Syllabus for pre-Ph.D. Coursework -2023

PHYSICS

As per Kalyani University (Minimum Standards and Procedure for Award of Ph.D. Degree) Regulations, 2022, the pre-Ph.D. Coursework consists of four papers, each with 4 credits (total 16 credits). The course work shall be treated as prerequisite for Ph.D. preparation.

The structure of the course will be as follows:

Paper - CW1: Research Methodology (A)

Quantitative Method (Numerical methods);

Computer Application: Programming languages (Fortran), Application package (Mathematica / Matlab, Origin);
Training (Material preparation and different characterization techniques, Basic instruments (XRD, Electron & Atomic microscopes, Spectroscopic techniques), Experimental data analysis technique);
Field Work,

Research Ethics, etc.

Marks Allotted: ***50*** *[Term End Exam. (30) + Internal Assessment (10) + Viva-voce Exam. (10) =50]*

Credits Allotted: ***04***

Paper - CW2: Research Methodology (B)

Review of Published research, Documentation/ submission of Reports on Review work and Presentation.
Marks Allotted: ***50*** *[Review Report (30) + Presentation (10) + viva-voce (10) = 50]*

Credits Allotted: ***04***

Paper - CW3: Advanced Level Course on Subject (A)

Marks Allotted: ***50*** *[Term End Exam. (30) + Internal Assessment (10) + Viva-voce Exam. (10) =50]*

Credits Allotted: ***04***

Subject Specific Components (*choose one component*):

1. Computational Materials Science

Density functional theory (DFT): Basics of Quantum Chemistry. The Hartree-Fock Approximation, Hohenberg-Kohn theorems: First theorem, Second HK theorem, Kohn-Sham formalism, Exchange-correlation functionals, Local Density Approximations, Generalized Gradient Approximations, Hybrid functional, Van der Waals correlation functions, Basis sets, Density-functional perturbation theory: Perturbation in Kohn-Sham scheme, Lattice dynamics approach, Vienna ab-initio simulation package (VASP)

Molecular Dynamics (MD): Potential energy surface, pair potential approximation, advantages and limitations, phenomenological potential, buckinghan, morse, lennard-jones and berker, pseudo potentials, many-body potentials, Model for MD calculation, initial value, isothermal equilibrium, boundary, nano-design and nano-construction, solution of the equation of motion, verlet, gear-predictor, and other methods, efficient force field computation, force derivation, list method, cell algorithm, scalable parallel procedure. Lammps simulation package. OVITO, VMD

2. Theoretical Atomic Collision Physics

Many Electron Atoms and Ions: The Hamiltonian, Pauli principle and Slater determinant, Shell structure of atoms, Classification of atomic levels

N-electron problem: Thomas Fermi model, Hartee-Fock method, Correlation and Configuration Interaction

Inner-Shell Vacancy Production Induced by Point Charge Particles: Protons and Alpha Particles: Theoretical Models, Total Cross Section Measurements, Characteristic Spectra, Extensions and Deviations

Heavy Ion Induced Inner-Shell Ionization: General Considerations, High-Energy Limit, Theoretical Developments (BEA, PWBA, SCA, ECPSSR, ECUSAR, CSC), Comparison of Auger and X-Ray Cross section Data: Fluorescence yields in Heavy Atom Collisions, Level Matching Effects, Electron capture and ionization in collisions of multiply charged ions.

3. Crystal-Field Theory

a) Hydrogen atom problem, s-, p-, d- orbital wave functions, wave-mechanical picture of covalent and ionic bonding, Valence Bond and Molecular Orbital Theory, sp^n hybridization, Ligand-Field Theory for 3d-group of elements, weak and strong-field cases, application to d^n orbitals for octahedral and tetrahedral symmetry- Orgel model, Jahn-Teller distortion.

Overlapping integrals, Crystal-field theory for rare-earth elements, Van Vleck Susceptibility, Schottky Specific heat, Nuclear quadrupolar and hyperfine properties.

b) **Molecular symmetry**: Reflection, Inversion, Rotational Reflection symmetry; Symmetry elements, Point groups, Space group, Classes, and representation, Character Tables; Direct product, Double groups, idea of Kramer's degeneracy.

c) **Molecular Magnetism**: Single Molecule Magnet (SMM), Single-Ion Magnet (SIM).

4. Nanofluids

Definition; Different types of Nanofluids; Fabrication, Stability of Nanofluids; Experimental results on thermos-physical properties of Nanofluids; Effect of particle size, particle shape, volume concentration and temperature on the thermos-physical properties of Nanofluids; Experimental and theoretical analysis of nanofluids based on high temperature-heat transfer fluid with enhanced thermal properties. Theoretical investigations on different Nanofluids; Molecular Dynamics Simulation (MDS) study of Nanofluids; Thermal conductivity and viscosity of nanofluids using Molecular Dynamics studies; Applications-Current & Future.

5. Quantum Field Theory

Principle of variation and Euler-Lagrangian equation, Real Scalar fields, Field decomposition and Hamiltonian in terms of the Number Operator, Field quantization, Complex Scalar fields, Noether's theorem, Clifford algebra and Gamma matrices, Dirac field theory, Basics of Abelian and Non-Abelian Gauge theory, Basics of QED, Self-interaction, Wick's Theorem, Normal ordering and Weyl ordering, S-Matrix formulation, Feynman Diagrams (Tree level), Decay Width and Cross-section calculation for some physical process and Standard Model of Particle physics, Amplitude calculation.

