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Non-equilibrium All-atoms Molecular Dynamics Simulations of Free and Tethered DNAs in Nano-channel Shear Flows[1] GUAN WANG[2], WILLIAM SANDBERG, Lab for Computational Physics and Fluid Dynamics, Naval Research Laboratory — The CHARMM equilibrium biomolecular dynamics software has been extended to handle non-equilibrium molecular dynamics (NEMD) problems. Biomolecules, both free and wall-tethered, have been simulated in the all-atom style in a water-filled nanochannel shear flow. The new methods and computational codes were demonstrated by carrying out NEMD simulations of tethered dsDNAs on gold surfaces. We investigated the diffusion coefficient and the velocity autocorrelation function in selected regions in the direction of shear. The fluidic forces on tethered ss/ds-DNAs and the tilting angles were also calculated. The tethering of the linker molecule (6-mercapto-1-hexanol) to perfect Au(111) surfaces was parameterized based on density functional theory calculations. Force field parameters were incorporated into the CHARMM database. Gold surfaces are simulated in a Lennard-Jones style model that was fitted to the Morse potential model of bulk gold.

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