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Asymmetric Breathing Motions of Nucleosomal DNA and the Role of Histone Tails

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The most important packing unit of DNA in the eukaryotic cell is the nucleosome [1]. It undergoes large-scale structural re-arrangements during different cell cycles [1,2]. For example, the disassembly of the nucleosome is one of the key steps for DNA replication, whereas reassembly occurs after replication. Thus, conformational dynamics of the nucleosome is crucial for different DNA metabolic processes. We perform three different sets of atomistic molecular dynamics (MD) simulations of the nucleosome core particle at varying degrees of salt conditions for a total of 0.7 microseconds simulation time. We find that the conformational dynamics of the nucleosomal DNA tails are oppositely correlated from each other during the initial breathing motions [3]. Furthermore, the strength of the interaction of the nucleosomal DNA tail with the neighboring H2A histone tail modulates the conformational state of the nucleosomal DNA tail. With increasing salt concentration, the degree of asymmetry in the conformation of the nucleosomal DNA tails decreases as both tails tend to unwrap. This direct correlation between the asymmetric breathing motions of the DNA tails and the H2A histone tails, and its decrease at higher salt concentrations, may play a significant role in the molecular pathway of unwrapping. [1] McGinty, R. K, Tan, S. Chemical Reviews 115, 2255 (2015). [2] Muller, M. M, Muir, T. W. Chemical Reviews 115, 2296 (2015). [3] Chakraborty, K., Loverde, S.M. Journal of Chemical Physics 147, 165101 (2017).