On Brownian dynamics simulations of semiflexible wormlike chains

*Jizeng Wang

Key Laboratory of mechanics on Disaster and Environment in Western China, the Ministry of Education, and School of Civil Engineering and Mechanics, Lanzhou University, Lanzhou 730000, China

*Corresponding author: jzwang@lzu.edu.cn

This study is aimed to creat our own mini-software on Brownian dynamics simulations for single charged semiflexible polymers and polymer networks in various complex solution microenviroments and under various loading conditions, where numerical simulation plays an indispensable role in complementing theory and experiments. In this software, each single singsemiflexible polymer is modelled as a discrete wormlike chain consisting of a string of virtual spherical beads connected by either extensible elastic springs or inextensible rods with length varying according to the confinement intensity of the chain. Complex potential enviroments, electrostatic and hydrodynamic interactions are taken into account. Rich functions of the mini-software and several bechmark simulation examples are demonstrated.

Keywords: Semiflexilbe wormlike chain, polymer network, Brownian dynamics simulations, software