Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Computational Analysis of DNA-Mediated Crystallization of Binary Colloidal Superlattices TALID SINNO, RAYNALDO SCARLETT, MARIE UNG, JOHN CROCKER, University of Pennsylvania — Colloidal self-assembly provides a potential avenue for the design of novel devices with unique optical and structural properties. Colloidal systems also provide useful insights into fundamental mechanisms of phase transitions such as crystal nucleation, growth and melting that are otherwise difficult to probe in atomic systems. A promising approach for realizing highly tunable colloidal assembly is to graft single-stranded DNA oligomer brushes onto the surfaces of particles in order to create attractive interactions between them. Using this approach, micro- and nanoscale particles have now been successfully assembled into several crystalline phases, including ordered, binary superlattice structures. Here, we apply Monte Carlo simulations and free energy calculations to generate a detailed picture for the assembly binary superlattice crystals. The interparticle potential used to perform the calculations was generated specifically for DNA-mediated interactions and verified by measurements. We develop a pseudo-phase diagram for the binary superlattice system which includes both thermodynamic and kinetic influences. The predictions of the pseudo-phase diagram are validated using direct simulations of crystal nucleation. Finally, we discuss recent findings related to diffusionless transformations in growing superlattice crystals that may be important in experiments aimed at growing these structures.

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Date submitted: 19 Nov 2010 Electronic form version 1.4