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Design of Bicontinuous Donor/Acceptor Morphologies for Use as Organic Solar Cell Active Layers DYLAN KIPP, Univ of Texas, Austin, JORGE MOK, RAFAEL VERDUZCO, Rice Univ, VENKAT GANESAN, Univ of Texas, Austin — Two of the primary challenges limiting the marketability of organic solar cells are i) the smaller device efficiency of the organic solar cell relative to the conventional silicon-based solar cell and ii) the long term thermal instability of the device active layer. The achievement of *equilibrium* donor/acceptor morphologies with the characteristics believed to yield high device performance characteristics could address each of these two challenges. In this work, we present the results of a combined simulations and experiments-based approach to investigate if a conjugated BCP additive can be used to control the self-assembled morphologies taken on by conjugated polymer/PCBM mixtures. First, we use single chain in mean field Monte Carlo simulations to identify regions within the conjugated polymer/PCBM composition space in which addition of copolymers can lead to bicontinuous equilibrium morphologies with high interfacial areas and nanoscale dimensions. Second, we conduct experiments as directed by the simulations to achieve such morphologies in the PTB7 + PTB7-*b*-PNDI + PCBM model blend. We characterize the results of our experiments via a combination of transmission electron microscopy and X-ray scattering techniques and demonstrate that the morphologies from experiments agree with those predicted in simulations. Accordingly, these results indicate that the approach utilized represents a promising approach to intelligently design the morphologies taken on by organic solar cell active layers.

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