An Integrated Post-B. Sc. Ph. D. Program in Chemical Sciences

2005

Jointly Conducted By

S. N. Bose National Centre for Basic Sciences, Kolkata

And

Indian Association for the Cultivation of Science, Kolkata

INTRODUCTION

In an unusual development in interinstitutional scientific collaboration in our country, S. N. Bose National Centre for Basic Sciences (SNBNCBS) and the Indian Association for the Cultivation of Science (IACS) will jointly run a Post B. Sc. integrated Ph. D. program in Chemical Sciences, starting from the academic session 2005-2006. The program will be multidisciplinary, including not only the traditional branches of chemistry, like inorganic chemistry, organic chemistry and physical chemistry, but will also have wide coverage of the areas like material sciences, molecular biology, biochemistry, bio-informatics along with other areas of science, namely, physics, mathematics, electronics and scientific computation. The present day scientific activities are advancing in a direction that needs simultaneous familiarity of the researchers with different disciplines of science like physics, chemistry, biology, mathematics and computation. In this broad perspective, it is hoped that the students trained in this integrated program will become researchers and scientists with broad, dynamic and integrated minds, with diverse capabilities to pursue research in any direction so that they can lead the upcoming researches at an international level.

The program is meant for the students after their Bachelor's degree, especially for talented and motivated students who wish to pursue a career in research and development in the areas of science and technology having multidisciplinary character. Admission to the course would be based on a written examination, followed by an oral examination of the short-listed candidates. The entire entrance test will be jointly conducted by SNBNCBS and IACS. The program begins with 4 semesters of a two-year M. Sc., each semester comprising 18 weeks. After successful completion of these four semesters, the students will receive an M. Sc. degree in Chemical Sciences, provided they attain the eligibility criteria. Students with Chemistry, Physics and Mathematics at the B. Sc. level would be eligible to compete. They will be provided with a scholarship from the very beginning, up to the completion of Ph.D.

The program should develop strong intellectual and manual skills in the students. Great care would be taken in designing the laboratory courses. Student initiatives would be an essential part of the learning process. Consequently, the total number of students needs to be restricted to 15 every year. A teaching laboratory would be set up to accommodate 30 students so that the first year and second year M. Sc, students can work together. However, considering the practical constraints, admission will be restricted to only 10 students in the first year.

The required funding for the course including student scholarships and running costs will be equally shared by SNBNCBS and IACS. Although the program will be conducted jointly by SNBNCBS and IACS, it will be a multi-institutional one with faculty members drawn from several institutions, even outside Calcutta. A major part of the teaching program will be shared between SNBNCBS and IACS.

It is hoped that the program would complement the traditional university system of education and revitalize chemical sciences, giving a boost to multidisciplinary research in our country.

Course Structure for M.Sc.

First Year

Semester I

Course Number	Course Title	L+T - P
CH411	Mathematical Methods	3 - 0
CH412	Quantum Chemistry	3 - 0
CH413	Equilibrium and Non-Equilibrium Thermodynamics	3 - 0
CH414	Organic Chemistry: Structure & Dynamics	3 - 0
CH415	Inorganic Chemistry I	3 - 0
CH416	Electronics & Instrumentation	1 - 3
CH 417	Laboratory	1 - 4
	Total Contact Hours per week	24
	Total Credits	24

Semester II

Course Number	Course Title	L+T - P
CH421	Symmetry in Chemistry	3 - 0
CH422	Elements of Chemical Biology	3 - 0
CH423	Molecular Structure and Dynamics by Single and Multi-photon Spectroscopy I	3 - 0
CH424	Inorganic Chemistry II	3 - 0
CH425	Synthetic and Biological Chemistry	3 - 0
CH426	Numerical Methods and Computer Programming	2 - 2
CH 427	Laboratory	1 - 4
	Total Contact Hours per week	24
	Total Credits	24

Notes:

1. "L+T" means 3 hours of lecture are followed by 1 hour of tutorial
2. "P" means practicals
3. For every course, course credits are equal to the number of contact hours per week

Second Year

Semester III

Course Number	Course Title	L+T - P
CH511	Equilibrium & Non-Equilibrium Statistical Mechanics	3 - 0
CH512	Chemical Dynamics of Atoms, Molecules and Soft Condensed Matter	3 - 0
CH513	Molecular Structure and Dynamics by Single and Multi-photon Spectroscopy II	3 - 0
CH514	Elective I	3 - 0
CH515	Elective II	3 - 0
CH516	Research Project (With Seminar)	0 - 12
	Total Contact Hours per week	27
	Total Credits	27

Semester IV

Course Number	Course Title	L+T - P
CH521	Chemistry and Physics of Materials	3 - 0
CH522	Equilibrium and Non-Equilibrium Electrochemistry	3 - 0
CH523	Elective III	3 - 0
CH524	Elective IV	3 - 0
CH525	Research Project Continued (With seminar)	0 - 16
	Total Contact Hours per week	28
	Total Credits	28

Suggested Electives:

1. Electronic Structure and Properties of Materials
2. Chemistry and Physics of Polymers
3. Small Scales in Space and Time
4. Structure, Properties and Design of Drugs
5. Structure, Folding and Function of Proteins
6. Electrochemical Technology
7. Bioinformatics in Chemistry
8. Advanced Quantum Chemistry
9. Advanced Numerical Methods

   Etc.

New electives may come in from year to year. Each elective would have a package of courses to choose from.

COURSE CONTENTS

FIRST YEAR : SEMESTER I

CH 411: Mathematical Methods

Ch-1:(3 Lectures) Function: functions, limits, continuity, Integral and differential calculus of one and two variables, Mean Value Theorems, Improper Integrals, Convergence of Integrals.

Ch-2:(4) Infinite series and sequences: convergence and divergence of infinite series, Tests of convergence, alternate series, Taylor series and application, Asymptotic expansion and application, Fourier sine and cosine series and applications,

Ch-3:(2) Functions defined as integrals: Gamma, Beta and error functions, exponetial integrals, elliptic integrals, Dirac delta functions

Ch-4:(4) Linear algebra and Vector spaces: Matrices, Rank of a Matrix, Complex Inner Product Spaces, Orthogonal and Unitary Transformations, Eigenvalues and Eigenvectors and application, Change of Basis, Diagonalization of Matrices.

Ch-5:(5) Complex variables: Limits, continuity, Differentiations, Cauchy-Reimann equations, Complex integrations, Residues and Cauchy residue theorem. Laplace inversion, Evaluation of real, definite integrals,

Ch-6:(4) Differential equation: Methods of solution, Laplace transformation method, Power series method, Fourier expansion methods.

Ch-7:(3) Orthogonal polynomials: Orthogonal polynomials, Legendre and Hermite polynomials, Sturm-Liouville Theory, Eigenfunction Expansions.

