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The role of stacking interactions in the folding dynamics of DNA hairpins MARTA SALES-PARDO, Northwestern University, JON WIDOM, Northwestern University, LUIS AMARAL, Northwestern University — To gain a deeper insight into cellular processes such as transcription and translation, one needs to uncover the mechanisms controlling the configurational changes of nucleic acids. As a step toward this aim, we present here a novel mesoscopic-level computational model that provides a *new window* into nucleic acid dynamics. We validate the model by studying DNA hairpins, single-stranded molecules with two complementary segments ("stems") linked by a non-complementary "loop." Our model reproduces experimental observations and enables us to monitor the configurational dynamics of hairpins, providing clear evidence of a "zipping" process in the closing toward the native configuration. In addition, our model allows us to demonstrate that there is a preferred zipping pathway for folding which is both the most frequent and the fastest way for the hairpin to fold. Most importantly, our model allows us to tune the importance of the different interactions in the nucleotides and uncover the role of stacking interactions as the driving force in the zipping dynamics.

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