CY247 Introduction to Molecular Thermodynamics

Credit: 3-0-0-3 Approval: Approved in 2nd Senate

Elective or Core: Elective

Prerequisite: Consent of the faculty member

Students intended for: B. Tech. 2nd year Semester: Odd/Even: Even

Course objective:

The course shows how basic understanding of probability can be used to predict the outcome of events and how, in particular, when dealing with a huge number of events, simple ideas of probability predict outcomes that are for all practical purposes totally certain e.g. why it is that chemical reactions approach equilibrium and why the natural unpredictability of random events makes equilibrium a dynamic state. But to understand what's really going on, one has to start with the idea of energy. Although the concept of energy itself would not be enough to explain why some chemical reactions occur and some do not. For that we need to add the concept of entropy, which is a measure of all possible ways energy can be distributed. Entropy is actually the key to understanding, what is going on in real chemical processes. Unlike energy, Entropy is not conserved, and that fact alone drives natural processes in the direction "forward in time."

Course content:

- Probability, Distributions, and Equilibrium: Distributions, Relative Probability and Fluctuations, Equilibrium, Most Probable Distribution, Le Chˆatelier's Principle, Equilibrium Amounts and Equilibrium Constants. [6 hrs]
- Energy Levels in Real Chemical Systems: Real Chemical Reactions, The Quantized Nature of Energy, Distributions of Energy Quanta in Small Systems, Probability of a Particular Distribution of Energy, Most Probable Distribution, Energy Level Separation, Fraction of reactive Particles. [6 hrs]
- First Law of thermodynamics, - bonding and internal energy:
- Internal Energy, Chemical Bond, Mean Bond Dissociation Energies and Internal Energy, Using Bond Dissociation Energies to Understand Chemical Reactions, The "High-Energy Phosphate Bond" and Other Anomalies, Beyond Covalent bond, Modern View of Bonding. [8 hrs]
- Entropy and the second law: Energy Does Not Rule, Entropy Comparisons Are Informative, Standard Change in Entropy for a Chemical. [4 hrs]
- Enthalpy and the surroundings: Enthalpy vs. Internal Energy, High Temperature Breaks Bonds. [2 hrs]
- Gibbs Energy and Equilibrium Constant: The Second Law - Again, Concept of equilibrium, The "Low Enthalpy/High Entropy Rule", Quantitative Look at Melting Points,Vapor Pressure, Barometric Pressure, and Boiling, Isomerization Reactions, Experimental Data Can Reveal Energy Level Information, Application to Real Chemical Reactions. [8 hrs]
- Applications of Gibbs Energy - Phase Changes: Evaporation, Boiling, Sublimation, Vapor Deposition, Solubility, Impure Liquids. [2 hrs]
- Applications of Gibbs Energy - Electrochemistry: Electrical Work Is Limited by the Gibbs Energy, Gibbs Energy and Cell Potential, Actual Cell Voltages and the Nernst Equation. [6 hrs]

Text & Reference Books:

Introduction to Molecular Thermodynamics: R. M. Hanson and S. Green, University Science Books, 2008.

Molecular Thermodynamics, D. A. Mcquarrie and J. D. Simon, University Science Books, 1999.

Molecular Thermodynamics, Richard E. Dickerson, W. A. Benjamin, 1969.

Molecular Thermodynamics: A Statistical Approach, James W. Whalen, 1991.