

MAR12-2011-008272

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Structural Diversity of DNA-Coated Particle Assemblies

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Custom designed nanoparticles (NP) or colloids with specific recognition offer the possibility to control the phase behavior and structure of particle assemblies for a range of applications. One approach to realize these new materials is by attaching DNA to a core particle; the hybridization of double-stranded DNA between particles results in the spontaneous assembly of higher-order structures. Control of the assembled state can be achieved by adjusting several parameters, including sequence selectivity, DNA link orientation, DNA length and flexibility, and the balance between the length of links and non-specific repulsive interactions. I will discuss the results of a coarse-grained molecular model for DNA-linked nanoparticles that helps to rationalize experimental findings and demonstrate new routes to control the assembled structure. We examine how the number and orientation of strands affects the structure, phase behavior, and dynamics. We show that it is possible to realize unusual phase diagrams with many thermodynamically distinct phases, both amorphous and crystal. We further examine the parameters that control the pathways of assembly, which are critical to avoid kinetic bottlenecks. Finally, we discuss strategies to create highly anisotropic structures using both isotropic and anisotropic core units.