

DNA micromechanics and macromolecular organization

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Encoded in the strings of DNA bases that make up the genomes of living species are codes that regulate, control, and describe all sorts of biological processes. The underpinnings of these codes lie in the base sequence-dependent micromechanical properties of DNA, which determine the degree to which the long, threadlike molecule fluctuates and how it responds to the proteins that control its processing and govern its packaging. In order to understand the mechanisms by which DNA base sequence and tightly bound proteins control the biophysical properties of the long, threadlike molecule, we have developed a coarse-grained model, in which the DNA base pairs are treated as rigid bodies subject to realistic, knowledge-based energy constraints, and computational techniques to determine the minimum-energy configurations, intrinsic dynamics, and looping/cyclization propensities of these molecules. The presentation will highlight some of the unique, sequence-dependent spatial information that has been gleaned from analyses of the high-resolution structures of DNA and its complexes with other molecules and illustrate how this information can be used to gain new insights into sequence-dependent DNA polymeric behavior.