Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

The Role of Interaction Heterogeneity in the Self-Assembly of DNA-Functionalized Colloids TALID SINNO, IAN JENKINS, JOHN CROCKER, Univ of Pennsylvania — Heterogeneity is generally considered to be a detrimental factor for the self-assembly of colloidal particles into ordered structures. While this is well-established for certain types of heterogeneity such as size polydispersity, here we show, using a combination of equilibrium and non-equilibrium simulations, that heterogeneity in the pairwise interaction strength among a collection of particles may in fact be useful for nucleation of crystalline phases. In particular, we consider interaction heterogeneities that may arise from density variations of DNA oligomers grafted on the surface of sub-micron spherical particles to drive self-assembly. The beneficial impact of interaction heterogeneity is shown to arise from a synergistic combination of two effects. First, we employ umbrella sampling simulations to show that heterogeneity strongly lowers the free energy barrier associated with the nucleation of crystals by the formation of strongly-bound small clusters. Concurrently, non-equilibrium growth simulations show that variations in the interaction strength between particles inhibit gelation and polycrystallinity by keeping the number of such nuclei low, allowing individual nuclei to grow unhindered.

Talid Sinno
Univ of Pennsylvania

Date submitted: 22 Nov 2016 Electronic form version 1.4