaluate the density of states	Lecture Group Discussion	
	4	Band structure of metals, Band structure of semiconductors and insulators.	4	To study the band structure of materials	Lecture with PPT Illustration	
II	**High Temperature Superconductivity**					
	1	High temperature superconductors: Cuprates, charge carriers	5	To understand basic concepts of super-conductors and charge carriers	Lecture with PPT Illustration	Evaluation through: quiz, short questions Descriptive

	2	Structure and doping of $La_{2-x}Ba_xCuO_4$ – Preparation and structure of $YBa_2Cu_3O_{7-x}$, More layer-like cuprate superconductors ($Bi_2CaSr_2Cu_2O_8$)	6	To study the Y123 super-conductors	Lecture cum Discussion	answers Formative assessment (I CIA)
	3	Applications of high temperature superconductors in microwave technology – superconducting aerials	3	To understand the high temperature super-conductivity in applied level.	Lecture with PPT Illustration	
III	**Modern Crystal growth Techniques**					
	1	Vapour growth (physical and chemical) ,Crystal growth by hydrothermal method, Introduction , Growth apparatus, Determination of growth parameter, Growth techniques.	2	To understand the techniques of crystal growth	Lecture Discussion	Evaluation through: quiz, short questions Descriptive answers Formative assessment (I and II CIA)
	2	Electro crystallization: Introduction, Electrochemical potential, Diffusion, Crystallization mechanism	4	To understand the crystallization mechanism	Lecture with PPT Illustration	
	3	Double layer, Faradaic and Non-Faradaic system, Equilibrium exchange current density i_0 , Non – equilibrium current density ,Over potential	5	To understand the Current density in Faradaic and Non-Faradaic system	Lecture and Group Discussion	
	4	Multinuclear multilayer deposition - Gel growth – Technology of Epitaxy	2	To understand the gel and epitaxial growth	Lecture cum Discussion	
IV	**Sensor Materials and Applications**					
	1	Sensor, signals and systems – Sensors classification – Radar sensors – ultrasonic sensors – Hall effect sensors	4	To know about the various types of sensors	Lecture cum Discussion	Evaluation through: quiz, short questions Descriptive answers Formative assessment (II CIA)
	2	Thin film sensors – liquid level sensors – Concepts of pressure – Optoelectric sensors – Basic flow dynamics – Microflow sensors – Fibre optic – Micro phone	6	To understand the Thin film sensors and their applications	Lecture and Group Discussion	

	3	Concept of Humidity – Optical hygrometer – semiconductor pn junction sensor – Acoustic temperature sensors – Chemical sensors characteristics – Specific Difficulties	3	To understand the concept of humidity and its applications	Lecture with PPT Illustration	
	4	Classification of Chemical sensing mechanism – Enhanced Catalytic gas sensor – Smart chemical sensors. Materials - Surface processing.	2	To understand the different types of chemical sensors	Lecture and Group Discussion	
V	**Characterization of Materials**					
	1	X-ray diffraction - Scanning electron microscopy - Transmission electron microscopy, Scanning probe microscopy	5	To analyze the structural and surface properties	Lecture with PPT Illustration	Evaluation through: quiz, short questions Descriptive answers Formative assessment (II CIA)
	2	Thermo gravimetric Analysis – Differential Thermal Analysis - Differential Scanning Calorimetry – Microthermal Analysis	5	To understand the thermal properties	Lecture and Group Discussion	
	3	Spectroscopy of semiconductors; excitons-Infra red surface spectroscopy - Raman spectroscopy- Electron spectroscopy	5	To understand the spectroscopic techniques	Lecture and Group Discussion	

Course Instructor: Dr. S.Sonia **Head of the Department: Dr.S.Mary Delphine**

Semester - I
Principles and Methods of Crystal Growth (In-depth paper)
Subject code: MPP184

No of hours per week		No of credits	Total no of hours	Marks
Contact	Library			
3	4	6	90	100

Objectives

1. To understand the basic concepts and theories of crystal growth.
2. To develop the ability to preparing crystals with preferred orientation.

