Indian Institute of Technology Kanpur

Proposal for a New Course

Course Number: ChE6XX

Structure: *Two* Lectures per week each of 1hr 15mins duration. (3-0-0-9)

Duration of the Course: Full Semester

Proposing Department: Chemical Engineering

Other Departments/IDPs which may be interested in the proposed course: Chemistry, Sustainable Energy Engineering

Other Faculties Interested in Teaching this Course: Indranil S. Dalal (CHE), Harshwardhan H. Katkar (CHE), Nishanth Nair (CHM)

Proposer: Vishal Agarwal

Course Description:

Objectives: The goal of the course is to acquaint students with the fundamentals of chemical kinetics, rare-event simulations, and reaction rate theories. The course will thoroughly cover the underlying theory and the assumptions made in it, even though the focus will be on applications. This is because understanding this material is essential to being an intelligent practitioner.

Title: "*Chemical Kinetics: Reaction Rate Theories and Rare-Event Simulations*"

Course Contents and Lecture-wise Breakup*:

Introduction: Stoichiometry and reaction progress variables. (1 lecture)

Thermodynamics of Chemical Reactions: Chemical potential, equilibrium constant, determination of equilibrium composition, effect of reaction conditions on equilibrium yields, statistical mechanics of equilibria in ideal gasses. (10 lectures)

Reaction Path: Concept of potential energy surface, saddle point and minimum energy path (MEP), saddle point searching algorithms: coordinate-driving, Cerjan-Miller and Nudged Elastic Band (NEB). Tutorials (or project) on saddle-point searches on 2D analytical potentials. (6+2 lectures)

Reaction Rates: Rate laws, reaction mechanisms, micro-kinetic modelling, degree of reaction control, heterogeneous catalysis, flux across a dividing surface, collision theory, RRKM, transition state theory (TST), variational and harmonic TST, correlation-flux theories. (12 lectures)

Rare-Event Simulations: Free-energies, Monte carlo and molecular dynamics, importance sampling, umbrella sampling, reactive flux and reaction rates from simulations. Tutorials (or project) on computation of rates from rare-event simulations. (6+3 lectures)

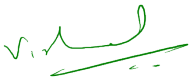
* Each lecture is assumed to be of 50 minutes duration.

Pre-requisites: ChE221 or equivalent, CHM102 or equivalent, MTH102 or equivalent and ChE331 or equivalent

Expected Enrolment: $\sim$ 10-30

- **Useful References**
  - "*Chemical Kinetics*", Keith J. Laidler, Pearson Education, 1987, ISBN: 8131709728.
  - "*Chemical Dynamics in Condensed Phases: Relaxation, Transfer, and Reactions in Condensed Molecular Systems*", by Abraham Nitzan, OUP Oxford, 2013, ISBN: 9780199686681.
  - "*Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics*", by Niels Engholm Henriksen and Flemming Yssing Hansen, Oxford University Press, 2019, ISBN: 9780198805014.
  - "*Introduction to Computational Chemistry*", Frank Jensen, Wiley, 2017, ISBN: 9781118825990.
  - "*Introduction to Modern Statistical Mechanics*", David Chandler, Oxford University Press, Sep 1987. ISBN-10: 0195042778, ISBN-13: 9780195042771.
  - "*Statistical Mechanics*", Donald A. McQuarrie, University Science Books, June 2000, 2nd Edition, ISBN-13: 978-1-891389-15-3.
  - "*Statistical Mechanics: Theory and Molecular Simulation*", by Mark Tuckerman, Oxford University Press, 2011, ISBN: 9780198525264.
  - "*Chemical Dynamics in Condensed Phases: Relaxation, Transfer, and Reactions in Condensed Molecular Systems*", by Abraham Nitzan, OUP Oxford, 2013, ISBN: 9780199686681.

Dated: June 20, 2024 Proposer: 

Dated: June 20, 2024 DPGC Convener: 

The course is approved / not approved

Chairman, SUGC/SPGC

Dated:_____