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Chemical physics of DNA packaging in a nucleosome core particle ANDREW SPAKOWITZ, BARIZ SUDHANSHU, Stanford University — The fundamental unit of packaged DNA, the nucleosome core particle, contains 146 base pairs of DNA wrapped 1.7 times around a cationic protein complex called the histone octamer. A string of nucleosomes is organized into higher-order structures at several hierarchical levels to form chromatin, a remarkable complex that is compact yet maintains accessibility for gene expression. We develop a theoretical model of the nucleosome core particle in order to extract detailed quantitative information from single-molecule measurements of a single nucleosome under tension. We employ the wormlike chain model to describe the DNA strand as a thermally fluctuating polymer chain. The chain adsorbs on a spool that represents the histone octamer. This model is directly compared to single-molecule experiments conducted in Carlos Bustamante's lab; we find good agreement between our theory and the experimental data. Our model reveals the mechanism that underlies structural transitions that are apparent in the experimental measurements and predicts the conditions where these transitions occur. We proceed to construct a free energy surface to predict the dynamic response in a single-molecule experiment with a time-dependent rate of unwinding the nucleosome. The combination of single-molecule experiments and our theoretical modeling gives detailed information about the specific interactions between DNA and histone proteins.

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