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Ordering Nanoparticles with Polymer Brushes SHENGFENG CHENG, Virginia Polytechnic Institute and State University, MARK STEVENS, GARY GREST, Sandia National Laboratories — Ordering nanoparticles into a desired super-structure is crucial for their technological applications. We use molecular dynamics simulations to study the assembly of nanoparticles with polymer brushes randomly grafted to a plane surface and with varying densities. In the starting state, the nanoparticles are mostly dispersed in the solvent that wets the polymer brush. After the solvent is evaporated, the nanoparticles either enter the brush or straddle the top of the brush, depending on the strength of the nanoparticle/brush interaction. In the case of engulfed nanoparticles, a 2-dimensional array is only formed when the brush density is finely tuned to accommodate just a single layer of nanoparticles. When the brush density is higher or lower than this optimal value, the packing of nanoparticles shows large fluctuations in space and its quality diminishes. In the case of weak nanoparticle/brush interactions, a hexagonal packing with almost no defects is always found as long as the brush density is higher than some critical value. We also report an interesting healing effect of nanoparticles weakly interacting with the brush that can make a low-density brush more uniform.

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