DNA Looping in the Presence of Divalent Counterions, a Simulation Study using a Coarse-grained Model of DNA

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Abstract: DNA looping is an important structure in many biological contexts such as in nucleosome structure, in viral DNA packaging, and present in all aspects of DNA metabolism, including transcription, replication, and recombination. The elastic energy of DNA is an important contribution to the total free energy of the system and there has been many works trying to understand the elastic behavior of DNA. Experimental results for looping of DNA chain with 60 or more nucleotide base pairs (bp) is consistent with the worm-like chain (WLC) model of DNA with proper persistence length. However, for shorter DNA chain, the looping behavior deviates significantly from the WLC result and suggests a possibility of formation of permanent kinks in the DNA chain to relax the elastic stress. In the presence of high valence counterions such as Mg^{+2}, the kink behavior starts at an even larger chain length (about 100bp). In this work, a simulation study of a DNA coarse-grained model is presented to understand the role of divalent counterions in the looping of DNA. It is shown that kinks are transiently formed when DNA loop but they are not permanent in longer DNA chain. However, divalent counterions can stabilize and make the kinks appear permanent.

This work is supported financially by the Vietnam National Foundation for Science and Technology Development (NAFOSTED) contract 103.02-2012.75 and the US National Science Foundation grant CBET-1134398.

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