Abstract Submitted
for the MAS17 Meeting of
The American Physical Society

Computational study of DNA-mediated self-assembly using coase-grained model RUNFANG MAO, JEETAIN MITTAL, Lehigh Univ — The ability to rationally design and synthesize complex nano-, micro-, and hierarchically structured materials with tunable functionality represents a holy grail that holds exciting promise for revolutionizing materials applications spanning catalysis, molecular sensing, drug delivery, molecular and charge manipulation, and beyond. Such applications hinge upon precise control over morphology, topology, material connectivity, and function, and demand accommodation of a wide range of materials compositions spanning organic, inorganic, and hybrid structures. One of the most promising approach to achieve such unprecedented control over colloidal self-assembly is to use DNA-mediated interactions between particles functionalized with partially complementary DNA sequences. In general, DNA functionalized particles have several adjustable parameters: the hybridization interaction strength, temperature, DNA chain length and so on. Using molecular dynamics simulations of a coarse-grained model developed specifically to study such systems, we show that variations in these key factors leads structure from amorphous to crystallization. In addition, the optimized design parameters that favored crystallization is carefully investigated.

Runfang Mao
Lehigh Univ

Date submitted: 28 Sep 2017 Electronic form version 1.4