Teaching Plan
Total Hours: 90 (Including Seminar & Test)

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment /Evaluation
I	**Fundamentals of Crystal Growth**					

	1	Importance of crystal growth, Classification of crystal growth methods, Basic steps: Generation, transport and adsorption of growth reactants	4	To understand the basic concepts and mechanisms of crystal growth	Lecture with PPT Illustration	Evaluation through Short Test
	2	Nucleation: Kinds of nucleation Classical theory of nucleation: Gibbs Thomson equations for vapour and solution	3	To understand the Process involved in nucleation	Lecture Discussion	Multiple Choice questions
	3	Kinetic theory of nucleation Becker and Doring concept on nucleation rate Energy of formation of a spherical nucleus Statistical theory on nucleation: Equilibrium concentration of critical nuclei, Free energy of formation	8	To evaluate the parameters involved in nucleation	Group Discussion	Formative assessment
II	**Theories of Crystal Growth**					
	1	An introductory note to Surface energy theory Diffusion theory and Adsorption layer theory Concepts of Volmer theory, Bravais theory, Kossel theory and Stranski's treatment	5	To understand the theories involved in nucleation	Lecture with PPT Illustration	Evaluation through Open Book
	2	Two-dimensional nucleation theory: Free energy of formation, Possible shapes and Rate of nucleation Mononuclear, Polynuclear and Birth and Spread models Modified Birth and Spread model	6	To identify the free energy formation of nucleation and rate of nucleation	Lecture cum Discussion	Formative assessment (CIA I)
	3	Crystal growth by mass transfer processes: Burton, Cabrera and Frank (BCF) bulk diffusion model Surface diffusion growth theory	3	To distinguish the bulk and surface diffusion theory	Group DIscussion	
III	**Experimental Crystal Growth-Part-I: Melt Growth Techniques**					
	1	Basics of melt growth, Heat and mass transfer	2	To understand the processes of crystal growth	Lecture Discussion	Evaluation through Open Book
	2	Conservative growth processes: Bridgman-Stockbarger method Czochralski pulling method	4	To understand the techniques of crystal growth	Lecture with PPT Illustration	Formative assessment (CIA I)
	3	Kyropolous method Non-conservative processes: Zone-refining Vertical and horizontal float zone methods	5	To understand the Kyropolous method of crystal growth	Group DIscussion	

	4	Skull melting method Vernueil flame fusion method	2	To understand the various methods of crystal growth	Lecture Discussion	
IV	**Solution Growth Techniques**					
	1	Growth from low temperature solutions: Selection of solvents and solubility Meir's solubility diagram Saturation and supersaturation	4	To know about the growth of crystals at low temperature	Lecture Discussion	Open Book Evaluation Formative assessment I and II
	2	Metastable zone width Growth by restricted evaporation of solvent, slow cooling of solution and temperature gradient methods Crystal growth in Gel media: Chemical reaction and solubility reduction methods	6	To understand the reactions involved in crystal growth	Group Discussion	
	3	Growth from high temperature solutions: Flux growth Principles of flux method Choice of flux	3	To understand the growth of crystals at high temperature	Lecture with PPT Illustration	
	4	Growth by slow evaporation and slow cooling methods Hydrothermal growth method	2	To grow single crystals by hydrothermal method	Group Discussion	
V	**Vapour Growth Techniques**					
	1	Basic principles Physical VapourDoposition (PVD): Vapour phase crystallization in a closed system	3	To describe the crystal formation by PVD	Lecture with PPT Illustration	Evaluation through Open Book Formative assessment I and II
	2	Gas flow crystallization Chemical Vapour Deposition (CVD): Advantageous and disadvantageous	3	To describe the crystal formation by PVD	Group Discussion	
	3	Growth by chemical vapour transport reaction: Transporting agents, Sealed capsule method, Open flow systems Temperature variation method: Stationary temperature profile	6	To understand the temperature varying method of crystal growth	Group Discussion	
	4	Linearly time varying temperature profile Oscillatory temperature profile	2	To evaluate the time-temperature profile	Lecture discussion	

Course Instructor: Dr. M.Priyadharshini Head of the Department: Dr.S.Mary Delphine

Semester - I

C4: Research Trends in Nanoscience and Technology (In-depth paper)

Subject Code: MPP185

No of hours per week		No of credits	Total no of hours	Marks
Contact	Library			
3	4	6	90	100

Objectives

1. To understand the basic properties, structure and behavior of nanoparticles.

2. To study the various nanostructures and their properties.

CO No.	Course outcomes Upon completion of this course the students will be able to:	PSO addressed	CL
CO- 1	List the basic properties of nanoparticles (size, shape, density melting, boiling point)	PSO-2	R
CO- 2	Explain the technique involved in measuring different properties of nanoparticles	PSO-2	U
CO- 3	Apply different methods used to control the structure of nanoparticles	PSO-3	Ap
CO -4	Explain the characteristics and behaviour of nanoparticles in dispersed system	PSO-2	U
CO- 5	Utilise different characterization methods to estimate physical properties of nanoparticles	PSO-4	An
CO- 6	Describe the procedure for studying physical properties	PSO-5	C

Modules

Total contact hours:45 (Including lectures, assignments and tests)

