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A United Atom Model for Simulation of DNA from Angstroms to Microns in Length THOMAS KNOTTS IV, NITIN RATHORE, JUAN DE PABLO, Department of Chemical and Biological Engineering - University of Wisconsin-Madison — For several years, single molecule pulling experiments have given insights into the stability of DNA. Many descriptions of DNA, from atomistic to continuum, have proven successful at reproducing observed behavior. We have found, however, that there is no suitable model for several problems of interest, including viral packaging of 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 molecular level of detail. Emerging technologies require that mesoscopic models of DNA be developed, capable of describing length scales in the 5 to 500 nm range. One of the main challenges is to preserve a coupling between the phenomena seen at longer length scales (e. g. a persistence length of 50 nm) while incorporating the features needed for smaller scales (e. g. charge effects, geometry, and base specificity). We have developed a coarse grain description of DNA which reduces the complexity of a nucleotide to three interaction sites. The model is capable of describing sequence information, bubble formation, and salt effects in simulations of DNA up to a few microns in length. The predictions are in remarkable, quantitative agreement with experiment, and shed light into the coupling of multiple length scales and interactions to yield unique behaviors and functions.

Thomas Knotts IV
Department of Chemical and Biological Engineering & University of Wisconsin-Madison

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