Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Patterned Substrates to Direct Self-Assembly of Particle Monolayers MARK FERRARO, THOMAS TRUSKETT, ROGER BONNECAZE, The University of Texas at Austin — As current lithographic techniques approach practical engineering limits for resolution, directed self-assembly of nanoparticles becomes an attractive scalable nanomanufacturing process for creating ordered arrays of particles at a variety of length scales that could be used both as patterning agents and functional materials. However the roles of interparticle forces and external fields on directed self-assembly of particles is not well understood. In this presentation density functional theory (DFT) and Monte Carlo (MC) simulations are used to explore the use of larger scale patterned substrates to drive smaller scale directed self-assembly of particle monolayers. Square patterned substrates with varying energy barriers at length scales N-fold the final desired particle pitch are considered (N>1). Ranges of N, bulk density and patterned substrate field strength are identified that disrupt the entropically favored hexagonally close-packed lattice and promote square lattice formation for hard-spheres. Monte Carlo simulations are then employed to verify the predictions from DFT and to further analyze the self-assembly process. These DFT and MC results are used to discuss and define the energetically and kinetically accessible spaces for non-hexagonal lattice formation.

Mark Ferraro
The University of Texas at Austin

Date submitted: 15 Nov 2013 Electronic form version 1.4