First Semester 2015-2016

Course Handout Part II

Date: 03/08/2015

In addition to part -I (General Handout for all courses appended to the timetable) this portion provides detail course description.

Course No. : **CHEM G553**
Course Title : **Advanced Physical Chemistry**
Instructor-in-charge : PRASHANT UDAY MANOHAR

1. Course Description: Structure: Principles and techniques of quantum mechanics, applications to atomic and molecular structure and spectroscopy, statistical thermodynamics, Equilibrium: The laws of Thermodynamics, applications to phase equilibrium, reaction equilibrium, and electrochemistry; Dynamics: Molecular motion in gases and liquids, reaction rate laws, mechanisms and rate theories of complex reactions, molecular reaction dynamics, surface processes, electron transfer dynamics.

Scope and Objective of the Course: The course aims at covering topics in advanced areas of physical chemistry, with the broad classification of the entire subject into three domains viz., structure, equilibrium and dynamics. Starting with fundamental principles and their application, the ultimate purpose of this course will be to understand the recent developments in experimental and theoretical physical chemistry before starting formal research in any of the chemistry areas. Areas of current interest such as femtochemistry, nanomaterials will be covered.

2. Text Book:

T1. Peter Atkins and Julio de Paula, *Atkins' Physical Chemistry*, 9th Ed., Oxford University Press, N.Delhi (2006).
T2. Ira N. Levine, *Physical Chemistry* 5th edition. Tata McGraw Hill, New Delhi, (2009).

Reference Books:

R1. Donald A. McQuarrie and John D. Simon, *Physical Chemistry, A Molecular Approach*, Viva Books Pvt. Ltd., N.Delhi, (2005).

3. Course Plan:

Lect. No.	Topic	Learning objectives	Ref. to text book sections
1-5	Quantum theory: introduction and principles	The failures of classical physics, wave-particle duality, wavefunction, Born interpretation, operators, The Schrodinger equation, uncertainty principle,	T1. 7.1-7.7
6-8	Quantum theory: techniques and applications	Translational, vibrational, rotational motion	T1. 8.1-8.9
9-11	Atomic structure	The structure and spectra of hydrogen atoms, the structures of many-electron atoms, the spectra of complex atoms	T1. 9.1-9.10
12-14	Molecular structure	Valence bond theory, molecular orbital theory, the molecular orbitals for polyatomic systems	T1. 10.1-10.8

15-19	Spectroscopy	Introduction to spectroscopy, Pure rotation spectra, rotational Raman spectra, the vibrations of diatomic molecules, the vibrations of polyatomic molecules, electronic transitions, magnetic resonance.	T1. 12.1-12.16; 13.1-13.6; 14.1-14.16
20-21	The properties of Gases	the state of gases; gas laws, the van der Waals equation, the principle of corresponding states	T1. 1.1-1.4
22-23	The first law of thermodynamics	The internal energy, enthalpy, adiabatic changes, standard enthalpy of formation, the Joule-Thompson effect	T1. 2.1-2.12
24-25	The second law of Thermodynamics	Entropy, the third law of thermodynamics, the Gibbs energies	T1. 3.1-3.9
26-27	Material equilibrium	Material equilibrium, thermodynamic properties of non-equilibrium systems, entropy and equilibrium, Gibbs and Helmholtz energies, Maxwell relations, calculations of changes in state functions, chemical potentials and material equilibrium, phase equilibrium, reaction equilibrium.	T2. 4.1-4.9
28	One-component phase equilibrium	Phase rule, phase equilibrium, Clausius-Clapeyron equation,	T2. 7.1-7.5
29-30	Solutions	The thermodynamic description of mixtures, the properties of solutions, activities, electrolyte solutions, Debye-Huckel theory of electrolyte solutions	T2. 9.1-9.8, 10.1-10.4, 10.6-10.8
31-32	Chemical equilibrium	Ideal gas reaction equilibrium, shifts in ideal gas reaction equilibria	T2. 6.1-6.6
33-35	Statistical thermodynamics: the concepts and applications	The distribution of molecular states, the internal energy and the entropy, thermodynamic functions and molecular partition function	T1. 15.1-15.7; 16.1-16.8
36-38	Kinetics	Molecular motions in gases and liquids, diffusion, empirical chemical kinetics, accounting for the rate laws, the kinetics of complex reactions	T1. 21.1-21.12; 22.1-22.8; 23.1-23.7
39	Molecular reaction dynamics	Reactive encounters, Transition state theory, the dynamics of molecular collisions, electron transfer in homogeneous systems	Lecture note + Study material
40	Processes at solid surfaces	The growth and structure of solid surfaces, the extent of adsorption, heterogeneous catalysis, processes at electrodes	Lecture note +

			Study material

The numbers of lectures shown above is notional. The students will have to resort largely to self-study, which will be followed by presentations and discussion. Extensive problem solving will be an integral part of the learning process. The instructor will provide references from recent literature in specific advanced areas.

4. Evaluation Components:

Components	Weightage (%)	Date/Time/Venue
Mid Semester Test	30	5/10 4:00 - 5:30 PM
Assignments + Seminars+ Term Papers	30	Continuous
Comprehensive Examination	40	2/12 AN

Assignments and Seminars: Assignments will be given periodically to supplement the material discussed in the class. These will include problem sets. Students will also have to deliver seminars on various topics related to the course and present at least one term paper on a topic of latest development in the field.

5. Chamber Consultation Hours: will be announced in the class.

6. Notices: Notices, if any, concerning the course will be displayed on the Nalanda/Chemistry Dept. Notice Board

Instructor-in-charge
CHEM G553