Dissipative Particle Dynamics Studies of Rod-Coil Polymer Nanocomposites\textsuperscript{1} CHARLES STARBIRD, DONGSHENG ZHANG, ARTHI JAYARAMAN, University of Colorado at Boulder — Organic solar cell efficiency depends strongly on the morphology within the active layer consisting of donor (e.g., conjugated polymer) and acceptor (e.g., fullerene derivative) materials. Higher device efficiency can be obtained if the donor-acceptor morphology has high interfacial area, small domains, and continuous pathways. One way to control donor-acceptor morphology is via copolymerization of the conjugated “rod” polymer and an acceptor “coil” block. Past theory and experimental studies have characterized the phase behavior of pure rod-coil block copolymers. In this talk we will present dissipative particle dynamics simulation studies of composites of symmetric rod-coil block copolymers and nanoscale additives of varying selectivity (rod-, coil- and non-selective). With increasing volume fraction of non- and rod- selective nanoadditives we see a shift in the liquid crystalline and microphase transitions to lower temperatures, and new morphologies (e.g. helical twists in rod block domain and zig-zag lamellae) not seen in pure symmetric rod-coil polymers. These shifts in phase transition are explained by where the nanoadditives reside, which in turn is dictated by where the system can maximize enthalpic gain and minimize loss of nanoadditive translational entropy.

\textsuperscript{1}DOE Early Career Award DE-SC0003912

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Date submitted: 01 Dec 2011