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Theory and Simulation Studies of Effect of Entropic and Enthalpic Driving Forces on Morphology in Polymer Grafted Particle Filled Nanocomposites TYLER MARTIN, Chemical and Biological Engineering - University of Colorado at Boulder, Chemical and Biomolecular Engineering - University of Delaware, ARTHI JAYARAMAN, Chemical and Biomolecular Engineering - University of Delaware, Materials Science and Engineering - University of Delaware — 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 it is important to have design rules that relate molecular features to morphologies of the composite. Using theory and simulation, we previously studied polymer nanocomposites with homopolymer grafted particles in a homopolymer matrix with chemically identical graft and matrix polymers. Specifically, we found that increasing the polydispersity in grafted chain lengths or decreasing the graft and matrix chain flexibility stabilizes the dispersed phase of polymer nanocomposites, due to increased wetting of the grafted layer by matrix chains. We now explore composites with chemically different graft and matrix polymers, that allow us to tune in enthalpic driving forces in addition to the entropic driving forces for particle dispersion/aggregation. We vary the grafting density, composition of the graft and matrix polymers, and strength of the attractive interactions between the grafts and matrix monomers, to study their impact on the phase behavior and structure of polymer grafted particles in a polymer matrix.

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