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Zip-DNA: A Novel DNA Structure Formed Under Mechanical Stress ALEXANDER BALAEFF, IVAN MIKHAILOV, MALAKHAT TURABEKOVA, University of Central Florida, STEPHEN CRAIG, DAVID BERATAN, Duke University — Zip-DNA is a novel DNA structure predicted by molecular dynamics simulations of forced DNA extension. In the zip-DNA form, the Watson-Crick hydrogen bonds are broken and nucleobases from the opposite DNA strands interdigitate with each other, forming a continuous single-base aromatic stack. The B-Zip DNA structural transition is proposed to be responsible for the famous overstretching plateau on the force-extension curve of DNA. The simulations show that zip-DNA may either self-assemble from force-melted DNA strands or evolve from B-DNA through an earlier recognized S-DNA. Zip-DNA is shown to be consistent with multiple experimental observations; notably, the S-DNA transition state is shown to be a highly disordered state consistent with experimentally measured thermodynamic characteristics of DNA extension. We predict that zip-DNA possesses increased molecular conductivity compared to the B-DNA form and, therefore, may find applications in molecular electronics. A conductive state of a stretched non-complementary double-stranded DNA would, if detected, become a "smoking gun" experiment validating the existence of zip-DNA.

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