Ph.D. COURSE WORK

Ph.D. students at SNBNCBS are required to do course work 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

Course Work: Credit Requirements, number, duration, syllabus, minimum standards for completion, etc.

6.1. The credit assigned to the Ph.D. course work shall be a minimum of 08 credits and a maximum of 16 credits.

6.2. The course work shall be treated as 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.

6.3. All candidates admitted to the Ph.D. programme shall be required to complete the course work as advised by their supervisors during the initial one or two semesters.

6.4. 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 Course Work – 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 atleast 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 in our website from time to time.

Ph.D. PROGRAMME IN CHEMICAL SCIENCES

COURSE STRUCTURE & SYLLABUS

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 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*			

COURSE DESCRIPTION IN OUTLINE

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:

1. Programming in FORTRAN by Rajaraman.
2. 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:

1. Solid state phyics by Ashcroft-Mermin
2. 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:

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 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 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 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:

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 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:

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 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:

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 628: 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 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:

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 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:

1. H. Eyring, SH Lin and SM Lin, Basic Chemical Kinetics
2. T Palmer and P L Bonner, Enzymes: Biochemistry, Biotechnology, clinical chemistry
3. R. D. Levine and R. B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity. New York: Oxford Univ. Press, 1987.
4. David Chandler, Nonequilibrium systems
5. N G Van Kampen, Stochastic Processes
6. Zwanzig, Nonequilibrium phenomena
7. Nitzan, Chemical dynamics
8. I. R. Epstein: An Introduction to Nonlinear Chemical Dynamics: Oscillations, Waves, Patterns, and Chaos
9. 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:

1. *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.*
2. *McQuarrie, Nonequilibrium systems*
3. *R. Zwanzig, Nonequilibrium phenomena*
4. *Nitzan, Chemical dynamics*
5. *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 modelling, fold recognition and ab-initio approaches. Exercise: Visualisation and analysis of protein structure (Tool: VMD/Pymol/Chimera etc), homology modelling (Tool: Modeller).
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 (Leap frog 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:

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

CB 691: PROJECT RESEARCH (SEMESTER – I)

CB 692: PROJECT RESEARCH (CONTINUED IN SEMESTER – II

AMITABHA LAHIRI
SENIOR PROFESSOR & DEAN (ACADEMIC PROGRAMME)
S N BOSE NATIONAL CENTRE FOR BASIC SCIENCES