Computational Design Tools for Directed Self-Assembly of Particles on Surfaces

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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. Manipulation of interparticle forces and external fields provide powerful means to direct self-assembly of particles, but the rational design is lacking. Here we develop computational tools based on density functional theory (DFT), Monte Carlo and molecular dynamics (MD) simulations to design larger scale patterned substrates to drive smaller scale precision directed self-assembly of particle monolayers. The technique is demonstrated with square patterned substrates with varying energy barriers at length scales N-fold the final desired particle pitch (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. The effects of interparticle forces and other geometries of patterned substrates are also discussed. The DFT tool is also shown to be a powerful inverse design tool where larger scale patterns and interparticle forces are determined to achieve desired 2D structures, such as the Kagome or honeycomb lattices.