Course Structure and Syllabus

Integrated Ph.D. in Physical Sciences

In Collaboration with the

University of Calcutta

and

Ph.D. Programme

CENTRE FOR
S. N. BOSE NATIONAL
BASIC SCIENCES 1986
1894-1974
विज्ञानेन परिपश्यन्ति धीराः

S. N. Bose National Centre for Basic Sciences

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INTEGRATED Ph.D. PROGRAMME IN PHYSICAL SCIENCES (IPhD-PH)

The Integrated PhD Programme in Physical Sciences (IPhD-Ph) at the S. N. Bose National Centre for Basic Sciences (SNBNCBS) in collaboration with the University of Calcutta (CU) is monitored by a Board of Studies comprising representatives from both SNBNCBS and CU, and eminent faculty members from other academic institutions as per CU rules. The duration of this course is 2+5 = 7 years. A student seeking admission to this course must have passed B.Sc. with Physics and Mathematics securing at least 60% marks in the main subject. Final selection will be made on the basis of national level written tests e.g. JEST/ NGPE or other standard national level eligibility tests followed by a personal interview/Counseling. The candidate must also possess other qualifications as may be prescribed by the Academic Council (AC) from time to time. After admission the candidates shall have to register with CU, and as per rules, students coming from Universities other than CU shall have to submit a migration certificate.

Syllabus and Course Structure:

The syllabus and course structure approved by the Students' Curriculum and Research Evaluation Committee (SCREC) of SNBNCBS is monitored by the Board of Studies strictly following the UGC guidelines issued from time to time.

The description in the following pages is an attempt to provide a basic outline of the material to be covered. But of course the detailing out and the point of view is one to be decided upon by the teacher. The same is true regarding the suggested textbooks. Generally one expects that attempts will be made to suggest to the students even at the level of the basic courses (in the first two semesters) the linkages with more advanced courses to come later, and to indicate how the core material relates to more recent applications. Furthermore, efforts may be made to establish connectivity to other courses going on concurrently or to those that are to come subsequently, to impart the sense of organic unity of the physical sciences. Emphasis will be placed on tutorials and in having examples of the material covered in the lectures to concretize the underlying ideas and facilitate the application of basic principles to solving problems.

FIRST SEMESTER COURSES & SYLLABI

L=Lectures T=Tutorials P=Practicals in hours per week & C=Credit points

PAPERS FOR 1ST SEMESTER (AUGUST – DECEMBER)

Course No.	Course Title	L	T	P	C
PHY 401	Mathematical Methods	3	1	-	4
PHY 403	Classical Dynamics	3	1	-	4
PHY 405	Quantum Mechanics I	3	1	-	4
PHY 407	Computational Methods in Physics	2	-	2	4
PHY 491	Basic Laboratory I	-	2	6	8

Examination: 2nd week of December

Semester Break: 4th week of December

PHY 401. MATHEMATICAL METHODS I

• **Linear spaces and algebra of linear transformations**: Axiomatic definition of a linear space with examples, dual spaces, inner product spaces, definition of an associative algebra with examples, vector space homomorphisms with examples, Algebra of linear transformations, matrices, characteristic roots and associated properties, canonical form of matrices, general definition of hermitian and unitary operators with examples. *[3 Lecture Hours]*

• **Group Theory**: Definition of a group (examples); subgroup (examples); normal subgroups and quotient groups (examples); homomorphisms (examples), permutation groups, orthogonal, unitary, pseudo-orthogonal groups; definition of a Lie algebra with examples; structure constants, adjoint representation; SU(2) and SO(3) groups as Lie groups, Lie algebra of their generators, homomorphism between SU(2) and SO(3); Poincare group and its algebra. *[10 Lecture Hours]*

• **Functions of a complex variable**: Review of complex numbers; definition of a complex function; continuous functions; differentiability; definition of an analytic function; Cauchy-Riemann equations; the exponential function; the trigonometric functions; the hyperbolic functions; multivalued functions and principal branch; power series for log(1+z); zeros and poles of functions; classification of singularities; Cauchy's theorem; analytic continuation; Cauchy's integral formula; Laurent expansion, calculus of residues, Conformal mapping. *[15 Lecture Hours]*

• **Metric spaces, Hilbert spaces, Green's functions, Boundary value problems**: Definition and some examples of a metric space; open sets; closed sets; convergence; completeness; compactness; continuous mappings; spaces of continuous functions; Euclidean and unitary spaces; Hilbert space, the Schwarz inequality; orthogonal complements (basic theorems); orthonormal sets; Bessel's inequality, Riesz-Fischer theorem; the adjoint of an operator; Hermitian and self-adjoint operators;

normal and unitary operators; projections. Sturm-Liouville theory, Green's functions, Laplace and Fourier transforms, Boundary and Initial value problems. *[12 Lecture Hours]*

Suggested Textbooks:

- *Brown and Churchill : Complex variables and applications*
- *Dennery and Krzywicki : Mathematics for Physicists*
- *E. Kreyzig : Engineering Mathematics*
- *G.B. Arfken, H.J. Weber, Mathematical Methods for Physicists*

PHY 403. CLASSICAL DYNAMICS

- **Elementary Principles:** Mechanics of particles, system of particles, Constraints, D'Alembert's Principle, generalized coordinates *[3 Lecture Hours]*
- **Lagrange's Equations:** Principle of least action, Lagrange's equations of motion, Symmetries and conservation laws *[5 Lecture hours]*
- **Oscillations:** Small oscillations, normal modes, forced and damped oscillators *[6 Lecture Hours]*
- **Central Force:** Equivalent one-body problem, Virial Theorem, Orbits, Scattering *[8 Lecture Hours]*
- **Rigid body:** Rigid body rotations and Euler angles, algebra of rotation group, Torque-free motion of a rigid body *[6 Lecture Hours]*
- **Hamilton Equations of Motion:** Legendre transformation, Hamilton's equations of motion,Concept of a phase space, Poisson brackets and its properties, Hamilton's equations of motion, Constants of motion, Liouville's theorem *[6 Lecture Hours]*
- **Canonical Transformations:** Generating functions, generators of symmetries, Hamiltonian as generator of time translation, Hamilton-Jacobi equation *[3 Lecture Hours]*
- **Continuous systems and fields:** Lagrangian and Hamiltonian for a free scalar field, general variation of the action, derivation of Euler-Lagrange equation, Noether's theorem, energy momentum tensor and conservation equation, Euler-Lagrange equations for pure electromagnetic theory and Maxwell's equations *[6 Lecture Hours]*

Suggested Textbooks:

- *H. Goldstein : Classical Mechanics, 2nd edition.*
- *John L. Synge and Byron A. Griffith : Principles of Mechanics, 3rd Edition.*
- *L. D. Landau and E. M. Lifshitz : Mechanics (Volume I of - A course of Theoretical Physics).*
- *E.C.G.Sudarshan and N. Mukunda : Classical Mechanics - a modern perspective.*

PHY 405. QUANTUM MECHANICS I

- **Mathematical preliminaries:**
  - Vector spaces: Definition, Dirac notation, inner product, Hilbert space, orthonormal basis, Gram-Schmidt construction, dual vectors, Cauchy-Schwarz inequality;
  - Linear operators: Definition, algebra, inverse, adjoint, Hermitian, unitary, projection operator, matrix representation, eigenvalue, eigenvector, complete set of commuting operators, functions and derivatives of operators;
  - Continuous basis: x-basis, delta function, -i d/dx, p-basis, Fourier transform;

  [10 Lecture Hours]
- **Quantum Mechanics:**
  - Formulation in terms of postulates, Schrödinger equation, stationary states, evolution operator, time independent systems, non-relativistic wave equation, 1-d oscillator in operator formulation, relation with wave functions;
  - Ehrenfest theorem, parity, 1-d potentials, square well, periodic potential, Dirac comb, 1-d scattering *[8 Lecture Hours]*
- **3-d systems:**
  - Central potential, angular momentum operator algebra, eigenvalues, eigenvectors, spherical harmonics, free particle, spherical oscillator, Hydrogen atom, operator methods; *[7 Lecture Hours]*
- **Identical particles:**
  - Multiparticle states and Hilbert space, bosons and fermions; *[6 Lecture Hours]*
- **Continuous Symmetry transformations:**
  - Translation, rotation, general structure, internal symmetries, conserved charge, gauge symmetry and coupling with electromagnetic field, Aharonov-Bohm effect

  [6 Lecture Hours]
- **Spin:**
  - Stern-Gerlach experiment, operator algebra and representation, Zeeman effect;
  - Addition of angular momentum, **L** + **S.** *[4 Lecture Hours]*

Suggested Textbooks:

- *R. Shankar: Principles of Quantum Mechanics*
- *A. Bohm: Quantum Mechanics: Foundations and Applications*

PHY 407. COMPUTATIONAL METHODS IN PHYSICS

- **Computational Language (FORTRAN / C / Python)**
  - Basic Linux commands and vi editor commands.
  - Constants and variables; variable types and declarations, and arithmetic expressions.
  - Read and write statements, logical expressions.
  - IF, Arithmetic IF, IF-THEN-ELSE statements.
  - GO TO, Computed GO TO statements.
  - DO loops, nested DO loops.

- Functions and subroutines.
- Arrays, 1-2-3 dimensionals.
- Formatted input / output statements.
- Precision – single, double, quartic.
- xmgrace and gnuplot *[10 Lecture Hours]*

- **Simple Problems to Practice the Language**
  - Finding the largest number in a set of numbers.
  - Sum of some numbers except one of them.
  - Arranging numbers in increasing / decreasing order.
  - Test if the given number is prime; generating all prime numbers up to a given number.
  - Mean, variance standard deviation of a given set of numbers.
  - Factorial of a given number.
  - Generating the Fibonacci series.
  - N atoms, each has two spin states. Enumerate all possible microstates, estimation of the energy of each of these states, distribution of magnetisation and energy.
  - Converting a decimal number into a binary.
  - Matrix operations *[10 Lecture Hours]*

- **Numerical Techniques**
  - Error in computation – definition and source of errors, propagating and control of errors.
  - Root finding for polynomial equations, Bisection method and Newton-Raphson method, or use any other two methods.
  - Interpolation, extrapolation – Polynomial interpolation or any other method.
  - Numerical integration – Midpoint rule and Trapezoidal rule or any two other methods.
  - Solving linear equations – Gauss elimination methods and Iterative solution methods.

[10 Lecture Hours]

- **Simulation Techniques**
  - Random number generation.
  - Monte Carlo (MC) method, Importance Sampling.
  - Estimate of (i) the value of π, (ii) area of an annular ring and (iii) Integration of simple functions using MC.
  - Biased and unbiased Random walks in one and two dimensions, probability distribution, dispersion, mean-square-distance, exponents.
  - Simple example of simulations using Monte Carlo method. *[10 Lecture Hours]*

Suggested Textbooks:

- *Numerical Recipes in C/Fortran: The Art of Scientific Computing By William H. Press et al.*
- *Monte Carlo Simulation in Statistical Physics: An Introduction by Kurt Binder, Dieter Heermann.*
- *Computer Programming In Fortran 90 and 95 By V. Rajaraman*

PHY 491. BASIC LABORATORY I

The aim of this course is to develop a temperament among the students so that they feel confident enough in setting up experimental arrangements for investigating physical problems. Instead of specifying a set of pre-existing equipment and already set-up experiments, this curriculum gives emphasis to the universal principles and underpinnings of experimental techniques through a laboratory based hands-on course and design of experiments.

Electronics Experiments:

As a first step towards this goal it is necessary to introduce the working principles of basic measuring instruments and sensors and how they can be used to measure and to control different physical variables. For this purpose it is essential that the students become familiar with the principles and practice of electronics. Accordingly, one of the components of this course is Electronics which will be superposed on the part devoted to the investigation of physical phenomena in order to avoid compartmentalisation. For convenience experiments with this component are carried out in the very beginning.

1. **Measurement of Thevenin parameters (V[TH] and R[TH]) of a DC power supply (Battery).**
    - Plot V[load] versus R[load] curve and mark slope and stiff regions.
    - In the slope region measure V[load] for at least two different R[load] and characterize V[TH] and R[TH].
    - In the stiff region measure I[Load] for at least two different R[Load] and characterize V[TH] and R[TH].
    - Measure V[TH] by using a multimeter and compare with the estimated value of V[TH] and comment.

2. Characterization of semiconductor diodes and designing of transformer based full wave rectifiers.

- Draw three characterization curves of two rectifier diodes (Germanium, Silicon) and one Zener diode.
- Estimate turn ratio of a transformer by measuring voltage ratio (primary and secondary).
- Construct a Full wave rectifier and measure input and output waveforms of the rectifier.

3. Characterization of a Zener Regulated DC power supply.

- Measure V[C], V[rms], g and PIV of a full wave rectifier and compare them with their calculated values.
- Design a R-C filter and measure p-p ripple voltage and compare with calculated value.
- Design a Zener regulator after the above filter and measure load dependency and load regulation (voltage).

4. Characterization of an n-p-n transistor and designing of fixed biased CE transistor amplifier.

- Draw base and collector characteristic curves of an n-p-n transistor in the CE configuration.
- Mark saturation, cutoff and active regions and determine Q point for best transistor operation.
- Design a simple fixed biased CE amplifier with the estimated Q point. Determine current gain and compare with the specified value.

5. Use of a transistor as an electronic switch and designing a memory unit (R-S flip flop).

- Use a transistor as a switch to operate a LED in the output with low frequency input.
- By using high frequency square wave input measure t[on] and t[off].
- Design a R-S flip-flop and complete its truth table with S as input. Catch a bit from a low frequency pulse train.

6. Use of IC 741 as an adder, amplifier, integrator, differentiator.

Suggested References:

- Price, Analog Electronics (Prentice Hall)

- Hickman, Analog Electronics (Newnes)
- Bogart, Electronic Devices and Circuits (Universal Book Stall)
- Streetman, Solid State Electronic Devices (P/H/I)
- Horowitz and Hall, The Art of Electronics (Cambridge)

Optics Experiments:

The other important component of this course is Optics. The details of the experiments on Optics are listed below.

1. Experiments related to Laser beam characteristics, such as:

- To study the intensity distribution of a Laser beam
- Determination of spot size and the angle of divergence of a given Laser source.
- Measurement of the absorption coefficient (Beer-Lambert Law) of a material (supplied) using Laser light.

2. Experiments related to interference, such as:

- To determine the wavelength of He-Ne Laser by Michelson Interferometer

3. Experiments related to diffraction, such as:

- To measure the number of lines in a transmission grating using a Laser.
- To measure the wavelength of a He-Ne laser using a grating.

4. Experiments related to polarization, such as:

- To study circularly polarized light by a quarter wave plate.
- To verify Malus's law and to determine the Verdet constant of a given crystal.
- To demonstrate Faraday effect
- To demonstrate the electro-optic effect

5. Experiments related to Spectroscopy:

- Construction of a simple spectrometer using a white light source and a grating as major components.
- Measurement of absorption spectra of a given liquid sample.
- Validation of Beer-Lambert's Law of molecular absorption from the setup.

6. Experiments using fiber optics, such as:

- To measure the numerical aperture of an optical fiber.
- To measure the attenuation in an optical fiber.
- To measure the bending loss in a fiber.

7. **Experiments using ultrasonic grating:**

- To determine the wavelength and velocity of ultrasonic waves in a liquid by studying the diffraction through the ultrasonic grating.

SECOND SEMESTER COURSES & SYLLABI

L=Lectures T=Tutorials P=Practicals in hours per week & C=Credit points

PAPERS FOR 2ND SEMESTER (JANUARY – MAY)

Course No.	Course Title	L	T	P	C
PHY 402	Electromagnetic Theory	3	1	-	4
PHY 404	Statistical Mechanics	3	1	-	4
PHY 406	Quantum Mechanics II	3	1	-	4
PHY 408	Electronics & Instrumentation	2	-	2	4
PHY 492	Basic Laboratory II*	-	2	6	8
PHY 494	Project Research I (Summer)**	-	-	8	8

Examination: 2nd week of June

Semester Break: June & July (Project Research I)

*For these laboratory based courses tutorials involve discussions on the underlying theory and methodology of the experiments. Each such course would occupy eight lab-hours distributed over two days in each week. In the Summer following the Second Semester students will start taking up projects to enable him or her to develop an integrated research attitude towards physics.

