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Capturing electrostatic interactions explicitly with the 3SPN model for DNA GORDON S. FREEMAN, DANIEL M. HINCKLEY, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — The "Three Sites Per Nucleotide" (3SPN) model for nucleic acid simulation provides a powerful tool for computational studies of biological phenomena. Previously, this model has relied on an implicit representation of the surrounding ionic environment at the level of Debye-Hückel theory. In this work, we eliminate this limitation and implement an explicit representation of ions, both monovalent and divalent. The coarse-grain ion-ion and ion-phosphate$_{DNA}$ potential is adapted after the model of Lenart *et al.* and parameterized to reproduce the key features in the local structure and organization of ions in the bulk and in the presence of DNA. The parameters of the previous generation of 3SPN (3SPN.1) have been modified to reproduce melting temperatures observed experimentally employing a biased parallel tempering scheme. The resulting model is capable of reproducing the local structure observed in fully detailed atomistic simulations as well as the melting temperature of DNA reported experimentally for a range of DNA oligonucleotide lengths, CG-content, Na^+ concentration and Mg^{2+} concentration. The usefulness of the model is demonstrated in the context of confinement of dsDNA within a viral capsid and the exploration of pathways between dehybridized and hybridized DNA.

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