Course: Discipline Specific Elective

Semester	**5**
Paper Number	**HCHDS5012T (60 MARKS) & HCHDS5012P (40 MARKS)**
Paper Title	**Discipline Specific Elective 1 : PHYSICAL CHEMISTRY**
No. of Credits	**Theory-04, Practicals-02**
Theory/Composite	Composite
No. of periods assigned	Th: 4 Pr: 3
Name of Faculty member(s)	Dr. Asish K. Nag Dr. Rina Ghosh Dr. Indranil Chakraborty Dr. Rahul Sharma
Course description/objective	***Theory:*** ***Crystal Structure*** Discussion on crystal structure is the starting point of material science where arrangement of atoms in crystals and the symmetry of their arrangement is introduced. Basic principles of X-ray diffraction and interpretation of the pattern will be dealt with for crystals like NaCl and KCl. Students will realise that X-ray diffraction leads to information about the structures of metallic, ionic and molecular solids, and rationalisation of results in terms of atomic and ionic radii will be discussed. ***Statistical Thermodynamics*** The microscopic viewpoint of thermodynamics will be dealt with. Statistical Thermodynamics provides the link between the microscopic properties of matter and its bulk properties. Two key ideas will be introduced here i) The Boltzmann distribution which predicts the population of states in systems at thermal equilibrium and introduction to the partition function. ii) Interpretation of the partition function will be introduced and its calculation for some simple cases will be dealt with. Students will learn how to extract thermodynamic information from the partition function. ***Special Topics*** Certain topics will be introduced which are required for a wholesome understanding of the subject at the UG level. The Third law, emphasising the concept of absolute entropies. Mean energies of modes of motion, heat capacities of substances and residual entropies will be discussed. Finally, students will develop an insight into macromolecular assemblies, with their characterisation in terms of molar mass, sizes and shapes. A range of influences will be considered, beginning with a structureless random coil and ending with structurally precise forces that operate in biological assemblies. ***Practical:*** The objective in this advanced course is to enable the students to develop skills in Computational Chemistry. The course will be offered in two sections i) To enable students to write source codes in FORTRAN 77/90. For this, they will learn how to develop program logic through flowcharts, compile simple programs, usage of dimensioned variables, usage of subroutines and functions, plotting of functions using gnuplot. ii) After they become conversant with writing source codes, they will learn how to tackle numerical problems related to whatever they have learnt in

	Chemistry. For this, they will be exposed to the techniques of Numerical Analysis covering methods of integration, differentiation, linear fitting, interpolation and extrapolation.
Syllabus	Annexure DSE 1
Texts	
Reading/Reference Lists	**Theory:** 1. Castellan, G. W. *Physical Chemistry*, Narosa 2. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill 3. Moore, W. J. *Physical Chemistry*, Orient Longman 4. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press 5. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry*: A Molecular Approach, Viva Press 6. Engel, T. & Reid, P. *Physical Chemistry*, Pearson 7. Nash, L. K. *Elements of Statistical Thermodynamics*, Dover 8. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas 9. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill 10. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc. 11. Seymour, R. B. & Carraher, C. E. *Polymer Chemistry: An Introduction*, Marcel Dekker, Inc. 12. Odian, G. *Principles of Polymerization*, Wiley **Practical:** 1. The Art of Programming Through Flowcharts & Algorithms: by A. B. Chaudhuri, Firewall Media 2. Algorithm, Pseudocode and Flowchart: Learn Algorithm in Simple Steps: by J. Rawal, P. Rawal and B. Singh,BelTReady 3. Computer Programming Logic Using Flowcharts: by J. Farrell, Boyd & Fraser Pub. Co. 4. Fortran 77 and Numerical Methods: by C. Xavier, New Age International (P) Ltd, New Delhi 5. Computer Programming in Fortran 77: by V. Rajaraman, PHI Learning Pvt. Ltd., New Delhi 6. Introduction to Fortran 77: by Gunther Lemprecht, Viewweg+TeubnerVerlag 7. Professional Pragrammer's guide to Fortran 77: by Clive G. Page, University of Leicester, U.K. 8. Computers in Chemistry: by K. V. Raman, Tata McGraw Hill Publishing Company Ltd., New Delhi 9. Mathematics for Physical Chemistry: by D. A. McQuarrie University Science Books 10. Mathematics for Physical Chemistry: by R. Mortimer, Elsevier 11. Chemical Calculations: by P. Yates, CRC Press 12. Physical Chemistry on a Microcomputer: by J. H Noggle, Little Brown & Co. 13. Numerical Recipes in Fortran 77: by W. F. Vetterling, G. A.Teukolsky,B. P. Flannery and W. H. Press, CUP 14. Gnuplot in ActionUnderstanding Data with Graphs: by Philipp K. Janert, Manning Publications.