Ch-8:(4) Partial differential equation: Examples, chain rule, Laplace equation in Cartesian and polar form, one and two dimensional wave equations, Heat equations,

Ch-9:(4) Vectors: Definitions, dot product, cross product, vector fields, Differentiation, line integrals, surface integrals, Divergence Theorem, Stokes Theorem, Tensors(qualitative concepts), summation convention and co-ordinate transformation.

Ch-10:(4) Nonlinear Differential equations: Phase plane, fixed points, linear stability analysis, vanderPol oscillator and limit cycle, Population dynamics.

Ch-11:(3) Probability and Statistics: Laws of probability: compound events, mutually exclusive events and statistically independent events. Mean and standard deviation of Binomial distribution, Poisson distribution and Gaussian distribution.

Ch-12:(2) Curvilinear Coordinates: Plane Polar Coordinates, Vectors in Plane Polar Coordinates, Cylindrical Coordinates, Spherical Coordinates, Curvilinear Coordinates.

Reference Books:

1. Applied Mathematics for Scientist and Engineers, Pipes and Harvill, MCGraw Hill, 1971

2. Mathematical Methods for Scientists and Engineers, D. A. McQuarrie University of California, Davis

3. Mathematical methods for Physicist, Arfken and Weber, Academic, 1995

4. Advanced Engineering Mathematics, Kreyszig (Wiley).

5. Methods of Mathematical Physics, Courant and Hilbert Wiley, 1989.

CH 412 Quantum Chemistry

Sequence of events/phenomena which establish that (i) both radiation and matter have wave-particle duality and (ii) physical variables can be discrete/quantized.

Elementary classical mechanics, using linear harmonic oscillator(LHO) as an example. Trajectories in configuration space and phase space. Lagrange's and Hamilton's equations of motion. Poisson's bracket.

Classical wave equation. Plane-wave solutions. De Broglie matter waves.

Operators. Linear Operators. The eigenvalue problem; occurrence of quantization, bounded and unbounded systems, discrete and continuous eigenvalue spectra.

Commutation relations, commuting and non-commuting operators, eigenfunctions.

Probability distribution(weighting function) and expectation value.

Operations of observation and their properties; parallelism with commuting/non-commuting eigenoperators. "Small" and "large" systems; origin of uncertainty and connection to commutation relations.

Postulates of quantum mechanics and their interpretations. Schroedinger equation and various interpretations of equation, energy spectrum, wave functions(Hilbert space), operators and Dirac notation(vectorial analogy). Hermitian operators. Acceptability conditions restricting energy values. Proof of Uncertainty Principle. Parity of eigenfunctions.Madelung- De Broglie fluid-dynamical interpretation. Brief discussion on alternative ways of obtaining Schroedinger equation(classical wave equation, action principle, Brownian motion, etc). Ehrenfest theorem. Heisenberg equation of motion.

Applications to one-, two- and three-dimensional systems, degeneracy, Jahn-Teller effect. LHO(in terms of ladder/creation-annihilation operators), rigid rotor(including electron in a ring), hydrogen atom(ladder operators). One-dimensional periodic potential; Bloch theorem, band structure.

Angular momentum in quantum mechanics in terms of ladder operators. Electron spin; Pauli spin matrices. Spin and magnetic field. Exchange; Slater determinant. Spin-orbit coupling. Spectral term symbols.

Approximate methods : Time-independent and time-dependent perturbation theories ; their applications. The variation principle for ground and excited states. Linear variation method and its applications : MO theory, VB theory, Hueckel MO theory; Hartree, Hartree-Fock and Hartree-Fock-Roothaan methods. Electron correlation. Configuration interaction; natural orbitals. Born-Oppenheimer approximation. Semi-empirical methods.

Electron density. Density matrices; exchange-correlation hole. Virial and Hellmann-Feynman theorems. Force concept in chemistry. Electrostatic potential and its significance in quantum biochemistry/pharmacology.

Elementary introductions to density functional theory(including Thomas-Fermi-Dirac-Weizsaecker theory), coupled cluster theory, Moeller-Plesset perturbation theory.

Brief introduction to time-dependent quantum mechanics; time-dependent variation principle.

Suggested Books

1. I. N. Levine, Quantum Chemistry, Prentice-Hall-India.
2. D.W. McQuarrie, Quantum Chemistry, Oxford University Press.
3. P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press.
4. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover.
5. F. L. Pilar, Elementary Quantum Chemistry, McGraw-Hill (1968).
6. R. McWeeny and B.T. Sutcliffe, Methods of Molecular Quantum Mechanics, Academic Press.

7. P. W. Atkins, Quanta : A Handbook of Concepts, Oxford University Press.

8. G. C. Schatz and M.A. Ratner, Quantum Mechanics in Chemistry, Prentice Hall.

9. F. Schwabl, Quantum Mechanics, Narosa Publishing House

10. L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Butterworth-Heinemann.

Etc.

CH 413: Equilibrium and Non- equilibrium Thermodynamics

A. Equilibrium Thermodynamics

1. Concept of thermodynamic equilibrium: Thermal, Mechanical and Chemical Equilibrium (3 lectures)
2. Formal relationships: Euler equation; Gibbs-Duhem relation (2 lectures)
3. Maximum work Theorem: Maximum Entropy an Minimum Energy principle; Legendre transformation and thermodynamic potentials; Minimum principles of potential (6 lectures)
4. The Maxwell relations and simple applications (2 lectures)
5. Stability condition for thermodynamic potential (2 lectures)
6. First order phase transition; Clausius-Clapayron equation; Gibbs Phase rule (3 lectures)
7. Thermodynamics in the neighborhood of the critical point with emphasis on scaling and universality (3 lectures)
8. Thermodynamics of small systems: Emphasis on interfacial energy (NVT ensemble) (2 lectures)

Books:

1. H. B. Callen, ***Thermodynamics & Introduction to Thermostatistics***
2. T. C. Hill, ***Thermodynamics of small systems***
3. K. G. Denbigh, ***Principles of Equilibrium Thermodynamics***

B. Non-Equilibrium Thermodynamics

1. Conservation laws; entropy production and 2nd law of thermodynamics (3 lectures)
2. Flux and thermodynamic force; Phenomenological equations; Onsager's reciprocal relations (4 lectures)
3. Stationary states; states with minimum entropy production; Glansdorf-Prigogine inequality (3 lectures)
4. Boltzmann equation, hydrodynamics, H-theorem (2 lectures)
5. Applications: Unimolecular reactions; Ion transport in Biological systems; spinodal decomposition (3 lectures)
6. Bifurcation and symmetry breaking: Turing pattern in autocatalytic systems; Brusselator; Predator-prey model; morphogenesis (4 lectures)

Books & References:

1. S. R. de Groot and P. Mazur, ***Non-equilibrium Thermodynamics***
2. I. Prigogine, ***Introduction to thermodynamics of irreversible processes***, Interscience Publishers; 2d, rev. ed edition (1961)
3. I. Prigogine, ***From Being to Becoming: Time and complexity in the physical sciences***, Freeman, San Francisco, 1980.
4. D. Mcquarrie, ***Statistical Mechanics***, Harper, NY, 1976.
5. H.J. Kreuzer, ***Nonequilibrium Thermodynamics and its Statistical Foundations***, Clarendon, 1981, Oxford
6. D Avnir, ***Fractal Approach to Heterogeneous Chemistry: Surfaces Colloids and Polymers***, John Wiley & Sons, NY, 1989.
7. J Keizer, ***Statistical Thermodynamics of Nonequilibrium Processes***, Springer-Verlag, Berlin, 1987.

