Characterization of Charge Transport Networks in Non-fullerene Bulk Heterojunction Thin Films

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Despite their excellent photoelectron-accepting capability and guasi-isotropic intermolecular charge transport, fullerene derivativess have limited absorption in the red and near-IR of the solar spectrum and contribute negligibly to organic photovoltaic (OPV) device photocurrent. A large effort exists to explore nonfullerene small-molecule acceptors that broaden the range of absorbed solar light, however, there is a fundamental lack of understanding between the chemical structure of small-molecule acceptors and the hierarchical morphology of bulk-heterojunction (BHJ) thin films. Two photophysical processes that dictate device performance - charge separation and transport - depend intimately on the hierarchical length scales of phase separation and interpenetrating polymer/small molecule networks. We have used a combination of synchrotron X-ray scattering and transmission electron microscopy to begin elucidating the relationship between blend film microstructure and small molecule chemical structure by using chemical series that interrogate the influence of molecular excluded volume and connectivity as well as self-assembly. To relate the microstructure to charge transport through the small-molecule domains, we have used dark current measurements in diode-configuration devices to investigae the formation of the percolated charge-transport network We find that the film morphology depends sensitively on the combination of polymer host microstructure and small molecule chemical structure, and that the viability of both to efficiently function in photovoltaic devices must be evaluated on an equal footing.