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Polymer Functionalized Nanoparticles in Polymer Nanocomposites

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Significant interest has grown around the ability to control spatial arrangement of nanoparticles in a polymer nanocomposite to engineer materials with target properties. Past work has shown that one could achieve controlled assembly of nanoparticles in the polymer matrix by functionalizing nanoparticle surfaces with homopolymers. This talk will focus on our recent work using Polymer Reference Interaction Site Model (PRISM) theory and Monte Carlo simulations and GPU-based molecular dynamics simulations to specifically understand how heterogeneity in the polymer functionalization in the form of a) copolymers with varying monomer chemistry and monomer sequence, and b) polydispersity in homopolymer grafts can tune effective interactions between functionalized nanoparticles, and the assembly of functionalized nanoparticles.