Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Effect of bending stiffness and confinement on a polymer chain under tension PETER POIER, CHRISTOS N. LIKOS, RICHARD MATTHEWS, University of Vienna — Type II topoisomerase are enzymes that (un)knot DNA. There is experimental evidence that a certain type II topoisomerase preferentially cleaves adenine (A) and thymine (T) rich regions of the DNA. It is believed that AT-rich sequences are more flexible than random ones. This raises the question of whether the flexibility of the preferred cleavage sites of topoisomerase II could play an important role in the regulation of knotting. With this motivation we study the effect of the bending stiffness and confinement on the free-energy cost of a knot in a polymer chain under tension. For the polymer chain we use a coarse-grained model. Via thermodynamic-integration we calculate the change of the free-energy cost of a knot due to modifications of the bending stiffness. The free-energy cost exhibits a minimum at a non-zero value for the bending stiffness. Our simulations suggest that this minimum is related to a suppression of the bending at the points where the strands of the polymer cross in the knotted region. We study how the minimum of the free-energy cost is affected by changing the knot type and introducing a two dimensional confinement for the polymer chain. The results of this work might be of importance for the localization of knots in DNA.

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Date submitted: 12 Nov 2013 Electronic form version 1.4