4cb Self-Assembly of Anisotropic Tethered Nano Building Blocks

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The advent of nanometer size building blocks provides unique opportunities to create novel materials with specific functionality and physical properties. Self-assembly may prove to be a viable means by which large numbers of nano building blocks can be arranged into such materials with order on several length scales. However, to realize the potentially revolutionary opportunities of bottom up assembly, new strategies are needed to induce the building blocks to self-assemble into predetermined target structures. Here I describe computer simulations in which we use anisotropy as a means to impart assembly "instructions" to nanoparticles. Using simple coarse-grained models we have developed and mesoscopic simulation methods such as Brownian dynamics and dissipative particle dynamics, I present our results of simulations demonstrating how tether number and placement, nanoparticle geometry, solvent selectivity, and tether length impact the final self-assembled structures of tethered rods, spheres, triangular plates, and disks [1-5]. Our studies show that anisotropy indeed can be used to induce the self-assembly of target structures with organization on multiple length scales.

[1] Zhang ZL, Horsch MA, Lamm MH, Glotzer SC, Tethered nano building blocks: toward a conceptual framework for nanoparticle self-assembly, Nano Lett. 2003, 3(10), 1341-1346 [2] Horsch MA, Zhang ZL, Glotzer SC, Tethered Nanoparticles: A New Class of "Macromolecule" for Bio-inspired Materials, Mat. Res. Soc. Symp. Proc., 2004, EXS-1, H2.5.1 [3] Horsch MA, Iacovella CR, Zhang ZL, Glotzer SC, Self-organization of nanoscopic building blocks into ordered assemblies, Mat. Res. Soc. Symp. Proc., 2004, 818, M10.5.1 [4] Horsch MA, Zhang ZL, Iacovella CR, Glotzer SC, Hydrodynamics and microphase ordering in block copolymers: Are hydrodynamics required for ordered phases with periodicity in more than one dimension?, JCP, 2004, 121(22), 11455-11462 [5] Horsch MA, Zhang ZL, Glotzer SC, Self-Assembly of Polymer-Tethered Nanorods, (submitted), 2005