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Entropic force of cone-tethered polymers interacting with a planar surface

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Computer simulations are used to characterize the entropic force of one or more polymers tethered to the tip of a hard conical object that interact with a nearby hard flat surface. Pruned-enriched-Rosenbluth-method (PERM) Monte Carlo simulations are used to calculate the variation of the conformational free energy, F, of a hard-sphere polymer with respect to cone-tip-to-surface distance, h, from which the variation of the entropic force, $f \equiv |dF/dh|$, with h is determined. We consider the following cases: (1) a single freely-jointed tethered chain, (2) a single semiflexible tethered chain, and (3) several freely-jointed chains of equal length each tethered to the cone tip. The simulation results are used to test the validity of a prediction by Maghrebi {\it et al.} (EPL, {\bf 96}, 66002(2011); Phys. Rev. E {\bf 86}, 061801 (2012)) that $f \propto (\gamma_\infty - \gamma_0)h^{-1}$, where γ_0 and γ_∞ are universal scaling exponents for the partition function of the tethered polymer for $h = 0$ and $h = \infty$, respectively. The measured functions $f(h)$ are generally consistent with the predictions, with small quantitative discrepancies arising from the approximations employed in the theory. In the case of multiple tethered polymers, the entropic force per polymer is roughly constant, which is qualitatively inconsistent with the predictions.

Keyword-1

polymer

Keyword-2

computer simulation

Keyword-3

entropy

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