

# Supplementary Information: Excluded volume effects on semiflexible ring polymers

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## Experimental Preparation

Atomic force microscopy was used to image DNA molecules of different lengths. The three longest chains with with flexibilities  $L/l_p=18.3$ , 30 and 40 were standard plasmids pUC19 (2686 bp), pBR322 (4361 bp), and pSH1 (5930 bp). The shorter chains with  $L/l_p=12.4$  and 4.6 were generated by using T4 DNA ligase to circularize DNA fragments (676 bp and 1769 bp) obtained from the restriction of pUC19 by endonuclease RsaI. The three largest rings were nicked to suppress any supercoiling  $\sigma$ . The two mini-circles were not nicked but their short size ensures that most of them are at their elastic energy minimum without supercoiling  $\sigma = 0$ . pUC19 and pBR322 plasmids as

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well as enzymes were purchased from Fermentas, plasmid pSH1 was provided by S.M Lewis. All DNA preparations were diluted in 1 mM Tris-HCl buffer, pH 7.8, to a final DNA concentration of 1  $\mu\text{g/ml}$ , and  $\text{MgCl}_2$  was added in the DNA solution to a final concentration of 5 mM. For imaging, 10  $\mu\text{l}$  solution were deposited for 10 minutes on a freshly cleave mica surface, rinsed with 3 ml deionized water, and dried under air flow. Images were taken with a Nanoscope III (Veeco) operated in tapping mode (150 to 300 kHz) in air with silicon ultrasharp non-contact tips of a nominal tip radius of  $<10$  nm (NT-MDT Co., Zelenograd, Moscow, Russia). The images were only flattened using the Nanoscope III program. Finally, the two dimensional coordinates of the molecules were recorded using the tracing module of *Ellipse*.<sup>1</sup> The tracked positions  $\vec{r}_i$ ,  $i \in [1, N]$ , along the polymer's contour are then used to calculate size and shape parameters based on the discretized version of the radius of gyration tensor

$$Q_{ij} = \frac{1}{N} \sum_{i=1}^N \vec{r}_i \vec{r}_i - \frac{1}{N^2} \sum_{i=1}^N \vec{r}_j \sum_{i=1}^N \vec{r}_j. \quad (1)$$

## Simulations

To sample the conformations of two dimensional, semiflexible ring polymers Metropolis Monte Carlo simulations is employed. The polymer ring of length  $L$  and persistence length  $l_p$  is discretized as a two dimensional closed polygon of  $N$  segments of length  $a$ ,  $L = Na$ , and direction  $\vec{t}_i$ . The energy associated with each single configuration is given by the discretized version of the wormlike chain model

$$\mathcal{H} = Nk_B T \frac{l_p}{L} \sum_{i=1}^N (1 - \vec{t}_i \vec{t}_{i+1}), \quad (2)$$

with imposed periodic boundary conditions  $\vec{t}_{N+1} = \vec{t}_1$ . The persistence length  $l_p$  is chosen to be the established value for DNA of  $l_p = 50\text{nm}$ .

New configurations are obtained by standard crankshaft move<sup>2</sup> as follows: Two arbitrary vertices of the polymer are selected randomly. A pivot axis is drawn between these two vertices and all segments between them are rotated by 180 degrees around the axis. Finite thickness is imple-

mented by discarding conformations in which tubes of diameter  $d$  around each segment overlap.

The correlation between subsequent polymer configurations is estimated by using the autocorrelation function for the polymer's squared radius of gyration

$$\chi(t) = \frac{1}{t_{max} - t} \sum_{t'=0}^{t_{max}-t} R_g^2(t' - t) R_g^2(t) - \left( \frac{1}{t_{max} - t} \right)^2 \left( \sum_{t'=0}^{t_{max}-t} R_g^2(t + t') \right) \left( \sum_{t'=0}^{t_{max}-t} R_g^2(t) \right), \quad (3)$$

resulting in a correlation time of

$$\tau = \frac{\chi(0)}{\chi(t_{max})}. \quad (4)$$

In our simulations the correlation time has been largely overestimated by values of  $10^6$  for phantom chain simulations and  $10^8$  for simulations with finite thickness.

## References

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