Chemically-controlled DNA nanoswitch

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In order to understand the stabilizing interactions in B-DNA and supramolecular systems inspired by DNA, we have analyzed a stack of two identical base pairs at a distance of 3.4 Å.[1] Our analyses provide detailed insight into the role and relative importance of the various types of interactions, such as hydrogen bonding, π-π stacking interactions, and solvation.[2] Interestingly, we can show that all stacked base pairs benefit from a stabilization by 6-12 kcal/mol if stacked base pairs are twisted from 0° to the mutually twisted stacking configuration that occurs in B-DNA. We also show that so-called "diagonal interactions" in the stacked base pairs are crucial for understanding the stability of B-DNA, in particular, in GC-rich sequences. Such analysis provides further insight for building a chemically-controlled nanoswitch based on the GC Watson-Crick pair,[3] a supramolecular complex that can be switched in terms of bond strength and shape through substitution, even under microsolvation.[4]

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