ChE 494 MOLECULAR & MACROMOLECULAR ENGINEERING

Term: Spring 2019 Instructor: *Vivek Sharma*

The goal of the course to develop a comprehensive understanding of physicochemical principles underlying (or needed for) molecular and macromolecular engineering of the macroscopic optical, mechanical and transport properties of materials. We shall rely on the use of (a) the principles of statistical mechanics that will be introduced as part of the course, (b) a close reading of a few papers and selections from classic textbooks, and (c) curiosity-driven extra reading, primarily focused on polymers, liquid crystals and other soft materials.. Familiarity with basic chemical engineering concepts (thermodynamics and transport phenomena typically taught at the undergraduate level) shall be assumed. We will discuss molecular and macromolecular basis of structure-property relationships, as well as how such relationships are deciphered in the macroscopic measurements that involve interaction with light with matter, or response to imposed mechanical stresses and other external fields. Though some overlap with an elective taught on Fizzics and Interfacial Phenomena by the instructor can be expected, the course will be significantly different in content, coverage and emphasis.

Lectures on Wednesday and Friday, 4-5:15 PM.

Course Outline

(A few topics will be added or altered based on the class participation and performance)

- **Molecular reality of matter**. Motivation for Molecular & Macromolecular Engineering of Materials including Complex Fluids. Historical overview: From Lucretius to Boltzmann & Perrin. Intermolecular Forces. Brownian Motion. Random Walks & Gaussian Chains. (Week 1)
- **Classical Statistical Mechanics:** Newtonian, Lagrangian and Hamiltonian mechanics. Microcanonical, canonical and grand canonical ensembles. Ideal Gas. Virial Expansion. Kuhn chain, Persistence length and Entropic Elasticity. Phase Transitions and Critical Phenomena. Curie Law. Ising Model. (Week 2-4)
- **Surface Forces and Thermodynamics of interfaces**: Gibbs and Langmuir adsorption equations. Charged interfaces and electrostatic double layer theory. Debye-Hückel approximation. Disjoining pressure. Dispersion forces. DLVO and Non-DLVO colloidal forces. (Weeks 5)
- **Molecular and Macromolecular Thermodynamics**: Review of Solution Thermodynamics, Bragg-Williams and Flory-Huggins Theory. Real Polymers & Excluded Volume Interactions. Polyelectrolytes and Coacervation. Gelation. Phase Separation: Nucleation & Growth *vs.* Spinodal Decomposition. (Week 6-7)
- **Hard *vs.* Soft Matter:** Order, Dislocations, Defects, and Microstructure. Crystal Structure. Liquid Crystals and Quasi-crystals. Pair-Correlation functions and Structure Factor. Optics: Birefringence, Dichroism, and Scattering Theory (X-ray, Light & Neutron). (Week 8-9)
- **Molecular Origin of Mechanical and Transport Properties:** Drude Model and Fermi Gas. Phonons and Plasmons. Elasticity, Viscosity, Plasticity, Conductivity, Thermal Diffusivity, Viscoelasticity. Anisotropic Transport properties. Frank Elasticity in Liquid Crystals. Curvature Elasticity. (Week 10-11)
- **Molecular and Macromolecular Dynamics**: Fluctuation-Dissipation Theorem. Stokes Drag, Stokeset and Hydrodynamic Interactions. Bead-Spring models (Rouse/Zimm). Fluctuations and Blob models for Semi-dilute Solutions. Entangled Polymer Dynamics. Dynamics of Polyelectrolytes. (Week 12-13)
- **Molecular & Macromolecular Engineering of Complex Fluids:** Applications in Energy, Water, Medicine, Cosmetics, Coatings, Adhesives or Bio-inspired Materials (Week 14)
- **Individual project and presentation, and two term papers.**