**In the case of Project-based Courses "P" indicates the number of interaction hours per week.

PHY 402. ELECTROMAGNETIC THEORY

- **Review of Electrostatics & Magnetostatics:** Gauss' law, Green function, multipole expansion, electrostatics of macroscopic media; magnetostatics, vector potential, magnetic moment, magnetostatics of macroscopic media, magnetic materials, energy in static fields. *[8 Lecture hours]*
- **Maxwell's equations:** Maxwell's equations, Gauge invariance of Maxwell Eq.s; energy, momentum, and angular momentum in E-M fields; conservation law. *[5 Lecture hours]*
- **Lorentz Invariance of Maxwell's equations:** Special Relativity; Lorentz transformations; 4-vectors; 4-vector potential and the electromagnetic field tensor; Maxwell eq. in covariant form; transformation of electric and magnetic fields; field of a uniformly moving charge; Lorentz force law in covariant form. *[6 Lecture Hours]*
- **Electromagnetic Waves:** Plane EM waves, Boundary conditions, Wave polarization, laws of optics; normal and anomalous dispersion. low frequency behaviour and conductivity, Propagation through anisotropic and chiral media. *[6 Lecture Hours]*
- **Radiation:** Radiation from an accelerated charge, retarded and advanced potentials, radiation from oscillating source; dipole radiation; quadrupoles; radiated power, Point charges. *[7 Lecture Hours]*

- **Potentials and Fields:** Scalar and Vector Potentials, Liénard-Wiechert potentials, Gauge transformations, Field of a moving charge; radiation from accelerated charge; Thomson scattering. *[7 Lecture Hours]*

- **Wave guides**: EM Waves in Coaxial and Rectangular Wave Guides, Resonant Cavities. *[6 Lecture Hours]*

- **Scattering:** Differential cross-section; Rayleigh's law; scattering in media; Born approximation; blue sky; density fluctuations. *[5 Lecture Hours]*

Suggested Textbooks:

- *J.D. Jackson, Classical Electrodynamics*
- *J.R. Reitz, F.J. Milford & R.W. Christy, Foundations of Electromagnetic Theory*
- *Landau, L. D., and E. M. Lifshitz. Classical Theory of Fields*
- *Griffiths, David J. Introduction to Electrodynamics*

PHY 404. STATISTICAL MECHANICS

- **Review of the laws of thermodynamics:** Need for statistical mechanics. *[2 Lecture Hours]*

- **Probability and statistics:** Random walks, Gaussian and Poisson Distributions, Central Limit Theorem, Saddle point integration *[4 Lecture Hours]*

- **Distribution functions and phase space:** Liouville equation, mixing and ergodicity, Markov process and Master equation *[4 Lecture Hours]*

- **Ensembles:** Micro canonical, Canonical, Grand canonical. Partition function and connection with thermodynamic potentials, equivalence of different ensembles *[8 Lecture Hours]*

- **Formulation of quantum statistics:** quantum mechanical ensemble theory, density matrix, distinguishable and indistinguishable particles *[4 Lecture Hours]*

- **Quantum Ideal Gases:** Bose and Fermi Statistics, density of states, equation of state *[6 Lecture Hours]*

- **Ideal Fermi gas:** Analysis of equation of state and properties of $f_{3/2}(z)$ function, high temperature low density limit and Maxwell-Boltzmann form, low temperature high density limit and Fermi level. Landau diamagnetism, Pauli paramagnetism, white dwarf stars *[6 Lecture Hours]*

- **Bose gas:** Equation of state and properties of $f_{5/2}(z)$ function, Black body radiation, Phonons in solids, Bose-Einstein condensation *[4 Lecture Hours]*

- **Ising Model:** Definition, spontaneous magnetization, Bragg-William approximation, Bethe-Peierls approximation, exact solution of 1-d Ising model. *[4 Lecture Hours]*

- Basic ideas of phase transitions. *[2 Lecture Hours]*

- Cluster expansion *[2 Lecture Hours]*

Suggested Textbooks:
- M. Kardar, Statistical Physics of Particles
- R. K. Pathria & P. D. Beale, Statistical Mechanics
- L.E. Reichl, A Modern Course in Statistical Physics
- Kerson Huang, Statistical Mechanics

PHY 406. QUANTUM MECHANICS II

- Scattering theory - Born approximation and partial wave analysis. *[4 Lecture Hours]*
- Time independent perturbation theory. *[5 Lecture Hours]*
- Variational method *[5 Lecture Hours]*
- The WKB approximation. *[3 Lecture Hours]*
- Time independent perturbation theory (Fermi's Golden Rule). *[4 Lecture Hours]*
- Adiabatic and Sudden Approximations *[4 Lecture Hours]*
- Geometric Phases and the Bohm-Aharanov Effect. *[4 Lecture Hours]*
- Rotation group, Tensor operators and the Wigner-Eckart theorem. *[3 Lecture Hours]*
- Illustrations from atomic, molecular and nuclear physics. *[4 Lecture Hours]*
- Pure and Mixed states. Density Matrix formalism *[5 Lecture Hours]*

Suggested Textbooks:
- *Shankar : Quantum Mechanics*
- *Landau & Lifshitz: Quantum Mechanics*
- *Messiah, Quantum Mechanics I & II*
- *Davidov, Quantum Mechanics*
- *Sakurai : Modern Quantum Mechanics*
- *Cohen-Tannoudji, Diu & Lal¨oe, Quantum Mechanics II*
- *Ryder, Quantum Field Theory*
- *Flugge, Practical Quantum Mechanics*

PHY 408. ELECTRONICS & INSTRUMENTATION

Analog Electronics:

1. Semiconductor Devices Part I: Electron and hole concentrations in semiconductors; Band diagram of p-n junction; Current flow in a semiconductor: concept of drift current and diffusion current; Basic equations of semiconductor; current-voltage characteristics of a p-n junction diode; Dynamic diffusion capacitances; Ebers-Moll equation. *[6 lecture hours]*

2. Semiconductor Devices Part II: Metal-semiconductor junctions: Schottky barriers; Rectifying and ohmic contacts. Miscellaneous semiconductor devices such as Photodiodes (APD & PIN); Phototransistors; Tunnel diode; Gunn diode; Solar cell; LEDs and LDR. *[7 lecture hours]*

3. Amplifiers: Review of Op-Amp circuits, OP-AMP architecture, Constant current sources, Input stage of an Op-Amp, characteristics and parameters of OP-AMP circuit. MOS Capacitor and MOSFET Physics: Band diagrams, accumulation/inversion, HF/LF C–V responses, FET and MOSFET operation. *[7 lecture hours]*

4. Filter Circuit: L and π filters, iterative and image impedance of a network, symmetrical network, characteristic impedance and propagation constant of a network. Development methods of different constant-K filters, such as high-pass, low-pass, band-pass, and band-stop filter circuits.
[5 lecture hours]

Digital Electronics

1. Combinational logic gates: Karnaugh mapping, Minimization or reduction techniques of Product of Sum (POS) and Sum of Products (SOP) expressions of 2, 3 and 4 variables Boolean expression, Logical implementations, Revision of Flip-Flop circuits, Conversion of Flip-Flops.
[4 lecture hours]

2. Registers: Shift Register, Serial in Serial out, Parallel in Serial out, Parallel in parallel out registers, Bi-directional and Universal registers. *[2 lecture hours]*

3. Counter: Synchronous and Asynchronous counter, other different counters like modulo-, decade, ring and twisted ring counter and Up/Down Counter. *[2 lecture hours]*

4. Combinational circuits: MUX, De-MUX, Encoder, Decoder, comparator. Analog to Digital and Digital to Analog Conversion. *[3 lecture hours]*

Instrumentation and Techniques:

Scintillation and Solid-state Detectors; Measurement of time and energy using electronic signals from the detectors and associated instrumentation, Signal processing; Multi channel analyzer; Time of fight and Lock-in detection technique; Noise in electronic systems; Types of internal noises, noise measurement techniques. Electronic Gauges; Strain Gauge, Capacitative and Piezoelectric Sensors. Microcontroller for Instrumentation; interfacing with Sensors and Actuators. Production and measurement of high vacuum; Rotary, Diffusion, Turbo-molecular and Ion pump; McLeod, Pirani and Penning gauge. *[8 lecture hours]*

Suggested Textbooks:

- *Solid State Electronic Devices: Streetman & Banerjee*
- *Semiconductor Physics and Devices: Donald A. Neamen*
- *Physics of Semiconductor Devices: S.M. Sze & Kwok K. Ng*
- *Electronic Fundamental and Applications: J.D. Ryder*
- *Radiation, Detection and Measurement: G.F. Knoll*

- *Noise in Solid State Devices and Circuits: Albert Van der Ziel*
- *Digital Design: M. Morris Mano & Michael D. Ciletti*

PHY 492 BASIC LABORATORY II

As an essential component of this course is to introduce the student to the advanced techniques in electronics, the syllabus of which is given below:

Perform the following experiments with a proper truth table:

- Use the NAND gate to realize the functions of NOT, AND, OR and EX-OR gates. Indicate the corresponding Boolean operation.
- Design a digital voting machine (using NAND gates only) for three voters by following the Karnaugh Map optimization technique.
- Design digital circuits for a half adder and subtractor by using NAND gates only.
- Show a circuit diagram of a full adder by using NAND gates only. Explain the design and operation.
- Make a J-K flip-flop circuit by using NAND gates only. Show toggle and self oscillation (racing) in the output.
- Design a Master-Slave J-K flip-flop and show the output performance.

The other component of this course is to develop the innovativeness of the student to put to use the knowledge, attitudes and techniques acquired through the basic electronics and optics courses in the first semester, to conceive, design, build and implement projects for the measurement of say a physically interesting quantity or the experimental verification of some physical principle or the quantitative observation of some interesting phenomena etc.

The corresponding experiments are listed below:

- Frank-Hertz experiments.
- Hall effect
- Study of magnetic properties of ferro- and paramagnetic materials
- Determination of band gap in a semiconductor
- Millikan's oil drop experiments
- To study the I-V characteristics of the solar cell and hence determine the fill factor.
- Electron spin resonance experiments to determine Lande-g-factor
- Use of Geiger-Muller counters to determine the half-life of a radioactive source, etc.
- Dispersion relation in a periodic electrical circuit: an analog of monatomic and diatomic lattice vibration.

PHY 494 Research project I (Summer)

Summer Research project with a Faculty member of SNBNCBS (May– July)

THIRD SEMESTER COURSES & SYLLABI

L=Lectures T=Tutorials P=Practicals in hours per week & C=Credit points

PAPERS FOR 3RD SEMESTER (AUGUST – DECEMBER)

Course No.	Course Title	L	T	P	C
PHY 501	Atomic & Molecular Physics	3	1	-	4
PHY 503	Condensed Matter Physics	3	1	-	4
PHY 505	Advanced Quantum Mechanics & Applications	3	1	-	4
PHY 530 *	Soft Matter	3	1	-	4
PHY 507 *	Nuclear & Particle Physics	3	1	-	4
PHY 509	Project Research II	-	-	8	8

* Either PHY 505 or PHY 530 to be chosen as "Optional Elective".

Examination: 2nd week of December

Semester Break: 4th week of December

PHY 501. ATOMIC & MOLECULAR PHYSICS

1. Atoms: One electron system, significance of quantum numbers, space quantization, spin quantum number, orbital and spin angular momentum, Parity operator, time dependent perturbation theory, atoms in external field, many electron systems, Pauli exclusion principle, spin-orbit interaction, hyperfine structure. *[8 Lecture Hours]*

2. Molecule: Electronic structure of diatomic molecules: MO theory (Quantum mechanical approach to explain molecular bonds, B.O. approximation, foundation of the MO theory, approximation methods for the calculation of electronic wave function, LCAO and VB approach, hydrogen molecule ion, hydrogen molecule etc., their charge distribution and the concept of covalent and ionic bonds), shape of molecular orbitals, spectroscopic term symbols, MO diagrams of some diatomic molecules. *[9 Lecture Hours]*

2. Molecular Spectra: Electromagnetic spectrum, interaction of radiation with matter, general features of stimulated absorption, spontaneous emission and stimulated emission, selection rule. *[5 Lecture Hours]*

3. Rotational Spectroscopy: Moment of inertia of molecules, rotational spectra of rigid molecules, diatomic molecules as non-rigid rotors, prolate and oblate rotors, intensity of spectral lines. *[6 Lecture Hours]*

4. Vibrational spectroscopy: Harmonic and an-harmonic oscillators, ro-vibrational spectra, vibrations of polyatomic molecules, Transition matrix elements, IR spectroscopy: basic theory and design (techniques), normal coordinates and normal modes, application of group theory to molecular vibration, FTIR spectroscopy. *[7 Lecture Hours]*

5. Electronic spectroscopy: Electronic spectra of diatomic molecules, BO approximation, FC principle, dissociation energy, fine structures, Fortrat diagram. *[4 Lecture Hours]*

6. Laser spectroscopy: Basic principle of lasers, population inversion, the Einstein coefficients, line-shape functions, two level, three level and four level laser systems, optical gain, optical resonators, pulsed operation of laser: Q-switching and Mode locking; experimental techniques of Q-switching and mode locking, different laser systems: Ruby, CO2, dye and Semiconductor diode lasers. *[8 Lecture Hours]*

Suggested Textbooks:

- *'Physics of Atoms and Molecules' by B.H. Bransden and C.J. Joachain*
- *'Molecular Spectroscopy' by I. N. Levine*
- *'Laser Fundamentals' by W. T. Silfvast*

PHY 503. CONDENSED MATTER PHYSICS

● **Crystallography:** Crystal structure, Lattice types, Brillouin zones, Structure factor Space groups, Point groups, X-ray Diffraction, Reciprocal lattice, Bragg's law. *[5 lecture hours]*

● **Binding and cohesion in solids:** Van der Waals bonding, Ionic bonding, Covalent bonding, Metallic Bonding, Cohesive energy. *[5 lecture hours]*

● **Periodic potentials:** Electron levels in periodic potentials, Bloch's theorem, Kronig-Penney model, Free electrons and Nearly free electrons. *[4 lecture hours]*

● **Electronic Band Structure**: Elementary ideas of band structure of crystalline solids, tight binding approximation, Fermi surfaces of metals, density of states in 1D, 2D and 3D. *[6 lecture hours]*

● **Transport properties of solids:** Drude model, Sommerfeld theory, Boltzmann transport equation, thermal conductivity, Hall effect, Magnetoresistance, Relaxation time approximation, Fermi-Dirac distribution, Wiedemann-Franz law. *[7 lecture hours]*

● **Lattice vibrations and Phonons:** harmonic approximation, dispersion relations and normal modes in one-atomic and diatomic lattices, quantization of lattice vibrations and phonons. *[7 lecture hours]*

● **Superconductivity:** Introduction to Superconductivity, Ginzburg-Landau theory, London equations, concept of BCS theory, Meissner effect, Energy gap, Flux quantization, Critical temperature, Critical fields, Persistent currents. *[5 lecture hours]*

● **Semiconductors:** Introduction to Semiconductors, intrinsic and extrinsic semiconductors, concept of holes and effective mass, carrier concentrations.

