Supporting Information

Pan et al. 10.1073/pnas.1221581110

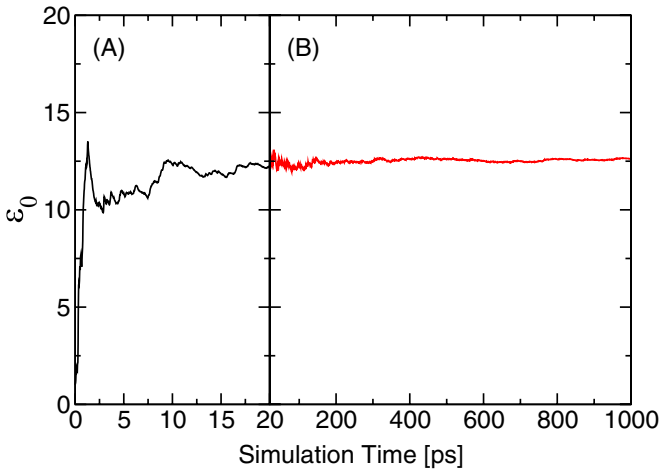

Fig. S1. Comparison between the results from the simple point charge extended (SPC/E) molecular dynamics (MD) simulations at 1,000 K and 0.88 g/cm^3, using (*A*) 128 water molecules for 20 ps and (*B*) 1,728 water molecules for 1 ns. The difference between the calculated dielectric constants, ε_0, by the simulations in *A* and *B* is less than 5%.

Table S1. Data for the static dielectric constant of water obtained from *ab initio* MD simulations

T, K	ϱ, g/cm^3	ε_0
1,000	0.88	15.0 (0.3)
	1.32	29.8 (0.7)
	1.57	39.4 (0.5)
2,000	1.13	9.73 (0.05)
	1.36	13.43 (0.05)

Within parentheses we report the result ranges in the last 5 ps of the running averages.