Rational Design of Block Copolymer Compatibilizers for Ternary Blend Polymer Bulk Heterojunction Solar Cells

In this talk, we discuss our recent work in the context of the use of block copolymers (BCP) as compatibilizers in ternary blend organic photovoltaic devices. While a number of earlier experimental studies have employed BCPs as a means to improve the long-term stability of the donor-acceptor based devices, in our work we pursued the hypothesis that the physico-electro-chemical properties of BCP compatibilizers may be targeted as a handle to modulate the morphology and device characteristics of such systems. In this regard, we developed coarse-grained computer simulation tools, despite being limited in their ability to capture complex interaction features and crystallization phenomena, to serve as a guide to narrow and/or identify parametric regions where morphologies desirable for better exciton and charge transport can be achieved. The output of such morphological predictions were combined with coarse-grained device simulation approaches to identify the overall photovoltaic properties of the ternary blends containing such BCP compatibilizers. Together, such computational studies served to connect the molecular structure and electronic properties of the BCP to the overall device properties and, thereby, enabled a rational molecular design of BCP compatibilizers for organic photovoltaic devices.

Tuesday, Oct. 4, 2016
Lecture at 4:00 p.m.
Room 1610, Engineering Hall
Refreshments will be served at 3:45 p.m.