ADVANCED THERMODYNAMICS AND MOLECULAR SIMULATIONS

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TYPE OF COURSE : New | Both | UG/PG
COURSE DURATION : 12 Weeks (18 Jan’ 21 - 09 Apr’ 21)
EXAM DATE : 25 Apr 2021

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 :
Dr. 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 working, 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 young scientist award and INSPIRE award from the Department of Science and Technology (India), and distinguished researcher award from 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 masters degree from NIT Warangal (India) and IIT Bombay (India), respectively.

COURSE PLAN :
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, advanced sampling strategies, practical tips, case studies.
Week 9: Molecular Dynamics (MD) Simulations: Numerical integration of equations of motion, temperature and pressure control, force-fields.
Week 10: Molecular Dynamics (MD) Simulations: Analysis and interpretation of results, efficiency and parallelization, MD software, practical tips, case studies.
Week 12: Non-equilibrium Simulations: Langevin equations, Brownian dynamics (BD), Kinetic Monte Carlo (kMC) simulations, and other methods.