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Energy Computation for nanopore DNA sequencing with an AFM[1] SHAHID QAMAR, Arizona State University, S. M. LINDSAY TEAM, P.M. WILLIAMS COLLABORATION — We are working on a technique to sequence the DNA with an atomic force microscope. Motivated by the experiment, we used an efficient technique to compute free energies of a DNA rotaxne molecule composed of a single strand DNA and a cyclodextrin molecule. Quantitative free energy computation involves milestoning technique with Arrhenius rate equation. The algorithm used computes the time scales of complex processes following the predetermined milestones along a reaction coordinate. A Markovian hopping mechanism was used. We performed the large scale molecular dynamics simulations at micro second level to compute the rare event kinetics which involves large scale distributed computational resources. We performed the molecular dynamics simulations for a DNA rotaxane in the absence of external force to compute the free energy differences among them. All the simulations were performed in aqueous solvent. The theoretical estimation of free energies qualitatively agrees with the experimental data obtained for nano pore DNA sequencing with an atomic force microscope. Initial results show the thermal fluctuations are dominant and the free energy differences between purine and pyrimidine is of the order of $1K_BT$ so the modification of DNA rotaxane is required to suppress the thermal fluctuations.

[1]NIH

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