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Effect of Backbone Design on Hybridization Thermodynamics of Oligo-nucleic Acids: A Coarse-Grained Molecular Dynamics Simulation Study AHMADREZA F. GHOBADI , Department of Chemical and Biomolecular Engineering, University of Delaware, Newark DE 19716, ARTHI JAYARAMAN , Department of Chemical and Biomolecular Engineering, Department of Material Science and Engineering, University of Delaware, Newark DE 19716 — DNA hybridization is the basis of various bio-nano technologies, such as DNA origami and assembly of DNA-functionalized nanoparticles. A hybridized double stranded (ds) DNA is formed when complementary nucleobases on hybridizing strands exhibit specific and directional hydrogen bonds through canonical Watson-Crick base-pairing interactions. In recent years, the need for cheaper alternatives and significant synthetic advances have driven design of DNA mimics with new backbone chemistries. However, a fundamental understanding of how these backbone modifications in the oligo-nucleic acids impact the hybridization and melting behavior of the duplex is still lacking. In this talk, we present our recent findings on impact of varying backbone chemistry on hybridization of oligo-nucleic acid duplexes. We use coarse-grained molecular dynamics simulations to isolate the effect of strand flexibility, electrostatic interactions and nucleobase spacing on the melting curves for duplexes with various strand sequences and concentrations. Since conjugation of oligo-nucleic acids with polymers serve as building blocks for thermo-responsive polymer networks and gels, we also present the effect of such conjugation on hybridization thermodynamics and polymer conformation.

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