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Flory theory or the two state cooperativity model: What describes backfolding of DNA in nanotubes? KEVIN DORFMAN, ABHIRAM MURALDIHAR, Univ of Minn - Minneapolis — Currently, there are two explanations available in the literature to describe the extension of semiflexible polymers, such as DNA, confined in nanotubes whose diameter is close to the persistence length. Almost a decade ago, Odijk (Phys. Rev. E, 2008, 77, 060901) used a Flory theory to derive a scaling law for the average extension of a semiflexible polymer confined in such a tube. More recently, Dai et al. (ACS Macro Lett. 1, 1046-1050) applied a two-state cooperativity model along the lines of the Zimm-Bragg model for helix coil transitions to explain the same phenomenon. Although the two theories are fundamentally different, there are simulation results supporting both approaches. In this talk, we will present results from Pruned-Enriched Rosenbluth Method (PERM) simulations of a discrete wormlike chain model, which show strong evidence supporting Odijk's Flory theory. Moreover, we will show that Odijk's scaling theory also predicts the contour length dependence of the chain extension. In contrast, we find that the cooperativity model predicts the average extension correctly only for the molecular weights used to parameterize the model.

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