Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Free Energy Change in the Complete Transport of All Water Molecules through a Carbon Nanotube

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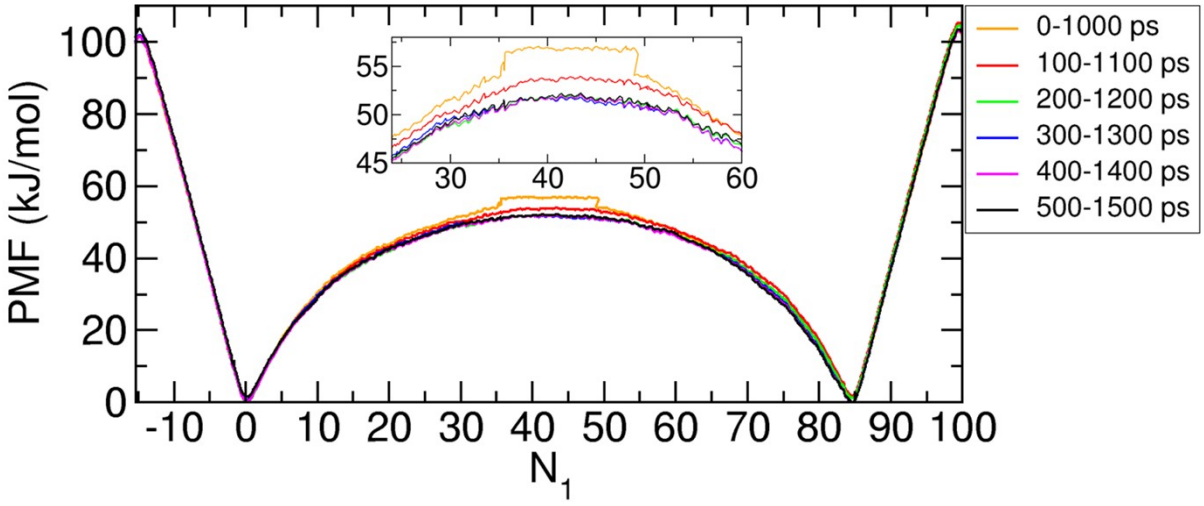

Figure S1. Convergence test of the PMF calculation for the case with 100 water molecules. Six PMFs were obtained by taking only a 1 ns trajectory from the total 1.5 ns trajectory of each sampling window, beginning at 0 ps, 100 ps, 200 ps, 300 ps, 400 ps, or 500 ps. As the beginning time for sampling is increased, the PMF converges. The inset shows the details of this convergence around $N_{1=}$ ~40.

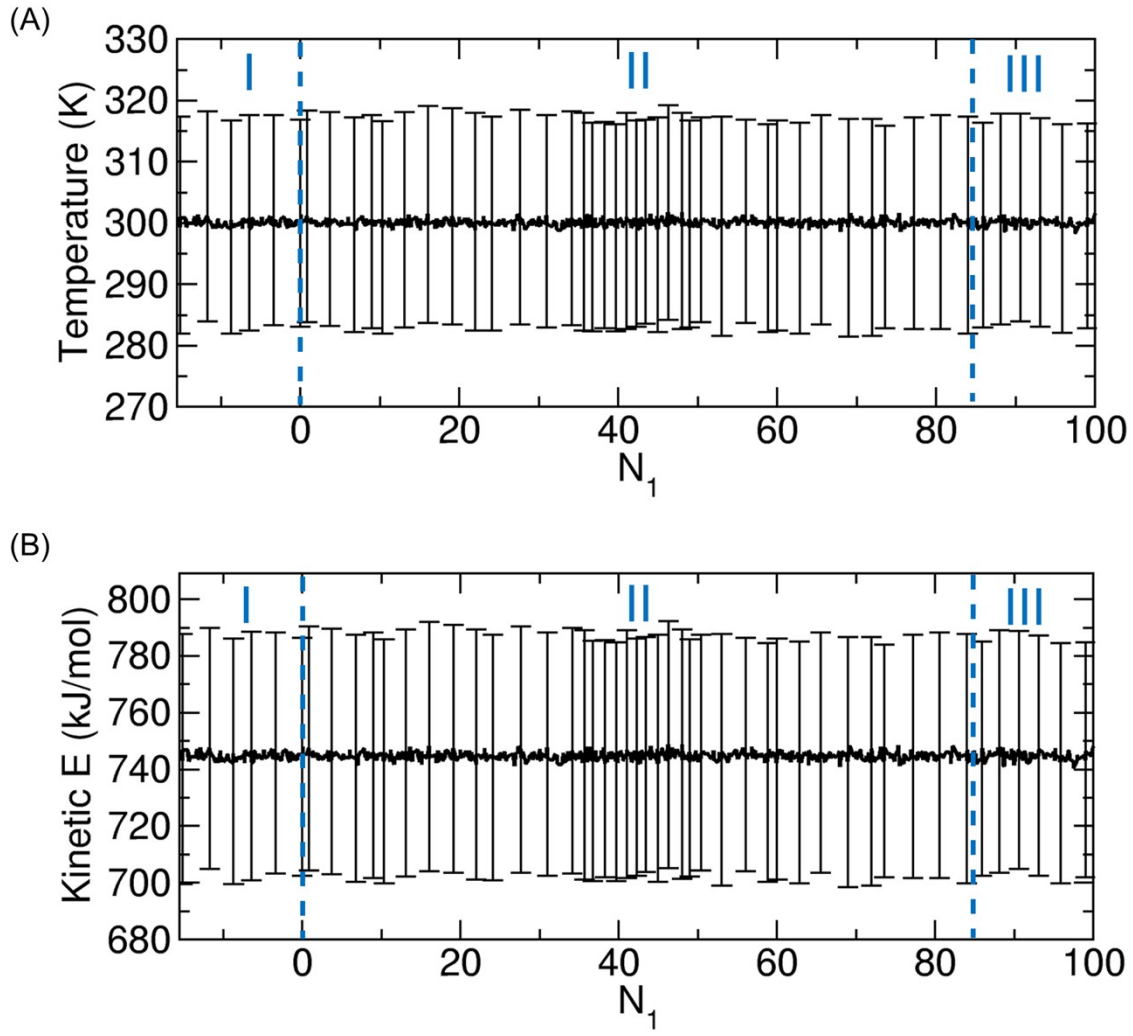

Figure S2. (A) Temperature as a function of N_1 for the case with 100 water molecules. (B) Kinetic energy (Kinetic E) as a function of N_1 for the case with 100 water molecules. The error bars represent standard deviations.