● **Magnetism**: Diamagnetism, Paramagnetism, Ferromagnetism, Antiferromagnetism. Curie's law, Hund's rules, Larmor diamagnetism, Pauli and van-Vleck paramagnetisms, Curie-Weiss law, Theory of magnetism, Magnetic ordering, Exchange interactions. *[6 lecture hours]*

Suggested Books:

- *Dekker, Solid State Physics*

- *Kittel, Introduction to Solid State Physics*
- *Ashcroft and Mermin, Introduction to Solid State Physics.*
- *Ziman, Principles of the Theory of Solids.*

PHY 505. ADVANCED QUANTUM MECHANICS AND APPLICATIONS

1. Non-relativistic Quantum mechanics *[27 lecture hours]*

A. Ground state of of Hydrogen atom
B. Ground state of Helium atom: (i) using perturbation theory, (ii) Using variation theory
C. Generalization of Hamiltonian for many particle systems: (i) Introduction of Second quantization theory, (ii) concept of Indistinguishability of particles, (iii) Permutation symmetry, (Anti) Symmetrization postulate; Bosons and Fermions
D. Concept of Bose-Einstein and Fermi-Dirac statistics.
E. Slater determinant for many body wave-function for two particle and many particle
F. Second quantization representation of many body Hamiltonian
G. Two site and two particle Hamiltonian of Hubbard model
H. Hole theory, anti-particles and charge conjugation.
I. Representation of Hilbert space and solution of Hamiltonian for two site and two particle
J. Mean field theory & exact solution

2. Relativistic Quantum Mechanics *[20 lecture hours]*

A. Klein-Gordon equation and failure of the probability interpretation.
B. The presence of negative energy states and stability problems.
C. Dirac equation and its Lorentz covariance, Poincar_e group/algebra, Pauli-Lubanski vector,
D. Casimir operators of Poincar_e algebra. Spin (½) particles.
E. Physical content, plane wave solutions and projectors, wave packets;
F. Problems in localization below Compton wavelength. Necessity for multi-particle theory.
G. Hydrogen-like atom, hyperfine structure, Lamb shift. Nuclear effects.
H. Free Dirac propagator, propagation in an arbitrary external electro-magnetic field. Relativistic corrections to Rutherford scattering.
I. Basic of Path Integral, Stationary phase approximations, Application in harmonic oscillator, Relation to Hilbert space formulation,

Suggested Books:

- Advanced Quantum Mechanics by F. Schwabl (Springer, 2000)
- Quantum Mechanics: Fundamentals by K. Gottfried and T-M. Yan (2nd Ed. Springer, 2003)
- Techniques and Applications of Path Integrations by L.S. Schulman (John Wiley and Sons,1981)
- Quantum Mechanics and Path Integrals, R.P. Feynman, A.R. Hibbs
- Quantum field theory and condensed matter:An introduction R. Shankar

- Quantum Theory of Many-Particle Systems:Alexander L. Fetter and John Dirk Walecka

PHY 530. SOFT MATTER

A. Soft matter systems: Brief introduction to colloids as a model soft matter system. Emphasis on large length and slow time scales. *[6 Lecture Hours]*

B. Statistical mechanics of interacting classical system:

Mean Field Theory in Variational approach. Application to Ising Model. Structural quantities of a liquid: Single point density, Pair correlation function, Structure factor and Direct correlation function. Connection to the Neutron scattering measurements.

Idea of functional derivatives (formula only). Kohn-Saam theorem for classical fluids: Grand partition function of a liquid as a functional of external potential. Classical density functional in Ramakrishnan-Yousuff form (statement only) and its application to freezing transition in colloidal systems using Alexander-Mc Tague form of Landau free for first order phase transitions. Examples of liquid to triangular lattice can be worked out. *[12 Lecture Hours]*

C. Dynamics: Auto-correlation functions and linear response theory. Langevin equation, the Over-damped limit: Brownian motion and implementation in computer simulations. Colloidal diffusion. Phenomenological equations of motion for conserved and non-conserved modes (statement only). Illustration for simple fluids. *[12 Lecture Hours]*

D. Any one of the following systems for illustration of soft matter behaviour

(i) Proteins as Bio-macromolecules: Proteins as a bio-macromolecule; Ramachandran plot; Free energy landscape for protein folding.

(ii) DNA as semiflexible polymer: Gaussian and self-avoiding polymer chain; semiflexible polymer and persistence length; introduction to polyelectrolyte models.

(iii) Polymer as Gaussian and self-avoiding chain; good solvent and bad solvent; polymer collapse. *[12 Lecture Hours]*

Suggested books:

- Donald Mc Quarie, Statistical Mechanics.
- Plischke and Bergerson: Equilibrium Statistical Mechanics
- Chaikin and Lubenski, Principles of Condensed Matter Physics
- Leninger, Biochemistry
- P. G. deGennes, Polymer physics
- Duncan J Shaw, Colloids and Surface Chemistry

PHY 507. NUCLEAR & PARTICLE PHYSICS

General properties of nuclei: nuclear size, nuclear radius and charge distribution, nuclear form factor, mass and binding energy, Angular momentum, parity and symmetry, Magnetic dipole moment and electric quadrupole moment. *[4 Lecture Hours]*

Two-body bound state: Properties of deuteron, Schrödinger equation and its solution for ground state of deuteron, rms radius, spin dependence of nuclear forces, electromagnetic moment and magnetic dipole moment of deuteron and the necessity of tensor forces. *[6 Lecture Hours]*

Two-body scattering: Experimental n-p scattering data, Partial wave analysis and phase shifts, scattering length, magnitude of scattering length and strength of scattering, Significance of the sign of scattering length; Scattering from molecular hydrogen and determination of singlet and triplet scattering lengths, effective range theory, low energy p-p scattering, Nature of nuclear forces: charge independence, charge symmetry and isospin invariance of nuclear forces. *[8 Lecture Hours]*

Nuclear structure: Liquid drop model, Bethe-Weizsäcker binding energy/mass formula, Fermi model, Shell model and Collective model. *[6 Lecture Hours]*

Nuclear reactions and fission: Different types of reactions, Quantum mechanical theory, Resonance scattering and reactions— Breit-Wigner dispersion relation; Compound nucleus formation and break-up, Statistical theory of nuclear reactions and evaporation probability, Optical model; Principle of detailed balance, Transfer reactions, Nuclear fission: Experimental features, spontaneous fission. *[6 Lecture Hours]*

Radioactive Decays: Alpha decay, Beta decay –Energy release in beta decay–Fermi theory of beta decay–Shape of the beta spectrum –decay rate Fermi-Curie plot–Fermi & G.T Selection rules – Comparatives half-lives and forbidden decays – Gamma decay-Multipole radiation – Angular momentum and parity selection rules – Internal conversion – Nuclear isomerism. *[4 Lecture Hours]*

Elementary particle Physics: Types and characteristics of interaction between elementary particles–Hadrons and leptons–Symmetry and conservation laws – CPT theorem–Gell-Mann-Nishijima formula-classification of hadrons –Quark model - symmetry classification of elementary particles- Parity non-conservation in weak interaction. Relativistic kinematics. *[10 lecture hours]*

Suggested Books:

- B. B. Cohen: Concepts of Nuclear Physics
- J. S. Lilley: Nuclear Physics
- M. K. Pal: Theory of Nuclear Structure
- R. R. Roy and B.P. Nigam: Nuclear Physics
- S. N. Ghoshal: Atomic and Nuclear Physics (Vol. 2)
- D. H. Perkins: Introduction to High Energy Physics
- D. J. Griffiths: Introduction to Elementary Particles
- D. C. Tayal: Nuclear Physics

PHY 509 PROJECT RESEARCH II

A six-month project shall be taken up by students under the supervision of a Project Guide.

FOURTH SEMESTER COURSES & SYLLABI

L=Lectures T=Tutorials P=Practicals in hours per week & C=Credit points

PAPERS FOR 4TH SEMESTER (JANUARY – MAY)

Course No.	Course Title	L	T	P	C
PHY 502	Project Research III	-	-	8	6
PHY 592	Methods of Experimental Physics	3	1	3	7
PHY 5xx	Elective 1*	3	1	-	4
PHY 5xx	Elective 2*	3	1	-	4
PHY 5xx	Elective 3*	3	1	-	4

* Reference to the list of optional courses given below. The student would be required to **choose at least one course from Part A (504, 506 & 508)**.

Part A

Course No.	Course Title	L	T	P	
PHY 504	Astrophysics & Astronomy	3	1	-	
PHY 506	Chemical Physics	3	1	-	
PHY 508	Biological Physics	3	1	-	

Part B

Course No.	Course Title	L	T	P	
PHY 510	Advanced Mathematical Methods	3	1	-	
PHY 512	Quantum Field Theory	3	1	-	
PHY 514	Advanced Statistical Physics	3	1	-	
PHY 516	Magnetism and Superconductivity	3	1	-	
PHY 518	Nonlinear Dynamics	3	1	-	
PHY 520	Optical Physics	3	1	-	
PHY 522	Correlated Electrons & Disorder	3	1	-	
PHY 524	Quantum Information Theory	3	1	-	
PHY 526	Theory of Elementary Particles	3	1	-	
PHY 528	Mesoscopic Physics	3	1	-	
PHY 530	Soft Matter	3	1	-	
PHY 532	General Relativity & Cosmology	3	1	-	

* In the case of Project-based Courses “P” indicates the number of interaction hours per week.

Examination: 2nd week of May

Semester Break: June & July

PHY 502. PROJECT RESEARCH III

A six-month project shall be taken up by students under the supervision of a Project Guide.

PHY 592. METHODS OF EXPERIMENTAL PHYSICS

Students will use some advanced level experimental techniques which are extensively used in experimental research. Some of them are listed below:

1. X-Ray and crystallography
2. Gamma Ray Spectroscopy.
3. Experiments on Observational Astronomy.
4. Experiments on Chemical thermodynamics/kinetics
5. Experiments on spectroscopy
6. Experiments on Thermal properties of matter.
7. Error analysis: Errors in observation and treatment of experimental data, estimation of error, theory of errors and distribution laws, least squares method, curve fitting, statistical assessment of goodness of fit.

"Advanced Laboratory" involving routine experiments [such as NMR, Mossbauer, X-Ray Diffraction, Electron Microscopy, Accelerators etc in the research laboratories of the participating institutions], shall be integrated into this course.

PHY 504. ASTROPHYSICS AND ASTRONOMY

Standard Theory of Cosmology: Simplifying assumptions of cosmology, the cosmological principle, Expansion of the Universe and redshift, Friedmann-Robertson-Walker models (closed, flat and open Universe), critical density, FRW solutions for simple equations of state of cosmic matter and radiation. Cosmological constant, de sitter Universe. *[4 lecture hours]*

Early Universe: Big bang model, Thermodynamics and thermal history of early universe, baryogenesis, Nucleosynthesis, relic neutrinos and microwave background radiation, Recent observational results. *[3 lecture hours]*

Dark Energy: Standard candles; Luminosity-Redshift relation – dimming of the brightness of the supernovae – a negative deceleration parameter q – an accelerated expansion: Agents driving acceleration – dark energy – Cosmological constant (ΛCDM model) – Λ -discrepancy between the predicted and the observed values: Quintessence models: Qualitative description of a presently accelerating universe – BAO, CMB, Hubble data *[4 lecture hours]*

Basic Background of Astronomy: Elementary radiative transfer equations , absorption and emission, atomic processes, continuum and line emission – Telescopes: Refracting and Reflecting telescopes, Ground-based and space-based observatories – Properties of telescope: Light gathering power and Angular resolution – Astronomical Instrumentation - Optical/IR filter-systems – Optical/IR detectors – X-ray detectors – Imaging camera and spectrometer. distance measurements – Hubble's law *[4 lecture hours]*

Astronomy: Spherical trigonometry – the Celestial sphere – Coordinate systems: Horizontal system; Equatorial system; Ecliptic system; Galactic system – Rising and setting of stars – Parallax – Astronomical time systems: Sidereal and Solar time – Concepts of Calendars *[3 lecture hours]*

Interstellar medium and formation of stars: Interstellar extinction law – theoretical extinction model and Mie scattering – nucleogenesis – Interstellar dust and Abundances – Molecular clouds – properties of molecular clouds – formation of protostars and stars – Jeans Instability: collapse of a spontaneous cloud and virial theorem – Kelvin-Helmholtz time scale *[5 lecture hours]*

Evolution of stars: Stellar energy sources – gravitational lifetime for a star – nucleosynthesis: lifetime for a star – evolution off the main sequence: Giant and supergiants – evolution of low and high mass stars – formation of heavy elements – Degenerate electron gas: White dwarf, Chandrasekhar limit, Neutron stars, Black hole *[5 lecture hours]*

Properties of stars: Continuous radiation from stars: Brightness of starlight – Electromagnetic spectrum – colors of stars – Stellar distances – stellar parameters: magnitude, luminosity, radius and their measurements *[4 lecture hours]*

The Sun: Elements of radiation transport theory – Basic structure: photosphere; chromosphere, corona – temperature problem of the corona – solar activity - Sunspots, Solar flares, Coronal mass Ejection (CME) *[4 lecture hours]*

Spectral Classifications of Stars: Spectral lines in stars – origin of spectral lines – line broadening: Doppler, thermal and collisions – Hydrogen spectral lines – Formation of spectral lines: excitation, ionization and recombination, Boltzmann Equation, Stimulated and spontaneous emission – Mass luminosity relation – Hertsprung-Russell diagram – Saha Ionization Equation – Ionized hydrogen regions *[5 lecture hours]*

Galaxies: Formation and classification: Active galaxies and Quasars – Density wave theory of the formation of spiral arms – Rotation curve: missing mass and dark matter – Quasars and active galactic nuclei, Milky Way Galaxy – Oort's constants – magnetic field *[4 lecture hours]*

Suggested Books:

- Norbert S. Schulz, From Dust To Stars: Studies of the Formation and Early Evolution of Stars, Springer-Verlag Berlin and Heidelberg GmbH & Co. K, 2005
- Physics of Astrophysics – F. Shu
- K. D. Abhayankar, Astrophysics: Stars And Galaxies, Universities Press, 2001
- H. Karttunen, P. Kröger, H. Oja, M. Poutanen, K. J. Donner (Eds.), Fundamental Astronomy, Springer Berlin Heidelberg New York, 2007

PHY 506. CHEMICAL PHYSICS

- Quantum Chemistry and the Nature of the Chemical Bond. *[5 lecture hours]*
- Chemical Kinetics and Thermodynamics. Order of the Reaction. Rate laws. *[5 lecture hours]*
- Mechanism of Chemical Reactions: (a) Collision Theory (b) Transition State Theory (c) Potential Energy Surface (d) Kramers Escape Rate. *[10 lecture hours]*
- Enzyme Reactions: Solution kinetics, characterization of enzymes, control mechanisms. *[5 lecture hours]*
- Electron Transfer: (a) Dynamical Electrochemistry (b) Electron Transfer (c) Quantum Models (d) Electron Charge Transfer in Proteins. *[10 lecture hours]*

Suggested books:

- *Nitzan, Chemical Dynam Basic Chemical Kinetics, John Wiley and Sons, 1980*
- *ics in Condensed Phases, OUP, 2006.*
- *H. Eyring, S H Lin, S M Lin,*

PHY 508. BIOLOGICAL PHYSICS

- **Molecular structure of biological systems:** this includes a brief introduction to molecular orbital theory, formation of various kinds of bonds, molecular excitation and energy transfer, thermal molecular movement, order and probability, molecular and ionic interactions: biological structures, interfacial phenomena and membranes. *[7 Lecture Hours]*

- **Energetics and dynamics:** Fundamental concept of thermodynamics, aqueous and ionic equilibrium in living cells, Fluxes, transport in biological systems, electric fields in cells, mechanical properties of biological materials, biomechanics and fluid behavior. *[6 Lecture Hours]*

- **Physical factors of the environment:** temperature, pressure, sound, mechanical oscillation, static and EM fields, ionizing radiation. *[4 Lecture Hours]*

- **Kinetics of biological systems:** systems theory, systems of metabolism and transport, model approaches to some complex biological processes. *[4 Lecture Hours]*

