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 CO_2.

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.

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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)

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