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**Molecular dynamics simulation of DNA base-pair opening by sharp bending** PEIWEN CONG, Singapore-MIT Alliance, National University of Singapore, LIANG DAI, Singapore-MIT Alliance for Research and Technology, National University of Singapore, JOHAN R.C. VAN DER MAAREL, JIE YAN, Physics, National University of Singapore — Many biological processes require sharp bending of DNA. According to worm-like chain model, the bending energy dominates the free energy cost of those processes containing DNA loops shorter than 40 nm, such as DNA wrapping around histones, Lac repressor looping and virus DNA packaging . However, several recent experimental observations suggest that the WLC model s not applicable under tight bending conditions. In full atom molecular dynamics simulations, a double stranded, 20 base-pairs DNA fragment is forced to bend by an external spring. It is found that one or two AT-rich regions are disrupted for sufficiently small end-to-end distance. The disrupted DNA base-pairs separate and usually stack with the neighbouring base-pairs to form a defect. It is shown that these defects are more bendable than the bending rigidity of the duplex in the regular B-form. The simulation suggests a curvature dependent, non-harmonic bending elasticity of the DNA backbone is necessary to describe the DNA conformation under tight bending conditions.

Peiwen Cong
Singapore-MIT Alliance, National University of Singapore

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