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Research paper

Brownian dynamics simulations of charged semiflexible polymers confined to curved surfaces

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ARTICLE INFO

Article history:
Received 3 May 2010
Received in revised form
12 November 2010
Accepted 12 November 2010
Published online 21 November 2010

Keywords:
Semiflexible polymer
Wormlike chain
Brownian dynamics
Surface confinement

ABSTRACT

As an extension of the generalized bead–rod model developed earlier by the authors, this paper proposes a method for Brownian dynamics simulations of charged semiflexible polymers confined to various curved surfaces such as spherical, cylindrical, ellipsoidal and toroidal. We model charged semiflexible polymers as discrete wormlike chains consisting of virtual beads connected by inextensible rods with length varying according to the characteristic radius of curvature of the confining surface. The long-range electrostatic interactions are incorporated via the Debye–Hueckel potential. The geometrical constraints associated with the inextensible rods are realized by the so-called linear constraint solver. For a semiflexible polymer chain confined to a spherical surface, an analytical expression for the winding number is obtained by using an existing exact closed-form solution of the mean-square end-to-end distance. The proposed simulation method is then validated against theoretical predictions for both charged and uncharged polymer chains under surface confinements.

1. Introduction

How geometrical confinements affect the statistical behaviors of polymers is a fundamental problem in polymer physics that underlies many important biological processes and technological applications. In particular, DNA/RNA packaging in viruses (Purohit et al., 2003) and eukaryotic cells (Calladine and Drew, 1997) make the genomic macromolecules compactly folded into geometrical confinements that are much smaller than their unconfined molecular sizes.

Theoretical investigations of confined polymer chains on curved surfaces have become an active research topic during the past decade. Mondescu and Muthukumar (1998) considered a Gaussian polymer chain confined to a curved surface. By using a diffusion equation and path-integral approach, they obtained the probability distribution function of the end-to-end vector as well as the mean-square end-to-end distance of the polymer chain. While the effect of geometrical confinement on a flexible polymer is primarily entropic, confining a semiflexible polymer involves both energetic and entropic effects, with the balance controlled by the stiffness of the chain and the length scale of the confinement. Based on the wormlike chain model for semiflexible polymers, Spakowitz and Wang (2003) developed a

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1751-6161/$ - see front matter
doi:10.1016/j.jmbbm.2010.11.008