Northeastern University
College of Engineering

Please join us for a
Special Chemical Engineering Seminar

Wednesday, February 27, 2013
108 West Village H
11:45 a.m. – 1:00 p.m.

"Dynamics of Polymer Solids and Fluids: Tales at Different Scales"

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ABSTRACT

Polymers are ubiquitous in our life. Properties and behaviors of these materials, however, are often not intuitively predictable because of the complexity in their structure and dynamics, which typically involve a wide range of length and time scales. Multiscale computer simulations play an important role in helping us understand these systems. In this talk, I will discuss two topics at entirely different length scales, corresponding to the two limits of the spectrum of scales relevant to polymer dynamics.

The first topic focuses on a polymer solid and its dynamics at the microscale (a few angstroms to a few nanometers). Using detailed molecular models, we study the diffusion motion of isolated solvent molecules in a glassy amorphous polymer. With the help of advanced simulation and analysis tools, a diffusion mechanism is statistically extracted from a large sample of molecular trajectories. Based on these insight, we set our next goal at developing predictive theories for materials screening and selection in a wide range of applications, including membrane-based separation and the manufacturing of polymer thin films.

The second topic focuses on a polymer solution and its behaviors in a macroscopic complex flow. Here, the polymer conformation is described at the continuum level, which is coupled with the momentum and mass balance of the flow. Numerical solutions of this coupled system are analyzed to investigate an experimentally-established phenomenon: polymer additives, at extremely low concentrations, can significantly reduce the energy consumption of turbulent flows. In particular, we propose a physical framework that offers a consistent explanation for a long-standing puzzle in this area: the origin of a universal upper limit for this polymer drag reduction phenomenon. These understanding will lead to innovative solutions for energy conservation in fluid transport.

BIOGRAPHY: Dr. Li Xi is currently a postdoctoral associate at the Massachusetts Institute of Technology and the Novartis-MIT Center for Continuous Manufacturing, working in the group of Prof. Bernhardt L. Trout. He received his B.S. in Chemical Engineering from Zhejiang University in China, and Ph.D. from University of Wisconsin-Madison, under the supervision of Prof. Michael D. Graham. His research interest focuses on adapting and combining a broad range of computational tools to tackle important problems in the areas of soft materials and complex fluids. His Ph.D. research focused on the flow behaviors of polymer solutions, including studies on both microfluidic and turbulent flows. Among his contributions in this area is a fundamentally new framework that explains the most important unsolved problem in polymeric turbulence. His current research at MIT concerns glassy amorphous polymers, and he has systematically delineated the mechanism by which solvent molecules travel through a glassy polymer matrix.

Refreshments will be served.