

Abstract Submitted
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Computer simulation of DNA translocation in functionalized conical nanopores¹ GUOQING HU, LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, BAO JIAO — As a powerful research tool to rapidly investigate the dynamic and structural properties of single biomolecules such as DNA and protein, solid-state single nanopores have attracted a great deal of scientific interests. In a typical setup, DNA molecule is driven electrokinetically and its translocation is conveniently detected via the ionic current measurement through single nanopores. One of challenges arising from solid-state nanopore DNA sequencing technique is the molecular selectivity and detection resolution. Tuning the geometry and surface property of nanopores helps create sensing devices that control transport of ions and molecules in electrolyte. Here we present molecular dynamics simulation method to study the ion transport and DNA translocation phenomena in conically shaped nanopores coated with single-stranded DNA molecules. Computer simulations characterize the effects of the effective nanopore diameter, conical pore geometry, ionic strength, surface charge, and applied biasing voltage on the ionic current and DNA translocation dynamics. The findings can be used to improve and optimize the experimental design for DNA detection in single nanopore devices.

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