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Conformational free energy of polymers under confinement

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An understanding of the physical properties of polymers in confined environments is essential for the development of nanofluidic devices for DNA analysis, as well as for understanding the organization of bacterial chromosomes. Theoretical treatments of the dynamical behaviour of confined polymers often employ analytical approximations of the conformational free energy. Monte Carlo (MC) computer simulation methods provide an effective means to directly measure the free energy for simple model systems and test these approximations. In this study, we employ MC simulations measure the free energy for linear, ring, and star polymers subject to cylindrical confinement. The free energy is measured as a function of intramolecular overlap along the cylinder axis, in the case of single-polymer systems, and intermolecular overlap for two-polymer systems. We examine the variation of the free energy functions with polymer length, stiffness and confinement dimensions. The results are compared with theoretical predictions using the de Gennes blob model, and we identify the parameter regime in which this scaling theory is valid. Finally, we discuss the relevance of the results to the following phenomena: the unfolding of cylindrically confined DNA, the arm-retraction relaxation mechanism of star polymers, and entropic separation of confined ring polymers.

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