128a Phase Diagrams of Self-Assembled Mono-Tethered Nanospheres from Molecular Simulation

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The rich phase behavior of polymer-tethered nano building blocks provides unique opportunities to control the self-assembly of novel structures and materials [1]. We perform Brownian dynamics simulations on model 3-D systems of mono-tethered nanospheres (TNS) to study the equilibrium morphologies formed by their self-assembly in a selective solvent. We present the temperature vs. concentration phase diagram for a system of TNS and propose a dimensionless scaling factor Fv (head-group volume/tether volume) that allows a comparison between the morphologies formed from TNS and traditional surfactants [2]. Nanoparticles are modeled as rigid objects and tethers are modeled as FENE chains. Our predictions show how several factors contribute to the equilibrium morphologies and demonstrate a general approach to manipulate the structure of a material on several length scales, potentially providing a method to design specific functionality into a material.

[1] Zhang Z-L, et al. Tethered Nano Building Blocks: Toward a Conceptual Framework for Nanoparticle Self-Assembly, Nano Letters 3, 1341-1346 (2003)

[2] Iacovella CR, et al. Phase diagrams of self-assembled mono-tethered nanospheres from molecular simulation and comparison to surfactants, preprint. (http://www.engin.umich.edu/dept/che/research/glotzer/documents/TNS_paper_submission.pdf)