Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

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.

Juan Araque
Rice University

Date submitted: 02 Dec 2007 Electronic form version 1.4