CH 414: Organic Chemistry: Structure and Dynamics

1. **Orbital Symmetry and Reaction Mechanism** **(12 L + 5 T)**

   Molecular orbitals (σ and π systems); Frontier orbital analysis of ionic reactions; Classification, characteristics and stereochemical outcome of pericyclic reactions - rationalisation using orbital symmetry principles

2. **Stereochemistry: Static and Dynamic Aspects** **(10 L + 3 T)**

   Symmetry and point groups; Stereocentre and stereoaxis configuration; Topicity; Conformational analysis; Conformation and reactivity

3. **Organic Spectroscopy** **(10 L + 3 T)**

   Nuclear magnetic resonance (NMR) and mass spectrometry (MS) - principles and applications; Applications of UV, IR, NMR and MS to structural and mechanistic problems

4. **Organic Photochemistry** **(5 L + 2 T)**

   Principles and reactions - photolytic cleavage, photoreduction, photooxidation, photoaddition, photorearrangement

5. **Radical Reactions** **(5 L + 2 T)**

   Principles and formation of carbon-halogen, carbon-carbon, carbon-nitrogen and carbon-oxygen bonds

Suggested Reading

1. J. March, *Advanced Organic Chemistry*
2. F. A. Carey & R. J. Sundberg, *Advanced Organic Chemistry (Part A)*
3. J. Clayden, N. Greeves, S. Warren & P. Wothers, *Organic Chemistry*
4. R. O. C. Norman & J. M. Coxon, *Principles of Organic Synthesis*
5. I. Fleming, *Pericyclic Reactions* (Oxford Chemistry Primer)
6. R. B. Woodward & R. Hoffmann, *The Conservation of Orbital Symmetry*
7. T. L. Gilchrist & R. C. Storr, *Organic Reactions and Orbital Symmetry*
8. D. Nasipuri, *Stereochemistry of Organic Compounds - Principles and Applications*
9. E. L. Eliel, S. H. Wilen & L. N. Mander, *Stereochemistry of Organic Compounds*
10. M. J. T. Robinson, *Organic Stereochemistry* (Oxford Chemistry Primer)
11. W. Kemp, *Organic Spectroscopy*
12. Silverstein & Schuster, *Spectrometric Identification of Organic Compounds (6^{th} Edn)*
13. J. W. Coxon & B. Halton, *Organic Photochemistry*
14. M. J. Perkins, *Radical Chemistry-The Fundamentals* (Oxford Chemistry Primer)

CH 415: Inorganic Chemistry- I

1. Periodicity- Trends in atomic size, ionization enthalpy, electronegativity, polarizability

2. Bonding models in inorganic chemistry- ionic and covalent bonds, VSEPR theory, The structure of solids; metals, insulators and semi-condutors

3. Acid- base concepts- Hard and soft acids and bases; non-aqueous solvents

4. Coordination chemistry- Bonding, spectra and magnetism

5. Lanthanides and actinides

6. Inorganic chains, rings and cages- Silicates; polyoxometallates; boron hydrides; carboranes; B-N, P-N and S-N rings

Text Books:

1. J.E.Huheey, E.A.Keiter and R.L.Keiter, "Inorganic Chemistry" 4 th Ed. Addison Wesley, 1993

2. D.F.Shriver and P.W.Atkins, 'Inorganic Chemistry ", 3 rd Ed ,OUP,

3. G.Wulfsberg, "Inorganic Chemistry", University Science Books, CA, U.S.A, Indian Ed. Viva Books, New Delhi, 2002

Reference books:

1. N.N.Greenwood and A.Earnshaw, "Chemistry of the Elements", Pergamon, 1997

2. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, " Advanced Inorganic Chemistry", 6 th Ed, John- Wiley, 1999

CH 416: Electronics and Instrumentation

1. **Measurement of Thevenin parameters (V_{TH} and R_{TH}) of a DC power supply (Battery).**
   - A. Plot V_{load} versus R_{load} curve and mark slope and stiff regions.
   - B. In the slope region measure V_{load} for at least two different R_{load} and characterize V_{TH} and R_{TH}.
   - C. In the stiff region measure I_{Load} for at least two different R_{Load} and characterize V_{TH} and R_{TH}.
   - D. 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 rectifier.**
   - A. Draw three characterization curves of two rectifier diodes (Germanium, Silicon) and one Zener diode.
   - B. Estimate turn ratio of a transformer by measuring voltage ratio (primary and secondary).
   - C. Construct a Full wave rectifier and measure input and output waveforms of the rectifier.

3. **Characterization of a Zener Regulated DC power supply.**
   - A. Measure V_C, V_{rms}, γ and PIV of a full wave rectifier and compare them with their calculated values.
   - B. Design a R-C filter and measure p-p ripple voltage and compare with calculated value.
   - C. 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.**
   - A. Draw base and collector characteristic curves of an n-p-n transistor in the CE configuration.

B. Mark saturation, cutoff and active regions and determine Q point for best transistor operation.
C. 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 electronic switch and designing a memory unit (R-S flip flop).**
    A. Use a transistor as a switch to operate a LED in the output with low frequency input.
    B. By using high frequency square wave input measure t_{on} and t_{off}.
    C. 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. **A Brief introduction to the DIGITAL ELECTRONICS would be given after completion of the above experimentations.**

List of Suggested Text Books:

1. Malvino "Electronic Principles" (Sixth Edition; Tata McGraw Hill)
2. R. A. Gayakwad "Op-Amps and Linear Integrated Circuits" (Third Edition; EEE)
3. Malvino "Digital Computer Electronics" (Second Edition; Tata McGraw Hill)
4. R. P. Jain "Modern Digital Electronics" (Tata McGraw Hill)
5. Jacob Millman, Christos C. Halkias "Integrated Electronics: Analog and Digital Circuits and Systems" (McGraw-Hill)

CH 417: Laboratory

- Experiments will be chosen from Chemistry, Physics and Biology and should be interdisciplinary in nature
- Experiments may vary from year to year depending upon the interests of the students and expertise of the instructor

COURSE CONTENTS

FIRST YEAR : SEMESTER II

CH 421: Symmetry in Chemistry

Symmetry as a mathematical concept ; geometry, profile, connectivity, fractals, cellular automata.

