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Molecular Dynamics Study of Polymer Separation Using a Nanofluidic Staircase FREDERICK PHELAN JR., CHRISTOPHER FORREY, National Institute of Standards and Technology (NIST) — The diffusive behavior of isolated polymer chains in a nanofluidic staircase has recently been studied experimentally [Strychalski et al., Macromolecules, 45(3), 1602, (2012); Stavis et al., Lab Chip, 12(19), 1174, (2012)] and by simulation [Phelan et al., in preparation, (2012)]. Chains are observed to exhibit spontaneous 1-D biased diffusion from regions of high to low confinement, without the use of external forces, under conditions where the local confinement lies in either the Odijk or de Gennes regimes. The transport mechanism is that of a Brownian motor, where the polymer free energy is used to generate directed transport using thermal fluctuations and the biased structural features of the device. The nanostaircase has potential for a number of applications in polymer measurement science and transport, an important one of which could be separations. To study this, we examine polymer separation in the nanofluidic staircase using the molecular dynamics simulation software LAMMPS. Length based separations of linear polymers as applicable to DNA separations are the main topic of the study, but the effect of more complex architectures such as branching are also examined.

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