- **Biomolecular structures and Nucleic acids:** Dihedral angles and base pair parameters along with different levels of structural organizations (descriptive only); water; carbohydrate and lipids; ATP. *[5 Lecture Hours]*

- **Biophysical experimental techniques:** Principles of Fluorescence, CD, NMR, X-Ray, crystallography, AFM, Single molecular spectroscopy etc. *[4 Lecture Hours]*

- **Molecular Dynamics simulation:** Verlet algorithm; PBC; Constraint systems; statistical analysis of data. *[5 Lecture Hours]*

- **Biological modeling:** Reaction-diffusion (or any other equivalent) systems for illustration. *[3 Lecture Hours]*

- **Introduction to Bio-informatics:** Data mining; sequence comparison and alignment. *[3 Lecture Hours]*

Suggested books:

- *Biological Physics: Energy, Information, Life by Philip Nelson*
- *Biophysics:* Roland Glaser
- *Biophysics: An Introduction by Rodney Cotterill*
- *Introduction to Molecular Biophysics by J.A. Tuszynski, M. Kurzynski*

PHY 510. ADVANCED MATHEMATICAL METHODS

1. Group Theory:

Basic definition of groups and subgroups. Homomorphism and isomorphism between groups, finite and infinite groups, conjugate classes, invariant subgroups and coset spaces. Representation of groups. unitary representation, character of a representation. Permutation group and Young' Tableaux. *[10 Lecture Hours]*

Elements of Lie Groups. unitary groups, orthogonal groups, homogeneous and inhomogeneous Lorentz groups, Wigner's little group and concept of helicity etc., conformal groups, symplectic groups. Local properties of Lie groups, infinitesimal group generators, Lie algebras, Adjoint representations, simple and semisimple Lie algebras, Casimir operators.
[7 Lecture Hours]

Elementary ideas of root vectors, Cartan subalgebra, graphical representations, weight vectors. Dynkin diagrams and Cartan matrices. *[3 Lecture Hours]*

2. Differential Geometry:

Concept of differentiable manifolds, tangent and cotangent spaces(one forms), tensors and tensor product spaces. *[5 Lecture Hours]*

Calculus of forms, exterior differentiation, Lie differentiation, covariant derivatives and connections, parallel displacements and geodesics. *[5 Lecture Hours]*

Torsion and curvature. Cartan's equations of structure and metric tensor. Symmetries of Riemann curvature tensor. *[5 Lecture Hours]*

Elementary theories of fibre bundles and connection between gravity and gauge theories.
[5 Lecture Hours]

Suggested books :

- *S. Mukhi & N. Mukunda, Introduction to topology, and differential geometry and group theory for physicists*
- *B. C. Hall, Lie Groups and representations*
- *Y. Choquet-Bruhat et al, Analysis, Manifolds & Physics*

PHY 512. QUANTUM FIELD THEORY

- Representation of Lorentz Group and SL(2,C): Relativistic notation, SU(2) and the rotation group, homogeneous and inhomogeneous Lorentz Group and their algebras, spinors. *[5 Lecture Hours]*
- Relativistic Covariant Equations - Klein Gordon, Dirac and Maxwell equations. *[2 Lecture Hours]*
- Quantization of free fields: Canonical and Path Integral Approach. Real scalar field, complex scalar field, Dirac field, electromagnetic field *[10 Lecture Hours]*
- Covariant quantisation of the Maxwell field. *[2 Lecture Hours]*
- Gauge Principle, interacting fields. *[5 Lecture Hours]*
- Feynman-Dyson Perturbation Expansion and Feynman Diagrams. *[10 Lecture Hours]*
- Quantum electrodynamics. Tree Level Calculations of Compton Scattering, Cross-section, Moller scattering. *[6 Lecture Hours]*
- Loops, Divergences, Regularization and Renormalization. *[10 Lecture Hours]*
- Anomalous magnetic moment of the electron and the Lamb-Shift. *[4 Lecture Hours]*

Reference books:

- *Quantum Field Theory by B. Hatfield*
- *Quantum Field Theory by L. Ryder*
- *Quantum Field Theory by Steven Weinberg*
- *Quantum Field Theory by Peskin & Schroder*
- *Quantum Field Theory and the Standard Model by Matthew D. Schwartz*

PHY 514. ADVANCED STATISTICAL PHYSICS

- **Critical Phenomena – General Concepts**: Order parameter, critical exponents, universality, scaling laws *[4 Lecture Hours]*
- **Mean Field Theory**: Weiss mean-field theory for Ising model, Landau theory, limitations of mean-field *[6 Lecture Hours]*
- **Landau–Ginzburg Theory**: Free energy functional, fluctuations, correlation functions, Ginzburg criterion *[5 Lecture Hours]*
- **Ising Model**: Exact solution in 1D, transfer matrix method; 2D Ising model (Onsager result overview) *[5 Lecture Hours]*
- **Renormalization Group (RG)**: RG flow, fixed points, ε-expansion, block spin transformations *[5 Lecture Hours]*
- **Superconductivity and Superfluidity**:Phenomenology, order parameters, second sound, two-fluid model *[5 Lecture Hours]*
- **Approach to Equilibrium – Transport Equations**:Boltzmann transport equation, molecular chaos assumption *[5 Lecture Hours]*

- **Langevin Dynamics**: Brownian motion, stochastic forces, fluctuation-dissipation theorem *[5 Lecture Hours]*
- **Master Equation and Fokker–Planck Equation**:Probability distributions, detailed balance, steady states *[5 Lecture Hours]*

Reference books:

- **R. K. Pathria & P. D. Beale** – *Statistical Mechanics*
- **N. Goldenfeld** – *Lectures on Phase Transitions and the Renormalization Group*
- **K. Huang** – *Statistical Mechanics*
- **M. Kardar** – *Statistical Physics of Particles* and *Fields*
- **J. P. Sethna** – *Statistical Mechanics: Entropy, Order Parameters and Complexity*
- **Chaikin & Lubensky** – *Principles of Condensed Matter Physics*

PHY 516. MAGNETISM AND SUPERCONDUCTIVITY

- Generalized Hamiltonians in condensed matter; symmetries; low-energy limits *[3 Lecture Hours]*
- Concept of effective theories; projection methods, renormalization, emergent behavior *[3 Lecture Hours]*
- Fundamentals of magnetism: localized moments, exchange interaction, spin Hamiltonians *[3 Lecture Hours]*
- Quantum magnetism: Heisenberg model, magnetic ordering, spin waves *[3 Lecture Hours]*
- Itinerant magnetism: Stoner model, RKKY interaction, spin-density waves *[4 Lecture Hours]*
- Introduction to superconductivity: discovery, zero resistance, Meissner effect *[3 Lecture Hours]*
- Experimental features: flux quantization, critical fields, type I & II superconductors *[4 Lecture Hours]*
- Phenomenological theories: London equations, Ginzburg–Landau theory, coherence length *[3 Lecture Hours]*
- Cooper pair problem: two-particle bound state in Fermi sea, instability of Fermi surface *[3 Lecture Hours]*
- BCS theory: Hamiltonian, variational ansatz, mean field approach *[3 Lecture Hours]*
- BCS ground state: Bogoliubov transformation, energy spectrum, gap equation *[3 Lecture Hours]*
- Critical temperature, specific heat, tunneling, isotope effect *[3 Lecture Hours]*
- BCS-BEC crossover: strong coupling limit, bosonic condensation of pairs *[3 Lecture Hours]*
- Interplay between superconductivity and magnetism: FFLO states, coexisting orders *[3 Lecture Hours]*
- High-Tc superconductivity and exotic phenomena: cuprates, spin fluctuations, outlook *[3 Lecture Hours]*

Reference books:

- M. Tinkham, *Introduction to Superconductivity*
- P. G. de Gennes, *Superconductivity of Metals and Alloys*
- J. R. Schrieffer, *Theory of Superconductivity*

- *A*. Altland & B. Simons, *Condensed Matter Field Theory*
- C. Kittel, *Introduction to Solid State Physics*
- D. C. Jiles, *Introduction to Magnetism and Magnetic Materials*

PHY 518. NONLINEAR DYNAMICS

- **Introduction to Dynamical Systems**Discrete and continuous time systems, flows and maps, phase space, orbits, fixed and periodic points, stability *[6 Lecture Hours]*
- **One-Dimensional Maps**Logistic map, tent map, Baker's map, graphical iteration, bifurcations, stability via derivatives *[6 Lecture Hours]*
- **Maps of the Circle**Circle maps, rotation number, winding number, periodicity and quasiperiodicity *[6 Lecture Hours]*
- **Linear Continuous-Time Systems**Solutions of linear ODEs, fixed point classification in 2D, nodes, saddles, centers, Hartman–Grobman theorem *[6 Lecture Hours]*
- **Bifurcations in Low-Dimensional Systems**Saddle-node, pitchfork, transcritical bifurcations, global phase portraits *[6 Lecture Hours]*
- **Periodic Orbits and Limit Cycles**Poincaré–Bendixson theorem, anharmonic oscillators, Hopf bifurcation, van der Pol oscillator *[6 Lecture Hours]*
- **Chaos and Sensitive Dependence**Sensitive dependence on initial conditions, Lyapunov exponents (qualitative), period doubling, strange attractors *[6 Lecture Hours]*

Reference books:

- Steven Strogatz – *Nonlinear Dynamics and Chaos*
- Robert Devaney – *An Introduction to Chaotic Dynamical Systems*
- Hirsch, Smale, Devaney – *Differential Equations, Dynamical Systems, and an Introduction to Chaos*
- Katok & Hasselblatt – *Introduction to the Modern Theory of Dynamical Systems*
- Wiggins – *Introduction to Applied Nonlinear Dynamical Systems and Chaos*

PHY 520. OPTICAL PHYSICS

- Classical Linear & Nonlinear Optics: Anharmonic oscillator model, nonlinear susceptibilities, absorption, dispersion, nonlinear wave mixing, coupled mode equations, phase matching, phase conjugation, optical bistability *[6 Lecture Hours]*
- Few-Level Atom Models (Semiclassical Theory): Two-level atom, optical Bloch equations, steady-state solutions, probe amplification, resonance fluorescence, semiclassical dressed states, coherent transients (optical nutation, photon echoes, SIT) *[6 Lecture Hours]*
- Quantized Atom-Field Interaction: Field quantization, Jaynes–Cummings model, vacuum Rabi oscillations, dressed states, collapses and revivals, spontaneous emission, Fermi Golden Rule, Wigner-Weisskopf theory, inhibition of emission *[6 Lecture Hours]*
- Nonclassical Light Generation: Quantum theory of four-wave mixing, parametric down-conversion, phase-matching, correlated photons, twin-beam generation *[6 Lecture Hours]*
- Coherent Control and EIT: Electromagnetically induced transparency (EIT), lasing without inversion (LWI), dark states, population trapping *[6 Lecture Hours]*

- Laser Theory: Spontaneous/stimulated emission, gain, population inversion, threshold, Doppler broadening, hole burning, Lamb dip, laser master equation (Scully–Lamb theory), photon statistics, linewidth, micromaser/microlaser *[6 Lecture Hours]*
- Classical & Quantum Optical Coherence: Young's double slit, mutual coherence, complex degree of coherence, van Cittert–Zernike theorem, HBT experiment, higher-order coherence, coherency matrix, Stokes parameters, Poincaré sphere *[6 Lecture Hours]*
- Quantum Coherence Functions à la Glauber: Coherent states, photon statistics (Poissonian, sub-Poissonian), antibunching, squeezed states *[6 Lecture Hours]*
- Atomic Motion in Laser Light: Laser cooling mechanisms, atom trapping, atom interferometry, BEC of trapped atoms, atom lasers, nonlinear atom optics, optical lattices *[6 Lecture Hours]*

Reference books:

- R. W. Boyd – *Nonlinear Optic*
- M. O. Scully & M. S. Zubairy – *Quantum Optics*
- L. Mandel & E. Wolf – *Optical Coherence and Quantum Optics*
- Y. Yamamoto & A. Imamoglu – *Mesoscopic Quantum Optics*
- H. J. Metcalf & P. van der Straten – *Laser Cooling and Trapping*
- P. Meystre & M. Sargent – *Elements of Quantum Optics*

PHY 522. CORRELATED ELECTRONS & DISORDER

Physics of Materials:

- **BAND INSULATORS vs CORRELATED INSULATORS:** Breakdown of independent electron description, Mott transition, Hubbard model, Limiting cases of Hubbard models - band limit & atomic limit, Hubbard sub-bands, Mott transitions in transition metal oxides, Mott insulators & charge transfer insulator, Zaanen-Sawatzky-Allen classification *[6 Lecture Hours]*
- **LARGE-U LIMIT:** Canonical transformation, t-J model, Super-exchange, Half-filled band: Heisenberg spin model, Antiferromagnetic Heisenberg model : spin waves, strange world of D=1 *[6 Lecture Hours]*
- **SOME INTERESTING SYSTEMS:** Band-width-control M-I transition systems: V2O3, RNiO3, NiS, etc; Filling control M-I transition systems: R_{1-x}A_{x}Ti(V)O3, High Tc superconducting cuprates, Quasi one-dimensional systems: Cu-O chain & ladder compounds, Double-exchange systems: R_{1-x}A_{x}MnO3 *[7 Lecture Hours]*
- **DISORDER INDUCED INSULATORS:** Anderson Localization, Scaling theory, Electron-electron interaction & disorder *[6 Lecture Hours]*

Electronic Structure of Materials:

- **BASICS:** Electrons in periodic potentials: Bloch's theorem, Kronig-Penney model, concept of energy bands; Density of states: Green's function, Tridiagonal matrices & Continued fractions, Singularities in DOS; Reciprocal lattice & Brillouin zone: Special k-points in BZ sampling *[7 Lecture Hours]*
- **EL-ION PROBLEM:** Adiabatic approximation (Born-Oppenheimer), Classical nuclei approximation (Ehrenfest Theorem), Hellman-Feynman force on nuclei *[4 Lecture Hours]*
- **MANY-ELECTRON PROBLEM:** Hartree approximation: LCAO method; Hartree-Fock approx: Slater-determinantal wavefunction & its properties, Hartree-Fock equation, Fock

operator, Energy of the ground state, Koopman's theorem; Going beyond Hartree-Fock: absence of correlation in H-F theory, Basics of MCI and Perturbative (Moller-Plesset) methods; Density Functional Theory: Energy as a functional of density, Thomas-Fermi theory, Hohenberg-Kohn Theorem, Kohn-Sham Equation, LDA for the exchange-correlation function *[8 Lecture Hours]*

- **MOLECULAR DYNAMICS METHODS IN ELECTRONIC STRUCTURE:** Introduction to MD methods: Deterministic vs. Stochastic methods, Connection to statistical mechanics & thermodynamics, Finite difference algorithms for solving eqns. of motion, running and controlling MD simulations, Limitations & errors in MD simulation; Tight-binding MD: Equation of motion in TB-MD; Ab-initio (Car-Parrinello) MD: Basic concepts and effective Lagrangian, Equation of motion, Iterative solution of Kohn-Sham equation *[8 Lecture Hours]*

- **EXPERIMENTAL MANIFESTATION OF ELECTRONIC STRUCTURE:** Theory of photoemission, Core-levels and Final states, Satellites, Valance band, Band structure, Surface states and surface effects *[3 Lecture Hours]*

References:

- Patrik Fazekas -- Lecture notes on Electron Correlation & Magn.
- Imada, Fujimori, Tokura -- Metal-Insulator Transitions, Review. Mod. Phys. vol 70, pg 1039 (1998)
- P.A. Lee & T.V. Ramakrishnan -- Disordered electronic system, Review. Mod. Phys. vol 57, pg 287 (1985)
- Fulde -- Electron correlation in Molecules and Solids
- *Ashcroft & Mermin -- Solid State Physics*
- *Grosso & Pastore-Parravicini -- Solid State Theory*
- *Kaxiras -- Electronic Structure of Solids*
- *Sutton -- Electronic Structure of Materials*
- *Fulde -- Electron correlation in Molecules and Solids*

