ChE Special Guest Seminar
Professor Scott Milner

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Chemical Engineering
Penn State University
University Park, PA

Host: Professor Elizabeth Podlaha-Murphy

Semiconducting polymers for photovoltaics: theoretical challenges for molecular design

Wednesday, March 30th
Shillman 305
11:45am-1:00pm

Sponsored by the Department of Chemical Engineering

Arguably the most pressing technological problem of this century is the replacement of fossil fuels with renewable energy sources, to avoid the worst effects of global warming. Solar electric power is the most promising of many options for renewable energy, and great progress is being made in installing current technology on a meaningful scale. At the same time, there is growing interest in a new generation of "soft" photovoltaic materials, which exploit recent decades of progress in polymer synthesis and morphological control. Among these materials are semiconducting diblock copolymers, in which donor and acceptor polymer blocks self-assemble to create nanoscale domains with plentiful interfaces for exciton separation. Design of these polymers for best device performance leads to critical new challenges for polymer materials theory. Unlike conventional polymers, these new polymers are semiflexible, which has profound consequences for their morphology. Using a combination of molecular dynamics simulations and self-consistent field theory, we can predict how semiflexible polymers are strongly aligned near substrates and interfaces, which may improve transport properties in thin-film devices. And unlike conventional semiconductors, electronic transport properties are strongly influenced by molecular disorder. Combining density functional theory, coarse-grained tight binding models, and atomistic MD simulations, we can make testable predictions of how conformational disorder effects electronic structure and ultimately transport in these promising materials.

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. Milner was selected as a 2015-16 Fellow of the Radcliffe Institute for Advanced Studies at Harvard University.