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Understanding the Structure and Phase Behavior of Model DNA-Linked Nanoparticles by Monte Carlo Simulations. JUAN ARAQUE, Rice University, ATHANASSIOS PANAGIOTOPOULOS, Princeton University, MARC ROBERT, Rice University — The high specificity and selectivity of DNA hybridization makes nucleic acid recognition a powerful tool for bottom-up assembling approaches. Here, we propose a coarse-grained model to address the question of how nanoparticles tethered with single stranded DNA self-assemble in solution. Our approach employs a computationally efficient discretization of hard-core interactions and a high-coordination lattice, in combination with parallel tempering and multicanonical Monte Carlo simulations. This simplified model of DNA strands not only accounts for all physically relevant interactions, but also enables a significant reduction of the problem dimensionality. We discuss the effects of a number of system parameters and assembling architectures on the equilibrium structures and phase behavior. In addition, we establish the relation of these results with experimental observations.

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