PHY 524. QUANTUM INFORMATION THEORY

Foundations of quantum theory: states, observables, measurement, dynamics. Spin-half systems and photon polarizations, qubits versus classical bits. Pure and mixed states, density matrices. Orthogonal measurements, positive operator valued measures. Unitary evolution, extension to superoperators. Master equation and decoherence. Quantum measurement. *[20 lecture hours]*

Quantum entanglement: Bell's theorems. Classical information theory, entropy. Quantum information theory, quantification of entanglement, communication complexity. Quantum cryptography and teleportation. Turing machines, reversible computation, universal logic gates and circuits. Quantum computers and circuits. Quantum algorithms: search, FFT, prime factorisation. Quantum simulations. Quantum error correction and codes. Faulttolerant quantum computation. Physical implementations: ion traps, quantum dots, cavity QED, NMR. *[25 lecture hours]*

Reference books:

- *J. Preskill, http://www.theory.caltech.edu/people/preskill/ph229*
- *Peres, Quantum Theory: Concepts and Methods.*

PHY 526. THEORY OF ELEMENTARY PARTICLES

- **Preliminaries:** Relativity – notation, kinematics; Particles as fields, Lagrangians and interactions; Examples of scattering and decay processes; Scattering cross-section and decay rate calculation *[6 Lecture Hours]*

- **Groups and Symmetries:** Definition of a group, matrix groups, direct product; Lie group, generator, Lie algebra, representation; SU(2) & SU(3), their representations, graphical representation; Internal symmetries and particles as representation; Symmetries and interactions *[8 Lecture Hours]*

- **PCT:** P,C,T in QM; P,C,T for Klein-Gordon, Dirac and Maxwell Equations (all as classical fields); P,C,T for quantum fields and their interactions; P,C,T violating terms in the Lagrangian *[8 Lecture Hours]*

- **SU(2):** Isospin and SU(2), nucleons, pions, composites; Isospin in scattering and decay processes; Isospin violations in electromagnetic and weak interactions; Isospin of strange particles, charge and I3 *[5 Lecture Hours]*

- **SU(3):** Isospin, Hypercharge and SU(3), quarks; Eightfold way, octets and decuplet for mesons and baryons; Existence of color *[4 Lecture Hours]*

- **Strangeness:** Strangeness selection rules; Weak interactions and strangeness; K decays and mixing; CP, long and short K; Strangeness oscillations *[4 Lecture Hours]*

- **Weak Interactions:** P violation, helicity and left-handed particles; Weak interactions of quarks; V-A interactions; CP violation *[5 Lecture Hours]*

Reference books:

- *O. M. Boyarkin: Advanced particle physics*
- *P. B. Pal: An introductory course of particle physics*
- *A. Bettini: Introduction to elementary particle physics*
- *T. P. Cheng and L. F. Li: Gauge theory of elementary particle physics.*
- *Halzen and Martin: Quarks and Leptons*

PHY 528. MESOSCOPIC PHYSICS

- History of the subject, fabrication techniques, and basic introduction to different material systems such as semiconductors, metals, and insulators. Semi-classical theory, Electronic structure, effective mass approximation. *[6 Lecture Hours]*
- Quantum transport regimes: Diffusive and Ballistic transport
    - Diffusive transport: different energy and length scales, Quantum coherent transport in diffusive medium, weak localization, weak anti-localization, universal conductance fluctuations, Aharonov-Bohm effect, Strong localization, Persistent currents in mesoscopic systems. *[10 Lecture Hours]*
    - Ballistic transport: Landauer formalism, Landauer-Buttiker approach to conductance, Comparison with Kubo formalism, violation of Onsager reciprocity relations, conductance quantization in point contacts, conductance quantization in modulated quantum wires. *[6 Lecture Hours]*

- Integral and fractional Quantum Hall effect *[6 Lecture Hours]*
- Quantum dots, electronic states in quantum dots, Hund's rule in a quantum dot, transport across quantum dots (capacitance approach), Kondo problem in a quantum dot, level statistics in a quantum dot *[6 Lecture Hours]*
- Definition of mesoscopic superconductivity in terms of Ginzburg-Landau theory, Ginzburg-Landau limit and London limit, phase transitions- magnetization and heat capacity of mesoscopic superconductors *[6 Lecture Hours]*

Optional/Elective topics: *[12 Lecture Hours]*

- Breit-Wigner and Fano resonance, delay time for resonances, Friedel sum rule, Levinson's theorem.
- Luttinger liquid in 1D.
- Noises in mesoscopic systems, Nyquist-Johnson noise, shot noise, 1/f noise
- Random Matrix theory
- Introduction to Qubits, Charge- and spin Qubits, Superconducting Qubits
- Andreev Reflection, Josephson effect
- Mesoscopic semiconductor devices
- Low-dimensional topological materials
- Different experimental techniques to probe mesoscopic systems: Optical, SPM, transport, etc.

References:

- Electronic Transport in Mesoscopic Systems, Supriyo Datta, Cambridge University Press
- Quantum Transport: Atom to Transistor, Supriyo Datta, Cambridge University Press
- Semiconductor Nanostructure, Thomas Ihn, Oxford University Press
- Quantum Transport: Introduction to Nanoscience, Yuli V. Nazarov, Yaroslav M. Blanter, Cambridge University Press

PHY 532. GENERAL RELATIVITY & COSMOLOGY

The Equivalence Principle: Non-Inertial frames and non-Euclidean Geometry, General Coordinate transformations and the general covariance of physical laws. *[5 Lecture Hours]*

Geometrical Basis: Contravariant and covariant vectors; Tangent vectors and 1-forms; Tensors – product, contraction and quotient laws, Wedge product – closed forms, Levi-Civita Symbol, Tensor densities, the invariant volume element. The Parallel Transport and affine connection, Covariant derivatives, Metric tensors, raising and lowering of indices, Christoffel connection on a Riemannian Space, Geodesics, Space-time curvature, curvature tensor Commutator and Lie derivatives, Equation for deviation, Symmetries of the curvature tensor, Bianchi Identities, Isometries and Killing Vectors. *[5 Lecture Hours]*

Einstein's Equations: Energy-Momentum Tensor and conservation laws, Einstein's equation, Hilvert's variational principle, Gravitational energy-momentum pseudo-tensors. Newtonian Approximation, Linearized field equations, Gravitational Waves, gravitational radiation. Principles of gravitational wave detectors – LISA, LIGO, VIRGO. *[10 Lecture Hours]*

Simple Solutions and Singularities: Static, Spherically symmetric space-time, Schwarzschild's exterior solution, Motion of perihelion of Mercury, Bending of Light, Gravitational Red-Shift Radar Echo delay. Black Holes; Kruskal –Szekeras diagram; Schwarzschild's interior solution;

Tolman-Oppenheimer-Volkov equation, Collapse of Stars, Kerr Metric, Reissner-Nordstrom metric, Kerr-Newman metric. Weyl's postulate and the cosmological (Copernican) principle, Robertson Walker metric, Anisotropies, vorticity and shear, Raychoudhury equation, Singularity theorems of Hawking and Penrose. *[10 Lecture Hours]*

Cosmology: Important models of the Universe; Red shift and expansion; Bigbang theory, Early Universe, and decoupling, neutrino temperature, nucleosynthesis, relative abundances of hydrogen, helium, deuterium, Radiation and matter dominated phases, Cosmic microwave background radiation, its isotropy and anisotropy properties, COBE and WMAP experiments; CMBR anisotropy as a hint to a large scale structure formation. Dark matter, Dark energy models. *[10 Lecture Hours]*

Reference books:

- Relativity: special, general, and cosmological, W. Rindler
- General Theory of Relativity: Robert Wald
- Gravitation and cosmology : principles and applications of the general theory of relativity, Steven Weinberg
- General Relativity : Lewis Ryder

SUBSEQUENT SEMESTERS

Subsequent semesters will be essentially devoted to research activities in the chosen topics and from time to time courses on Special Topics at an advanced level will be offered to broaden and deepen the base of the research scholars.

The actual courses offered will vary from year to year depending on the choice of specialization made by the students in consultation with the Students' Curriculum and Research Evaluation Committee (SCREC), availability of teachers, and topicality of the subject etc.

This updated Course Structure has been approved by the Academic Council and the Board of Studies for the Integrated Ph.D Programme (IPhD) in a meeting held on 5th May 2011 at the S N Bose National Centre for Basic Sciences and submitted to the University of Calcutta for inclusion as regular curriculum for the M.Sc. in Physical Sciences being the first two years of the Integrated Ph.D Programme in Physical Sciences (IPhD-Ph).

Integrated PhD Programme in Physical Sciences (IPhD-Ph)

In Collaboration with the

UNIVERSITY OF CALCUTTA

Examination Regulations

1. **Examination:** There shall be four examinations in the M.Sc course in the span of two years.

   Examination I: On completion of the course specified for first semester (December).

   Examination II: On completion of the course specified for second semester (May).

   Examination III: On completion of the course specified for third semester (December).

   Examination IV: On completion of the course specified for fourth semester (May).

NOTE:

- The medium of instruction and examination shall be English.
- No candidate shall be permitted to proceed to the next semester unless s/he has secured at least 50% marks in the aggregate in the examinations prescribed for the previous semesters.
- The course structure and the scheme of examination shall be reviewed from time to time by the Board of Studies.
- **Attendance:** Students will be considered eligible for taking the examinations I, II, III and IV only when s/he has pursued a regular course of study by attending not less than 90% of both theory and practical classes in relation to the course prescribed for each of the semesters separately.

M.Sc. EXAMINATION IN PHYSICAL SCIENCES

Scheme of Examination: Proposed in line with the pattern followed at the University of Calcutta

Semester	Midsem	Endsem	Project	Total
I	125 (25 x 5)	125 (25 x 5)	-------	250
II	125 (25 x 5)	125 (25 x 5)	-------	250
III	125 (25 x 5)	125 (25 x 5)	-------	250
IV	125 (25 x 5)	125 (25 x 5)	-------	250
TOTAL				**1000**

Compulsory Project Research

Semester	Programme
I	-------------------
II	Summer Programme – Project Research I (8 weeks in May-July)
III	Project Research II – Full Semester
IV	Project Research III – Full Semester
TOTAL	

1st Semester

Course No.	Course Title	Midsem	Endsem	Total
PHY 401	Mathematical Methods	25	25	50
PHY 403	Classical Dynamics	25	25	50
PHY 405	Quantum Mechanics I	25	25	50
PHY 407	Computational Methods in Physics	25	25	50
PHY 491	Basic Laboratory I	25	25	50
				250

2nd Semester

Course No.	Course Title	Midsem	Endsem	Total
PHY 402	Electromagnetic Theory	25	25	50
PHY 404	Statistical Mechanics	25	25	50
PHY 406	Quantum Mechanics II	25	25	50
PHY 408	Electronics & Instrumentation	25	25	50
PHY 492	Basic Laboratory II*	25	25	50
				250
PHY 494	Summer Research Project I (8 weeks)[1]		Unsatisfactory/Satisfactory/Good/Outstanding	

3rd Semester

Course No.	Course Title	Midsem	Endsem	Total
PHY 501	Atomic & Molecular Physics	25	25	50
PHY 503	Condensed Matter Physics	25	25	50
PHY 505 *	Advanced Quantum Mechanics & Applications	25	25	50
PHY 530 *	Soft Matter	25	25	50
PHY 507	Nuclear & Particle Physics		50	50
PHY 509	Project Research II	25	25	50
				250

* Either PHY 505 or PHY 530 to be chosen as “Optional Elective”.

[1] The conversion of Grades into marks – U = <37.5, S = 37.5-40, G = 41-45, O = 46-50. Pass Marks – 37.5 (75%).

4th Semester

Course No.	Course Title	Midsem	Endsem	Total
PHY 502	Project Research III		50	50
PHY 592	Methods of Experimental Physics	25	25	50
PHY 5xx	Elective 1*	25	25	50
PHY 5xx	Elective 2*	25	25	50
PHY 5xx	Elective 3*	25	25	50
				250
GRAND TOTAL				**1000**

Project Based Course

Course No.	Course Title	Semester	Report writing	Presentation	Total
PHY 509	Project Research II	3rd	25	25	50
PHY 502	Project Research III	4th	25	25	50
					100

Note: The project research is part of the whole curriculum and is compulsory to all students. The students are required to score at least 75% in each of the three Project Research Papers.

- **Mid Semester Examination must be conducted through "Written Test".**

2. **PhD Programme and evaluation of the PhD thesis:** The following guidelines towards monitoring of the doctoral research shall be strictly adhered to -

2.1 After successful completion of the first four semesters (two-year M.Sc), the student shall appear for a qualifying test[2] before she/he may be admitted as a Junior Research Fellow. The successful candidate shall enroll with a Supervisor from SNBNCBS for pursuing her/his Doctoral Research. S/he shall also complete the course work as per UGC guidelines.

2.2 The Supervisor shall constitute a Thesis Committee (3/4 members including one external expert as per SNBNCBS rules) after completion of the first year of Junior Research Fellowship. The JRF shall submit a broad outline on the thesis and present her/his plan before the committee.

2.3 After completion of 24 months of the Junior Research Fellowship, the student shall appear in a Comprehensive Examination (mode of examination shall be as per guidelines framed by the SCREC), and, if succeeds, shall be upgraded to Senior Research Fellow (SRF).

[2] The qualifying test includes a written test followed by an interview [Pass Mark – 60%; to qualify as JRF, the basis would be – 50: 50 – Written Test: Interview].

2.4 Within two years of JRF, the Student is expected to register with CU as a Doctoral Student. The monitoring of the progress shall continue through the Annual Thesis Committee meetings.

2.5 At the end of the work, the student shall present her/his work in an Open Thesis Colloquium which will be attended by the members of the Thesis Committee and other members of the academic community.

2.6 If the Thesis Colloquium appears to be satisfactory to the members of the Thesis Committee, the student is permitted to submit the **Extended Abstract of the Thesis** (as per CU rules).

2.7 Subsequent to the above, the CU rules shall prevail for PhD registration, Thesis submission, reviewing etc. and the students are to adhere to strictly the steps required to be complied with at CU offices.

11. **Eligibility for entering into the PhD Programme**.

11.1 The admission to the programme shall entail a candidate qualifying in the national level written tests [Section 4 above] followed by an interview. The candidates who meet the qualifying criteria – a) qualifying marks in B.Sc; (b) qualifying in the national level written test/s; (c) qualifying in the interview will be admitted to the Programme. However, the competent authority may relax/modify some of the criteria if there is a requirement.

11.2 A candidate who would obtain 60% and above marks in the 1st, 2nd, 3rd and 4th semesters and at least 75% marks in the respective project work, will be allowed to sit for the qualifying Examination[3] for continuing with the Doctoral Research. The successful candidates will be allowed to carry on their work for Ph.D. degree in the related programme under the guidance of particular supervisor/s. They will also be declared as having passed M.Sc. Examination.

12. All eligible candidates will be awarded an M.Sc. Degree in Physics. Candidates who will not qualify as mentioned above (Section 11.2) will be issued an M.Sc. completion certificate. Other eligible candidates who will be continuing PhD shall receive the M.Sc certificate after completion of the Comprehensive Examination.

13. Minimum Pass Marks and Classification of Successful Candidates:

(a) **[Pass Marks: 50%]** In order to qualify for the degree of M.Sc., a candidate must secure at least 50% marks in aggregate in theory, practical and in the project work.

(b) **First Class**: **60% or above** marks in the aggregate of all the examinations.

Second Class: **50% or above** marks in the aggregate of all the examinations.

