Ordering of Nanoparticles Mediated by End-Functionalized Triblock Copolymers

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Using molecular dynamics simulations we show that triblock copolymers, designed to have specific affinity for nanoparticles at the chain ends, can successfully mediate assembly of nanoparticle/copolymer composites. We present a detailed investigation of the phase diagram of these nanocomposites as a function of both nanoparticle size and concentration. We find a rich phase diagram with a number of distinct ordered structures. Next to phases such as hexagons or gyroids, regularly observed in copolymer solutions and melts, we find a novel square columnar phase of two interpenetrating line-lattices of micellar cylinders and aligned nanoparticles. We argue that this phase is a realization of the packing problem of binary mixtures of disks. Our study suggests that combining nanoparticles with functionalized block copolymers can provide a simple and efficient tool for assembling novel materials with nanometer scale resolution.