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Effect of Graft Polymer Architecture on the Grafted Layer Structure in Polymer Functionalized Nanoparticles.[1] KEVIN MODICA, TYLER MARTIN, ARTHI JAYARAMAN, University of Delaware, Newark — Tailoring the physical and chemical features of the graft polymer chains in polymer functionalized nanoparticles allows one to tune the grafted layer structure and control the assembly/dispersion of the nanoparticles. While past theoretical and experimental studies have established the underlying polymer physics in polymer functionalized nanoparticles containing linear homopolymer grafts, much less is known about how non-linear polymer architecture impacts the grafted layer structure. Recent advances in synthesis of polymers with complex new architectures has inspired us to look into the effect of graft polymer architecture on the grafted layer and inter-particle interactions. In this talk, we present our recent theory and simulation studies on comb polymer grafted nanoparticles (CPGPs). We use Langevin dynamics to investigate the effect of particle curvature, backbone grafting density, and sidechain length and spacing within comb graft polymers on the grafted layer of a single CPGP in an implicit solvent. We also use PRISM theory to calculate the effective inter-particle interactions in explicit solvent and linear homopolymer matrix as a function of the comb graft polymer design.

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