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simulation of the DNA force-extension curve GREGORY SHINABERRY, IVAN MIKHAYLOV, ALEXANDER BALAEFF, University of Central Florida — A molecular dynamics simulation study of the force-extension curve of double-stranded DNA is presented. Extended simulations of the DNA at multiple points along the force-extension curve are conducted with DNA end-to-end length constrained at each point. The calculated force-extension curve qualitatively reproduces the experimental one. The DNA conformational ensemble at each extension shows that the famous plateau of the force-extension curve results from B-DNA melting, whereas the formation of the earlier-predicted novel DNA conformation called 'zip-DNA' takes place at extensions past the plateau. An extensive analysis of the DNA conformational ensemble in terms of base configuration, backbone configuration, solvent interaction energy, etc., is conducted in order to elucidate the physical origin of DNA elasticity and the main interactions responsible for the shape of the force-extension curve.

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