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The effect of fluid density on the transport of particles in nanochannels ZHIGANG LI, GERMAN DRAZER, Department of Chemical and Biomolecular Engineering, Johns Hopkins University — Understanding particle transport in nanochannels is crucial for the development of micro and nanofluidic devices. In this work, we investigate the effect of fluid number density on the transport of particles in nanochannels, by means of molecular dynamics simulations. Specifically, we examine the motion of a Lennard-Jones nanoparticle, under the action of a constant external force, in a Platinum nanochannel that contains a Lennard-Jones fluid. In the limiting case of a nanochannel free of fluid molecules the particle adsorbs to the surface of the nanochannel and moves at a very low velocity, due to dry friction with the wall. As the number density of the fluid increases the mobility of the nanoparticle is greatly enhanced, due to the formation of adsorbed fluid layers on the surface of both the nanochannel and the particle, which substantially reduce friction between the particle and the wall. Then, if the number density of the fluid is increased further the particle mobility drops, due to viscous drag. In fact, there is an optimal value at low fluid densities, at which the particle mobility can be significantly enhanced. We also examine the existence of a second peak at higher densities, when the fluid density is high enough to prevent the adsorption of the nanoparticles, and how these phenomena depend on the fluid-solid molecular interactions.

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