Evaluation	**Theory: 60 marks**	**Practical: 40 marks** *(Continuous Assessment)*
	CIA: 10 End-Sem: 50	Internal Assessment Exams: 30 Viva (End Sem): 8 Attendance: 2
Paper Structure for the End Sem **Theory Exam** (50 marks)	6 (SIX) Questions (each of 10 marks) will be set and the students will have to answer any 5 (FIVE). Each of the Questions (10 marks) will consist of 2 or 3 parts (of 2/ 3/ 4/ 5)	

DSE -1: ADVANCED PHYSICAL CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory (60 Lecturers)

a) Crystal Structure **(20 Lectures)**

Bravais Lattice and Laws of Crystallography: Types of solid, Bragg's law of diffraction; Laws of crystallography (Haüy's law and Steno's law); Permissible symmetry axes in crystals; Lattice, space lattice, unit cell, crystal planes, Bravais lattice. Packing of uniform hard sphere, close packed arrangements (fcc and hcp); Tetrahedral and octahedral voids. Void space in p-type, F-type and I-type cubic systems

Crystal planes: Distance between consecutive planes [cubic, tetragonal and orthorhombic lattices]; Indexing of planes, Miller indices; calculation of d_{hkl}; Relation between molar mass and unit cell dimension for cubic system; Bragg's law (derivation)

Determination of crystal structure: Powder method; Structure of NaCl and KCl crystals

b) Statistical Thermodynamics **(20 Lectures)**

Configuration: Macrostates, microstates and configuration; calculation with harmonic oscillator; variation of W with E; equilibrium configuration

Boltzmann distribution: Thermodynamic probability, entropy and probability, Boltzmann distribution formula (with derivation); Applications to barometric distribution; Partition function, concept of ensemble - canonical ensemble and grand canonical ensembles

Partition function: molecular partition function and thermodynamic properties, Maxwell's speed distribution; Gibbs' paradox, ; outline of Transition State theory (classical treatment).

c) Special selected topics **(20 Lectures)**

Specific heat of solid: Coefficient of thermal expansion, thermal compressibility of solids; Dulong –Petit's law; Perfect Crystal model, Einstein's theory – derivation from partition function, limitations; Debye's T^3 law – analysis at the two extremes

3^{rd} law: Absolute entropy, Plank's law, Calculation of entropy, Nernst heat theorem

Adiabatic demagnetization: Approach to zero Kelvin, adiabatic cooling, demagnetization, adiabatic demagnetization – involved curves

Polymers: Classification of polymers, nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers; Criteria for synthetic polymer formation; Relationships between functionality, extent of reaction and degree of polymerization; Mechanism and kinetics of step growth and copolymerization; Conducting polymers

PRACTICALS-DSE -1 LAB: Advanced Physical Chemistry

(60 Lecturers)

Computer Programming using Fortran and Introduction to numerical methods

1. Introduction to Algorithms and flowcharts
2. Introduction to Fortran
    a. Datatypes: integer, real, double precision, complex, character, logical
    b. Operators: Arithmetic, logical, character, assignment
    c. Input/Output statements: read, write, file manipulation
    d. Carriage Control: if-then-else-endif, goto, do loop
    e. Inbuilt functions
    f. Arrays and their manipulation
    g. User defined functions
    h. Subroutines
3. Numerical Methods and their applications in chemistry (any four methods)
    a) Root finding of equations
    b) Numerical differentiation: difference formula for 1st and 2nd derivative
    c) Numerical Integration: Trapezoidal rule and Simpson's formula
    d) Least square method: linear case
    e) Interpolation
    f) Matrix manipulation: matrix product, Gaussian elimination and the Gauss-Siedel method
4. Introduction to gnuplot and visualization of data using it.