

SUPPLEMENTRY INFORMATION

Fickian diffusion of single file water molecules confined inside SWCNT

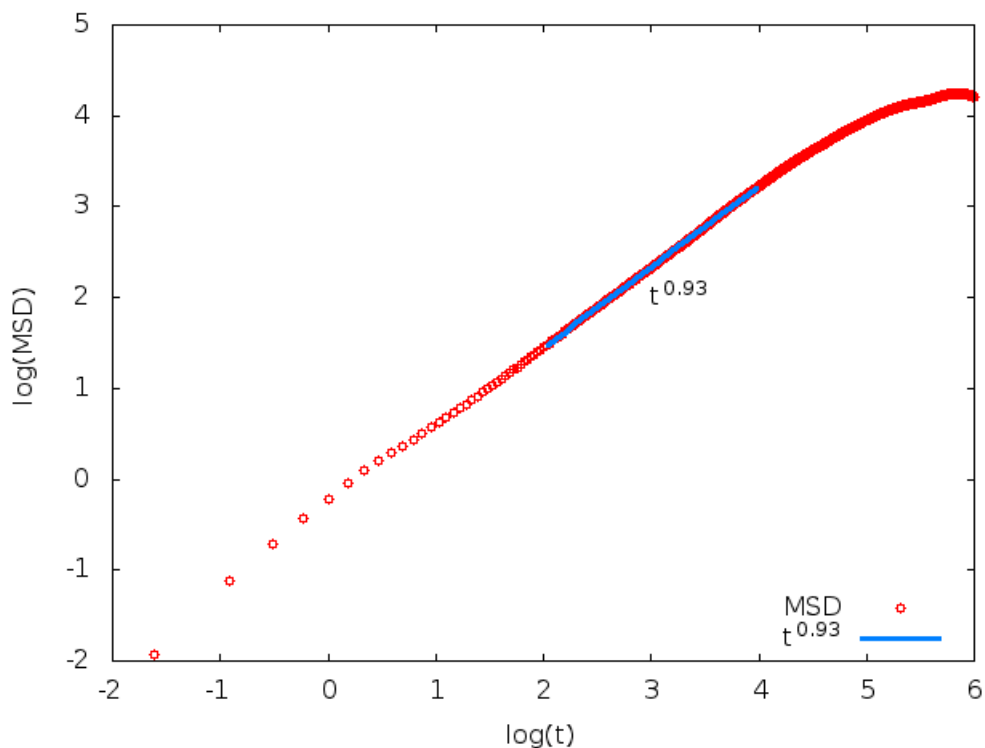


FIG. 1. Log-log fit for MSD of single file water molecules confined inside (6,6) SWCNT. Slope of the curve (0.93) shows water molecules have normal diffusion.

Effect of thermostat on the translational diffusion

Thermostat used to simulate NVT ensemble may have some unwanted effect on the dynamical properties of simulated water molecules. To calculate the effect thermostat on translational diffusion, we compare mean square displacement computed in NVT ensemble (Brensen thermostat) with NVE ensemble (without any thermostat). Our result shows that with appropriate coupling constant, translational diffusion behavior is almost same.

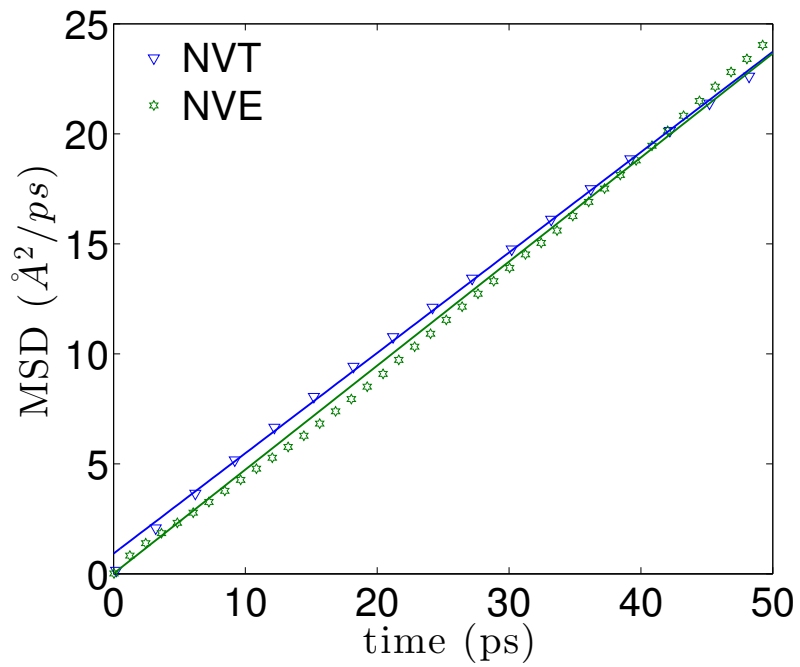


FIG. 2. Comparison of MSD from NVT and NVE ensemble for TIP3P water model at $T = 300$ K.