Semester	5
Paper Number	C3CH230532T/ C3CH230532P
Paper Title	Physical Chemistry 4
No. of Credits	4
Theory/Composite	Composite
No. of periods assigned	Theory: 3 Practicals: 3
Name of Faculty member(s)	Rina Ghosh Indranil Chakraborty Rahul Sharma
Course description/objective	Theory: 1. Description of the thermodynamic properties of reactions that take place in electrochemical cells in which, progress of the reaction drives electrons through an external circuit. Thermodynamic arguments can be used to derive an expression for the electrical potential of such cells and the potential can be related to their composition. The definition of standard potentials is important in this context, in order to predict the equilibrium constants. 2. Quantum mechanical application for the theories of bonding considered for diatomic molecules are introduced as is the variational principle. 3. Study of surfaces is a very important aspect of any comprehensive understanding of chemical reaction dynamics. In solids, the extent to which a surface is covered and variation of the extent of coverage with pressure and temperature is an aspect to be investigated. In liquids, presence of a surface tension requires as rather involved approach from the thermodynamic point of view. Practical: 1. Various numerical methods are introduced and applied to solve problems encountered in physical chemistry.
Syllabus	Annexure Core Course
Reading/Reference Lists	Theory:

	1. Atkins, P. W. & Paula, J. de Atkins', Physical Chemistry, Oxford University Press. 2. Castellan, G. W. Physical Chemistry, Narosa. 3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva. 4. Levine, I. N. Physical Chemistry, Tata McGraw-Hill. 5. Rakshit, P.C., Physical Chemistry, Sarat Book House. 6. Moore, W. J. Physical Chemistry, Orient Longman. 7. Mortimer, R. G. Physical Chemistry, Elsevier. 8. Engel, T. & Reid, P. Physical Chemistry, Pearson. 9. Ball, D. W. Physical Chemistry, Thomson Press. 10. Vemulapalli, G. K, Physical Chemistry, Prentice Hall India. 11. Glasstone, S, Thermodynamics for Chemists, EWP. 12. Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata McGraw-Hill. 13. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press. 14 Nag, A. K, Physical Chemistry Vol. 1, 2, McGraw Hill. 15. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods Wiley. 16. Sears, F. W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition. 17. Metiu, H., Physical Chemistry: Thermodynamics, Taylor and Francis. 18. Kaufman, M., Principles of Thermodynamics, Taylor and Francis. 19. Honig, J. M., Thermodynamics, Academic Press. 20. Levine, I. N. Quantum Chemistry, PHI.

	21. Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford. 22. Eisberg, R., Resnick, R, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 2ed, Wiley. 23. Griffiths, D. J., Introduction to Quantum Mechanics, Cambridge India. 24. Adamson, A. W., Gast, A. P., Physical Chemistry of Surfaces, Wiley. 25. Hiemenz, P. C., Rajagopalan, R., Principles of Colloid and Surface Chemistry, Marcel Dekker. Practicals: 1. Mathematics for Physical Chemistry: by D. A. McQuarrie University Science Books 2. Mathematics for Physical Chemistry: by R. Mortimer, Elsevier 3. Chemical Calculations: by P. Yates, CRC Press 4. Physical Chemistry on a Microcomputer: by J. H Noggle, Little Brown & Co. 5. Numerical Recipes in Fortran 77: by W. F. Vetterling, G. A.Teukolsky,B. P. Flannery and W. H. Press, CUP 6. Hildebrand, F. B., Introduction to Numerical Analysis: Second Edition (Dover Books on Mathematics), Dover 7. Boas, M. L., Mathematical Methods in the Physical Sciences 3e, Wiley 8. Riley, K. F., Hobson, M. P., Mathematical Methods for Physics and Engineering: A Comprehensive Guide, Cambridge University Press	
Evaluation	Theory: 60 Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3) Semester Exam: 45	Practical: 40 CA: 38; Attendance:2
Paper Structure for the End Semester Theory Examination	Answer THREE out of FOUR questions of 15 marks each.	

Annexure Core Course

Electrochemical Cell *(12 Lectures)*

1. Electrical work output: thermodynamic consideration
2. Basic electrostatics
3. Potential difference
4. Electrochemical potential
5. Galvani potential difference at electrode-solution interface
6. Choice of positive and negative electrodes
7. Types of electrodes
8. Coupling of electrodes: electrochemical cell
9. Measuring cell potential
10. Reversible, irreversible cells
11. Electrochemical cells
12. Electrodes
13. Constructing electrochemical cell: liquid-liquid junction and salt bridge
14. Nernst equation for electrode potential: significance
15. Cell potential: its significance
16. Thermodynamics of Galvanic cell
17. Solubility product of a sparingly soluble salt
18. Tabulating standard electrode potential: SHE scale
19. Reference electrode
20. Potentiometric determination of pH of a solution: quinhydrone and glass electrode
21. Concentration cell: electrode and electrolyte concentration cell
22. Electrolyte concentration cell with transference

Quantum Chemistry IV *(12 lectures)*

1. Diatomic Molecules
2. Separation of electronic and nuclear motion
3. LCAO-MO treatment of H_2^+
4. Bonding and Anti-bonding orbitals
5. Extension to H_2
6. Comparison of LCAO-MO and VB treatments of H_2 and their limitations
7. Dissociation energy
8. Two-centre integrals
9. Valency
10. Approximations in Quantum Chemistry
11. Born-Oppenheimer (B.O.) approximation

Liquid state *(12 Lectures)*

1. Intermolecular forces in liquid.
2. reactivity of a surface molecule.
3. Vapour pressure of a liquid: boiling point.
4. Variation in vapour pressure of a liquid with pressure.
5. Surface tension: force per unit length and energy per unit area interpretation.
6. Liquid drop on a solid surface: contact angle.
7. Variation of shape of the drop: interplay of surface tension between different phases.
8. Shape of liquid meniscus in a capillary.
9. Adhesive and cohesive forces in determining the liquid meniscus in a capillary.
10. Surface energy.
11. Excess pressure: Young and Laplace equation.
12. Capillarity phenomenon.
13. Spreading of liquids: spreading coefficient and Dupre equation.
14. Temperature dependence of surface tension.
15. Measurement of surface tension.

Practicals:

Introduction to Computer Programming and Numerical Methods
Introduction FORTRAN 77 / FORTRAN 90 /C programming:
User defined functions
Subroutines
Numerical Methods and their applications in chemistry
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) Matrix manipulation: matrix product, Gaussian elimination and the Gauss-Siedel method
f) Numerical interpolation
g) Extrapolation of data
h) Richardson's method

Mathematica/Python: Continued
Algebraic and numerical calculations using symbolic manipulation programs–Use of Mathematica for simple manipulations.