DNA organisation under confinement: hints from topology.

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Abstract

Nanodevices are increasingly used to investigate the impact of spatial restraints on the statics and dynamics of polymers and biopolymers. DNA is ideally suited for such studies both for its applicative potential (nanoconfinement can be used to sort, sieve and sequence DNA) and because its elastic properties can be exploited to elucidate issues of primary interest in polymer science. In fact, the width of presently available confining nanodevices (a channel, a slit, a pit etc.) can be set to compete with one or more of the characteristic lengths of a DNA molecule and hence allow for probing different physical regimes.

Natural questions that may arise in this context are the following:

Which are the effects of geometrical confinement on the metric and topological properties of linear and circular DNAs ?

Is there any relation between the topology-based features of the confined DNA and the multiple scaling regimes (de Gennes, Odjik) conjectures for its average extension ?

Here we present a theoretical study of several aspects of DNA under confinement. This is based on a suitable mesoscopic model of dsDNA which can be studied by advances Monte Carlo simulations and scaling analysis. The results obtained either for nano-slits and nano-channels reveal an interesting characterization of the metric crossover behaviour in terms of knotting probability and complexity of the knot population.

Finally we show that the topological properties of the DNA molecules confined into nano-slits and nano-channles have two major differences compared to three-dimensional confinement as viral capsids. Firstly, the overall knotting probability is nonmonotonic for increasing confinement and can be largely enhanced or suppressed compared to the bulk case by simply varying the slit or channel trasversal dimension. Secondly, the knot population consists of knots that are far simpler than for three-dimensional confinement. The results suggest that nanoslits and nanochannels could be used in nanofluidic setups to produce DNA rings having simple topologies (including the unknot) or to sevie DNA rings according to their knotted state.

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