Approval: 6th Senate Meeting

Course Name : Molecular Physical Chemistry for Engineers

Course Number : CY 248

Credit : 3-0-0-3

Prerequisites : None.

Students intended for : B. Tech. 2nd year

Elective or Compulsory : Elective

Semester: Odd/Even : Odd

Objectives: This course will deal with the behaviour of material from the molecular point of view. After a brief introduction to the fundamentals of thermodynamic, this course will cover three core areas of physical chemistry -- quantum chemistry, statistical mechanics, and kinetics.

Outline:

Unit 1. Brief Review of Elementary Thermodynamics:
Introduction, Application of Gibbs free energy, Calculation of an Equilibrium Constant that cannot be Measured Conveniently. 4 lectures

Unit 2. Introduction to Quantum Theory & Applications

Introduction, one dimensional problems, Observing Vibrations and Rotations of Molecules by Spectroscopy, Infrared Spectroscopy, Electronic Excitations in Molecules. 10 lectures

Unit 3. Statistical Mechanics—Fundamental Ideas and Applications

Introduction, Statistical Occupation of Energy Levels, Boltzmann Distribution Function, Ensembles, Molecular Partition Function, Connecting the Molecular Partition Function to the Internal Energy and Entropy, Boltzmann Law on entropy, Applications of the Partition Function to Chemical Thermodynamics Problems. 12 lectures

Unit 4. Chemical Reactions
Introduction, Collision Theory—Reactive Hard-Sphere Molecules, Transition State Theory of Chemical Reaction Rates, Connection of Transition State Theory to Collision Theory, unimolecular reactions, RRKM theory. 16 lectures

Textbook:

- Molecular Physical Chemistry for Engineers - John T. Yates and J. Karl Johnson.

References:

- Molecular Physical Chemistry - A Concise Introduction: K. A. McLauchlan.
- Physical Chemistry: A Molecular Approach, D. Mcquarrie and J. Simon.
- Physical Chemistry: Understanding our Chemical World : P. M. S. Monk.
- The Physical Basis of Chemistry: S. Warren.
- Physical Chemistry: R. J. Silbey, R. A. Alberty, M. G. Bawendi.
- Physical Chemistry: P. Atkins and J. de Paula.