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Numerical study of linear and circular model DNA chains confined in a slit: metric and topological properties

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Advanced Monte Carlo simulations are used to study the effect of nano-slit confinement on metric and topological properties of model DNA chains. We consider both linear and circularised chains with contour lengths in the 1.2--4.8 μm range and slits widths spanning continuously the 50--1250nm range. The metric scaling predicted by de Gennes' blob model is shown to hold for both linear and circularised DNA up to the strongest levels of confinement. More notably, the topological properties of the circularised DNA molecules have two major differences compared to three-dimensional confinement. First, the overall knotting probability is non-monotonic for increasing confinement and can be largely enhanced or suppressed compared to the bulk case by simply varying the slit width. Secondly, the knot population consists of knots that are far simpler than for three-dimensional confinement. The results suggest that nano-slits could be used in nano-fluidic setups to produce DNA rings having simple topologies (including the unknot) or to separate heterogeneous ensembles of DNA rings by knot type.

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