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Control of nanoparticle formation using the constrained dewetting of polymer brushes THOMAS LEE[1], School of Chemsitry, The University of Sydney, Camperdown, NSW 2006, Australia, SHAUN C. HENDY, MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Physics, University of Auckland, Auckland 1142, New Zealand, CHIARA NETO, School of Chemsitry, The University of Sydney, Camperdown, NSW 2006, Australia — We have used coarse-grained molecular dynamics simulations to investigate the use of pinned micelles formed by the constrained dewetting of polymer brushes to act as a template for nanoparticle formation. The evaporation of a thin film containing a dissolved solute from a polymer brush was modeled to study the effect of solubility, concentration, grafting density, and evaporation rate on the nucleation and growth of nanoparticles. Control over particle nucleation could be imposed when the solution was dilute enough such that particle nucleation occurred following the onset of constrained dewetting. We predict that nanoparticles with sizes on the order of 1 nm to 10 nm could be produced from a range of organic molecules under experimentally accessable conditions. This method could allow the functionality of organic materials to be imparted onto surfaces without the need for synthetic modification of the functional molecule, and with control over particle size and aggregation, allowing for the preparation of surfaces with useful optical, pharmaceutical, or electronic properties.

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