(c) **Backlog Cases/Supplementary Examinations** – Students cannot continue with the next semesters if they have accumulated more than 2 (two) backlogs at a time. They can clear the backlogs through Supplementary Examinations. For any particular subject, a student can sit for the examination three times – first, the main semester examination; then, if unsuccessful, can avail of two special chances to clear the backlog/s. They will be given two chances to clear the backlog –

- the first Supplementary Examination will be held within 3 (three) months from the publication of the semester result, i.e. during the ensuing Mid-semester examination;

[3]

- The second Supplementary Examination will be held along with the regular main semester examination.
- At the time of the fourth semester, the student has to clear it preferably within 3 (three) months from the publication of the semester result and then qualify for joining the PhD Programme. However, the Competent Authority may permit the candidate to appear in the qualifying examination, and if successful, provisionally join a Supervisor.

COORDINATOR, IPHD PROGRAMME
S N BOSE NATIONAL CENTRE FOR BASIC SCIENCES

Ph.D. PROGRAMME

IN

PHYSICAL SCIENCES

Ph.D. PROGRAMME in PHYSICAL SCIENCES

ABOUT Ph.D. COURSEWORK

Ph.D. students at SNBNCBS are required to do coursework as mandated by UGC. Relevant points from 2016 regulations of UGC are quoted below. They are also required to take additional courses as stipulated by SNBNCBS as outlined in the section 'PhD Course Work – Current Session'.

University Grants Commission (Minimum Standards and Procedure for Award of M.PHIL./PH.D. Degrees) Regulations, 2016

Coursework: Credit Requirements, number, duration, syllabus, minimum standards for completion.

- The credit assigned to the Ph.D. course work shall be a minimum of 08 credits and a maximum of 16 credits.
- The coursework shall be treated as a prerequisite for Ph.D. preparation. A minimum of four credits shall be assigned to one or more courses on Research Methodology which could cover areas such as quantitative methods, computer applications, research ethics and review of published research in the relevant field, training, field work, etc. Other courses shall be advanced level courses preparing the students for Ph.D. degree.
- All candidates admitted to the Ph.D. programme shall be required to complete the coursework as advised by their supervisors during the initial one or two semesters.
- A Ph.D. scholar has to obtain a minimum of 55% of marks or its equivalent grade in the UGC 7-point scale (or an equivalent grade/CGPA in a point scale wherever grading system is followed) in the course work in order to be eligible to continue in the programme and submit the dissertation/thesis.

PhD Coursework – Current Session

Uniform Course Structure is being formulated for all PhD scholars. The course guideline is as follows:

i. External course requirement: As per UGC requirement, one subject is to be chosen from the list of courses approved by the University.
ii. Internal course requirement: As per Centre's requirement, one subject is to be chosen from the approved courses by the Centre from time to time.
iii. The scholars have to fulfill the above mentioned criteria [(i) & (ii)] which is mandatory for upgradation as Senior Research Fellow.
iv. All JRF students including IPhD students are required to take one Centre's required course.
v. The Centre's required courses cannot be one of IPhD semester I or II courses. However they can be one of IPhD semester III or IV courses, and any of the departmental courses that are at least of the III Semester IPhD level.
vi. Supervisors may however advise their PhD students to audit some of the IPhD semester I or II courses if necessary.

* Future updates regarding internal courses will be notified on our website from time to time.

COURSE STRUCTURE & SYLLABI

List of courses approved by the University

L=Lectures T=Tutorials P=Practicals in hours per week & C=Credit points

Course No.	Course Title	L	T	P	C
PHY 601	Research Methodology	4	-	-	4
PHY 602	Review of the topical Research	4	-	-	4
PHY 603 / 503	Condensed Matter Physics	4	-	-	4
PHY 604 / 504	Astrophysics	3	1	-	4
PHY 605 / 505	Quantum Physics (Application)	3	1	-	4
PHY 606	Computational Methods in Physics	3	1	-	4
PHY 607 / 507	Nuclear & Particle Physics	4	-	-	4
PHY 608	Classical Mechanics & Electromagnetism	4	-	-	4
PHY 609	Numerical Methods				
PHY 610 / 510	Mathematical Methods	3	1	-	4
PHY 611	High Energy Astrophysics around compact stars	4	-	-	4
PHY 612 / 512	Advanced Quantum Field Theory	4	-	-	4
PHY 614 / 514	Statistical Physics	3	1	-	4
PHY 616 / 516	Advanced Condensed Matter Physics I – Magnetism & Superconductivity	4	-	-	4
PHY 618 / 518	Nonlinear Dynamics	3	1	-	4
PHY 620 / 520	Optical Physics	3	1	-	4
PHY 622 / 522	Advanced Condensed Matter Physics II – Correlated Electrons & Disorder	4	-	-	4
PHY 624 / 524	Quantum Information Theory	3	1	-	4
PHY 626 / 526	Theory of Elementary Particles	3	1	-	4
PHY 628 / 528	Mesoscopic Physics	3	1	-	4
PHY 630 / 530	Soft Matter	3	1	-	4
PHY 632 / 532	General Relativity & Cosmology	3	1	-	4
PHY 691	Project Research (Semester - I)	-	-	8	8
PHY 692	Project Research (Continued in Semester - II)	-	-	8	8
	Total hours of contact per week	*16*			
	Total credits	*16*			

* The syllabi of the courses starting with Course Code No. 5XX are available in IPhD Course Curriculum. The syllabi for Courses with Code No. 6XX will include the syllabi of Courses with Code No. 5XX plus additional special/advanced topics that will be decided by the concerned teachers.

DEAN (ACADEMIC PROGRAMME)
S N BOSE NATIONAL CENTRE FOR BASIC SCIENCES

PHY 601. RESEARCH METHODOLOGY

1. Define Research and Methodology; Types of research methods available; Describe Experiments, Theory and Computation/ Simulation in general terms; Spell out explicitly (with a few examples) the connection among them. *[4 Lecture Hours]*

2. Define Library Research, Field Research and Laboratory Research; Explain Sample Survey, Sample Collection and/or Preparation, Data Analyses, Hypothesis, Modeling, Interpretation, and Conclusion. *[2 Lecture Hours]*

3. Error in Data Analyses and Ways to Report Error; Statistical Analyses of Collected Data; Importance of Error Analyses in Experimental/Numerical Study. Validity, Reliability and Reproducibility of Measured/Acquired Data. *[6 Lecture Hours]*

4. Accuracy and Precision in Measurements/ Predictions. Selectivity and Specificity of a Method Developed; Generalization and External Validity; Internal Validity and Inter-relationship between measurements and the underlying theory/hypothesis. *[6 Lecture Hours]*

5. Formulation of a Research Problem: Motivation, Induction, Hypothesis, Deduction, Observation and Conclusion *[2 Lecture Hours]*

6. Scientific Reporting of Data/Observation/Prediction; Difference between Magazine or Newspaper Reporting, and Science Journal Reporting; Expression Skill Development and Nurturing. *[2 Lecture Hours]*

7. Plagiarism – Self and External. Ethics, Attitude, Discipline and Holistic Approach to Research; Implication of Research Tenure on Personality Development. Importance of Focus, Challenge and Self-belief in Research. *[2 Lecture Hours]*

8. Research and Society – Coupling and Necessary Aloofness. Relevance to "Old fashion" Indian Philosophy of High Thinking. Basic Scientific Research, Translational Research, Technology Development and Elements of Commerce. *[2 Lecture Hours]*

9. Specific Experimental, Theoretical and Simulation Techniques for Decoding the Systems Around; Interconnection Between Theory and Experiments. Computer Languages Necessary for Machining a Scientific Problem, and Relevant Data Collection; Examples of a few commercially available software; Popular Numerical Techniques and Libraries (For example, MATLAB). *[16 Lecture Hours]*

PHY 602. REVIEW OF THE TOPICAL RESEARCH

Goal of the review – History of the subject – development of the subject: theoretical and experimental – alternative models and theories – pros and cons of various models and theories if any – the relevance of the topical research from the perspective of the subject – Possible ways to develop the research topic further.

PHY 603. CONDENSED MATTER PHYSICS

- Binding and cohesion in solids. Bonds and bands.
- Crystal Structure, X-ray Diffraction, Reciprocal Lattice.
- Periodic potentials, Bloch's Theorem, Kroning Penney Model, Free electrons and nearly free electrons; tight binding approximation.
- Elementary ideas of band structure of crystalline solids.
- Concept of holes and effective mass; density of states; Fermi surface; explanation of electronic behaviour of metals, semi-conductors and insulators.
- Lattice vibrations, harmonic approximation, dispersion relations and normal modes, quantization of lattice vibrations and phonons. thermal expansion and need for anharmonicity.
- Transport properties of solids. Boltzmann transport equation. Wiedemann-Franz law. Hall effect.
- Superconductivity: Phenomenology, penetration depth, flux quantization etc. Josephson effect.
- Semiconductors: intrinsic and extrinsic, carrier mobility etc.
- Thermal properties of solids.
- Magnetism in solids.
- Optical and Dielectric Properties.

Reference Books:

- *Dekker, Solid State Physics*
- *Kittel, Introduction to Solid State Physics*
- *Ashcroft and Mermin, Introduction to Solid State Physics.*
- *Ziman, Principles of the Theory of Solids.*

PHY 604. ASTROPHYSICS

Basic Background of Astronomy: Elementary radiative transfer equations , absorption and emission, atomic processes, continuum and line emission – Telescopes: Refracting and Reflecting telescopes, Ground-based and space-based observatories – Properties of telescope: Light gathering power and Angular resolution – Astronomical Instrumentation - Optical/IR filter-systems – Optical/IR detectors – X-ray detectors – Imaging camera and spectrometer. distance measurements – Hubble's law *[6 lecture hours]*

Coordinate Systems: Spherical trigonometry – the Celestial sphere – Coordinate systems: Horizontal system; Equatorial system; Ecliptic system; Galactic system – Rising and setting of stars – Parallax – Astronomical time systems: Sidereal and Solar time – Concepts of Calendars

[5 lecture hours]

Interstellar medium and formation of stars: Interstellar extinction law – theoretical extinction model and Mie scattering – nucleogenesis – Interstellar dust and Abundances – Molecular clouds – properties of molecular clouds – formation of protostars and stars – Jeans Instability: collapse of a spontaneous cloud and virial theorem – Kelvin-Helmholtz time scale – Protostellar systems: disks, bipolar outflows *[6 lecture hours]*

Stellar structure: Equations for hydrostatic equilibrium –polytropic stars – Lane Emden equations and its solutions – stellar interior *[4 lecture hours]*

Evolution of stars: Sources of stellar energy: Fusion reactions (p-p) chain, CNO Cycle, triple alpha reactions – formation of heavy elements – evolution of low mass and high mass stars, Chandrasekhar limit, Neutron stars and Blackholes – Hertzsprung-Russell diagram

[5 lecture hours]

Stellar properties: Continuous radiation from stars: Brightness of starlight – Electromagnetic spectrum – colors of stars – Stellar distances – stellar parameters: magnitude, luminosity, radius and their measurements *[3 lecture hours]*

Spectral Classifications of Stars: Spectral lines in stars – origin of spectral lines – line broadening: Doppler, thermal and collisions – Hydrogen spectral lines – Formation of spectral lines: excitation, ionization and recombination, Boltzmann Equation, Stimulated and spontaneous emission – Mass luminosity relation – Hertsprung-Russell diagram – Saha Ionization Equation – Ionized hydrogen regions
[6 lecture hours]

Binary Stars: Different types of binary stars, Importance of binary systems, Accretion and gravitational radiation (basic ideas) *[4 lecture hours]*

Galaxies: Formation and classification: Active galaxies and Quasars – Density wave theory of the formation of spiral arms – Rotation curve: missing mass and dark matter – Quasars and active galactic nuclei, Milky Way Galaxy – Oort's constants – magnetic field *[5 lecture hours]*

Suggested Books:

- Norbert S. Schulz, From Dust To Stars: Studies of the Formation and Early Evolution of Stars, Springer-Verlag Berlin and Heidelberg GmbH & Co. K, 2005
- K. D. Abhayankar, Astrophysics: Stars And Galaxies, Universities Press, 2001
- H. Karttunen, P. Kröger, H. Oja, M. Poutanen, K. J. Donner (Eds.), Fundamental Astronomy, Springer Berlin Heidelberg New York, 2007
- B. Basu, An Introduction to Astrophysics
- Radiative processes in Astrophysics: G. Rybicki and A. Lightman
- Physics of Astrophysics – F. Shu

PHY 605. QUANTUM PHYSICS (FORMAL)

The formal structure of quantum mechanics, Schroedinger equation, matrix formulations, application to simple systems, angular momentum, perturbation theory, variational techniques, and WKB approximations.

R. Shankar, Quantum Mechanics

L.D Landau and E. M Lifshitz, Course of Theoretical Physics

PHY 606. COMPUTATIONAL METHODS IN PHYSICS

Introduction to Fortran programming and basic numerical methods will be imparted to the students through lectures and projects based on the numerical analysis of elementary physical problems illustrating such techniques.

This course will involve lectures on advanced numerical techniques and projects based on the numerical analysis of advanced physical problems illustrating such techniques.

PHY 607. NUCLEAR & PARTICLE PHYSICS

General properties of nuclei: nuclear size, nuclear radius and charge distribution, nuclear form factor, mass and binding energy, Angular momentum, parity and symmetry, Magnetic dipole moment and electric quadrupole moment. *[4 Lecture Hours]*

Two-body bound state: Properties of deuteron, Schr ̈odinger equation and its solution for ground state of deuteron, rms radius, spin dependence of nuclear forces, electromagnetic moment and magnetic dipole moment of deuteron and the necessity of tensor forces. *[6 Lecture Hours]*

Two-body scattering: Experimental n-p scattering data, Partial wave analysis and phase shifts, scattering length, magnitude of scattering length and strength of scattering, Significance of the sign of scattering length; Scattering from molecular hydrogen and determination of singlet and triplet scattering lengths, effective range theory, low energy p-p scattering, Nature of nuclear forces: charge independence, charge symmetry and isospin invariance of nuclear forces. *[8 Lecture Hours]*

Nuclear structure: Liquid drop model, Bethe-Weizs ̈acker binding energy/mass formula, Fermi model, Shell model and Collective model. *[6 Lecture Hours]*

Nuclear reactions and fission: Different types of reactions, Quantum mechanical theory, Resonance scattering and reactions— Breit-Wigner dispersion relation; Compound nucleus formation and break-up, Statistical theory of nuclear reactions and evaporation probability, Optical model; Principle of detailed balance, Transfer reactions, Nuclear fission: Experimental features, spontaneous fission.

[6 Lecture Hours]

Radio Active Decays: Alpha decay, Beta decay –Energy release in beta decay–Fermi theory of beta decay–Shape of the beta spectrum –decay rate Fermi-Curie plot–Fermi & G.T Selection rules – Comparatives half-lives and forbidden decays – Gama decay-Multi pole radation – Angular momentum and parity selection rules – Internal conversion – Nuclear isomerism. *[4 Lecture Hours]*

Elementry particle Physics: Types and characteristics of interaction between elementary particles–Hadrons and laptons–Symmetry and conservation laws – CPT theorem–Gell-Mann-Nishijima formula-classification of hadrons –Quark model - symmetry classification of elementary particles- Parity non-conservation in weak interaction. Relativistic kinematics.

[10 lecture hours]

Suggested Books:

- B. B.Cohen: ConceptsofNuclearPhysics
- J. S. Lilley: Nuclear Physics
- M. K. Pal: Theory of Nuclear Structure
- R. R. Roy and B.P. Nigam: Nuclear Physics

- S. N. Ghoshal: Atomic and Nuclear Physics (Vol. 2)
- D. H. Perkins: Introduction to High Energy Physics
- D. J. Griffiths: Introduction to Elementary Particles
- D. C. Tayal: Nuclear Physics

PHY 608. CLASSICAL MECHANICS & ELECTROMAGNETISM

Lagrangian treatment, Variational principle, Hamiltonian structure, Canonical transformations, Hamilton Jacobi theory, Spatial relativity, Electromagnetism from a least action principle, potential theory, retarded and advanced potentials, waves.