Unit	Section	Topics	Lecture hours	Learning outcome	Padagogy	Assessment/Evaluation
I	**Basic properties and measuring methods of nanoparticles**					
	1.	Size effect and properties of Nanoparticles , Particle size, Particle shape, Particle density	2	To define the basic properties of nanoparticles.	Lecture, discussion	Short test, Seminar, Formative assessment (I)
	2.	Melting point, surface tension, wettability,	4	To understand the size effect.	Lecture	
	3.	Specific surface area and pore Crystal structure Surface characteristics	4	To list out the properties of nanoparticles	Lecture	
	4.	Mechanical property, Electrical properties, Magnetic properties, Optical property of nanoparticle	8	To recall the techniques involved in measuring different properties of nanoparticles	Self study	
II	**Structural control of nanoparticles**					

	1.	Particle size ,Gas phase Liquid phase,Solid phase	5	To understand the structural effects on nanoparticles synthesized with different phases.	Lecture,	Short test, Assignment, Seminar, Formative assessment (I & II)
	2.	Supercritical hydrothermal, Particle shape,Gas phase, Liquid phase,Solid phase	6	To apply hydrothermal method to control structure of nanoparticles	Lecture, Discussion,	
	3.	Supercritical hydrothermal, Composite structure, Pore structure, Nanoparticle design for DDS.	7	To differentiate Supercritical hydrothermal method from hydrothermal method	Self study	
III	**Characteristics and behavior of nanoparticles and its dispersion systems**					
	1.	Introduction of nanoparticle dispersion and aggregation behavior, Single nanoparticle motion in fluid,Brownian diffusion	5	To Explain the characteristics and behaviour of nanoparticles in dispersed system	Lecture,	Short test, Seminar, Formative assessment (II) Seminar,
	2.	Adsorption properties wettability of nanoparticle surface, Interaction between the particles aggregation behavior	5	To be able to know adsorption properties	Lecture, Discussion,	
	3.	Characterization and control Characterization and control Simulation of colloidal particle Simulation of colloidal particle	8	To understand about colloidal particle	Self study .	
IV	**Control of nanostructure of materials**					
	1.	Nanoparticles arranged structures ,Photonic fractal Electrophoresis, Nanopore structure	5	To control the characteristics and behaviour of nanoparticles in dispersed system	Lecture	
	2.	Nanocomposite structure			Lecture	
		Catalytic microstructure Percolation structure Insitu polymerisation	4	To understand about Nanocomposite polymerisation	Lecture, PPT	Short test, Seminar, Formative assessment (II & III)
	3.	ECAP process,Structure control of nanoparticles, Self-assembly. Fabrication of organic materials,Fabrication of inorganic materials	9	To understand about Fabrication of materials	Self study	

V	**Evaluation methods for properties of nanostructured materials**					
	1.	Functionality of nanostructures and their characteristic evaluation Mechanical properties Strength, fracture Creep test	5	To apply different characterisation methods to estimate Mechanical properties	Lecture Discussion	Short test, Seminar, Formative assessment (III)
	2.	Thermo physical properties Electric properties Thermoelectric properties Electrochemical properties	4	To apply different characterisation methods to estimate Thermoelectric , Electrochemical properties	Lecture, Discussion	
	3.	Characteristics of sensor Magnetic properties Optical properties Photonic crystal	9	To apply different characterisation methods to estimate Magnetic ,Optical properties	Self study	

Course Instructor: Dr. R.Krishna Priya Head of the Department: Dr.S.Mary Delphine

Semester I

C4: Electronic Structure Calculations for Solids (In depth paper)

Subject Code: MPP186

No of hours per week		**No of credits**	**Total no of hours**	**Marks**
Contact	Library	5	45	100

Objective

1. To emphasize the use of first principles in the theoretical calculations of electronic structure in the understanding of structural, cohesive, optical and vibrational properties of solids under high pressure.

2.To improve the computational skill and the theoretical calculations for providing scientific advances and discoveries which play a key role in the future employability and worldwide progress of students.

Course Outcomes

CO	**Upon completion of this course the students will be able to :**	**PSO addressed**	**CL**
CO- 1	**Identify** the eigen values and eigen functions of materials using theoretical calculations	PSO-4	R
CO- 2	**Discuss** the probability of occupancy of an electron in an energy state at various pressures by electronic structure calculation	PSO-1	U
CO- 3	**Analyse**the crystal parameters to investigate electronic and structural phase transition in crystalline materials.	PSO-3	An
CO -4	**Apply** the FP-LMTO method in the Basic theories of electronic	PSO-2	Ap

	structure		
CO- 5	**Explain** the phenomenon of Metallizaton, superconductivity and Fermi surfacein materials.	PSO-5	U
CO -6	**Compare** the various band structure methods suitable for metals, semiconductors and insulators using recent reprints (KI,RbI, CsI, CsBr and alkali halides)	PSO-2	E
CO -7	**Develop** a deeper research experience in electronic structure calculations	PSO-6	C

