

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Manipulating assembly of nanoparticles by polymer tethers

ZHENLI ZHANG, MARK HORSCH, CHRISTOPHER IACOVELLA, SHARON GLOTZER — A major challenge in nanoscience and nanotechnology is the ability to control and guide the self-assembly of nano building blocks into target structures in a predictable way. In this talk, we use molecular simulation to show how polymer tethers can be used to manipulate the assembly of nanoparticles into various one-dimensional, two-dimensional, and three-dimensional structures. We present results on the self-assembly of polymer-tethered nanospheres, nanorods, and more exotic shapes, and present temperature versus concentration phase diagrams for the nanosphere and nanorod systems. For polymer-tethered nanorods we predict tetragonally perforated lamellar and honeycomb phases, which have been observed experimentally but have not been predicted by any previous theory. We also predict a new phase—a racemic mixture of hexagonally ordered chiral cylinders that self-assemble from these achiral building blocks. For the system of polymer-tethered nanospheres we predict that in contrast to flexible amphiphiles, the nanospheres are locally ordered and there is an increase in the local ordering with an increase in concentration or relative nanoparticle diameter. [1] Zhang, Mark A. Horsch, Monica H. Lamm, and Sharon C. Glotzer, *Nano Lett.*, 3(10), 1341-1346, 2003. [2] Mark A. Horsch, Zhenli Zhang and Sharon C. Glotzer, *Phys. Rev. Lett.*, 95(5), 056106, 2005. [3] Christopher R. Iacovella, Mark A. Horsch, Zhenli Zhang and Sharon C. Glotzer, *Langmuir*, 21(21), 9488, 2005.

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Date submitted: 05 Dec 2005

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