INTRODUCTION TO POLYMER PHYSICS-IITR

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INTENDED AUDIENCE : For undergraduate/postgraduate students in Polymer Science and Engineering, Chemical Engineering, Physics, Materials Science and Engineering, and Chemistry.

PRE-REQUISITES : Following courses are desired but not mandatory: Undergraduate courses in computer programming, thermodynamics, fluid mechanics/solid mechanics/continuum mechanics, and engineering mathematics/calculus.

INDUSTRIES APPLICABLE TO : Polymer and plastic Industries.

COURSE OUTLINE :

This course is an introduction to the physics of polymers, designed for senior undergraduate and postgraduate students. We will discuss statistical-mechanical, thermodynamic, and continuum theories for the structure, dynamics, and rheology of polymeric materials. Emphasis will be on developing a conceptual understanding of the theoretical and simulation methods employed in the study of polymers, and their application to specific systems. This course can be of potential interest to students studying in various disciplines including polymer science, chemical engineering, physics, chemistry, and materials science.

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 01 : Macromolecules and Life, Molecular flexibility, Classification of polymers, Types of polymerization, Average molecular weights and polydispersity, Concept of universality

Week 02 : Random walk models in polymer physics: 1-D random walk (drunkard walk), 2-D random walk on a lattice, freely jointed chain, modified freely jointed chain, freely rotating chain

Week 03 : Elastic energy of polymer chain, bead-spring model, ideal polymer chain and finite extension models, radius of gyration, pair correlation function, scattering experiments

Week 04 : Review of programming concepts, Monte Carlo simulations of a polymer chain, Importance Sampling, Metropolis criteria, Practical aspects of Monte Carlo simulation

Week 05 : Excluded volume interaction. Flory theory in good solvent, bad solvent, and theta solvent. Monte Carlo simulations in good solvent and bad solvent regime.

Week 06 : Concentrated polymer solutions. Review of Solution thermodynamics: Mixing and phase separation, osmotic pressure, chemical potential, thermodynamic origin of diffusion.

Week 07 : Lattice model of solutions, Flory-Huggins theory of polymer solutions, Definition of partition function and free energy, binodal and spinodal curve, critical point, extension to polymer blends and melt

Week 08 : Brownian motion, Correlation functions, Time translational invariance and time reversal symmetry, Brownian motion of a free particle, Einstein relation

Week 09 : Brownian motion in a potential field, Introduction to Molecular Dynamics and Brownian Dynamics

Week 10 : Rouse model of polymer chain, normalized coordinates and basis functions, Rouse modes, problems with Rouse model

Week 11 : Review of continuum mechanics: equations of motion, stress tensor, deformation tensor, deformation gradient tensor, constitutive relations of solids, liquids, and rubber. Microscopic definition of stress tensor.

Week 12 : Experimental rheology: rheometers, linear viscoelasticity, superposition principle, relaxation modulus, storage modulus, loss modulus.