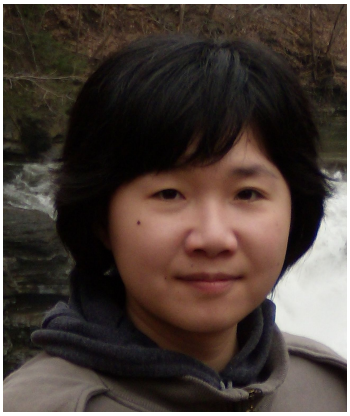
Department of Chemical Engineering Seminar Series

Predictive Theoretical Modeling of Complex Fluids: From Advanced Functionalized Materials to Targeted Vascular Drug Delivery



Hsiu-Yu Yu
Postdoctoral Researcher
Department of Anesthesiology and Critical Care
Department of Chemical and Biomolecular Engineering
University of Pennsylvania

Monday, February 2, 2015
Seminar: 4:00-5:00 p.m.
Physics/Astronomy Auditorium (PAA) A118
Reception: 3:30 p.m. – PAA A118 Lobby

Abstract

Theoretical modeling provides insights into fundamental understanding of many complex systems ranging from hybrid nanocomposites to biological fluids. In this talk, I will demonstrate the application of classical theoretical modeling in two nanoparticle systems. In the first example, the equilibrium structure and the transport properties of solvent-free nanoparticle-organic hybrid materials (NOHMs) are investigated by a classical density-functional approach for model hard spheres with tethered bead-spring oligomers. Through rigorous, first-principle formulation and minimization of the system free energy, the predicted material properties not only agree with relevant molecular dynamics simulations and experiments, but further guide the advanced applications such as carbon capture using NOHMs. In the second example, the binding of ligand-functionalized nanocarriers to specific receptor proteins in targeted vascular drug delivery is studied using a combined framework of generalized Langevin equations and dynamical density-functional theory. Specifically, the effects of red-blood-cell-driven margination, glycocalyx resistance, receptor protein relaxation, hydrodynamic interactions, and thermal fluctuations on the nanocarrier-cell adhesion landscape are characterized. This enables the determination of the nanocarrier attachment/detachment rates under different physiological conditions in targeted drug delivery, and may be used to predict the biodistribution.

Speaker Biography

Hsiu-Yu Yu is a postdoctoral researcher in the Department of Chemical and Biomolecular Engineering at the University of Pennsylvania. She received her B.S. and M.S. degrees in Chemical Engineering from National Taiwan University in 2004 and 2006, respectively. She earned her Ph.D. degree in Chemical Engineering from Cornell University in 2012 under the supervision of Professor Donald L. Koch. Her thesis investigated the fundamental properties of solvent-free nanoparticle-organic hybrid materials using classical density-functional theories. Subsequently, she joined Professor Ravi Radhakrishnan's lab at Penn developing next-generation pharmacodynamic models for drug delivery. Dr. Yu's primary research interests are utilizing statistical mechanics and fluid mechanics with engineering models to understand how macroscopic properties of complex fluids are related to microscopic physics, and applying the understanding to drive the innovation toward advanced applications.