468c Simulation of Friction in Nanoconfined Fluids for an Arbitrarily Low Shear Rate

Jerome P. Delhommelle and Peter T. Cummings

Molecular dynamics (MD) simulations are a valuable tool to characterize the microscopic mechanisms underlying friction. However, the lowest shear rate accessible by current MD methods is at least 4 order of magnitude larger than those typically used in experiments. Using the transient-time correlation function, we show how MD simulations can be extended to study systems subjected to a realistic shear rate. We demonstrate the usefulness of this approach by studying the frictional response of a simple fluid confined to a film of about 5 molecular diameters.