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Molecular Dynamics Simulations of Nanopropulsion Engine JAN-MICHAEL CARRILLO, University of Connecticut, JUNHWAN JEON, Vanderbilt University, ANDREY DOBRYNIN, University of Connecticut — We have performed molecular dynamics simulations of a nanoscale size engine - nozzle. The engine consists of an end capped cylindrical pore with polymerization sites located on the cap surface. These polymerization sites power the engine by polymerizing chains inside a cylindrical pore. The molecular dynamics simulations are performed with explicit solvent in NVT-ensemble with a Nose-Hoover thermostat. The explicit solvent models hydrodynamic interactions between the engine and its surrounding. The explicit solvent also provides a supply of monomers for the polymerization reaction. Addition of a monomer to a growing polymer chain occurs when a monomer is within a capture radius from the polymerization site. The polymerization induces chain compression, which results in the pressure gradient throughout the length of the nozzle propelling it forward. There is a linear relationship between the average velocity of the nozzle and the chain polymerization rate with a proportionality coefficient dependent on the nozzle geometry such as nozzle length or radius and effective friction brought about by the nozzle itself and the monomers within the nozzle. We compare the motion of the nozzle in solutions and near adsorbing surfaces.

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