Syllabus
Department of Chemistry
FCH 650 – Graduate Studies
Statistical Physics and Chemistry of Macromolecules
Polymer Physical Chemistry

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Spring, 2011

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Pre-requisites:

This 3-credit course is primarily intended for graduate students who have already gained some exposure to the field of polymer science. The official pre-requisites are: (i) a semester of undergraduate physical chemistry (thermodynamics), and: (ii) an introductory course at the early graduate/advanced undergraduate level that explores the basic properties of polymeric materials. Prior familiarity with statistical mechanics is not required, but is very helpful.

Exceptionally well-prepared undergraduates in their senior year who satisfy the above pre-requisites may also enroll (and frequently do enroll) for this course, subject to the consent of the instructor.

Meeting Time: (Spring, 2011):

The class will meet in Room 148, Baker Laboratory, from 3:30 P.M. to 4:50 P.M., on Tuesdays and Thursdays.

Textbook and Other Readings:

The required textbook for this course is *Polymer Chemistry*, 2nd Edition, by P.C. Hiemenz and T.P. Lodge, Taylor & Francis, (2007).

The textbook will be supplemented by an extensive series of lecture notes compiled and provided by the instructor.

Other useful readings (that in many instances are representative of the level of detail/rigor in which subjects will be covered in this course) include the following volumes: *Scaling Concepts in Polymer Physics*, by P.G. de Gennes, (1979); *The Physics of Polymers*, by G.R. Strobl, (1997); *The Theory of Polymer Dynamics*, by M. Doi and S.F. Edwards, (1986); *Polymeric Liquids and Networks: Structure and Properties*, by W.W. Graessley, (2003); and: *Fundamentals of Statistical and Thermal Physics*, by F. Reif (1965).

Grading and Evaluation:

The grade for this course will be based upon four (4) homework assignments that are due at various points during the semester. Additionally, there will be a take-home final assignment/examination. Each of these five components is assigned equal weightage in determining the grade.

Goals and Objectives for the course:

The primary objective of this course is to acquaint graduate (and well-prepared undergraduate) students with key aspects of the physical science of macromolecules, and with the language (both verbal and mathematical) that is employed in this field. Emphasis is placed upon the mathematics and derivations that are the foundation for a number of important results and pieces of scientific vocabulary that are widely used in interpreting experimental measurements, as well as upon the limitations that accompany the use of these tools. Completion of this course should prepare students to directly approach the primary research literature (including in areas that are not addressed directly during the class) with a discerning and critical eye.

Detailed listing of subject matter to be covered:

Introduction to Statistical Mechanics:

Review of thermodynamics; Euler's theorem for homogeneous functions and the Gibbs-Duhem relations; the information-theoretic definition of entropy; introduction to ensembles and calculation of ensemble averages.

Chain Dimensions and Chain Statistics:

Random walks, ideal and self-avoiding, in two and three dimensions; Radius of gyration, end-to-end vectors; mean-field argument for the Flory exponent.

Freely-jointed, freely-rotating, and persistent/worm-like chains; different definitions and possible physical interpretations of the persistence length; chain swelling following mean-field approach for the coil expansion factor.

Light Scattering and Correlation functions:

Light scattering methods to determine radii of gyration, molecular weights, and virial coefficients. Scattering by fractal architectures and aggregates. Zimm plot. Introduction to dynamic light scattering and the measurement of diffusion coefficients. Introduction to Fourier transform and Green's function methods; the convolution theorem, correlation functions, and Dirac delta functions.

Thermodynamics and Solution Properties:

Identification of semidilute crossover, static scaling theory; results for the mesh size, coil dimensions, and osmotic pressure in semidilute solutions, from scaling arguments.

Flory-Huggins theory for thermodynamics, and compressible generalizations thereof (*e.g.*, the Sanchez-Lacombe model). Connections with related work in "simple" (small molecule) liquids.

Interfaces in solutions and blends; motivation for the square-gradient term, and its use in calculating density profiles and interfacial tension in strong segregation limit.

Rubber Elasticity:

Ideal rubbers, elastomers, calculation of stress-strain behavior and moduli based on fixed junction model. Stress-optical rule.

Dynamics:

Viscoelasticity; general expression for stress tensor for harmonic chains. Unentangled melts and solutions, Rouse and Zimm models; calculation of diffusion constants and viscosity with and without hydrodynamic interactions.

Entangled polymers and reptation; calculation of diffusion constants and dynamic moduli from tube model.

The Glass Transition:

Basic phenomenology of the glass transition; free volume and Adams-Gibbs theories for the temperature dependence of viscosity, relaxation times, and tracer diffusion; relationship to semi-empirical constructs *e.g.* the WLF/VFT equation and temperature-time superposition principle.

Rod-Like Polymers and Liquid Crystals:

Excluded volume considerations for rods, relation to percolation threshold in suspensions of rigid particles/macromolecules; Onsager theory for isotropic-nematic transition; Rotational diffusion and intrinsic viscosity.

Charged Polymers:

Linear polyelectrolytes: Manning condensation and the electrostatic persistence length.

Brownian Motion and Linear Response Theory: (*if time permits*):

Description of Brownian motion based upon the Langevin and Smoluchowski equation approaches; Stokes-Einstein relation; linear response theory and the relation between transport coefficients and time-correlation functions (Green-Kubo relations); causality and the Kramers-Kronig relations; Markov processes and the master equation.