

Abstract Submitted
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Characterization of DNA Translocation and Detection in Functionalized Nanopores YALING LIU, Lehigh University, ABHIJIT RAMACHANDRAN, QINGJIANG GUO — Functionalized nanopores have been used in selective detection of DNA. While the interaction between a bare nanopore and a DNA has been analyzed extensively, little is known for that of a functionalized nanopore. This work focuses on studying the DNA translocation dynamics and mechanism of DNA sequencing in a functionalized nanopore through a coarse-grained molecular dynamics model. Physical properties of chemically modified nanopores, i.e., the effective pore diameter under different bias voltages are characterized. The DNA translocation dynamics under different nanopore coatings and different bias voltages are studied. The simulation results reveal that molecular selective translocation largely lies on the flexibility and orientation of the coating molecules and their interaction with the translocating DNA. This research supports rational designs of DNA transportation- and manipulation-based diagnostic systems.

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