Ph.D. PROGRAMME IN PHYSICAL SCIENCES
COURSE STRUCTURE & SYLLABUS

List of courses approved by the University

Fifth Semester

Course No.	Course Title	L	T	P	C
PHY 501	Research Methodology	4	-	-	4
PHY 502	Review of the topical Research	4	-	-	4
PHY 503	Condensed Matter Physics	4	-	-	4
PHY 504	Computational Methods in Physics	3	1	-	4
PHY 505	Classical Mechanics & Electromagnetism	4	-	-	4
PHY 506	Quantum Physics (Formal)	4	-	-	4
PHY 507	Mathematical Methods - I	3	1	-	4
PHY 508	Numerical Methods	3	1	-	4
PHY 509	Relativity & Cosmology	4	-	-	4
PHY 510	Astrophysics	4	-	-	4
PHY 511	High Energy Astrophysics around compact stars	4	-	-	4
PHY 591	Project Research – Part I	-	-	8	8
	Total hours of contact per week	*16*			
	Total credits	*16*			

Sixth Semester

Course No.	Course Title	L	T	P	C
PHY 601	Advanced Condensed Matter Physics – Magnetism & Superconductivity	4	-	-	4
PHY 602	Advanced Condensed Matter Physics – Electronic Structure & Physics of Materials	4	-	-	4
PHY 603	Statistical Physics	3	1	-	4
PHY 604	Quantum Physics (Application)	3	1	-	4
PHY 410/610	Non-Linear Dynamics	3	1	-	4
PHY 411/611	Optical Physics	3	1	-	4
PHY 413/613	Quantum Information Theory	3	1	-	4
PHY 414/614	Theory of Elementary Particles	3	1	-	4
PHY 415/615	Mesoscopic Physics	3	1	-	4
PHY 691	Project Research (Two semesters) – Part II	-	-	8	8
	Total hours of contact per week	*16*			
	Total credits	*16*			

* The syllabi of the courses starting with Course Code No. 4XX are available in IPhD Course Curriculum. The syllabi for Courses with Code No. 6XX will include the syllabi of Courses with Code No. 4XX plus additional special/advanced topics that will be decided by the concerned teachers.

BISWAJIT CHAKRABORTY
PROFESSOR & DEAN (ACADEMIC PROGRAMME)
S N BOSE NATIONAL CENTRE FOR BASIC SCIENCES

COURSE DESCRIPTION IN OUTLINE

Fifth Semester Syllabus

PHY 501 RESEARCH METHODOLOGY: 4-0-0-4

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.

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

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.

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.

5. Formulation of a Research Problem: Motivation, Induction, Hypothesis, Deduction, Observation and Conclusion

6. Scientific Reporting of Data/Observation/Prediction; Difference between Magazine or Newspaper Reporting, and Science Journal Reporting; Expression Skill Development and Nurturing.

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.

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.

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).

PHY 502 REVIEW OF THE TOPICAL RESEARCH: 4-0-0-4

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 503 CONDENSED MATTER PHYSICS: 4-0-0-4

- 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.

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 504 COMPUTATIONAL METHODS IN PHYSICS: 3-1-0-4

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 505 CLASSICAL MECHANICS & ELECTROMAGNETISM: 4-0-0-4

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.

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

PHY 506 QUANTUM PHYSICS (FORMAL): 4-0-0-4

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 507 MATHEMATICAL METHODS – I: 3-1-0-4

- 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.

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 508 NUMERICAL METHODS: 3-1-0-4

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.

1. Programming in FORTRAN by Rajaraman.
2. Numerical Recipe by Press, Shapiro and Teukolski
3. Numerical methods for Scientists and Engineers by HM Antia

PHY 509 RELATIVITY & COSMOLOGY: 4-0-0-4

The Equivalence Principle: Non-Inertial frames and non-Euclidean Geometry, General Coordinate transformations and the general covariance of physical laws.
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, rasing 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 survature tensor, Bianchi Identities, Isometries and Killing Vectors.
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, Gravitaional Waves, Gravitaional radiation. Principles of gravitational wave detectors – LISA, LIGO, VIRGO
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.
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 and Dark energy: need for them and possible models.

1. *Relativity: special, general, and cosmological, W. Rindler*
2. ***General Theory of Relativity: Robert Wald***
3. *Gravitation and cosmology: principles and applications of the general theory of relativity, S. Weinberg*
4. *Relevant reviews from current journals as reading matter*

PHY 510 ASTROPHYSICS: 4-0-0-4

Basic Background and Instrumentations: Elecmentary radiative transfer equations, absorption and emission, atomic processes, continuum and line emission, Optical and radio telescopes, Fourier Transform methods, detectors and image processing, Distance measurements in astronomy, Hubble's law, modern observational techniques.

