393h A New Model for Simulation of Long DNA

Thomas A. Knotts, Nitin Rathore, and Juan J. De Pablo

Over the past several years, single molecule force spectroscopy experiments have provided important insights into the mechanical and conformational stability of DNA. Several descriptions of DNA, from atomistic to continuum, have proven valuable for interpreting the observed behavior. We have found, however, that there is no suitable model for several problems of interest, including various aspects of viral packaging of DNA, bubble formation in double-stranded DNA, and microarray interactions, where the size of the molecules prohibits atomistic representations, but continuum and linear bead-spring models do not contain the required level of molecular detail. In an effort to bridge this gap of length-scales in the multi-scale modeling of DNA, we have developed a united-atom-type description which reduces the complexity of a nucleotide to three beads, one representing the phosphate, one the nitrogen base, and one the sugar. Other beads are also added to represent counterions in solution. This description allows sequence information and base stacking phenomena to be incorporated into the model but permits simulation of DNA molecules that are hundreds of nanometers in length. Following a description of the model, results will be presented on its ability to reproduce experimental findings on the thermal and mechanical stability of DNA. With the model thus validated, results, obtained from Density of States Monte Carlo methods will be presented describing hybridization and how stretching of single stranded DNA affects this process. This latter effect has implications for optimization of DNA microarrays.