Suggested Books:

- *H. Goldstein, Classical Mechanics*
- *J. D Jackson, Electrodynamics*

PHY 609. NUMERICAL METHODS

Basic programming in Fortran, Numerical methods of finding roots of an equation (Bisection method, Newton's method), Numerical methods of solving set of linear equations(Gauss elimination method, Thomas method), Numerical method of integration (Gregory-Newton expansion, Trapezoidal rule, Simpson's rule),Numerical method of differentiation, Numerical method of solving differential equation (Euler's method, Runge-Kutta method).

In addition to the above, some lectures at a more advanced level will be offered.

Suggested Books:

- *Programming in FORTRAN by Rajaraman.*
- *Numerical Recipe by Press, Shapiro and Teukolski*
- *Numerical methods for Scientists and Engineers by HM Antia*

PHY 610. MATHEMATICAL METHODS – I

- Vector analysis, Green, Gauss and Stokes theorems.
- Linear vector spaces and linear operators. Matrices & eigenvalue problem.
- Theory of complex variables, Cauchy-Riemann conditions, Cauchy integral theorem, Taylor-Laurent expansion, classification of singularities, analytic continuation, theorem of residues and evaluation of definite integrals and series.
- Ordinary differential equations and series solution. Sturm-Liouville problem and orthogonal functions, special functions.
- Green's functions for self-adjoint differential operators and eigenfunction expansion. (Laplace, Poisson, Diffusion, Wave equation etc to be discussed).

In addition to the above, some lectures at a more advanced level will be offered.

Suggested Books:

- *G. Arfken, Mathematical Methods for Physicists*
- *I.N. Sneddon, Special Functions of Mathematical Physics & Chemistry*
- *P.K. Chattopadhyay, Mathematical Physics*
- *E. Kreyszig, Advanced Engineering Mathematics*
- *Mathews and Walker, Mathematical Physics*
- *P. Dennery & A. Kryzwicki, Mathematics for Physicists*
- *C.M. Bender & S.A. Orszag, Advanced Mathematical Methods for Scientists & Engineers*
- *E. Butkov, Mathematical Physics*
- *R.W. Churchill & J.W. Brown, Com*

PHY 611. HIGH ENERGY ASTROPHYSICS AROUND COMPACT STARS

Astrophysics of compact stars: Black Holes, Neutron Stars and White Dwarfs;
Accretion processes on these objects: Transonic Flows, Outflows and origin, acceleration and collimation of jets; Radiative Properties of the accretion flows; Observational Evidence for compact stars.
Data Analysis: Observations of high energy radiation from compact objects; satellite data and their analysis

Suggested Books:

- *Accretion Power in Astrophysics - J. Frank*
- *Theory of Transonic Astrophysical Flows – S. K. Chakrabarti*
- *Accretion Processes in Astrophysics – (Physics Reports) S.K. Chakrabarti*
- *Black Holes, Neutron Stars and White Dwarfs: Physics of Compact Objects by Shapiro and Teukolsky*

PHY 612. ADVANCED QUANTUM FIELD THEORY

- Path integral quantization of free fields: Real scalar field, complex scalar field, Dirac field, electromagnetic field *[10 Lecture Hours]*
- Connection of path integral approach to QFT with Statistical Mechanics, Finite temperature field theory *[5 Lecture Hours]*
- Fadeev-Popov method *[5 Lecture Hours]*
- Perturbation Expansion and Feynman Diagrams through path integral approach for interacting scalar fields, Dirac fields, quantum electrodynamics *[10 Lecture Hours]*
- Loops, Divergences, Regularization and Renormalization *[5 Lecture Hours]*
- Anomalous magnetic moment of the electron and the Lamb-Shift *[5 Lecture Hours]*

Suggested Books:

- *Quantum Field Theory by B. Hatfield*
- *Quantum Field Theory by L. Ryder*
- *Quantum Field Theory by Steven Weinberg*
- *Quantum Field Theory by Peskin & Schroder*

PHY 614. STATISTICAL PHYSICS

Foundations, micro-canonical, canonical and grand canonical ensembles, non-interacting systems, interacting systems, phase transitions, quantum statistics, BEC, Quantum Hall, magnetism, superconductivity.

PHY 616. ADVANCED CONDENSED MATTER PHYSICS I

– MAGNETISM & SUPERCONDUCTIVITY

Generalized Hamiltonian of Condensed Matter Physics and origin of various "effective theories"; Introduction to phenomenon of Superconductivity; Experimental features; Various phenomenological theories; Cooper's one pair problem; Gateway to microscopic theories--- BCS Fermion pairing theory and BSB Bose Condensation theory; BCS ground state; Mean field treatment of BCS Hamiltonian; Gap equation and its solution; Equation for critical temperature; Brief applications of BCS theory to various experiments; Brief introduction to exotic phenomena like interplay of superconductivity and magnetism, high temperature superconductivity etc.

In addition to the above, some lectures at a more advanced level will be offered.

Suggested Books:

- *"Theory of Superconductivity" by J.R. Schrieffer.*
- *"Solid State Physics" by N. Ashcroft and N.D. Mermin.*
- *"Introduction to Solid State Physics" by C. Kittel.*
- *"Quantum Theory of Solids" by C. Kittel.*
- *"Quantum Theory of Many Particle Systems" by G.D. Mahan.*
- *"Elementary Excitations" by D. Pines*

PHY 622. ADVANCED CONDENSED MATTER PHYSICS II

– CORRELATED ELECTRONS & DISORDER

Physics of Materials:

Metals (M) and Insulators (I)

A. BAND INSULATORS vs CORRELATED INSULATORS

- Breakdown of independent electron description
- Mott transition
- Hubbard model
- Limiting cases of Hubbard models - band limit & atomic limit, Hubbard sub-bands
- Mott transitions in transition metal oxides
- Mott insulators & charge transfer insulator, Zaanen-Sawatzky-Allen classification

B. LARGE-U LIMIT

- Canonical transformation
- t-J model, Super-exchange
- Half-filled band : Heisenberg spin model
- Antiferromagnetic Heisenberg model : spin waves, strange world of D=1

C. SOME INTERESTING SYSTEMS

- Band-width-control M-I transition systems: V_2O_3, $RNiO_3$, NiS etc
- Filling control M-I transition systems: $R_{1-x}A_{x}Ti(V)O_3$
- High Tc super-conducting cuprates
- Quasi one-dimensional systems: Cu-O chain & ladder compounds
- Double-exchange systems: $R_{1-x}A_{x}MnO_3$

D. DISORDER INDUCED INSULATORS

- Anderson Localization
- Scaling theory
- Electron-electron interaction & disorder

References:

- Patrik Fazekas -- Lecture notes on Electron Correlation & Magn.
- Imada, Fujimori, Tokura -- Metal-Insulator Transitions, Review. Mod. Phys. vol 70, pg 1039 (1998)
- P.A. Lee & T.V. Ramakrishnan -- Disordered electronic system, Review. Mod. Phys. vol 57, pg 287 (1985)
- Fulde -- Electron correlation in Molecules and Solids

Electronic Structure of Materials

A. BASICS

1. Electrons in periodic potentials
   - Bloch's theorem
   - Kronig-Penney model
   - concept of energy bands
2. Density of states
   - Green's function
   - Tridiagonal matrices & Continued fractions
   - Singularities in DOS
3. Reciprocal lattice & Brillouin zone
   - Special k-points in BZ sampling

B. EL-ION PROBLEM

4. Adiabatic approximation (Born-Oppenheimer).
5. Classical nuclei approximation (Ehrenfest Theorem).
6. Hellman-Feynman force on nuclei.

C. MANY-ELECTRON PROBLEM

7. Hartree approximation
   - LCAO method
8. Hartree-Fock approx.
   - Slater-determinantal wavefunction & its properties
   - Hartree-Fock equation
   - Fock operator
   - Energy of the ground state
   - Koopman's theorem
9. Going beyond Hartree-Fock (introductory)
   - Absence of correlation in H-F theory
   - Basics of MCI and Perturbative (Moller-Plesset) methods
10. Density Functional Theory
    - Energy as a functional of density : basic concepts
    - Thomas-Fermi theory
    - Hohenberg-Kohn Theorem
    - Kohn-Sham Eqn.
    - LDA for the exchange-correlation function

D. MOLECULAR DYNAMICS METHODS IN ELECTRONIC STRUCTURE

11. Introduction to MD methods
   - Deterministic vs. Stochastic methods
   - Connection to statistical mechanics & thermodynamics
   - Finite difference algorithms for solving eqns. of motion
   - running and controlling MD simulations
   - Limitations & errors in MD simulation
12. Tight-binding MD
   - Eqn of motion in TB-MD
13. Ab-initio (Car-Parrinello) MD
   - Basic concepts and effective Lagrangian
   - Eqn of motion
   - Iterative solution of Kohn-Sham eqn

<u>E. EXPERIMENTAL MANIFESTATION OF ELECTRONIC STRUCTURE</u>
   - Theory of photoemission
   - Core-levels and Final states
   - Satellites
   - Valance band
   - Band structure
   - Surface states and surface effects

References:

- *Ashcroft & Mermin -- Solid State Physics*
- *Grosso & Pastore-Parravicini -- Solid State Theory*
- *Kaxiras -- Electronic Structure of Solids*
- *Sutton -- Electronic Structure of Materials*
- *Fulde -- Electron correlation in Molecules and Solids*

PHY 691. PROJECT RESEARCH (SEMESTER - I)

Projects shall be taken up by students under the supervision of a Research Guide.

PHY 692. PROJECT RESEARCH (CONTINUED IN SEMESTER - II)

Continuation of the fifth semester project under the supervision of a Research Guide.

DEAN (ACADEMIC PROGRAMME)
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Ph.D. PROGRAMME

IN

CHEMICAL SCIENCES

Ph.D. PROGRAMME in CHEMICAL SCIENCES
COURSE STRUCTURE & SYLLABI

List of courses approved by the University

L=Lectures T=Tutorials P=Practicals in hours per week & C=Credit points

Course Code	Course Title	L	T	P	C
CB 621	Numerical Methods	3	1	0	4
CB 622	Condensed Matter Theory	3	1	0	4
CB 623	Advanced Equilibrium Statistical Mechanics	3	1	0	4
CB 624	Physical Chemistry: Experiments & Theory	3	1	0	4
CB 625	Instrumental Methods of Analysis	3	1	0	4
CB 626	Fundamentals of Biophysics	3	1	0	4
CB 627	Molecular Physics and Spectroscopy	3	1	0	4
CB 628	Stochastic Processes in Physics and Chemistry	3	1	0	4
CB 629	Dynamics near and far away from Equilibrium Systems	3	1	0	4
CB 630	Mathematical Methods	3	1	0	4
CB 631	Advanced Numerical Methods & Simulation	3	1	0	4
CB 632	Chemical Dynamics	3	1	0	4
CB 633	Liquids	3	1	0	4
CB 634	Quantum Statistical Process in Dynamics	3	1	0	4
CB 635	Non-equilibrium Statistical Mechanics	3	1	0	4
CB 636	Mesoscopic Physics	3	1	0	4
CB 637	Classical & Quantum Stochastic Process	3	1	0	4
CB 638	Nonlinear Spectroscopy	3	1	0	4
CB 639	Radiation Matter Interaction	3	1	0	4
CB 640	Study of Bio-Macromolecules	3	1	0	4
CB 641	Surfaces & Interfaces	3	1	0	4
CB 691	Project Research (Semester – I)	-	-	8	8
CB 692	Project Research (Continued in Semester – II)	-	-	8	8
	Total hours of contact per week	*16*			
	Total credits	*16*			

CB 621: NUMERICAL METHODS

Basic programming in Fortran, Numerical methods of finding roots of an equation (Bisection method, Newton's method), Numerical methods of solving set of linear equations (Gauss elimination method, Thomas method), Numerical method of integration (Gregory-Newton expansion, Trapezoidal rule, Simpson's rule), Numerical method of differentiation, Numerical method of solving differential equation (Euler's method, Runge-Kutta method).

Reference Books:

- *Programming in FORTRAN by Rajaraman.*
- *Numerical methods by Sujit Kumar Bose.*

CB 622: CONDENSED MATTER THEORY

Drude's model, Sommerfelds theory of free electrons, entropy calculation, Electron in a periodic potential, Bloch's theorem, Almost free electron approximation, Tight binding approximation, group velocity of an electron in a periodic potential, effective mass tensor, reciprocal lattice, density of states as a surface Integral.

Reference Books:

- *Solid state phyics by Ashcroft-Mermin*
- *Theory of properties of metals and alloys by Mott and Jones.*

CB 623: ADVANCED EQUILIBRIUM STATISTICAL MECHANICS

1. Statistical Mechanics of an Interacting System. 1-d Ising Chain, 2nd virial expansion for real gas & Limitations.
2. Structural quantities of a liquid, Single point density, Pair correlation function. Structure factor.
   Thermodynamics of a liquid in terms of pair correlation function.
3. Mean Field Theory in Variational approach.
4. Grand partition function of a liquid as a function of external potential. Direct correlation function. Classical density functional theory. Application to freezing and screening in colloids.
5. Basic algorithm of Monte Carlo, Molecular Dynamics and Brownian Dynamics Simulation.

Reference Books:

- *Equilibrium Statistical Mechanics by Plischke & Bergerson.*
- *Theory of Simple Liquids by Hansen and McDonald*
- *Complete Simulation of Liquids by Allen & Tildesley*

CB 624: PHYSICAL CHEMISTRY: EXPERIMENTS & THEORY

1. Rate & Order of Reaction, Determination of Rate Equation, Various types of first order reaction, Principles of Microscopic Reversibility and Detailed Balance, Flow Reactors, Effect of Temperature, Mechanism of Chemical Reactions, Relation between rate constants for the forward and backward reactions, molecularity of a reaction (uni, bi & tri), Unbranched & Branched Chain reaction, Analyses of Complex Reaction Systems and Solution of Coupled Linear Rate Equations.

2. Simple Collision Theory of Bimolecular Reactions, Potential Energy Surfaces, Theoretical Calculations of a Rate Constant, Transition State Theory, Hinselwood's modification, Rice-Ramsperger-Kassel-Marcus Theory (a small touch) Thermodynamic Formulation of TST, Molecular Beam Experiments, Principles of Photochemistry, Rates of Intramolecular Processes, Quenching, Intermolecular processes, Chemical Reactions and their Quantum Yields, Flash Photolysis, Femtosecond Transition State Spectroscopy, Small discussions on Photosynthesis and Photochemical Cell.

3. Kinetics in the Liquid Phase: Small discussion on Liquid Structure including radial distribution function and structure factor, Viscosity of a Liquid, Diffusion, Mobility of an Ion, Encounter Pairs, Diffusion Controlled Reactions in Liquids, Relaxation Time for a one step reaction, Rate constants for elementary reactions in water, Acid and Base Catalysis, Kinetic Salt effect, Enzyme Catalysis (Michaelis-Menten Kinetics), Stern-Volmer description, Electrochemical Kinetics; Kinetics of the Hydration of CO2.

4. Relation Between Diffusion and Brownian Motion, Thermodynamic view of diffusion, diffusion equation, diffusion probabilities, Statistical view of diffusion, Random walk, Einstein-Smoluchowski equation, Ion conductivities and ion-ion interaction, expression for diffusion in terms of force autocorrelation and velocity auto-correlation functions

5. Kramers' theory for simple chemical reaction in liquid, energy and diffusion dominated regimes, viscosity (friction dependence); Breakdown of Kramers' theory as revealed by time domain laser spectroscopy, fractional viscosity dependence of cis-trans isomerization of stilbene. Grote-Hynes Theory for the observed fractional viscosity dependence and the related debate.

6. Solvation as an example of non-reactive dynamics, time scales for solvation in simple liquids and dynamical solvent control on reaction rates. Factors that determine the fast response and its coupling to the environment, time scales found in trapped solvents and solvents (water) near macromolecular surfaces; Supercritical solvents and its difference (structure & dynamics) with solvents at ambient condition, solvation in ionic liquids.