Symmetry in chemical sciences explored through group theory and topology.

Significance of symmetry concepts in bringing about conceptual unification and universalization across microscopic, mesoscopic and macroscopic systems and phenomena. Linkages with quantum mechanics.

Elements of group theory in chemistry : Symmetry operations and their associated algebra. Dipole moment and optical activity. Group, subgroup, symmetric(permutation) group, simple group, semi-simple group, colour(magnetic/Shubnikov)group, point group, space group. Isomorphism and homomorphism. Properties of groups. Schoenflies notation for point groups. Hermann-Maugin notation for space groups. Generating elements of a group. Elementary theory of representations of groups; transformation operators, function spaces, invariant subspaces. Equivalent, reducible and irreducible representations. Character tables(grand orthogonality thorem, other theorems/relations involving irreducible representations and characters). The reduction of a representation; projection operators. Notations for character tables for point groups. Definition of an algebra. Direct product group; direct product representation. Representations and quantum mechanics. The vanishing of integrals. Applications of group theory to bonding, structure and reactivity as well as other properties : Symmetry-adapted MOs of small and medium-size molecules(e.g., benzene, MX_6, etc), Mulliken-Walsh correlation diagrams. Molecular vibrations(normal modes and normal coordinate analysis).“Proof”of Jahn-Teller theorem; first- and second-order Jahn-Teller effects. Selection rules for single- and two-photon spectroscopy of various types, intensity “borrowing”, magnetic dipole selection rules. Woodward-Hoffmann and FMO approaches to reactivity. Symmetry selection for transition states and reaction paths. Symmetry and other properties.

Elements of chemical topology : Topology of electron density, critical points, atoms in molecules. Graph theory and molecular descriptors of various kinds; their correlations with various properties and applications to the design of different types of materials, e.g., pesticides, catalysts, drugs,etc.

Fractals, deterministic chaos and their applications in chemistry, e.g., Brownian motion, electrolysis, heterogeneous catalysis, protein folding, reaction mechanisms. Applications of cellular automata in chemistry.

Suggested books :

1. D. M. Bishop, Group Theory in Chemistry, Dover.
2. F. A. Cotton, Chemical Applications of GroupTheory, John Wiley.
3. J. M. Hollas, Symmetry in Molecules, Chapman
4. I. Hargittai and M. Hargittai, Symmetry Through the Eyes of a Chemist, Plenum Press.
5. M. Tinkham, Group Theory and Quantum Mechanics, McGraw-Hill.
6. C. D. H. Chisholm, Group Theoretical Techniques in Quantum Chemistry, Academic Press.
7. M. Hamermesh, Group Theory and Its Applications to Physical Problems, Dover.
8. R. F. W. Bader, Atoms in Molecules, Oxford University Press.

9. A. T. Balaban (Editor), Chemical Applications of Graph Theory, Academic Press.

10. N. Trinajstic, Chemical Graph Theory, Vols. I and II, CRC Press.

11. J. Devillers and A.T. Balaban(Eitors), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach.

12. B. Mandelbrot, The Fractal Geometry of Nature, W.H. Freeman.

13. W. G. Rothschild, Fractals in Chemistry, John Wiley.

14. Willi-Hans Steeb, Nonlinear Workbook, World Scientific.

(This book connects cellular automata, neural networks, chaos, fractals,etc.).

CH422 Elements of Chemical Biology

Topics (Headings)	Topics (Description)
Chemical principles of life	1. Chemical principles that govern the processes driving living systems 2. Chemistry of carbohydrates, lipids and hormones 3. Chemistry of amino acids, peptides and proteins 4. Chemistry of Heterocycles: nucleosides, nucleotides and nucleic acids
Principles governing recognition and catalysis in biological systems	Enzyme action: transition state theory, examination of the kinetics of single and multi-substrate enzyme reactions, kinetics and mechanisms of reversible and irreversible inhibition with special reference to potent inhibitor design, allosterism.
Fundamentals of cell biology	1. Structure and function of cell organelles. 2. Modern aspects of molecular basis of cell function: cell migration, secretion, division and intercellular communication. 3. Metabolomics
Introduction to modern genetics	Basic concepts of genetics, in depth analysis of genetic mechanisms, genetic exchange, mutagenesis, chromosome mapping and introduction to Genomics
Macromolecular structure-function relationships	1. Structure of macromolecules: Proteins, DNA, RNA. 2. Methods of structure determination: CD-ORD, Fluorescence, X-ray crystallography, NMR. 3. Proteomics: Principles of Mass Spectrometry and its application in solving biological problems. 4. Introduction to Capillary electrophoresis, HPLC, 2D Gel electrophoresis.
Supramolecular assemblies	Chromosome structure and function, nucleosomes, ribosomes and biological membranes

Introduction to Molecular biology	1. Foundations of Molecular Biology. Replication: chemistry and topology, DNA recombination and DNA damage. 2. Transcription: mechanisms in prokaryotes and eukaryotes, RNA splicing, RNA editing and RNA interference. 3. Translation: protein biosynthesis, genetic code, gene expression and its regulation
Computation in biology	1. Applications of computer science in solving biological phenomena 2. Modeling of macromolecular structure, interactions and dynamics 3. Introduction to biocomputing algorithms and bioinformatics

Recommended books:

Biochemistry:
1. **Lehninger, Nelson, Cox**
2. **Voet, Voet**
3. **Stryer**

Biophysical Chemistry:
1. **Cantor, Schimmel**
2. **Tinoco, Wang**
3. **van Holde**

Molecular Biology of the Cell:
1. **Baltimore, Lodish, Darnell**
2. **Alberts**

Genetics:
1. **Suzuki**
2. **Russell**
3. **Gardener**
4. **T.A.Brown**

Enzymes:

Alan Fersht

CH423: Molecular Structure and Dynamics by Single & Multi-photon Spectroscopy I

1. **Rotational & Vibrational Spectroscopy:** Intensity & width of a spectral line (general features), electromagnetic spectrum and classification of spectral regions, experimental procedure (with a layout of a typical absorption /emission spectrometer), Beer-Lambert law, Einstein's coefficient of spontaneous emission, transition moments and selection rules (general discussion); types of rotors, Pure rotational spectra, rotational energy levels, Stark effect, Appearance of rotational spectra, Rotational Raman spectra, selection rules for rotational Raman spectra, Stokes, Anti-Stokes and Rayleigh lines.Selection rules for vibrational spectrum, determination of anharmonicity from Morse potential, Birge-Sponar extrapolation, vibration-rotaion spectra and spectral branches, Normal modes and vibrations in polyatomic molecules, appearance of vibrational spectrum (for example, absorption spectra of amino acids), exclusion rule and active modes. Depolarization and resonance Raman spectroscopy. Two and multi-photon spectroscopy: Coherent Anti-Stokes Raman Spectroscopy and Raman Echo experiments. Relation between Raman Echo & Nuclear Spin Echo Experiments. Applications of CARS and Raman Echo Techniques.

