

## Séminaire

**Jeudi 23 mai 2024 à 10h30**  
**Amphithéâtre Henri Benoît**

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# Using Simulations to Predict Miscibility

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.

### Brief bio

Scott Milner joined the Chemical Engineering faculty at Penn State University in January 2008, where he holds the William H. Joyce Chair. He 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. His current research interests include semiconducting polymer structural and electronic properties, polymer membranes for water purification and energy storage, and solvation effects on reaction rates in electrocatalysis.

*Les personnes souhaitant rencontrer S. Milner sont priées de prendre contact avec A.N. Semenov.*