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Dynamic Origins of Entropic Force: Thermodynamic Theory vs. Molecular Dynamics Simulations

by

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The aim of this research is to study the dynamic origins of entropic forces acting on semi-confined polymer chains. We make use of Molecular Dynamics Simulations to study at first the global chain characteristics and relaxation times of fully confined chains. Our results infer that we need to go to higher values of N and stronger con- finement to reach the asymptotic limits of the relaxation times and the radial forces acting on the chain. We eventually move on to study the dynamics of semi-confined chains in two limiting cases. The results show that for both cases (infinite and finite walls at the open end of the nanopore), the pulling force is only dependent on the temperature T and the diameter D with $f_{pull} \sim \tilde{B}\, k_B T/D$. Our model proves to be in agreemement with the theoretical predictions which state that the two limiting cases should produce the same entropic force for given values of T and D. The value of $\tilde{B}$ is extracted it appears that for semi-confined chains the pulling force's coefficient is different than the universal model independent constant $B = 5.79$. Studies of the effect of the length of the tail outside the nanopore were also administered. The change of weights/concentrations of contacts and magnitudes of forces with the radial distance were deduced from the Green's function of a polymer near a plane and were found to match our simulation results, and a final expression was obtained from the weights that retrieves the force's dependence on D theoretically. Finally, we provide a brief comparison of our model to the ejection of a dsDNA from a bacteriophage T5.

Date: Friday, January 27, 2017
Place: Rm. 310
Time: 4:00 p.m.