2. **Electronic Spectroscopy**: Nature of the transition, Franck-Condon factor, Quantum yield and radiative processes, Fluoresecnce and Phosphorescence, life times, Jablonski diagrams and potential energy surfaces. Elementary ideas on laser action (including discussions on mode-locking, Q-switching, cavity-dumping etc.), types of lasers (solid state, gas, chemical, exciplex, dye & diode lasers) and their applications in Chemistry. Two and multi-photon laser microscopy. Applications of multi-photon spectroscopy in chemistry and biophysics. Spectroscopy.

3. **Dielectric Relaxation Spectroscopy**: Electric dipole moments (permanent and induced), polarization, polarizability, hyper-polarizability, frequency dependence of polarization, orientation and electronic polarizabilities. Permittivity, Debye equation and Clausius-Mossotti relation. Measurement of dipole moment and its connection to the dielectric permittivity. Langevin function and temperature dependence. Frequency dependence of the dielectric permittivity, real and imaginary parts, Debye semi-circle, relaxation times and Havriliak-Negami description of relaxation types. Novel interplay between the dielectric response and solvation in a medium.

Books & References:

1. R. S. Drago, '***Physical Methods for Chemists***' , Saunders College Publishing.
2. P. W. Atkins, '**Physical Chemistry**' ELBS
3. D. A. Long, '**Raman Spectroscopy**' , McGraw-Hill Inc.

4. G. Barrow, '***Introduction to Molecular Spectroscopy***', McGraw-Hill.
5. T. G. Spiro, '***Chemical and Biological Applications of Lasers***' , (Ed. C. B. Moore), Academic Press, NY.
6. Lakowicz et al, '*Two photon induced fluorescence intensity and anisotropy decays of diphenyl hexatriene in solvents and lipid bilayers*' in **J. Fluoresc**. 1992, volm.2, 247 – 258.
7. C. Xu and W. W. Webb, '*Multiphoton excitation of molecular fluorophore and nonlinear laser microscopy*' in " ***Topics in Fluorescence Spectroscopy", volm.5; Nonlinear and two photon induced fluorescence***' J. Lackowicz (Ed.), 1997, Plenum Press, NY.
8. P. R. Calis, '*Two Photon Induced Fluorescence' in* ***Annu. Rev. Phys. Chem***., 1997, volm. 48, pages 271 – 297.
9. C. J. F. Bottcher & P. Bordewijk (Eds.), '**Theory of Electric Polarization**', Elsevier, Amsterdam, 1978.
10. Barthel et al, ***J. Solution Chem***. 1995, volm. 24, page 1; ***Chem. Phys. Lett***., 1990, volm.165, page 390.
11. Powell – Crasemann
12. Schiff
13. M. El Sayed, ***Chem. Rev***. volm. 77, page 793, 1977.
14. C. J. F. Bottcher, ***Theory of Electric Polarization***.
15. P. W. Atkins, ***Molecular Spectroscopy***, Volm. I, II & III
16. Yariv, ***Quantum Electronics*** .

CH 424: Inorganic Chemistry- II

1. Cordination chemistry: Reactions, kinetics and mechanisms- Reaction types; labile and inert complexes; substitution in square-planar and octahedral complexes; Electron transfer reactions; photochemical reactions.

2. Main group organometallic compounds

3. Organometallic chemistry of the transition elements- 18- electron rule, carbonyls, nitrosyls, alkyls and open-chain hydrocarbon ligands, cyclic polyene complexes, Metal-metal bonding and metal clusters, catalysis by organometallic compounds

4. Bioinorganic chemistry- Essential and trace elements in biology; ion-pumps; dioxygen storage and transport; heme proteins; eletron transfer, respiration and photosynthesis; metalloenzymes

Text Books:

4. J.E.Huheey, E.A.Keiter and R.L.Keiter, "Inorganic Chemistry" 4 th Ed. Addison Wesley, 1993

5. D.F.Shriver and P.W.Atkins, 'Inorganic Chemistry ", 3 rd Ed ,OUP,

6. G.Wulfsberg, "Inorganic Chemistry", University Science Books, CA, U.S.A, Indian Ed. Viva Books, New Delhi, 2002

Reference books:

3. N.N.Greenwood and A.Earnshaw, "Chemistry of the Elements", Pergamon, 1997

4. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, " Advanced Inorganic Chemistry", 6 th Ed, John- Wiley, 1999

CH 425: Synthetic and Biological Organic Chemistry

1. Organic Synthesis: Synthetic Strategy (6 L + 2 T)

Retrosynthetic analysis; Disconnections; 'Natural reactivity' and 'umpolung'

2. Organic Synthesis: Synthetic Methodology (18 L + 6 T)

I. Reagents containing boron, silicon, phosphorus, sulfur
II. Organotransition metal reagents
III. Asymmetric synthesis
IV. Aromatic heterocycle synthesis

3. Supramolecular Chemistry (6 L + 2 T)

Molecular recognition; Biological recognition; Synthetic molecular receptors; Molecular self-assembly

4. Medicinal Chemistry (6 L + 2 T)

Drug-receptor interactions; Drug design and synthesis

5. Bioorganic Chemistry (6 L + 3 T)

Enzyme action; Oligonucleotide synthesis; Mechanisms in biological chemistry

<u>Suggested Reading</u>

1. F. A. Carey & R. J. Sundberg, *Advanced Organic Chemistry (Part B)*
2. J. Clayden, N. Greeves, S. Warren & P. Wothers, *Organic Chemistry*
3. R. O. C. Norman & J. M. Coxon, *Principles of Organic Synthesis*
4. W. Carruthers, *Some Modern Methods of Organic Synthesis*
5. S. Warren, *Organic Synthesis - The Disconnection Approach*
6. S. G. Davies, *Organotransition Metal Chemistry: Applications to Organic Synthesis*
7. L. S. Hegedus, *Transition Metals in the Synthesis of Complex Organic Molecules*
8. E. L. Eliel, S. H. Wilen & L. N. Mander, *Stereochemistry of Organic Compounds*
9. J. A. Joule & K. Mills, Heterocyclic Chemistry
10. D. Nasipuri, *Stereochemistry of Organic Compounds - Principles and Applications*
11. J. M. Lehn, *Supramolecular Chemistry - Concepts and Perspectives*
12. J. Saunders, *Top Drugs - Top Synthetic Routes* (Oxford Chemistry Primer)

CH426: Numerical Methods and Computer Programming

Theory : Total Contact Hours 18 x 2 = 36

1. **Programming Language**:

   Basic knowledge of Fortran 90 – Data statements, Logical and Arithmetic expressions, Operators, I-O statements, Implementation of Loops, Control Statements, Functions and Subroutines, Array manipulation, Processing Strings and Characters, Format Specifications, File processing, Derived types, Pointers and Structure Data Type.

