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Modeling the Forced Extension of Nicked DNA ALEXANDER BALAEFF, STEPHEN CRAIG, DAVID BERATAN, Department of Chemistry, Duke University — The design and study of DNA-based nanodevices has been a topic of considerable interest in the last decade. While the applications of classical continuous DNA structures have been thoroughly studied, nicked DNA structures, i.e., ones that contains breaks ("nicks") in one or both DNA backbone chains, have received much less attention. Recently, Kersey et al. (JACS, 2004) reported the force spectroscopy of long DNA chains with periodic nicks, self-assembled from short DNA oligomers. We attempt to model the experimental force-extension profiles in a series of steered molecular dynamics simulations. The simulated all-atom model of a basic unit of the long self-assembled chain, a 16bp-long DNA segment with a nick in the middle of one strand, is extended by applying either a constant force or a moving harmonic potential to the DNA ends. The computed force-extension profiles are compared to those for a non-nicked DNA; the dynamics of structural changes in the nicked DNA during the forced extension is discussed. A theoretical framework is established to link the extension and rupture in the simulated basic unit to the corresponding events in the long self-assembled chain.

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