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Loop Closure Dynamics of Flexible and Semi-flexible Polymer

JEN-FANG CHANG, YENG-LONG CHEN, Academia Sinica, INST. OF PHYS.,
ACADEMIA SINICA TEAM, RCAS, ACADEMIA SINICA TEAM — It is widely
believed that DNA looping due to multi-site DNA-binding proteins is important
for DNA transcription, replication, and recombination. The chain closure problem
has been studied in several Monte Carlo simulations to determine the chain closure
probabilities and the chain conformation to infer dynamic properties. In this work,
we investigate how the loop closure dynamics of flexible and semi-flexible polymers
depend on the polymer length and the reactive site position using Brownian dy-
namics simulation, accounting for hydrodynamic interactions. Our study examines
the probability of closing for two reactive sites along the chain and the shape of the
loop formed by closing. In addition, intrachain hydrodynamic interactions are found
to affect the diffusivity of circular chains compared to linear chains, in accord with
experimental observations. We also consider the dynamics of chain closing under
strong slit-like confinement as a function of slit height.

Jen-Fang Chang

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