ADVANCED THERMODYNAMICS AND MOLECULAR SIMULATIONS

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IIT Roorkee

TYPE OF COURSE : Rerun | Elective | UG/PG
COURSE DURATION : 12 Weeks (24 Jan' 22 - 15 Apr' 22)
EXAM DATE : 24 Apr 2022

PRE-REQUISITES : Basic UG course in thermodynamics or statistical mechanics

INTENDED AUDIENCE : First year postgraduate and fourth year undergraduate students in Chemical Engineering, Chemistry, Materials Science, Polymer Science, Nanotechnology, Mechanical Engineering

INDUSTRIES APPLICABLE TO : Pharmaceutical, FMCG, Chemical, and Oil companies.

COURSE OUTLINE :

This course aims to impart knowledge of advanced thermodynamics concepts and molecular simulation methods. Unlike the standard undergraduate chemical engineering thermodynamics, we will follow a rather physics-based treatment of thermodynamics based on statistical mechanics concepts and molecular theories. The thermodynamics part to be covered in first half of the course would be used in the discussion of molecular simulations to be covered in the second half of the course.

ABOUT INSTRUCTOR :

Prof. Prateek Jha is an associate professor in the Department of Chemical Engineering, IIT Roorkee, India. His research interests are in the areas of molecular simulations, drug delivery, polymer physics, and theoretical nanoscience. He has earned his PhD from Northwestern University, followed by a postdoctoral stint at University of Michigan-Ann Arbor on a collaborative project with The Dow Chemical Company. He has won several awards including institute research fellowship of IIT Roorkee awarded to outstanding young faculty, DST young scientist award, DST-INSPIRE award, and distinguished researcher award for his PhD work at Northwestern University. He was a finalist for Frank J. Padden Jr. Award for excellence in polymer physics research of the American Physical Society in 2012. He has earned his undergraduate and master's degree from NIT Warangal (India) and IIT Bombay (India), respectively.

COURSE PLAN :

Week 1: Introduction and scope of the course. Probability and distributions. Boltzmann approximation and concept of thermodynamic Equilibrium. Molecular origin of entropy.

Week 2: Laws of thermodynamics, thermodynamic functions, Legendre transformation, Maxwell relations.

Week 3: Averages and fluctuations, Method of Lagrange multipliers. Introduction to thermodynamic ensembles, partition function.

Week 4: Derivation of thermodynamic properties in different ensembles, definition of temperature.

Week 5: Phase equilibrium, Gibbs phase rule, mixing and phase separation, chemical potential, osmotic pressure.

Week 6: Lattice model of solutions, phase space and Hamiltonian. Theoretical basis of molecular simulations.

Week 7: Monte Carlo (MC) Simulations: Setting up a simulation, types of boundary conditions, detailed balance.

Week 8: Monte Carlo (MC) Simulations: Numerical implementation, analysis and interpretation of results, case studies.

Week 9: Practical Introduction to Particle Simulations, Molecular Dynamics (MD) Simulations: Numerical integration of equations of motion, force-fields.

Week 10: Molecular Dynamics (MD) Simulations: Temperature and Pressure Control, Analysis and interpretation of results, efficiency and parallelization, case studies.

Week 11: Methods to study phase behavior and coexistence; Methods for Free Energy Calculations: Thermodynamic integration, Widom's particle insertion method, umbrella sampling and other advanced strategies.

Week 12: Non-equilibrium and Mesoscale Simulations: Langevin equations, Brownian dynamics (BD), Kinetic Monte Carlo (kMC) simulations, and other methods; simulations of chemical reactions and quantum chemistry simulations.