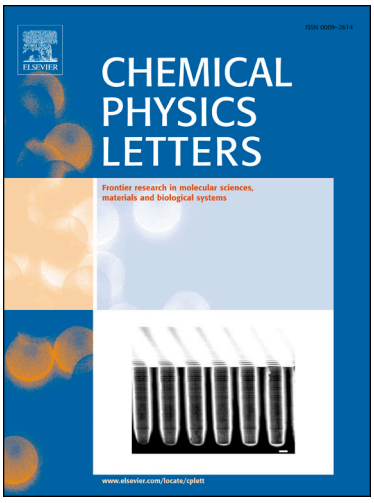

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Effects of solvent quality on contact formation dynamics of polymer chain

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ABSTRACT
We investigate the interplay effects of internal friction and solvent quality on the contact formation dynamics based on non-Markovian diffusion equation supplemented with an exponential sink term accounting for the electron transfer quenching. The mean contact formation time has been derived under Wilemski-Fixman approximation. We show that internal friction induces fractional viscosity dependence of looping time, which will be affected remarkably by solvent quality condition. Besides, internal friction promotes a diffusion-limited mechanism by slowing chain relaxation, while solvent quality being another key factor shifts the critical internal friction for the crossover of the transition from reaction to diffusion-limited regimes.

1. Introduction

Contact formation (cyclization) between the ends of a long polymer is a dynamical process with broad applications, which has been studied widely by experiments [1–3], theories [4–6], and simulations [7–9]. The kinetics of loop formation has become increasingly important, largely because of its biological relevance to DNA looping [10] as well as protein [11, 12] and RNA folding [13]. For example, the formation of loops and hairpins in DNA is important in gene expression and interactions of DNA with proteins and RNA, while the formation of contacts between residues (nucleotides) may be the key nucleating event in protein (RNA) folding. Particularly, the crucial problem of determining the rate of end-to-end collisions for polymer chains has received considerable attention so far. This problem arises in a number of different contexts. Diffusional search for certain native contacts has been proposed to be the rate limiting step in protein folding [14, 15]. In the past few years, experimentally, fluorescence quenching measurement based on triplet-triplet energy transfer has provided one type of novel means to probe loop closure times for a range of proteins [16–20] and DNA [21, 22]. By monitoring the triplet-triplet absorption, these experiments can obtain the effective contact formation rate k_{eff}, which is equal to the reciprocal of the mean contact formation time. The scheme for measuring the rate of contact formation was usually described by a two-step process [16, 18], wherein the donor and acceptor diffuse together with a rate k_D to form contact pair, and the acceptor either quenches the donor triplet state with a rate q or diffuses away. The observed effective contact

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