Abstract Submitted
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A hybrid molecular dynamics study of the translocation of DNA through entropic traps PETR HOTMAR, Florida State University — The interplay between thermal diffusion and electrophoretic migration of λ-phage DNA in entropic traps was studied using a hybrid molecular dynamics algorithm. The governing systems of field equations are discretized by finite differences on curvilinear overlapping grids with the solvent modeled as a continuum in unsteady creeping flow. Similar to Brownian dynamics, the polymer segments are coarse-grained into a bead-spring model that follows Langevin dynamics. The hydrodynamic interactions are captured on a semi-empirical level with localized force-transfer. We have established the non-monotonic dependence of electrophoretic mobility on chain length, which characterizes the transition from the free flowing to the trapping behavior. We further quantify the subtle effects of dielectrophoresis and induced-charge electroosmosis on the polymer dynamics.

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