PhD PROGRAMME IN PHYSICS

Syllabi Of Discipline Elective Courses

PAPER-I

<table>
<tr><td rowspan="2">DSE</td><td rowspan="2">NANOMATERIALS</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td colspan="6">Pre-requisite: Concepts of Quantum Mechanics, physics of semiconductors with good knowledge of the related topics incorporated in Post Graduate curriculum.</td></tr>
<tr><td colspan="6">Course Objective
(1) aims to have a broader concepts on the historical perspective and synthesis of nanomaterials via different techniques.
(2) aims to enhance knowledge about different characterization techniques.
(3) focuses on developing theoretical concepts about low dimensional structures.
(4) aims to enhance the knowledge on different softwares required to understand the behaviour of nanoparticles.</td></tr>
<tr><td colspan="6">Course Outcome:</td></tr>
<tr><td colspan="6">After successful completion of the course, the students will be able
CO1: to understand the historical perspectives of nanoparticles, synthesis, characterization tools, theoretical mechanics on low dimensional structures, and different softwares.
CO2: to apply the understanding on different theories of science to understand the characteristics of nanoparticles via ways of synthesis and characterization tools.
CO3: to distinguish synthesis procedures and characteristics of different nanoparticles.
CO4: to evaluate various parameters related to nanoparticles via softwares.</td></tr>
<tr><td colspan="5">Module 1: Historical perspective, synthesis of nanomaterials</td><td>15 hours</td></tr>
<tr><td colspan="6">History and development of Nanoscale science, fundamental concepts, examples of interesting nanoscience applications, Bottom up and Top down methods- Template-based synthesis: Electrochemical deposition, Electrophoretic deposition, colloid dispersion, melt or solution filling, Lithographic Techniques: Photolithography (Optical, UV, EUV), Electron beam lithography, Ion beam Lithography, X-Ray Lithography, Dip-pen lithography, Nonlithographic techniques: Plasma Arc discharge, sputtering, Thermal evaporation, Electron beam evaporation, Chemical vapour deposition, pulsed laser deposition, Molecular beam epitaxy, liquid phase epitaxy, Chemical bath deposition (CBD), Ion beam deposition(IBD), Vapour-liquid-solid(VLS) technique, Spray pyrolysis, biological synthesis.</td></tr>
<tr><td colspan="5">Module 2: Characterisation tools for nanomaterials</td><td>10 hours</td></tr>
<tr><td colspan="6">Chemical Characterisation- UV-Visible spectroscopy, Photoluminescence spectroscopy, Raman Spectroscopy, Fourier Transform Infrared Spectroscopy(FTIR), Secondary Ion Mass Spectrometry(SIMS), Energy Dispersive X-ray Spectroscopy(EDS)
Structural Characterisation: X-ray Diffraction(XRD), Scanning Electron Microscopy(SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM)</td></tr>
<tr><td colspan="5">Module 3: Quantum confinement and low dimensional structure, metal nanoparticles</td><td>10 hours</td></tr>
<tr><td colspan="6">Models of semiconductor quantum wells, quantum wires & quantum dots semiconductor heterostructures & quantum wells- confinement models & 2D electron gas, Energy band transitions</td></tr>
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in quantum wells, transition & excitonic effects in quantum wire, density of states (DOS), in various dimensions: 1D, 2D & 3D density of states of quantum well, quantum wire & quantum dots, application of semiconductor quantum dots, Quantum wells and Quantum wires, surface Plasmon resonance, metal nanoparticles core/shell nanoparticles, applications of semiconductor, metal & core/shell nanoparticles.		
Module 4: Modeling and simulation		**10 hours**
Modeling, need of modeling, simulation techniques, different simulation software: COMSOL, Multiphysics, CST Microwave Studio, MATLAB, analysis of characterization results by Origin software.		
Total Lecture hours		**45 hours**
Text Book(s)		
1.	Madhuri Sharon, *History of Nanotechnology: From Prehistoric to Modern Times*, (2019), Wiley-Scrivener.	
2.	Felipe Lopez- Saucedo, *Synthesis of Nanomaterials,* (2023), Bentham Science Publishers.	
3.	Sabu Thomas, *Microscopy Methods in Nanomaterials Characterisation*,(2017), Elsevier.	
4.	V. Tiwari, Modeling, *Characterisation and Production of Nanomaterials* (2015), Woodhead Publishing	
5.	George W. Hanson, *Fundamentals of Nanoelectronics*,(2008), Pearson Education.	
Reference Books		
1.	Mohammed Baalousha, Characterisation of Nanomaterials in Complex Environmental and Biological Media, (2015), Elsevier.	
2.	Gunter Schmid, *Nanomaterials: From Theory to Application*(2011), Wiley-VCH	

PAPER-II

DSE	Density Functional Theory	L	T	P	C
		2	0	2	3

Pre-requisite: Quantum Mechanics at Post Graduate Level

Course Objectives:

1. To provide knowledge about the basic formalism of density functional theory.
2. To apply density functional theory to investigate molecular properties.

