Séminaire

Jeudi 23 mai 2024 à 10h30

Amphithéâtre Henri Benoît

Scott Milner

Chem. Engineering, Pennsylvania State University

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.

Séminaire

Mardi 14 mai 2024 à 11h00
Amphithéâtre Henri Benoît

Scott Milner

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Predicting structural and electronic properties of donor-acceptor interfaces

Organic semiconducting polymers and oligomers are promising candidates for photovoltaic materials alternative to silicon. These materials are prepared as “bulk heterojunctions”, resulting from demixing of donor and acceptor chains. In operation, photons are absorbed to create excitons, which diffuse to a nearby donor-acceptor interface, where the difference in electron affinities helps to separate the exciton into free carriers, that must then transport to the electrodes. The materials are disordered, which complicates the prediction of electronic properties, such as the optical gap (energy to form an exciton), binding energy of excitons to the D-A interface, and structure and dynamics of polarons in the donor and acceptor phases. To predict these properties, two computational challenges emerge: 1) generating realistic nanoscale structures with simulations, and 2) computing electronic properties in the presence of disorder. In this talk, I will describe progress on both fronts: 1) fast simulations for stiff molecules that retain atomistic detail, and 2) DFT-parameterized tight-binding models that can describe excitons and polarons in the presence of disorder.

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