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Using Molecular Simulations to Link Chemical and Physical Features of Conjugated Polymers and Fullerene Derivatives to Bulk Heterojunction Morphology for Organic Photovoltaics HILARY MARSH, ERIC JANKOWSKI, ARTHI JAYARAMAN, University of Colorado at Boulder — The morphology of blends of conjugated polymers (electron donors) and fullerene derivatives (electron acceptors) strongly affects the charge transport, charge separation and the overall efficiency of organic photovoltaic devices. In this talk we will present coarse-grained molecular simulation studies to understand how molecular-level features such as alkyl side chain length, alkyl side chain spacing along thiophene polymer backbone and fullerene functionalization (and in turn miscibility with the conjugated polymer) affect the blend morphology. Our coarse-grained models are validated by reproducing neat polymer (without acceptors) morphologies observed in experiments, such as lamellae and hexagonally packed cylinders. Furthermore, for blends of conjugated polymers and fullerene derivatives, this work shows how conjugated polymer architecture and acceptor miscibility can be tuned to obtain new blend morphologies with features that are known to enhance efficiency of organic solar cells.

Hilary Marsh
University of Colorado at Boulder

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