Penn Engineering | Chemical and Biomolecular Engineering
University of Pennsylvania

Fall 2022 CBE Seminar Series

SCOTT MILNER

"Using Simulations to Predict Miscibility"

Wednesday
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3:30 PM
Wu and Chen Auditorium
Levine Hall

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The Pennsylvania State University

ABSTRACT

A key property of all fluid mixtures is the extent of miscibility, which is ultimately governed by packing of and interactions between species, but is challenging to predict from molecular structure. Atomistic simulations would appear to be well suited for such predictions, because with well-tuned interaction potentials, such simulations can reasonably represent the ensemble of configurations for a molecular mixture. However, while the system energy can be computed directly from atomic positions and velocities and averaged over a simulation trajectory, the entropy is a property of the ensemble as a whole, and cannot be so calculated. Thus special techniques are required to compute free energies and chemical potentials, on which miscibility depends. In this talk, I will describe a succession of methods developed over the last six years in my group to predict miscibility, first for idealized "bead-spring" polymer blends, then for real polymers of similar architecture, then for mixtures of real molecules of arbitrary structure. Besides presenting the methods themselves, I will describe how successive methods occurred to us as we struggled with the limitations of each, which serves as an illustrative example of progress in research.

BIO

Scott Milner joined the Chemical Engineering faculty at Penn State University in January 2008, where he holds the William H. Joyce Chair. Milner was a research physicist at ExxonMobil Corporate Strategic Research from 1989 to 2008. He received his Ph.D. in theoretical condensed-matter physics from Harvard University in 1986, after which he held postdoctoral positions at Exxon and AT&T Bell Labs before returning to Exxon in 1989. In 1993 Milner was awarded the John H. Dillon Medal of the American Physical Society for work on polymer brushes, copolymer mesophase ordering, and effects of flow on polymer solutions. He is an APS Fellow, served on the Executive Committee of the APS Division of Polymer Physics from 1999-2003, and as division councillor from 2006-2012. In 2015-16, Milner was a Fellow at the Radcliffe Institute at Harvard University.