Spectral Classifications of Stars: Saha's equation, Harvard system, Luminosity effect, Absolute and apparent luminosity relation, spectroscopic parallax

Evolution of Stars: Observational basis, protostars, disks, bipolar outflows, hydrostatic equilibrium, Sources of stellar energy, Gravitational Collapse, Fusion reactions (p-p) chain, CNO Cycle, triple alpha reactions, formation of heavy elements, Hertzsprung-Russell diagram, evolution of lowmass and high mass stars, Chandrasekhar limit, Pulsars, neutron stars and black holes

The Sun: Different layers of the Sun and their properties, Solar cycles, sunspots, solar corona and solar winds, expected and observed solar neutrino spectra, Possible resolution of the solar neutrino problem.

Binary Stars: Different types of binary stars, Importance of binary systems, Accretion, spectral properties of radiations from accretion flows and identification of black holes and neutron stars.

Galaxies: Formations and classification, Density Wave Theory of the formation of spiral arms, Rotation curves, missing mass and dark matter, Quasars and active galactic nuclei magnetic fields in the galaxy.

Cosmic Rays: Extensive air shower and Fermi's theory of high energy cosmic rays; Interaction of high energy cosmic rays with the CMBR background and the GZK cutoff, Cosmic ray experiments like HiRes, AGASA, Pierre Augur Observatory.

1. *M. Zeilik and S.A. Gregory, Introductory Astronomy and Astrophysics*
2. *B. Basu, An Introduction to Astrophysics*
3. *Radiative processes in Astrophysics: G. Rybicki and A. Lightman*
4. *Accretion Power in Astrophysics, J. Frank*
5. *Physics of Astrophysics – F. Shu*
6. *General relativity with Application to Astrophysics: N. Straumann*

PHY 511 HIGH ENERGY ASTROPHYSICS AROUND COMPACT STARS: 4-0-0-4

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

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

PHY 591 PROJECT RESEARCH – PART I

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

Sixth Semester Syllabus

PHY 601 ADVANCED CONDENSED MATTER PHYSICS – MAGNETISM & SUPERCONDUCTIVITY: 4-0-0-4

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.

(i) "Theory of Superconductivity" by J.R. Schrieffer.
(ii) "Solid State Physics" by N. Ashcroft and N.D. Mermin.
(iii) "Introduction to Solid State Physics" by C. Kittel.
(iv) "Quantum Theory of Solids" by C. Kittel.
(v) "Quantum Theory of Many Particle Systems" by G.D. Mahan.
(vi) "Elementary Excitations" by D. Pines

PHY 602 ADVANCED CONDENSED MATTER PHYSICS – ELECTRONIC STRUCTURE & PHYSICS OF MATERIALS: 4-0-0-4

- **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: V2O3, RNiO3, NiS etc
- Filling control M-I transition systems: R_{1-x}A_{x}Ti(V)O3
- High Tc super-conducting cuprates
- Quasi one-dimensional systems: Cu-O chain & ladder compounds
- Double-exchange systems: R_{1-x}A_{x}MnO3

D. DISORDER INDUCED INSULATORS
- Anderson Localization
- Scaling theory
- Electron-electron interaction & disorder

References:

1. Patrik Fazekas -- Lecture notes on Electron Correlation & Magn.
2. Imada, Fujimori, Tokura -- Metal-Insulator Transitions, Review. Mod. Phys. vol 70, pg 1039 (1998)
3. P.A. Lee & T.V. Ramakrishnan -- Disordered electronic system, Review. Mod. Phys. vol 57, pg 287 (1985)
4. 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 groundstate
- 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

1. Ashcroft & Mermin -- Solid State Physics
2. Grosso & Pastore-Parravicini -- Solid State Theory
3. Kaxiras -- Electronic Structure of Solids
4. Sutton -- Electronic Structure of Materials
5. Fulde -- Electron correlation in Molecules and Solids

PHY 603 STATISTICAL PHYSICS: 3-1-0-4

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

PHY 604 QUANTUM PHYSICS (APPLICATION): 3-1-0-4

Applications of quantum mechanics to atomic physics, condensed matter physics and nuclear physics.

PHY 691 PROJECT RESEARCH – PART II

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

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Ph.D. PROGRAMME IN CHEMICAL SCIENCES

DEPARTMENT OF CHEMICAL, BIOLOGICAL & MACROMOLECULAR SCIENCE (CBMS)

COURSE STRUCTURE & SYLLABUS

The current syllabus and the course structure aim at training students in different areas of frontier research leading to Ph.D. degrees keeping in mind the different academic backgrounds of the students. With this end in view the CBMS Department, SNBNCBS includes the detailed Syllabus prepared and approved in 2005 for training the Post B.Sc. Integrated Ph.D. students in Chemical Sciences. In addition to this, a few more advanced courses have been included. Every semester from this syllabus, the Departmental Faculty Committee shall announce the Courses typically suitable to the new intake of students.

