

Abstract Submitted
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Simulations of Single DNA Nucleotide Transport Through Nanoslits¹ BRIAN NOVAK, KAI XIA, DOREL MOLDOVAN, DIMITRIS NIKITOPoulos, Louisiana State University, Mechanical Engineering, STEVEN SOPER, Louisiana State University, Chemistry and Mechanical Engineering — Transport of single molecules in nano-scale geometries might be used to identify them via their flight times. The motion of nucleotides in aqueous NaCl solution flowing through atomically smooth nanoslits composed of disordered carbon atoms was studied using nonequilibrium molecular dynamics simulations. The fluid was driven by gravity-like forces or the nucleotide was moved electrophoretically. Velocities were on the order of 1 m/s or 3 m/s, respectively. The relatively hydrophobic base parts of the nucleotides adsorbed to the walls multiple times while moving along the slit. The bases tended to adsorb/desorb with the sugar end of the base contacting the surface last/first. The distance required for separation of the flight time distributions (required channel length) was 8.8 μm for the gravity case. In the electrophoretic case with this surface, the nucleotides moved nearly as fast while adsorbed as while desorbed which made the separation more difficult than in the gravity case.

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