

Abstract Submitted  
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**Using theory and simulation to link molecular features of nanoscale fillers to morphology in polymer nanocomposites** ARTHI JAYARAMAN, TYLER MARTIN, University of Colorado, Boulder — Polymer nanocomposites are a class of materials that consist of a polymer matrix embedded with nanoscale fillers or additives that enhance the inherent properties of the matrix polymer. To engineer polymer nanocomposites for specific applications with target macroscopic properties (e.g. photovoltaics, photonics, automobile parts) it is important to have design rules that relate molecular features to equilibrium morphology of the composite. In the first part of the talk I will present our recent theory and simulation work on composites containing polymer grafted nanoparticles, showing how polydispersity in graft and matrix polymers (physical heterogeneity) can be used to stabilize dispersion of the nanoparticles within a polymer matrix. In the second part of the talk I will present our recent work linking block-copolymer functionalization to the nanoparticle location in a polymer matrix consisting of homopolymer blends.

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