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Correlating microstructure, charge transport and device performance in small molecule organic photovoltaic cells

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Organic semiconductors continue to receive attention for use in photovoltaic cells (OPVs) due to their unique optoelectronic properties and compatibility with high-throughput processing. In these materials, the molecular excited state is a tightly-bound, electron-hole pair known as an exciton. Consequently, the generation of photocurrent requires the efficient dissociation of the exciton into its component charge carriers. Often, this is accomplished using a heterojunction between electron donating and accepting materials. In this work we explore the electrical and structural behavior of uniformly mixed films of boron subphthalocyanine chloride (SubPc) and C_{60} and their performance in OPVs. Device performance shows a strong dependence on active layer donor-acceptor composition with peak efficiency realized at 80 wt.% C_{60}. The origin of this unusual C_{60}-rich optimum composition is elucidated in terms of morphological changes in the active layer upon diluting SubPc with C_{60}. While neat SubPc is found to be amorphous, mixed films containing 80 wt.% C_{60} show clear nanocrystalline domains of SubPc. Supporting electrical characterization indicates that this change in morphology coincides with an increase in the hole mobility of the mixture, with peak mobility observed at a composition of 80 wt.% C_{60}. Cells constructed using this optimum ratio realize a power conversion efficiency of $(3.7\pm0.1)\%$ under 100 mW cm^{-2} simulated AM1.5G solar illumination.