Advanced Chemical Thermodynamics and Kinetics

Chemistry and Biochemistry

Instructor Name: Arijit Kumar De
Institute: IISER Mohali
Department: Chemical Engineering

Course Intro: : This course will cover classical/ macroscopic and statistical thermodynamics and kinetics developed to explain a variety of physico-chemical phenomena with applications in Chemistry. This course is designed as an advanced level course to the broad area of thermodynamics and kinetics and the lectures will be pitched at the level of advanced undergraduates (senior level) as well as graduate students.

Pre Requisites: : Any introductory course on Thermodynamics is preferred but not absolutely necessary
Core/Elective: : Elective
UG/PG: : Both
Industry Support : None

Reference : 1) D. A. McQuarrie, J. D. Simon, Physical Chemistry: A Molecular Approach, 1st Ed, University Science Books, California (1997). 2) P. W. Atkins, J de Paula, Physical Chemistry, 8th Ed, Oxford University Press, New Delhi (2006). 3) I. N. Levine, Physical Chemistry, 6th Ed, Mcgraw Hill Education (2011).

About Instructor: Arijit Kumar De completed his BSc (2003) with Chemistry major from University of Calcutta (WB, India) and MSc (2005) in Chemistry from IIT Kanpur (UP, India). He pursued his PhD with Debabrata Goswami at IIT Kanpur (2005-2010). He was a postdoctoral fellow at Lawrence Berkeley National Lab and University of California Berkeley (CA, USA) with Graham R. Fleming (2010-2014). In 2014, he joined IISER Mohali (PB, India) as an Assistant Professor in the Department of Chemical Sciences.

COURSE PLAN

SL.NO	Week	Module Name
1	1	Review of classical thermodynamics: Concept of entropy, Properties of Gibbs free energy, Phase equilibrium of one and two component system.
2	2	Ideal dilute solution: Binary solutions, The lever rule, Fractional distillation, Azeotropes.
3	3	Condensed phase equilibrium: Liquid-liquid, Liquid-solid and Gas-solid equilibria.
4	4	Non-ideal systems: Concept of activity, Activity of ions, Debye-Huckel theory.
5	5	Electrochemical phenomena: Electrical polarization: Dipole moment and Electrical double-layer, Colloids: Lyophobic and lyophilic colloids, Electrokinetic phenomena, Sedimentation, Flocculation and coagulation (Introduction to DLVO theory), Stability of colloids, Light scattering.
6	6	SurfaceInterface phenomena: Langmuir adsorption isotherm, Multilayer adsorption (BET isotherm), Introduction to mesophase: Micelles, Biological membranes & Liquid crystals, Surfactants: Critical micellar concentration, Introduction to Rheology.
7	7	Nernst-Simon theorem (third law of thermodynamics), Irreversible thermodynamics.
8	8	Transport phenomena: Review of kinetic theory of gases, Mean free path, Viscosity, Diffusion (Ficks laws), Introduction to electrical conductivity.
9	9	Review of basic concepts in chemical kinetics, Reaction mechanism, Kinetic measurements.
10	10	Advanced topics in chemical kinetics: Laplace transform, Oscillatory reactions, Introduction to Atmospheric chemistry.
11	11	Introduction to statistical thermodynamics, Molecular partition function, Boltzmann distribution.

12	12	Introduction to molecular reaction dynamics: Potential energy surface, Transition state theory, Unimolecular reactions (Lindemann-Christiansen model (Introductory discussion on Hinshelwood and RRKRRKM models).