Teaching Plan

Total contact hours: 90 (Including lectures, assignment and tests)

Unit	Module	Topics	Lecture Hours	Learning outcomes	Pedagogy	Assessment /Evaluation
I	**BASIC THEORIES OF ELECTRONIC STRUCTURE**					
	1	Zeroth Born-Oppenheimer approximation – Density functional theory	**4**	formulate Zeroth Born-Oppenheimer approximation	Discussion, derivation and PPT	Evaluation Class test, oral question Assignment , self work Formative assessment I
	2	Self interaction correction and optimized effective potentials – Gradient corrections	**4**	formulate different Formula for optimized effective potentials	Discussion, derivation and PPT	
	3	Local density approximation- Atomic sphere approximation-	**4**	formulate Local density approximation and Atomic sphere approximation	Discussion, derivation and PPT Seminar	
	4	Hartree approximation- Hartree-Fock approximation.	**3**	Derive Hartree approximation and Hartree-Fock approximation	Discussion, derivation and PPT	
II	**THE FP-LMTO METHOD**					
	1	The energy band problem - Partial waves for a single muffin-tin- The muffin-tin orbitals	**4**	Solve energy band problems	Problem solving and Derivation	Evaluation Class test, oral question Assignment , seminar Formative assessment I
	2	Independent muffin-tin orbitals- One center expansion and structure constants	**3**	Solve Solution of muffin-tin orbitals	Problem solving and Derivation	
	3	Korringa- Kohn - Rostoker (KKR) condition- Total energy and enthalpy determination	**4**	Solve total energy and enthalpy	Problem solving and Derivation Seminar	
	4	McMillan's formula-	**4**	Superconducting	Derivation ,	

		Superconducting transition temperature calculation.		transition temperature calculation.	PPT	
III	Five reprints of electronic structure calculations					
	1	Ab-initio calculations of physical properties of alkali chloride XCl (X = K, Rb and Li) under pressure Computational Condensed Matter 4 (2015) 6-12	**3**	Study on physical properties of alkali chloride XCl (X = K, Rb and Li) under pressure	Discussion and calculation	Evaluation Class test, oral question Assignment, seminar Formative assessment II
	2	Pressure dependence of structural phase transition and superconducting transition in CsI phys. stat. sol. (b) 236, No. 3, 614–624 (2003)	**3**	Obtain structural phase transition and superconducting transition in CsI	Discussion and calculation	
	3	Epitaxial diamond encapsulation of metal microprobes for high pressure experiments APPLIED PHYSICS LETTERS, VOLUME 77, NUMBER 21, 3400 (2000).	**3**	Discuss high pressure experiments	Discussion and calculation	
	4	Band structure,metallization and superconducting transition of CsBr under high pressure ChemXpress 8(3), 158-164, (2015). Electronic Band Structure and Metallization of KI and RbI under High Pressure stat. sol. (b) 233, No. 2, 339–350 (2002)	**6**	Apply Band structure, metallization and superconducting transition of CsBr , KI and RbI	Discussion and calculation Seminar	
IV	**PRESSURE INDUCED STRUCTURAL CHANGES**					
	1	Murnaghan's equation of state (EOS) – NaCl structure to CsCl	**4**	Derive Solution Of Murnaghan's equation of state	Derivation discussion and Problem solving	Evaluation Class test, oral question Assignment,

		structure pressure induced transitions				seminar Formative assessment II/III
	2	ZnS to NaCl andNaCl to CsCl transitions – BCC to FCC transitions	**4**	Define and derive BCC to FCC transitions	Derivation discussion, PPT	
	3	HCP to BCC transitions – Transitions in and from Wurtzite structures	**3**	Derive different types of HCP to BCC Transitions	Derivation discussion Seminar	
	4	Force theorem and elastic constants of solids.	**4**	Define , derive and apply Force theorem	Derivation discussion, PPT	
V	**METALLIZATON AND FERMI SURFACE**					
	1	Metallization in alkali halides – silver halides	**4**	Define and derive Basics Of Metallization	Derivation discussion, PPT	Evaluation Class test, oral question and program writing Assignment, Seminar Formative assessment III
	2	Group III-V compounds – Group II-VI compounds – Measurement of Fermi surface	**4**	Define and derive Measurement of Fermi surface	Derivation discussion, PPT	
	3	Bohr-Somerfield quantization rule – Oscillation of the Density of states at the Fermi energy	**3**	Define and Derive Density of states at the Fermi energy	Derivation discussion Seminar	
	4	Determination of Fermi surface – electronic and optical properties of Alkali metals and noble metals.	**4**	Study the electronic and optical properties of Alkali metals and noble metals.	Discussion, PPT	

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