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Free energy of a folded semiflexible polymer confined to a nanochannel of various geometries

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Monte Carlo simulations are used to study the conformational properties of a folded semiflexible polymer confined to a long channel. We measure the variation in the conformational free energy with respect to the end-to-end distance of the polymer, and from these functions we extract the free energy of the hairpin fold as well as the entropic force arising from interactions between the portions of the polymer that overlap along the channel. We consider the scaling of the free energies with respect to varying the persistence length of the polymer and the channel dimensions for confinement in cylindrical, rectangular and triangular channels. We focus on polymer behaviour in both the classic Odijk and backfolded Odijk regimes. We find the scaling of the entropic force to be close to that predicted from a scaling argument that treats interactions between deflection segments at the second virial level. In addition, the measured hairpin fold free energy is consistent with that obtained directly from a recent theoretical calculation for cylindrical channels. It is also consistent with values determined from measurements of the global persistence length of a polymer in the backfolded Odijk regime in recent simulation studies.

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