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End-Functionalized Triblock Copolymers as a Guide for Nanoparticle Ordering RASTKO SKNEPNEK, JOSHUA ANDERSON, MONICA LAMM, JOERG SCHMALIAN, ALEX TRAVESSET, Iowa State University and Ames Laboratory — 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. In this talk, we will 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 two striking features. The first is the existence of an unconventional square columnar phase of two interpenetrating line-lattices of micellar cylinders and aligned nanoparticles, and the second is a drastically enhanced stability of the gyroid phase. We interpret the origin of the square columnar phase by making an analogy to the packing of binary mixtures of disks. Based on the analysis of stretching of copolymers we argue that nanoparticles help stabilize gyroid order and drastically widen the region of its stability. 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.

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