Course Title **Physical Chemistry**

Course Code CH-802

Credit Hours 3-0

Prerequisite Nil

Course Objectives

This a conventional branch of chemistry which will be tailored to cater for modern trends of quantum mechanics, thermodynamics and solid states.

Course Outcomes

Students will be able to lean mathematics necessary for chemists and to apply it over certain physical phenomena. They will learn to explain that how quantum mechanics applies to subatomic particles using models and theories like black body radiation, photoelectric effect, de Broglie idea of duality and particle-in-a-box. They will be able to use quantum numbers and wavefunctions to describe electron configurations for atoms.

They will be able to use the thermodynamic variables to determine properties of a system and to calculate enthalpy changes and Gibbs free energy change and also their relation to the spontaneity and the direction of chemical reaction.

By the end of this course students will know the basis of solid state and crystalline materials as well as the characterization and dealing with X-ray Powder diffraction patterns. Students will be able to do Profile matching with the help of PCW (Powder Cell) program and certain crystallographic data available.

Course Contents

Course outline has been revised by realizing that we are having students with different fields of specializations (physical, organic, inorganic and analytical).

Quantum Mechanics: General Principles-(State of system, Quantum mechanical operators, time dependent wave functions), Blackbody Radiation, Einstein Explanation of the Photoelectric Effect with a Quantum Hypothesis, The Hydrogen Atomic Spectrum and S Series of Lines, The Rydberg Formula for all Lines in the

Hydrogen Atomic Spectrum, Louis de Broglie Postulated and experimental observation of these formulism, use of the Bohr Theory for Hydrogen Atom to Derive the Rydberg Formula, The Heisenberg Uncertainty Principle.

Cartesian and polar coordinates. Complex numbers. Derivation and integration. Operators (types), Eigen functions, Eigen values and operators.

The Schrödinger Equation for Finding Wave Function. The Schrödinger Equation to formulate an Eigen value Problem. Probabilistic interpretation of Wave Functions. The Energy of a Particle in a Box Is Quantized. Normalization (including integration) of wave function. Particle in three dimensional box, harmonic oscillator, rigid rotator. Treatment of many-electron atoms: Pauli's principle, Hund's rule, spin-orbit interaction. The Hartree-Fock method, Variational method, Perturbation theory. Calculations for butadiene.

Thermodynamics: State of a system, 0^{th} law, equation of state, Work, heat, first law, $\Delta H_r^{\,0}$ *calculations.* Heat capacity *(C_p and C_v).* Second law, spontaneous and non spontaneous reactions. Joule Thomson Effect and its coefficient (derivation and Applications), calculations. Entropy, Fundamental equation, absolute S, third law, Gibbs free energy, Thermodynamics of living systems. Helmholtz Energy (derivation and applications).

Solid State: Crystalline solids, Miller indices, lattice plans (hkl), Packing efficiency, Bravais Lattices, Crystal Structure, Crystal Defects, X-Diffraction, Properties of X-Rays, Production of X-rays (X-ray tube, Synchrotron), characteristic X-rays. X-ray Powder and Single crystal diffraction. Powder pattern. Structure factor. Peak position. Introduction to Powder Cell Program (Powder pattern matching), High-Score plus software for structural peaks indexing and other relevant parameters determination.

Recommended Books

1. R. Barrante, Applied Mathematics for Physical Chemistry, ISBN 0-13-741737-3
2. A. McQuarrie, Physical Chemistry, Physical Chemistry: A Molecular Approach, Viva books private limited, first South Asian Ed., 1998

3. R. Morales-Rodriguez, Thermodynamics - Fundamentals and Its Application in Science, , ISBN 978-953-51-0779-8, 554 pages, Publisher: InTech, Chapters published October 03, 2012, DOI: 10.5772/2615
4. P. Atkins and J. de Paula. *Physical Chemistry*. 7th ed. New York, NY: W.H. Freeman and Company, 2001. ISBN: 9780716735397.
5. L. F. del Castillo, P. Vera-Cruz, Thermodynamic Formulation of Living Systems and Their Evolution, *Journal of Modern Physics*, 2011, 2, 379-391.
6. A. R. West, Solid State chemistry and its Applications, John Wiley & Sons, Ltd. 2014
7. Cohen-Tannoudji, C., F. Laloë, and B. Diu. *Quantum Mechanics*. Vols. 1 and 2. New York, NY: John Wiley & Sons, 2006. ISBN: 9780471569527.
8. Silbey, R. Alberty, and M. Bawendi. *Physical Chemistry*. 4th ed. New York, NY: John Wiley & Sons, 2004. ISBN: 9780471215042.
9. J. Shackelford. *Introduction to Materials Science for Engineers*. 6th edition. Upper Saddle River, NJ: Pearson, 2004. ISBN: 9780131424869.