Course Outcome:

After successful completion of the course, the students will be able to

CO1: Build a strong theoretical foundation of density functional theory.

CO 2: Calculate molecular properties like energy, vibrational frequency, dissociation energy, charge etc. of simple molecules on the basis of density functional theory.

Module 1: FORMULATIONS OF DENSITY FUNCTIONAL THEORY	15 hours

1) Density matrices: Electron density, pair density, Fermi and Coulomb holes.
2) Thomas-Fermi model
3) Derivation of the Hohenberg-Kohn theorem
4) Kohn-Sham formalism
5) Different density 3unctional-LDA, GGA etc.
6) Concept of Basis set (STO-3G, 3-21G, 6-31G, 6-31G*, 6-31G**)

Module 2: APPLICATIONS OF DENSITY FUNCTIONAL THEORY	15 hours

1) Geometry optimization and vibrational frequencies of simple molecules.

2) Charges on the atomic centers in a molecule, Mulliken population analysis, Reactivity descriptors.

3) van der Waals interaction, Lennard-Jones potential, counterpoise correction for Ar_2.

4) Molecules exhibiting Hydrogen bond, counterpoise correction for $(HF)_2$.

5) Dissociation energies of $Ni(CO)_4$.

6) Potential energy surface

7) Force Fields

Total Lecture hours	30 hours (Theory)+ 30 hours (Practical)

Text Book(s)

1. A Chemist's Guide to Density Functional Theory, W. Koch, M.C. Holthausen Second edn., Wiley-VCH, 2001

2. Density Functional Theory An Advanced Course, E. Engel, R.M. Dreizler, Springer, 2011

Reference Books

1. Density-Functional Theory of Atoms and Molecules,Robert G. Parr and W. Yang, Oxford University Press, 1995.

PAPER-III

DSE	Numerical Programming in Physics	L	T	P	C
		2	0	1	3

Prerequisite: Basic Knowledge of Coding using Python.

Course Objectives:

1. This course aims to give the students an introductory course on the methods in numerical analysis to physics students with the addition of Python programming lab to better understand these methods.

2. To disseminate lectures on the numerical methods applied in finding the zeros of a function, curve fitting, numerical integration and numerical solution of ordinary differential equations and its associated applications in physical problems.

3. To analyze how the exact solution obtained using mathematical approximation in different models in physics differs from the numerical solution of the same.

Course Outcome:

1. To apply numerical methods to solve problems that could not be solved exactly using traditional methods as well as successfully fit a polynomial to a given dataset taking into consideration the aspects of overfitting and underfitting.

2. To understand how differential equations and definite integrals are solved computationally and also understand how the concept of singularity could be numerically handled in such methods.

3. To successfully apply numerical methods in different areas of physics such as polynomial fitting using a given dataset, the numerical simulation of the damped harmonic oscillator, simple pendulum and predator-prey model, etc.

Module 1: Zeros of an Equation, Polynomial Fitting and Linear Algebra	15 Hours

Zeros of an Equation - Bisection, Newton Raphson and Secant Method. *Polynomial Fitting* – Least Square Curve Fitting Procedure (straight-line and n^{th} order polynomial fitting) and Cubic Spline.	
Module 2: Numerical Integration and Solution of Ordinary Differential Equations (ODEs)	**15 hours**
Integration - Midpoint rule, Trapezoidal Method and Simpson's Rule – 1/3 and 3/8 Rule. *Solution of ODEs* - Picard's Method of Successive Approximation, Euler's Method and Runge-Kutta Method – 2^{nd} and 4^{th} order.	
Module 3: Applications in Problems of Physics	**15 hours**
Straight line/Polynomial fitting for a given dataset, Motion of a body in a straight under constant acceleration, Numerical solution of the Simple and the Damped Harmonic Oscillator, Numerical solution of the Simple Pendulum with or without using approximation, Numerical Solution of the Predator-Prey Model.	

Textbook (s)

1.	Numerical Analysis, R. L. Faires and J. D. Burden 9^{th} Edition, Cengage India Pvt. Ltd. (2012).
2.	Introductory Methods of Numerical Analysis 5^{th} Edition, S. S. Sastry, Prentice Hall India Learning Pvt. Ltd. (2012).

Reference Books

1.	Numerical Methods in Physics with Python 2^{nd} Edition, A. Gezerlis, Cambridge University Press (2023).