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DNA-based Brownian motor for directional nanoparticle delivery – computational design

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Abstract

Brownian particles subject to a periodic, asymmetric potential can be transported in a specific direction along the potential by repetitively switching the potential on and off. In this work, we design a DNA-based Brownian motor for directional transport of positively charged nanoparticles along a single, long double-stranded DNA (dsDNA) with elaborately designed flexibility variation. We prove its realization by Brownian dynamics simulations of coarse-grained models. A periodic and asymmetry potential for nanoparticle binding is constructed along a single dsDNA by a novel strategy that utilizes variation in sequence-dependent DNA flexibility. Directional and processive motion of nanoparticles is achieved by changing salt concentration repetitively over several cycles to switch the asymmetric potential on and off. This work suggests that dsDNA molecules with elaborately designed flexibility variation can be used as a molecule-scale guide for spatial and dynamic control of nanoparticles for future applications.