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DNA Self-Assembly and Computation Studied with a Coarse-grained Dynamic Bonded Model

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We study DNA self-assembly and DNA computation using a coarse-grained DNA model within the directional dynamic bonding framework {[}C. Svaneborg, Comp. Phys. Comm. 183, 1793 (2012){]}. In our model, a single nucleotide or domain is represented by a single interaction site. Complementary sites can reversibly hybridize and dehybridize during a simulation. This bond dynamics induces a dynamics of the angular and dihedral bonds, that model the collective effects of chemical structure on the hybridization dynamics. We use the DNA model to perform simulations of the self-assembly kinetics of DNA tetrahedra, an icosahedron, as well as strand displacement operations used in DNA computation.

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