

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Simulations of Nanoparticle Ordering in Polymer Brush/Solvent Mixtures GARY S. GREY, SHENGFENG CHENG, MARK J. STEVENS, Sandia National Laboratories — Organizing nanoparticles into a desired super-structure is crucial for their technological applications. We present molecular dynamics simulations of the assembly of nanoparticles during the evaporation of solvent from 3-component mixtures of nanoparticles and solvent in contact with an end-grafted polymer brush. The organization of nanoparticles strongly depends on their interaction with polymer chains. For relatively weak attraction between the nanoparticles and brush, the nanoparticles straddle the brush surface and form an ordered lattice. For a strong attraction between the nanoparticles and polymer, the nanoparticles are engulfed inside the brush and the packing quality diminishes, because the lateral diffusion of the nanoparticles is suppressed. The opposite trend is observed in the case in which the polymer chains are not grafted to a substrate. In this case, a layer of nanoparticles is entrapped in the concentrated polymer film at the interface and assemble into a close-packed hexagonal lattice for strong mutual attraction, while for weak interactions the nanoparticles are mostly dispersed in the relatively solvent-rich solution below the interface and remain disordered.

Gary S. Grest
Sandia National Laboratories

Date submitted: 09 Nov 2012

Electronic form version 1.4