

Abstract Submitted
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Stability of the double gyroid phase to nanoparticle polydispersity in polymer tethered nanosphere systems¹ CAROLYN PHILLIPS, CHRISTOPHER IACOVELLA, SHARON GLOTZER, University of Michigan — Recent simulations have shown that aggregating nanospheres functionalized with polymer “tethers” can self-assemble to form the double gyroid phase also seen in block copolymer and surfactant systems. Within the gyroid domain, the nanoparticles pack in icosahedral motifs, stabilizing the gyroid phase in a small region of the phase diagram[1]. We study the impact of nanoparticle polydispersity on the properties of the double gyroid phase [2]. Here we show that a low amount of polydispersity lowers the energy of the phase. A large amount of polydispersity raises the potential energy of the system, disrupts the icosahedral packing, and eventually, destabilizes the gyroid. A study of binary gyroids indicates that the inclusion of a small population of either smaller or larger nanospheres encourages low-energy icosahedral clusters. Using a new measure for determining the volume of a component in a microphase-separated system based on the Voronoi-tessellation, we show that polydispersity compacts the gyroid domain and lowers the average coordination of the nanospheres. [1] Iacovella, et al., PRE, 2007 [2] Phillips, et al., “Stability of the double gyroid phase to nanoparticle polydispersity in polymer tethered nanosphere systems, preprint.

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