[Semester I & II – Fall (August – December) & Spring (January – May)]

[L – Lecture; T – Tutorial; P – Practical; C - Credit]

Course Code	Course Title	L	T	P	C
CB 521	Numerical Methods	3	1	0	4
CB 522	Condensed Matter Theory	3	1	0	4
CB 523	Advanced Equilibrium Statistical Mechanics	3	1	0	4
CB 524	Physical Chemistry: Experiments & Theory	3	1	0	4
CB 525	Instrumental Methods of Analysis	3	1	0	4
CB 526	Fundamentals of Biophysics	3	1	0	4
CB 527	Molecular Physics and Spectroscopy	3	1	0	4
CB 528	Stochastic Processes in Physics and Chemistry	3	1	0	4
CB 529	Dynamics near and far away from Equilibrium Systems	3	1	0	4
CB 530	Mathematical Methods	3	1	0	4
CB 531	Advanced Numerical Methods & Simulation	3	1	0	4
CB 532	Chemical Dynamics	3	1	0	4
CB 533	Liquids	3	1	0	4

CB 534	Quantum Statistical Process in Dynamics	3	1	0	4
CB 535	Non-equilibrium Statistical Mechanics	3	1	0	4
CB 536	Mesoscopic Physics	3	1	0	4
CB 537	Classical & Quantum Stochastic Process	3	1	0	4
CB 538	Nonlinear Spectroscopy	3	1	0	4
CB 539	Radiation Matter Interaction	3	1	0	4
CB 540	Study of Bio-Macromolecules	3	1	0	4
CB 591	Project Research (Semester – I)	8	8	-	-
CB 592	Project Research (Continued in Semester – II)	8	8	-	-
	Total hours of contact per week	*16*			
	Total credits	*16*			

Fifth Semester Syllabus

COURSE DESCRIPTION IN OUTLINE

CB 521: 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:

1. Programming in FORTRAN by Rajaraman.
2. Numerical methods by Sujit Kumar Bose.

CB 522: 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:

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

CB 523: 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:

1. Equilibrium Statistical Mechanics by Plischke & Bergerson.
2. Theory of Simple Liquids by Hansen and McDonald
3. Complete Simulation of Liquids by Allen & Tildesley

CB 524: 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 CO_2.

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:

1. *J. I. Steinfeild, J. S. Francisco and W. L. Hase,* ***Chemical Kinetics and Dynamics****, Englewood Cliffs, NJ: Prentice Hall, 1989*
2. *R. D. Levine and R. B. Bernstein,* ***Molecular Reaction Dynamics and Chemical Reactivity****. New York: Oxford Univ. Press, 1987.*
3. *R. B. Bernstein,* ***Chemical Dynamics via Molecular Beam and Laser Techniques****. New York: Oxford Univ. Press, 1982.*
4. *I. H. Seagal,* ***Enzyme Kinetics****. New York: Wiley-Interscience, 1975*
5. *R. A. Alberty and R. J. Silbey,* ***Physical Chemistry****. John Wiley and Sons*
6. *P. W. Atkins,* ***Physical Chemistry****, 5th Edition. ELBS with Oxford Univ. Press.*
7. *A. H. Zewail,* ***Science****, volm. 242, 1645 (1988).*
8. *G. R. Fleming and P. G. Wolynes,* ***Phys. Today****, volm.43, 36 (1990)*
9. *H. A. Kramers,* ***Physica****, volm.7, 284 (1940).*
10. *R. F. Grote & J. T. Hynes,* ***J. Chem. Phys****. Volm.73, 2715 (1980).*
11. *M. Maroncelli, J. McInnis, G. R. Fleming,* ***Science****, volm.243, 1674, (1989); Jimenez et al.,* ***Nature****, volm. 369, 471, (1994).*
12. *M. Gavrilla (Ed.),* ***Atoms in Intense Laser Fields****, Academic Press*

CB 525: 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:

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

CB 526: 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:

1. Biochemistry by Donald Voet and Judith G. Voet
2. Protein Structure and Function by George A. Petsko
3. Principles of Fluorescence Spectroscopy by J. Lakowicz

CB 527: 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:

1. Nitzan, Chemical Dynamics
2. Szabo and Oslund, Quantum Chemistry
3. May and Kuhn, Energy transfer and electron transfer
4. Louisell, Quantum Statistical Properties of Radiation
5. Mukamel, Principles of nonlinear spectroscopy

CB 528: STOCHASTIC PROCESSES IN PHYSICS AND CHEMISTRY

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.

