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Brownian dynamics simulation of a polymer chain in a solid-state nanopore attached to a molecular stop[1] CRAIG WELLS, ZACHERY HULINGS, DMITRIY MELNIKOV, MARIA GRACHEVA, Clarkson University — We study a nanopore inside a silicon dioxide membrane submerged in a KCl solution with a negatively charged polymer chain of varying lengths whose movement is described using Brownian dynamics. The polymer is attached to a molecule with a radius larger than that of the nanopore's which acts as a molecular stop, allowing the chain to thread the nanopore but preventing it from translocating. We found that the polymer chain's variation of movement along the nanopore decreased when increasing applied biases and chain lengths for portions of the chain closest to the molecular stop. The chain displacement within the pore is also compared to a freely translocating polymer where preliminary results show the free polymer having a greater variation in the radial direction. Overall, our preliminary results indicate that the radial direction of the polymer chain is dominated by the confinement in the narrow nanopore with restrictions imposed by the molecular stop and bias playing a lesser role. Understanding the interaction behavior of the polymer chain-stop molecule may lead to methods that decrease movement variation, facilitating an improvement on characterizing and identification of molecules.

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