MAR17-2016-020329

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Simulations of self-assembling DNA

JONATHAN DOYE, University of Oxford

The ability of complementary sequences of DNA to self assemble has been harnessed by DNA nanotechnology to create an extremely impressive array of DNA nanostructures. Even now, over ten years since Rothemund's first smiley-faced DNA origami appeared on the cover of Nature, it seems remarkable that such complex structures can form so easily. As probing the mechanisms of assembly is experimentally difficult, molecular simulations can potentially provide important microscopic insights. In this talk, I will describe our attempts to uncover the fundamentals of DNA self-assembly using oxDNA, a coarse-grained model of DNA developed in Oxford. Starting from a consideration of the hybridization of two strands to form a single duplex, I will consider the assembly of progressively more complex structures, including the protein-like folding of a single strand of DNA, DNA origami and DNA bricks. A particular emphasis will be on the complexities that arise from the polymeric and double helical nature of DNA, such as wrapping, threading, and kinetic traps where further assembly progress is topologically inhibited.