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:

1. David Chandler, Nonequilibrium systems
2. Van Kampen, Stochastic Processes
3. Zwanzig, Nonequilibrium phenomena
4. Nitzan, Chemical dynamics
5. Hangii, etal, Review of Modern Physics, 1990, Fifty years after Kramers Theory

CB 529: 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:

1. *McQuarrie, Nonequilibrium systems*
2. *R. Zwanzig, Nonequilibrium phenomena*
3. *Nitzan, Chemical dynamics*
4. *Epstein, Nonlinear dynamics and chaos in chemical systems*
5. *van Kampen, Stochastic Processes*

CB 530: 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 532: CHEMICAL DYNAMICS

1. 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.

2. 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.

3. 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.

4. 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.

References and Books:

*1. J. I. Steinfeild, J. S. Francisco and W. L. Hase, **Chemical Kinetics and Dynamics**, Englewood Cliffs, NJ: Prentice Hall, 1989*
*2. R. D. Levine and R. B. Bernstein, **Molecular Reaction Dynamics and Chemical Reactivity**. New York: Oxford Univ. Press, 1987.*
*3. R. B. Bernstein, **Chemical Dynamics via Molecular Beam and Laser Techniques**. New York: Oxford Univ. Press, 1982.*
*4. I. H. Seagal, **Enzyme Kinetics**. New York: Wiley-Interscience, 1975.*
*5. R. A. Alberty and R. J. Silbey, **Physical Chemistry**. John Wiley and Sons*
*6. P. W. Atkins, **Physical Chemistry**, 5th Edition. ELBS with Oxford Univ. Press.*
*7. A. H. Zewail, **Science**, volm. 242, 1645 (1988).*
*8. G. R. Fleming and P. G. Wolynes, **Phys. Today**, volm.43, 36 (1990)*
*9. H. A. Kramers, **Physica**, volm.7, 284 (1940).*
*10. . R. F. Grote & J. T. Hynes, **J. Chem. Phys**. Volm.73, 2715 (1980).*
*11. M. Maroncelli, J. McInnis, G. R. Fleming, **Science**, volm.243, 1674, (1989); Jimenez et al., **Nature**, volm. 369, 471, (1994).*
*12. M. Gavrilla (Ed.), **Atoms in Intense Laser Fields**, Academic Press*

CB 533: 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 535: NON-EQUILIBRIUM STATISTICAL MECHANICS

1. Stochastic Processes and Transition Probability; Random Walk: Master Equation of diffusion over a lattice; Time dependent correlation function, response function, Linear

response and susceptibility with illustration via harmonic oscillators; Fluctuation-Dissipation theorem.

2. Slow and fast degrees of freedom: Illustration via damped harmonic oscillator; Elementary idea of elimination of fast degree of freedom and noise; Langevin Equation of motion of Brownian particle and calculation of different correlation functions; Over damped dynamics with illustration from the Rouse Model of polymer chain.

3. Phenomenological formulation of equation of motion for conserved and nonconserved modes (model A and model B). Transport coefficient. Linearised hydrodynamics of simple fluids: diffusive and propagating modes.

References

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.

CB 540: STUDY OF BIO-MACROMOLECULES

The course content includes the following topics:

a. Introduction to macromolecules
1. Amino Acids and their structures
2. Nucleotides and their structures
3. Proteins
4. Nucleic acids

b. Biophysical characterization of macromolecules
1. Optical Spectroscopy
2. Fluorescence Spectroscopy
3. Mass Spectrometry
4. NMR Spectroscopy

c. Structural characterization of macromolecules
1. X-ray Crystallography
2. NMR Spectroscopy
3. Mass Spectrometry

d. Biochemical Studies of macromolecules
1. Protein Folding
2. Genetic Modification and oxidative stress
3. Role of water in biomolecules
4. Enzymes: polymerase, nuclease etc.

Reference books:

1. *Proteins: Structures and Molecular Properties by Thomas E. Creighton*
2. *Introduction to protein structure: Branden and Tooze*
3. *Crystallography made crystal clear: Gale Rhodes*
4. *Principles of nucleic acid structure: Stephen Neidle*
5. *Structure and Mechanism in Protein Science: A guide to enzyme catalysis and protein folding: Alan Fersht*

CB 591: PROJECT RESEARCH (SEMESTER – I)

CB 592: PROJECT RESEARCH (CONTINUED IN SEMESTER – II)

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