2. **Numerical Methods:**

   (a) Root finding of equations having numerical coefficients using Successive Bi-section and Newton Raphson method

   (b) Basic ideas of Interpolation – Newton's forward and backward interpolation, Lagrange method for unequal intervals

   (c) Numerical integration of a definite integral using Trapezoidal and Simpson's one-third rule

   (d) Statistical Description of Data

   (e) Fast Fourier Transform, Fourier and Spectral Applications

   (f) Numerical solution for a set of coupled ordinary differential equation – (i) Initial Value Problem: Runge Kutta Method, (ii) Boundary Value Problem: Relaxation Technique, Shooting Method

   (g) Partial Differential Equations (PDE): (i) Elliptic PDE – Static Boundary Value Problems, (ii) Parabolic PDE – Time Evolution or Dynamic Initial Value Problems, (iii) Hyperbolic PDE – Wave Propagation Problems

Practicals: Total Contact Hours 18 x 2 = 36

1. Familiarization with Unix operating system. Development of simple Fortran programs, compilation and execution.
2. Development of programs for physical problems using numerical techniques discussed in theory classes.

Suggested Textbooks:

1. ‘Computer Programming in Fortran 90 and 95’, V. Rajaraman, Prentice Hall of India, New Delhi (2003).
2. ‘Computing Methods for Scientists and Engineers’, L. Fox and D. F. Mayers, Clarendon Press (1968).
3. ‘Numerical Recipes in Fortran’, W. H. Press and S. A. Teukolsky, Cambridge University Press (1996).
4. ‘Numerical Methods for Scientists and Engineers’, H. M. Anita, Hindustan Book Agency (2002).

CH 427: Laboratory

- Experiments will be chosen from Chemistry, Physics and Biology and should be interdisciplinary in nature

- Experiments may vary from year to year depending upon the interests of the students and expertise of the instructor

COURSE CONTENTS

SECOND YEAR : SEMESTER III

CH 511: Equilibrium and Non-equilibrium Statistical Mechanics

A. Equilibrium Statistical Mechanics

1. Description of Ensembles and Thermodynamic Potentials. Illustration with Ideal diatomic gas: vibrational and rotational partition functions of hetero and homonuclear diatomic molecules; Calculation of equlibrium chemical constant. (6 lectures)

2. Ideal Bose Gas: Photon Statistics, Specific heat of insulators, and BE condensation. (3 lectures)

3. Ideal Fermi Gas: Specific heat ofd free electron gas (2 lectures)

4. Exact Solution of 1-D Ising model via Transfer Matrix; Mean Field Solution of 3-D Ising Model. (2 lectures)

5. Concept of order parameter through magentic phase transition; Landau theory for continuous phase transition and its connection to Mean Field solution of Ising model; First Order phase transition with illustration via Isotropic-Nematic phase transition. (3 lectures)

6. Elementary theory of Liquid Structures: Definitions of single particle density, two particle density, pair correlation function and structure factor; Relation between pair correlation function and structure factor; Experimental significance of structure factor; Equation of state of a liquid; Mean Field treatment of electrolyte solution. (5 lectures)

7. Qualitative description of phenomena near critical point: critical exponents in magnets, binary liquid, Carbon-di-oxide; Growing correlation and Role of fluctuations: Qualitative Illustration via 1-D and 3-D Ising Model. (4 lectures)

8. Computer Simulation: statement of basic algorithm of MC and MD. (The instructor may enecourage students to perform simulation on simple systems, for e.g., Ising system, Lennard-Jones fluid etc). (2 lectures)

B. Nonequilibrium 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. (7 lectures)

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. (4 lectures)

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. (4 lectures)

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.

CH 512 : Chemical Dynamics of Atoms, Molecules and Soft-Condensed Matter

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 auto-correlation 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**, 5^{th} 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

CH513: Molecular Structure and Dynamics by Single- & Mulphoton Spectroscopy II

1. **Nuclear Magnetic Resonance (NMR) Spectroscopy**: Magnetization vector & relaxation, NMR transition, Bloch equations, NMR experimental technique (with a schematic diagram of an NMR instrument), Transition probabilities. Chemical shift measurements and interpretation (with examples), interatomic ring currents. Effect of spin-spin splitting on spectrum, Non-equivalent protons, effects of bonds on spin-spin coupling, Scalar mechanisms for spin-spin coupling, Applications of spin coupling to structure determination. Double resonance and spin tickling experiments. Pulse techniques in NMR, Linewidths and rate processes, Determination of rate costants, activation enthalpies and reaction orders from NMR, nuclear Overhauser effect, 2-D NMR, NMR in liquid crystals and Solid State NMR.

2. **Electron Paramagnetic Resonance (EPR) Spectroscopy**: Basic principles, presentation of the spectrum, *g*-value, elementary ideas on hyperfine splitting. Brief discussions on anisotropies in g-factor and hyperfine splitting, EPR of triplet states, Nuclear Quadrupole interaction and line widths. Applications of EPR in determining the geometry of complexes and biological systems.

3. **Mass spectrometry, Ion Cyclotron Resonance and Photoelectron Spectroscopy**: Presentation of mass spectra, Interaction between a molecule and a high energy electron, Interpretation of mass spectra, Isotope effects, Molecular weight determination by field ionization technique, Estimation of heats of sublimation, Apperance potentials and Ionization potentials. Fourier Transform Ion Cyclotron Resonance Technique (brief discussion).

   Basic principles of Photoelectron spectroscopy; applications (discuss with PES spectra of gaseous N_2, NH_3, and NO). Elementary discussions (with examples) on Secondary Ion Mass Spectrometry, Electron energy loss spectroscopy, Scanning Tunneling Microscopy and Atomic Force Microscopy. Basic Ideas on Extended X-ray Absorption Fine Structre (EXAFS) and Xray Absorption Near-edge Structure (XANES). Applications of STM, AFM, EXAFS and XANES in Surface Science (Brief).

