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Molecular Simulations of DNA Hybridization in Solution and in Microarrays. JUAN ARAQUE, Rice University, ATHANASSIOS PANAGIOTOPOULOS, Princeton University, MARC ROBERT, Rice University — Nucleic acid hybridization describes a thermodynamic transition in which a single-stranded DNA molecule associates with its complementary sequence. A comprehensive understanding of the thermodynamic behavior of this process can be achieved by computer simulation. However, the collective behavior of DNA hybridization in solution and on grafted surfaces exhibits disparate time and length scales that make atomistic simulations technically unfeasible. We propose a coarse-grained model where DNA strands are described by the single-site bond-fluctuation model on a cubic lattice. Our approach incorporates physically relevant features such as the sequence and orientation dependence of base-stacking and base-pairing interactions. We perform parallel tempering Monte Carlo simulations of DNA oligomers in the canonical ensemble. We explore how chain length, interaction heterogeneity, chain stiffness, and surface density alter the location of the melting temperature and the width of the transition. The model allows the determination of the free energy change associated with the grafting of probe chains onto the array surface with respect to the free probes in solution. Overall, the thermodynamic behavior predicted is in qualitative agreement with experimental observations both in solution and in microarrays.

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