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Dynanimcal Properties of Water in Nanoconfinement[1] MICHAEL CHANDROSS, Sandia National Laboratories, CHRISTIAN D. LORENZ, Kings College London, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — We report the results of large-scale Molecular Dynamics (MD) simulations of water confined to sub-nanometer thicknesses. We vary the amount of water and the applied pressure to examine the effects on the structure and dynamics of the confined water. Calculations of two dimensional diffusion constants indicate that the water remains liquid-like in all cases. The water is subjected to shear to measure the viscosity and microscopic friction. We find that while the viscosity increases by as much as a factor of six for low coverage and high loads, there is still no evidence of ice-like layers being formed. Friction coefficients can only be calculated at high shear velocities due to the low viscosity of the water and are found to decrease with increasing amounts of water, similar to experimental results.

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