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Designing Functionalized Nanoparticles for Controlled Assembly in Polymer Matrix: Self consistent PRISM Theory and Monte Carlo simulation Study ARTHI JAYARAMAN, NITISH NAIR, University of Colorado at Boulder — Significant interest has grown around the ability to create hybrid materials with controlled spatial arrangement of nanoparticles mediated by a polymer matrix. By functionalizing or grafting polymers on to nanoparticle surfaces and systematically tuning the composition, chemistry, molecular weight and grafting density of the grafted polymers one can tailor the inter-particle interactions and control the assembly/dispersion of the particles in the polymer matrix. In our recent work using self-consistent Polymer Reference Interaction Site Model (PRISM) theory-Monte Carlo simulations we have shown that tailoring the monomer sequences in the grafted copolymers provides a novel route to tuning the effective inter-particle interactions between the functionalized nanoparticles in a polymer matrix. In this talk I will present how monomer sequence and molecular weights (with and without polydispersity) of the grafted polymers, compatibility of the graft and matrix polymers, and nanoparticle size affect the chain conformations of the grafted polymers and the potential of mean force between the grafted nanoparticles in the matrix.

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