

Abstract Submitted
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Molecular Dynamics simulations of polymer translocation through a nanoscopic pore MICHEL G. GAUTHIER, GARY W. SLATER, University of Ottawa — The detection of linear polymers translocating through a nanoscopic pore is an extremely promising idea for the development of new DNA analysis techniques; such systems are already studied experimentally. However, the physics of these macromolecules and the fluid that surround them at the nanoscopic scale is still not well understood. In fact, many theoretical models neglect both excluded volume and hydrodynamic effects. We use Molecular Dynamics simulations with explicit solvent to study the impact of hydrodynamic interactions on the translocation time of a polymer. In particular, we look at the effect of increasing the pore radius when only a small number of fluid particles are located in the pore as the polymer undergoes translocation. We also investigate the relaxation time of the polymer as function of its length and compare it to the translocation time for different initial conditions in order to test the quasi-equilibrium hypothesis of the translocation process.

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