Block Copolymer Compatibilizers for Morphological Control on the Equilibrium Structural Characteristics of Polymer/Fullerene Blends

DYLAN KIPP, VENKAT GANESAN, Univ of Texas, Austin — We develop a single chain in mean field model for the equilibrium morphologies of solar cells based on the homopolymer/block copolymer/fullerene blend. Using our model, we study the ability of the block copolymer compatibilizer to provide morphological control on the domain and interfacial characteristics of the equilibrium structures. We focus our efforts on the case of a semiflexible homopolymer and a semiflexible/flexible diblock copolymer as these are emblematic of the kinds of molecules used in photovoltaic applications. Our results reveal a novel progression of morphologies in transitioning the ternary composition space, the rigidity of the semiflexible chains, and the flexible block ratio of the diblock copolymer. To elucidate the morphologies, we first present a series of ternary phase diagrams and then use a simple morphological characterization scheme to evaluate the domain sizes and interfacial quantities characterizing our equilibrium structures.