

Abstract Submitted
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DNA in Nanochannels: A Multistage Free Energy Perturbation Approach¹ YANWEI WANG², Soochow University, DOUGLAS R. TREE, KEVIN D. DORFMAN, University of Minnesota-Twin Cities — Nanochannels are ideal platforms for studying the basic physics of confined polymers, using DNA as the model polymer. While the scaling laws for strong (Odijk) and weak (de Gennes) confinement were established decades ago, recent experiments and computer simulations have illuminated the complex physics arising between these limiting cases. To understand fully the transition region between the classical regimes of de Gennes and Odijk, it is necessary to examine the underlying free energy behavior of DNA in nanochannels. This presentation reports our studies on the confinement free energy and other properties of nanochannel-confined DNA by the multistage free energy perturbation (MFEP) technique. Emphases are focused on the methodology, the role of the aspect ratio of the channel on the confinement free energy and the force-extension relation of DNA confined in nanochannels.

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