

Abstract Submitted  
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**Icosahedral packing of polymer-tethered nanospheres and stabilization of the gyroid phase** C.R. IACOVELLA, A.S. KEYS, M.A. HORSCH, S.C. GLOTZER, Department of Chemical Engineering, University of Michigan — We present results of molecular simulations that predict the phases formed by the self-assembly of model nanospheres functionalized with a single polymer “tether,” including double gyroid, perforated lamella and crystalline bilayer phases. We show that microphase separation of the immiscible tethers and nanospheres causes confinement of the nanoparticles, which promotes local icosahedral packing that stabilizes the gyroid and perforated lamella phases. We present a new metric for determining the local arrangement of particles based on spherical harmonic “fingerprints,” which we use to quantify the extent of icosahedral ordering.

Sharon Glotzer  
Department of Chemical Engineering, University of Michigan

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