4. **Time Dependent Fluorescence Spectroscopy**: Time dependent shift of fluorescence emission peak of a dissolved fluorophore, Time correlated single photon counting (technique, outline with schematics), decay curves, construction of solvent correlation function from the observed time dependent frequency, Interpretation and comparison with the estimates from the continuum model. Determination of rotational diffusion by fluorescence depolarization, Implications of exponential and non-exponential decays. Brief discussions on ultra-fast decay and the relevant experimental techniques (fluorescence up-conversion, transient grating, 3-pulse photon echo peak shift , hole burning, etc.)

Books & References:

1. R. S. Drago, '***Physical Methods for Chemists***' , Saunders College Publishing
2. J. A. Pople et al. , '***High Resolution Nuclear Magnetic Resonance***' , McGraw-Hill, NY.
3. J. E. Wertz and J. R. Bolton, '***Electron Spin Resonance***', McGraw-Hill, NY
4. Mc. Millin, Drago & Nusz, ***J. Amer. Chem. Soc***., 1976, volm.98, 3120
5. Yang & Heuennekens, ***Biochemistry***, 1970, volm.9, 2127
6. J. Lakowicz, '***Principles of Fluorescence Spectroscopy***', **2nd Edition**, Kluwer Academic/ Plenum Publishers
7. G. R. Fleming, '***Chemical Applications of Ultrafast Spectroscopy***' , Oxford University Press, 1986
8. D. A. Wiersma, (Ed.) '***Femtosecond Reaction Dynamics***', North Holland, Amsterdam, 1994
9. A. H. Zewail, '***Femtochemistry:Ultrafast Dynamics of the Chemical Bond***', World Scientific, Singapore, 1994.

COURSE CONTENTS

SECOND YEAR : SEMESTER IV

CH 521: Chemistry and Physics of Materials

1. **Structure of Solids**: Periodicity, Fundamental lattice types (two & three dimensional), Index systems of crystal planes, Crystal structures and close packed arrangements, Examples of general interest, Direct Imaging (qualitative discussion on experiments such STM and TEM); Diffraction, Bragg's Law, Reciprocal Lattice Vectors, Diffraction Condition, Laue Equation & Brillouin Zones. (5 lectures)

2. **Crystal Vibrations & Phonons**: Vibrations with monatomic basis, Group velocity & its relation to sound velocity at long wavelength limit, Elastic Strains, Compliance & Stiffness Constants, Elastic Waves. Derivation of Force constants from experiments, Normal modes, Density of States in one & three dimensions, Debye T^3 Law, Einstein's modification and a general discussion on $D(\omega)$. (6 lectures)

3. Band Theory and Electronic Structure of Solids, Tight Binding Model (4 lectures)

4. Deviations from Ideal Crystals (descriptive): Crystal Defects, grain boundaries, dislocations, stacking faults and reactivity of solid due to the non-ideal structure; Glassy and amorphous materials, Alloys (7 lectures)

5. Tailor-making of materials with desired properties: (20 lectures)

A. Materials like liquid crystals /surfactant, microemulsions and micelles /colloids/polymer/membrane (to be covered in 10 lectures):

Liquid crystals: Chemical synthesis; ordering of phases: isotropic, nematic and smectic (descriptive); Maier-Saupe model for isotropic-nematic phase transition; anchoring.

Colloid: Chemical synthesis; colloidal phases (descriptive); screened Coulomb interaction in charged colloid, phase transition in colloids and colloids under shear (descriptive).

Polymer: Structural aspect – persistence length; Gaussian chain; Self avoiding walk; Theta solution; Rouse and Zimm model of dynamics (elementary level).

Surfactant, microemulsions and micelles : Chemical synthesis; structural properties and phase diagram (descriptive)

Membrane: Elementary idea of differential geometry; Helfrich free energy; Biological membranes (simple description of Mosaic model).

B. Superconducting Materials: Basic phenomenologies of type I and type II superconductors, BCS theory, phenomenology of high Tc superconductors
C. Quasi-one dimensional systems (phenomenology only)
D. Charge ordering systems (phenomenology)
E. Nanomaterials: Nanotubes, Fullerenes (descriptive)

References:

1. ***Solid State Chemistry & Its Applications*** by A. R. West (John Wiley & Sons)

2. ***New Directions in Solid State Chemistry*** by C N R Rao & J. Gopalakrishnan (John Wiley & Sons)

3. ***Crystal Chemistry and Physics of Metals and Alloys*** by W. B. Pearson (Wiley 1972)

4. ***Introduction to Crystal Geometry*** by M. J. Buerger (McGraw-Hill, 1971)

5. ***Phonons : Theory and Experiments*** by P. Bruesch (Springer 1987)

6. ***Structural Phase Transitions*** by A. D. Bruce and R. A. Cowley, (Taylor & Francis, 1981)

7. ***Thermal expansion of crystals*** by R. S. Krishnan (Plenum, 1980)

8. N. W. Ashcroft and N. D. Mermin, '***Solid State Physics***', Saunders College Publishing

9. de Gennes

10. T. C. Chaikin and T. C. Lubensky, '***Principles of Condensed Matter Physics***' , Cambridge University Press

11. Safran

CH 522: Equilibrium and Non-Equilibrium Electrochemistry

Electrolyte Solutions:

Equilibrium Aspects:
- Theory of Electrolytic Dissociation:
  - Arrhenius' Theory, Concept of Strong & Weak Electrolytes
- Theory of Ionic Interaction
  - Concept of Activity Coefficient & Ionic Strength
  - Debye Huckel Theory & Beyond
- Solvation and Hydration of Ions
  - Theory of Acids & Bases, Concept of Effective Size of Ions

Non-equilibrium Aspects:
- Electrical Conductance of Electrolytic Solutions
  - Conductivity & Conductometric Titrations
- Theory of Electrolytic Conductance
  - Debye-Onsager Theory
  - Wien Effect
  - Abnormal Mobility of Hydrogen and Hydroxide Ions
  - Conductance of Nonaqueous Electrolyte Solutions
- Diffusion Phenomena in Electrolytes
  - Fick's Law in Electrolyte Solutions

Electrode Related Electrochemistry

Equilibrium Aspects:
- Equilibrium Electrode Potentials
  - Electrodes of Various kind
  - Standard Electrode Potentials & Electrochemical Series
- Electrochemical Cells
  - Chemical cells
  - Concentration Cells
  - Potentiometric Titrations
- Theory of Electrode Potentials
  - Nernst Equation & Origin of EMF in Galvanic Cells
  - Theory of Electric Double Layer: Models & Thermodynamics
  - Electric Double Layer at the Surfaces of Colloids & Micelles

Non-equilibrium Phenomena:
- Electrolysis
  - Faraday's Laws, Electroanalysis
- Kinetics of Electrode Processes
- Concentration Polarization & Overvoltage
  - Mechanism of Electrochemical Overpotential
- Polarography

Miscellaneous & Modern Kinetic Aspects:
- Hydrogen Evolution in Electrolysis

Activated Barrier Crossing Processes in Electrode Processes
Electrodeposition of Metals from Metal Ion Solutions
Electrochemical Dissolution
Electrochemical Corrosion
Fuel Cells
Electron-Transfer Reactions
    Marcus Theory & Beyond

Books:

1. S. Glasstone, ***An Introduction to Electrochemistry***, Litton Educational Publishing, NY.
2. J. O'M Bockris & A. K. N. Reddy, ***Modern Electrochemistry***, Plenum Press, NY.
3. H. S. Harned and B. B. Owen, ***The Physical Chemistry of Electrolyte Solutions***, 3rd. Edition, Reinhold, NY.
4. H. S. Frank, ***Chemical Physics of Ionic Solutions***, Wiley, NY.
5. R. A. Robinson and R. H. Stokes, ***Electrolyte Solutions***, 2nd. Ed., Butterworth, London.

