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Molecular Dynamics Simulations of the Transport of Single DNA Nucleotides Through Nanochannels BRIAN NOVAK, DOREL MOLDOVAN, DIMITRIS NIKITOPOULOS, Mechanical Eng., STEVEN SOPER, Chemistry and Mechanical Eng., Louisiana State University — Transport of single molecules through nano-confined geometries can be used to identify them via their unique flight times. The movement of the nucleotides in aqueous solution flowing through nanochannels was studied using nonequilibrium molecular dynamics simulations. Initial 150 ns simulations of nucleotides in 89 mM NaCl solution in 3.0 nm slits with walls composed of disordered carbon atoms show well separated flight times for the nucleotides C and T. The fluid was driven by gravity-like forces to an average velocity of about 1.0 m/s. In contrast, the flight times for A and G are within one standard deviation of each other and the differences between A and T and between G and C are roughly two standard deviations. Our simulations show that the nucleotides are adsorbed and desorbed from the wall multiple times while moving along the channel. The evidence shows that the hydrophobicity of T is responsible for its longer residence times in contact with the also hydrophobic wall and longer flight time relative to C.

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