# ADVANCED CHEMICAL THERMODYNAMICS AND KINETICS

**Prof. Arijit Kumar De**
Department of Chemistry
IISER Mohali

**INTENDED AUDIENCE :** BSc/BS/ Int-MSc (BS-MS) - 3rd year BE/BTech/ Int-MTech - 2nd year MSc/Int-PhD - 1st/2nd year PhD – 1st year

**PREREQUISITES:** Any introductory course on Thermodynamics is preferred but not absolutely necessary
ABOUT THE COURSE: 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.

**ABOUT THE 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:**
**Week 1 :** Review of classical thermodynamics: Concept of entropy, Properties of Gibbs free energy, Phase equilibrium of one and two component system, Mixtures, Chemical equilibrium.
**Week 2 :** Molecular interactions: Dipole moment, Electrical polarization, Charge-dipole, Dipole-dipole and Dipole-induced dipole interaction, Dispersion interaction.
**Week 3 :** Transport phenomena: Viscosity, Diffusion (Ficks laws).
**Week 4 :** Review of chemical kinetics: Reaction mechanism, Kinetic measurements.
**Week 5 :** Advanced topics in chemical kinetics: Introduction to photochemistry, Kinetics of multicomponent systems: Combustion and Atmospheric chemistry.
**Week 6 :** Introduction to statistical thermodynamics: Molecular partition function, Boltzmann distribution.
**Week 7 :** Introduction to bimolecular reaction dynamics: Potential energy surface, Transition state theory.
**Week 8 :** Unimolecular reactions (Lindemann-Christiansen model (Introductory discussion on Hinshelwood and RRK/RRKM models).
**Week 9 :** Introduction to solution phase reaction dynamics: Cage effect, Diffusion controlled reactions, Polar solvation, Marcus theory of electron transfer.
**Week 10 :** Non-ideal solutions, Activity of ions (Debye-Huckel theory).
**Week 11 :** Electrochemistry: Insights into electrode processes, Ionic conductivity.
**Week 12 :** Lab demonstration (including illustrations): 1) Transport phenomena: Coefficient of viscosity, 2) Chemical kinetics: Hydrolysis of an ester, 3) Photochemistry: Degradation of a dye, 4) Reaction dynamics: Femtosecond pump-probe spectroscopy.