Rules and Regulations for the Two-Year M.Sc. Under the Integrated Ph.D. Program in Chemical Sciences :

Except the following, all other rules and regulations for the Integrated Ph.D. Program in Physical Sciences, including rules for Ph.D. will remain valid.

1. Admission :

1.1. Admission will be through an all-India entrance test consisting of both written and oral examinations. Only students with a minimum of 55% marks in the aggregate and who have completed B.Sc.with chemistry-physics-mathematics combination will be eligible for appearing at the entrance test. Application forms can be downloaded from the websites of S.N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata 700 098 and Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 032. They may also be published in national newspapers.

2. Duration of Semesters :

2.1. In an academic year, the first semester will begin in the middle of July. After 18 weeks, instruction will end in the middle of November. The end-semester examination and showing of answer scripts to the students will be completed by the end of November. The month of December will be a vacation period for the students.

2.2. The second semester will begin at the beginning of January. After 18 weeks, instruction will end in the middle of May. The end-semester examination and showing of answer scripts to the students will be completed by the end of May.The month of June will be a vacation period for the students who will rejoin by July 15 for the second academic year.

3. Faculty Advisor :

3.1. Upon admission, a group of 3-5 students will be assigned to a Faculty Advisor who will act as their friend, philosopher and guide during the first four semesters. Students should meet their Faculty Advisors at least once in a fortnight. Faculty Advisor will keep track of the students' academic progress, help them in their difficulties, advise them in exercising various options, offer career counseling and generally help them to tide over any difficulty, as far as possible. Faculty Advisors may or may not be subsequent M.Sc. Project Supervisor and/or Ph.D. Supervisors.

4. Instruction :

4.1. Each academic session will consist of two semesters. Each semester will have 18 weeks of instruction, excluding end-semester examination. The complete academic calendar for the year will be drawn up and displayed on the notice board(s). A copy of the academic calendar, course contents as well as rules and regulations will be given to every teacher and student.

4.2. Elective courses and experiments in the laboratory may change from year to year. Course contents may undergo dynamic evolution in course of time.

4.3. As far as possible, formal instruction should be for 5 days a week, with ample encouragement to the student for library work, self-study and regular habits of study.

4.4. In both theory and practical classes, student initiative will be an important element in the learning process.

4.5. Every theory course will have 3 hours of lectures followed by 1 hour of tutorial. Tutorial classes will involve *active participation* by the student in the form of problem-solving, problem-designing, discussion of test questions and assignments, discussion of problems concerned with lectures, etc. Students must avoid rote-learning.

4.6. The Instructor for a particular course will be responsible for maintaining the desired standard of the course and for evaluating the students' performance.

4.7. Every course is a distinct individual entity and the student has to pass every course.

4.8. In case of more than one teacher for a course, the teacher with the highest number of contact hours will be the teacher-in-charge who will coordinate the instruction and assessment in that course.

4.8. Experiments in the laboratory courses should be designed with great care. Every experiment should heighten the element of self-discovery by the student as well as be intellectually stimulating and exciting and exciting for the student to perform. As far as possible, experiments should integrate diverse concepts and be multidisciplinary in character.

4.10..Once the student has chosen an elective course, he/she cannot drop it.

4.11. All courses will run on the basis of credits. The number of credits for a particular course is equal to the number of contact hours per week for that course.

5. Research Project :

5.1. In the beginning of the second year, every student will be assigned to a Supervisor for the entire academic year. As far as possible, not more than one student will be assigned to any Supervisor.

5.2. Project work involves literature survey, formulation of the research problem, gathering of necessary materials, followed by actual research work. Every student will keep a day-to-day logbook/register for daily records of his/her work. The Supervisor will sign the logbook once in a fortnight.

5.3. Within the bounds of feasibility and practicality, students should be encouraged to give free rein to their imagination for the research problem. They should be encouraged to take up problems which are imaginative, exciting, novel, adventurous and exotic, even in the nature of "kite-flying". Such research problems might not lead to definite conclusions within the one-year duration.However, every student will submit an interim report of his/her project work at the end of third semester and a final project report at the end of fourth semester, for assessment.

6. Assessment :

6.1. In all theory and laboratory courses, assessment is fully internal and open. For every test/examination, the answer scripts will be shown to the students by the instructors concerned.

6.2. For project evaluation, an external examiner may be incorporated in the panel of examiners. In each semester, the student will deliver a seminar lecture which will be assessed by a panel of examiners. The final project assessment may be done through seminar lecture, poster presentation, etc.

6.3. The in-semester assessment will carry 50% of the total credits. The end semester assessment will carry the remaining 50% of the credits

7. Failures and Reappear Examinations :

7.1. If a students fails in a laboratory course, he/she will repeat the course.

7.2. If a student fails in a theory course in a semester, he/she will have a Reappear Examination in the first week of the next semester. If the student fails again, he/she will repeat the course. If the student fails again, he/she will have to leave the program.

8. Academic Program Monitoring and Execution Committee(APMEC) :

8.1. The APMEC will consist of 2-3 faculty members from SNBNCBS and 2-3 faculty members from IACS. All administrative work including the maintenance of records will be done at SNBNCBS. For smooth functioning, both the Convener and Secretary will be from SNBNCBS. From time to time, they will consult and keep in the picture the Director, SNBNCBS and the Director, IACS.

8.2. The APMEC will have the responsibilities for the smooth implementation of the 4-semester M.Sc. program in both letter and spirit.

8.3. The tenure of the first APMEC will be for 2 years. At the end of 2 years, 50% of the members will retire making way for new members. At the end of 4 years, the remaining 50% of the members will retire making way for new members. This process of change and continuity will continue.

9. Sharing of Ph.D. Students :

9.1. After successful completion of the 4-semester program, Ph.D. students will be shared between SNBNCBS and IACS on an equitable basis.