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(I) Polymers under extreme confinement: Insights from computer simulations

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In recent years, nanofluidic devices have proven extremely useful for characterizing the physical behaviour of biopolymers such as DNA confined to narrow channels and micron-sized cavities. Insight gleaned from experiments using nanochannels is valuable for applications such as optical mapping of elongated DNA. Likewise, studies of multiple DNA molecules in nanocavities have provided insight into the confinement-enhanced entropic force that tends to induce polymer segregation, an effect that likely contributes to segregation of chromosomes in replicating prokaryotes. While simple theoretical models can be used to explain the basic aspects of such behaviour, the experiments are often carried out under conditions where the system lies outside clearly defined scaling regimes. This can give rise to pronounced quantitative discrepancies between theory and experiment. In such cases, computer simulations can provide an effective means to bridge the divide between the theoretical predictions and experimental results. In this talk, I present the results of recent Monte Carlo simulation studies, most of which have been inspired by recent experiments on confined DNA. I examine the effects of channel shape and width on the tendency for single semiflexible chains to form structures such as backfolds and knots. I also examine polymer segregation behaviour of two-chain systems confined to channels or elongated cavities. A key aspect of this work is the explicit calculation of the variation of the configurational free energy with respect to some relevant system parameter such as knot size or inter-polymer overlap. Theoretical treatments typically employ analytical approximations of free energy functions. While the explicitly calculated free energy functions yield qualitatively similar scaling behaviour, the discrepancies between calculated and theoretical scaling exponents can be appreciable. Quantifying these discrepancies should be of value in the interpretation of experimental results.

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Keyword-2

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Keyword-3

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