7. Atoms and Molecules in Intense and Super-intense laser fields

References and Books:

- *J. I. Steinfeild, J. S. Francisco and W. L. Hase,* ***Chemical Kinetics and Dynamics,*** *Englewood Cliffs, NJ: Prentice Hall, 1989*
- *R. D. Levine and R. B. Bernstein,* ***Molecular Reaction Dynamics and Chemical Reactivity****. New York: Oxford Univ. Press, 1987.*
- *R. B. Bernstein,* ***Chemical Dynamics via Molecular Beam and Laser Techniques****. New York: Oxford Univ. Press, 1982.*

- *I. H. Seagal, **Enzyme Kinetics**. New York: Wiley-Interscience, 1975*
- *R. A. Alberty and R. J. Silbey, **Physical Chemistry**. John Wiley and Sons*
- *P. W. Atkins, **Physical Chemistry**, 5th Edition. ELBS with Oxford Univ. Press.*
- *A. H. Zewail, **Science**, volm. 242, 1645 (1988).*
- *G. R. Fleming and P. G. Wolynes, **Phys. Today**, volm.43, 36 (1990)*
- *H. A. Kramers, **Physica**, volm.7, 284 (1940).*
- *R. F. Grote & J. T. Hynes, **J. Chem. Phys**. Volm.73, 2715 (1980).*
- *M. Maroncelli, J. McInnis, G. R. Fleming, **Science**, volm.243, 1674, (1989); Jimenez et al., **Nature**, volm. 369, 471, (1994).*
- *M. Gavrilla (Ed.), **Atoms in Intense Laser Fields**, Academic Press*

CB 625: INSTRUMENTAL METHODS OF ANALYSIS

Fundamental of Electricity, Current , Voltage Power, conversion from AC to DC, Fundamentals of Optical system, Light sources and Detection system, Lens, Mirror, Grating, Fundamentals of Optical Absorption spectroscopy, Fundamentals of Optical Emission spectroscopy, Fundamentals of Fourier Transformed Infrared spectroscopy (FTIR), Fundamentals of Circular Dichroism Spectroscopy, Fundamentals of Time correlated single photon counting Spectroscopy, Fundamentals of Time correlated single photon counting Spectroscopy, Fundamentals of Femtosecond spectroscopy Transient absorption, Fundamentals of Femtosecond spectroscopy Optical upconversion, Data analysis of fluorescence anisotropy, various models, Data Analysis for the Solvation dynamics, TRANES, Data analysis for the Forsters Resonance energy transfer, Fundamentals of Densimetric and sonometric measurements, Data analysis of Densimetric and sonometric measurements.

Reference Books:

- *Electronic Principles by Malvino*
- *Instrumental Methods of Analysis by Willard, Merritt, Dean, Settle*
- *Principles of Fluorescence Spectroscopy by J. Lakowicz*
- *Time correlated single photon counting O'conor and Philips*
- *PhD thesis from Dr. Pal's Group*

CB 626: FUNDAMENTALS OF BIOPHYSICS

Biological Macromolecules (Structure Protein and Nucleic Acids), Spectroscopic Methods to study Biological Macromolecules (UV-VIS, Fluorescence, Circular Dichroism, NMR), Protein folding and application of FRET to protein folding, Enzymes: Reaction kinetics, mechanism and inhibition and measurement methodologies, Gene structure, modification, DNA damage and Cancer Biology, Receptor-ligand interactions and Signal transduction, Solvation, densimetric, sonometric methods to study biomolecular interaction, Fluorescence anisotropy to study microenvironments and charge transfer reactions in biological macromolecules.

Reference Books:

- *Biochemistry by Donald Voet and Judith G. Voet*

- *Protein Structure and Function by George A. Petsko*
- *Principles of Fluorescence Spectroscopy by J. Lakowicz*

CB 627: MOLECULAR PHYSICS AND SPECTROSCOPY

Born-Oppenheimer approximation; Franck-Condon factor, diabatic and adiabatic representation; nonadiabatic effects.
Potential energy surface; vibration and rotational motion on an electronic energy surface. Valence bond and molecular orbital theory.

Radiation-matter interaction; interaction of a two-level system with a single mode classical and quantum field; Calculation of absorption, fluorescence and Raman spectra of multimode two-state molecular system.
Electron transfer and energy transfer in molecular system.

Reference Books:

- *Nitzan, Chemical Dynamics*
- *Szabo and Oslund, Quantum Chemistry*
- *May and Kuhn, Energy transfer and electron transfer*
- *Louisell, Quantum Statistical Properties of Radiation*
- *Mukamel, Principles of nonlinear spectroscopy*

CB 628: STOCHASTIC PROCESSES IN PHYSICS AND CHEMISTRY

- **Introduction to probability theory:** Random numbers, Gaussian distribution; Central limit theorem [4 lecture hours]
- **Stochastic dynamics:** Langevin equation, Brownian motion, Ornstein-Uhlenbeck process. Markov jump processes and master equations. Fokker-Planck and Smoluchowski approaches to dynamical processes and their solutions for simple problems. [8 lecture hours]
- **Fluctuation-response formalism**: Onsager regression theorem; linear response theory; fluctuation-dissipation relations and spectra. [6 lecture hours]
- **Introduction to chemical reaction kinetics**: order of a reaction with examples; Microscopic theories of chemical reaction rates: Collision theory; transition state theory; Kramers theory; effect of diffusion in unimolecular reaction rate.

Reference Books:

- *David Chandler, Nonequilibrium systems*
- *Van Kampen, Stochastic Processes*
- *Zwanzig, Nonequilibrium phenomena*
- *Nitzan, Chemical dynamics*
- *Hangii, etal, Review of Modern Physics, 1990, Fifty years after Kramers Theory*

CB 629: DYNAMICS NEAR AND FAR AWAY FROM EQUILIBRIUM SYSTEMS

Brownian motion; introduction to probability theory; Gaussian distribution; Central limit theorem; Onsager regression theorem; linear response theory; fluctuation-dissipation relations and spectra; Langevin equation, Master equation, Fokker-Planck and Smoluchowski approaches to dynamical processes and their solutions for simple problems.
Oscillatory chemical reactions and population dynamics in simple system; An introduction to nonlinear dynamics; nonlinear feedback systems and nonequilibrium steady state; reaction-diffusion systems; Pattern formation in nonlinear dynamical system with simple diffusion.

Reference Books:

- *McQuarrie, Nonequilibrium systems*
- *R. Zwanzig, Nonequilibrium phenomena*
- *Nitzan, Chemical dynamics*
- *Epstein, Nonlinear dynamics and chaos in chemical systems*
- *van Kampen, Stochastic Processes*

CB 630: MATHEMATICAL METHODS

- Vector analysis, Green, Gauss and Stokes theorems.
- Linear vector spaces and linear operators. Matrices & eigenvalue problem.
- Theory of complex variables, Cauchy-Riemann conditions, Cauchy integral theorem, Taylor-Laurent expansion, classification of singularities, analytic continuation, theorem of residues and evaluation of definite integrals and series.
- Ordinary differential equations and series solution. Sturm-Liouville problem and orthogonal functions, special functions.
- Green's functions for self-adjoint differential operators and eigenfunction expansion. (Laplace, Poisson, Diffusion, Wave equation etc to be discussed).

References & Books:

- *G. Arfken, Mathematical Methods for Physicists*
- *I.N. Sneddon, Special Functions of Mathematical Physics & Chemistry*
- *P.K. Chattopadhyay, Mathematical Physics*
- *E. Kreyszig, Advanced Engineering Mathematics*
- *Mathews and Walker, Mathematical Physics*
- *P. Dennery & A. Kryzwicki, Mathematics for Physicists*
- *C.M. Bender & S.A. Orszag, Advanced Mathematical Methods for Scientists & Engineers*
- *E. Butkov, Mathematical Physics*
- *R.W. Churchill & J.W. Brown, Complex Variables & Applications*

CB 632: CHEMICAL DYNAMICS

Introduction to chemical reaction kinetics, order and molecularity of a reaction; potential energy surfaces, reaction coordinate, the activation energy.

Enzyme Kinetics, Lineweever-Burk Plot, Cooperativity, Hill coefficient, Ultrasensitivity in enzyme kinetics

Theory of chemical reaction: Collision theory; Transition state theory; Unimolecular reactions: Lindemann mechanism, RRKM theory.

Chemical reaction as scattering processes: the total and differential reaction cross sections, the rate constant and the reaction cross-section

Probabilistic reaction kinetics for small system, Chemical master equation, stochastic approach to reaction kinetics.

Reaction Rate Theory: Stochastic response function approch to chemical reaction, Onsager regression hypothesis and reaction rate; Fokker-Planck equation, Kramers' theory of activated rate, Energy diffusion limited rate; Reactions in liquid: Smoluchowsky equation of overdamped system, Diffusion limited reaction; viscocity and temperature dependence in gas and liquid phase reaction.

Reaction in ionic solution: Donan equilibrium, electron transfer reaction, Marcus theory of electron transfer, quantum theory of electron transfer reaction.

Driven chemical dynamics in flow system, nonequilibrium steady state of first order and second order reaction in a continuously stirred tank reactor.
Reaction dynamics in feedback system, stability of chemical reaction dynamics ; Reaction dynamics in open nonhomogeneous system; Reaction-diffusion equation; Activator and inhibitor dynamics; Turing pattern formation

Reference Books:

- H. Eyring, SH Lin and SM Lin, Basic Chemical Kinetics
- T Palmer and P L Bonner, Enzymes: Biochemistry, Biotechnology, clinical chemistry
- R. D. Levine and R. B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity. New York: Oxford Univ. Press, 1987
- David Chandler, Nonequilibrium systems
- N G Van Kampen, Stochastic Processes
- Zwanzig, Nonequilibrium phenomena
- Nitzan, Chemical dynamics
- I. R. Epstein: An Introduction to Nonlinear Chemical Dynamics: Oscillations, Waves, Patterns, and Chaos
- Hangii, etal, Review of Modern Physics, 1990, Fifty years after Kramers Theory

CB 633: LIQUIDS

A. Thermodynamics of liquids

1. Mean field theory of liquids
2. Density functional theory
3. Dynamics: correlation function (defn), conservation laws and diffusive motion
4. Basic Computer simulation: MC. MD and BD

B. Applications of liquid theory in chemistry

1.Basic ideas of absorption and fluorescence response of a dissolved solute, Relation between interaction and line-width

2.Connection between molecular motions in a liquid solvent and fluorescence and dielectric response; complexities associated with conducting liquids

3.Time-resolved measurements of reactive and non-reactive dynamics in liquids and their statistical mechanical (time-dependent) interpretations; confinement effects

4. Concept of friction, diffusive motions and experimental realizations

5. Heterogeneity (spatial and temporal) in liquids and its relation to non-hydrodynamic behavior: reflections from experiments, simulations and theory.

CB 635: NON-EQUILIBRIUM STATISTICAL MECHANICS

1. **Introduction to probability theory**: Gaussian distribution; Central limit theorem
2. **Stochastic Processes**: Transition Probability; Random Walk: Master Equation of diffusion over a lattice.
3. **Time dependent correlation function**: Properties, response function, Linear response and susceptibility with illustration via harmonic oscillators; Fluctuation-Dissipation theorem.
4. **Slow and fast degrees of freedom**: Illustration via damped harmonic oscillator; Langevin Equation of motion of Brownian particle and calculation of different correlation functions; Fokker-Planck and Smoluchowski approaches to dynamical processes and their solutions for simple problems.
5. **Phenomenological formulation** of equation of motion for conserved and non-conserved modes. Transport coefficient. Linearized hydrodynamics of simple fluids: diffusive and propagating modes.
6. **Dynamical systems:** Fixed points and bifurcations**.** Oscillatory chemical reactions and population dynamics in simple system; An introduction to nonlinear dynamics; nonlinear feedback systems and nonequilibrium steady state; reaction- diffusion systems; Pattern formation in nonlinear dynamical system with simple diffusion.

Reference Books:

- *Plischke and Bergerson, D. Chandler, D. McQuarrie, S. K. Ma (along with the textbook on Critical Phenomena), Chaikin and Lubensky, De Gennes (Scaling Concepts in Polymer), Hansen and McDonald, D. Forster, Boon and Yip.*
- *McQuarrie, Nonequilibrium systems*
- *R. Zwanzig, Nonequilibrium phenomena*
- *Nitzan, Chemical dynamics*
- *Epstein, Nonlinear dynamics and chaos in chemical systems van Kampen, Stochastic Processes*

CB 640: STUDY OF BIO-MACROMOLECULES

1. Basic structural biology: Building blocks of proteins, motifs of protein structures, theories of protein folding, basic concepts of experimental methods of structure determination, introduction to the central dogma of molecular biology, examples from enzyme catalysis and structure, membrane proteins, signal transduction, proteins of the immune system etc.
2. Structure prediction: Introduction to principles and methods for computational prediction and engineering of protein structures, methods to identify secondary structural elements, homology modeling, fold recognition and ab-initio approaches. Exercise: Visualization and analysis of protein structure (Tool: VMD/Pymol/Chimera etc), homology modeling (Tool: Modeler).
3. Docking: Introduction to computer aided drug designing, target identification and validation, lead optimization and validation, virtual screening. Exercise: molecular docking (Tool: Autodock).
4. Molecular mechanics and potential energy surface: Introduction to molecular mechanics, different types of interactions in polyatomic molecules, principles of development and validation of force fields (e.g. AMBER, CHARMM etc). Potential energy surface: Identification of stationary points, transition state search, energy optimization algorithm: steepest descent and conjugate gradient methods. (Tool: Gaussian, Gromacs).
5. Molecular dynamics simulation: Introduction, Integrators (Leapfrog and velocity Verlet algorithm), Potential truncation and shifted-force potentials, periodic boundary conditions, temperature and pressure control in molecular dynamics simulations, implicit and explicit solvation models. Basic analysis of molecular dynamics trajectories: radial distribution function, correlation functions etc (Tool: Gromacs).
6. Free energy calculation and enhanced sampling methods: Introduction to enhanced sampling methods and potential of mean force, umbrella sampling, metadynamics, replica exchange molecular dynamics. Binding free energy calculation using MM/PBSA and MM/GBSA methods. (Tools: Gromacs, Plumed, APBS etc).

Reference books:

- Understanding Molecular Simulation: From Algorithms to Applications by Daan Frenkel and Berend Smit
- Molecular Modelling: Principles and Applications by Andrew R. Leach
- Principles of Biochemistry by Lehninger

CB 641: SURFACES & INTERFACES

Introduction to Surface Science:

- Surface phenomena

- Adsorption, desorption, adsorption models

-Absorption vs. adsorption

-Special properties of surfaces and interfaces

-Electronic structure of surfaces – techniques for probing

Surface modification and its applications:

-Experimental characterization of surfaces

-Basic aspects of XPS, LEED, XAS, etc.

Nanoscale catalysis and applications

-Surface spectroscopy

-Microscopy tools for catalysis applications

-Catalysis at Nanoscale

-Surface science techniques at operando conditions

Books and References:

- 'Surface Science: An Introduction' by K. Oura, V.G. Lifshits, A.A. Saranin, A.V. Zotov and M. Katayama; Springer Science & Business Media, 2013.
- 'Physics of Surfaces and Interfaces' by Harald Ibach; Springer, 2006.
- 'Surfaces and Interfaces of Solid Materials' by Hans Luth; Springer, 2013.
- 'Heterogeneous Micro and Nanoscale Composites for the Catalysis of Organic Reactions' by Ali Maleki; Elsevier, 2021.
- 'Semiconductor Catalysis & Photocatalysis on the Nanoscale' by Olexsander L Stroyuk; Nova Science Publishers Inc; UK ed., 2011.

CB 691: PROJECT RESEARCH (SEMESTER – I)

CB 692: PROJECT RESEARCH (CONTINUED IN SEMESTER – II)

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