6. Energy and Power Storage Devices

Fundamentals of Batteries and Supercapacitors: An Overview; open circuit voltage and its Impact on the internal resistance of an energy storage device; Time delays in delivering or transferring energy; Complex models of Energy Storage Devices; Primary and secondary batteries.

Electrochemical Characterization techniques: Electrochemical Impedance Spectroscopy; Cyclic Voltametry; Transference number calculations; Galvanostatic Charge/Discharge Energy storage in electrical systems: Basic electrical components as in-circuit energy storage.

Technical specifications of Energy storage Devices: Energy and power density, Ragone plot. Rechargeable battery technologies: Battery terminology and fundamentals, Peukert's law and the battery capacity, C rate, Energy density, Power density of a battery, Cycle life, Cyclic energy density, Self-discharge rate, Charge acceptance, Depth of discharge, Battery discharge curves and related terminology, Overcharge, State of charge (SoC), State of health.

Lithium-based rechargeable batteries: Construction, Characteristics of different components; Charge and discharge characteristics.

Supercapacitors as power storage devices: Fundamental of Supercapacitors (SC); Characteristics of different SC components; Electric double layer capacitance and Pseudo capacitance.

Paper - CW4: Advanced level course on subject (B)

Marks Allotted: ***50*** *[Term End Exam. (30) + Internal Assessment (10) + Viva-voce Exam. (10) =50]*

Credits Allotted: ***04***

The paper will be based on Trans-disciplinary Components (*choose one component*):

1. Atomic Physics with Accelerators

Introduction to Accelerator Physics: Short Historical Overview, Main Components of Accelerator Facilities , Applications of Particle Accelerators, Principles of Particle-Beam Dynamics , Stability of a Charged-Particle Beam, Principles of Linear Accelerators , Charged Particles in Electric Fields, Electrostatic Accelerators, Electric Field Components (Electrostatic Deflectors, Electrostatic Focusing Devices, Iris Doublet, Einzellens), Acceleration by rf Fields (Microwave Linear Accelerators)

Semiconductor Diode Detectors: The Action of Ionizing Radiation in Semiconductors, Semiconductors as Radiation Detectors, Semiconductor Detector Configurations, Operational Characteristics, Germanium Gamma-Ray Detectors, Lithium-Drifted Silicon Detectors

Processing of experimental data: The presentation of physical quantities with their inaccuracies (measuring errors and uncertainties), Classification and propagation of errors, Binomial distribution; Poisson distribution; Gaussian or Normal distribution; Lorentzian distribution; the central limit theorem. Distribution function of a data series; the average and the mean squared deviation of a data series; estimates for mean and variance; $\square^2$ Test of a distribution; handling data with unequal weights. Fitting functions to data: Dependent and independent variables, method of least squares, fitting to a polynomial, minimizing $\square^2$ for Goodness of Fit, Linear-Correlation Coefficient. Numerical Methods: Polynomial Interpolation, Numerical Differentiation and Integration, Roots of Nonlinear Equations.

Scattering Experiments: Experimental Procedures, Electron Promotion Energies and High Energy Collisions, Cross Section Measurements: X-Ray Cross Sections, Auger-Electron Cross Sections. Spectral Measurements: Electron Spectra, X-Ray Spectra.

2. Material Characterization Techniques

Electron Microscopy: Interaction of electrons with solids, Scanning electron microscopy, Transmission electron microscopy and specimen preparation techniques, Scanning transmission electron microscopy, Energy dispersive spectroscopy, Wavelength dispersive spectroscopy.

Diffraction Methods: Fundamental crystallography, Generation and detection of X-rays, Diffraction of X-rays, X-ray diffraction techniques, Electron diffraction. Neutron diffraction.

Surface Analysis: Atomic force microscopy, scanning tunnelling microscopy, X-ray photo-electron spectroscopy, Surface plasmon resonance, X-ray reflectivity

Spectroscopy: Atomic absorption spectroscopy, UV/Visible spectroscopy, Fourier transform infrared spectroscopy, Raman spectroscopy, NMR

Thermal Analysis: Thermo-gravimetric analysis, Differential thermal analysis, Differential canning calorimetry, Thermo-mechanical analysis and dilatometry

Electrical characterization techniques: electrical resistivity, thermoelectric power, thermal conductivity, frequency dependent impedance and dielectric

Magnetic properties characterization: AC susceptibility, DC magnetization. VSM, SQUID.

3. General Relativity & Cosmology

: Basics of Tensor calculus, Riemann Tensor, Ricci Tensor, Covariant derivative, Parallel transport, Bianchi Identity, Einstein Tensor, Postulates of General Relativity, Lagrangian formulation and Einstein equation, Some applications of General theory of Relativity (Perihelion of Mercury, Red shift and Blue shift, Age of the universe etc.), Geodesic equation, FRLW solution of Einstein equation, Friedman equations, Basic concepts about Ray Chowdhury equation, Principles of Standard model of Cosmology, Hubble parameter, Early time and late time of the Universe, Coupling of EM field to gravity, Maxwell equation in curved space-time, Spherically symmetric black hole solutions of the Einstein equation (Schwarzschild BH, Reissner-Nordstrom BH), Basic concepts about Cosmological constant.