Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Hybridization Pathways and Mechanisms of Model DNA Oligonucleotides in Solution. JUAN ARAQUE, Rice University, ATHANASSIOS PANAGIOTOPOULOS, Princeton University, MARC ROBERT, Rice University — We propose a coarse-grained lattice model of short DNA strands to investigate the microscopic pathways and mechanisms of oligonucleoides hybridization in solution. The extent to which hybridization in solution conforms to two-state thermodynamics is also analyzed. Monte Carlo simulations with parallel tempering are performed to estimate the equilibrium population of single- and double-stranded states and the associated free-energy landscapes. Sequence complexity is shown to largely dominate the nucleation and helix propagation pathways. The two-state nature of the transition is found to exhibit strong sequence dependence. Although the model predictions are consistent with classical cooperativity signatures, stable intermediates appear, in violation of the two-state assumption.

Juan Araque
Rice University

Date submitted: 27 Nov 2007 Electronic form version 1.4