Supporting information:

Water Molecules in a Carbon Nanotube under an Applied Electric Field at Various Temperatures and Pressures

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Simulation results with the TIP4P water model are presented in Figure S1 to S6, and Table S1 to S6, as follows.

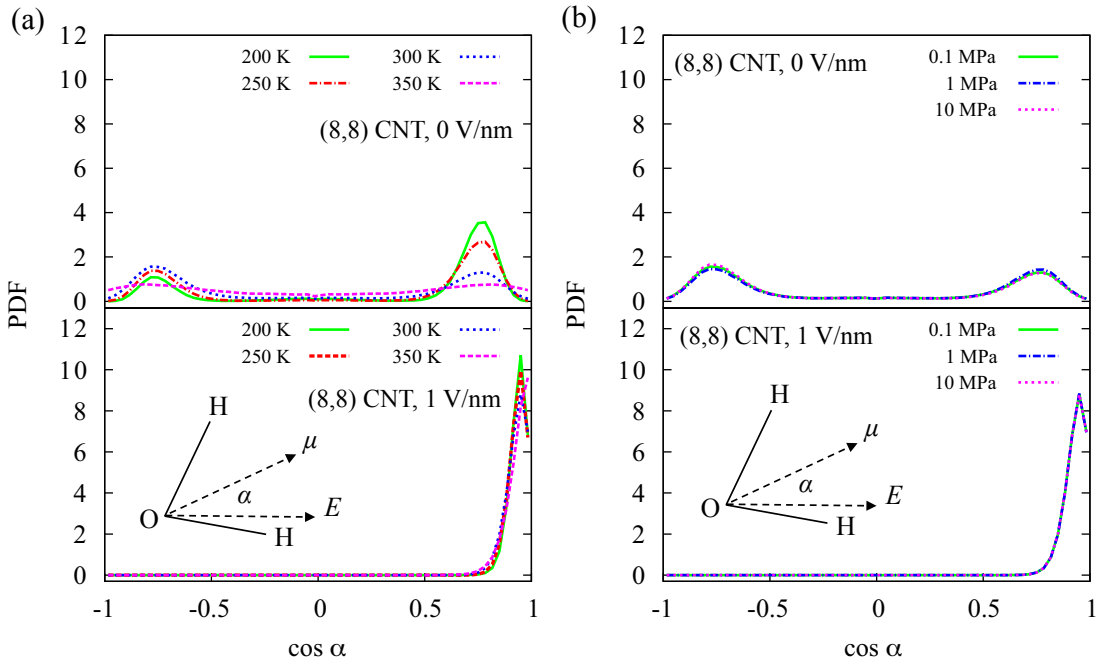

Figure S1. Orientation of the TIP4P water in (8,8) CNT: (**a**) at various temperatures from 200 K to 350 K and ambient pressure of 0.1 MPa. The applied electric field are 0 V/nm (top) and 1 V/nm (bottom). (**b**) at various pressures from 0.1 MPa to 10 MPa, T = 300 K, and E = 0 V/nm (top) and 1 V/nm (bottom).

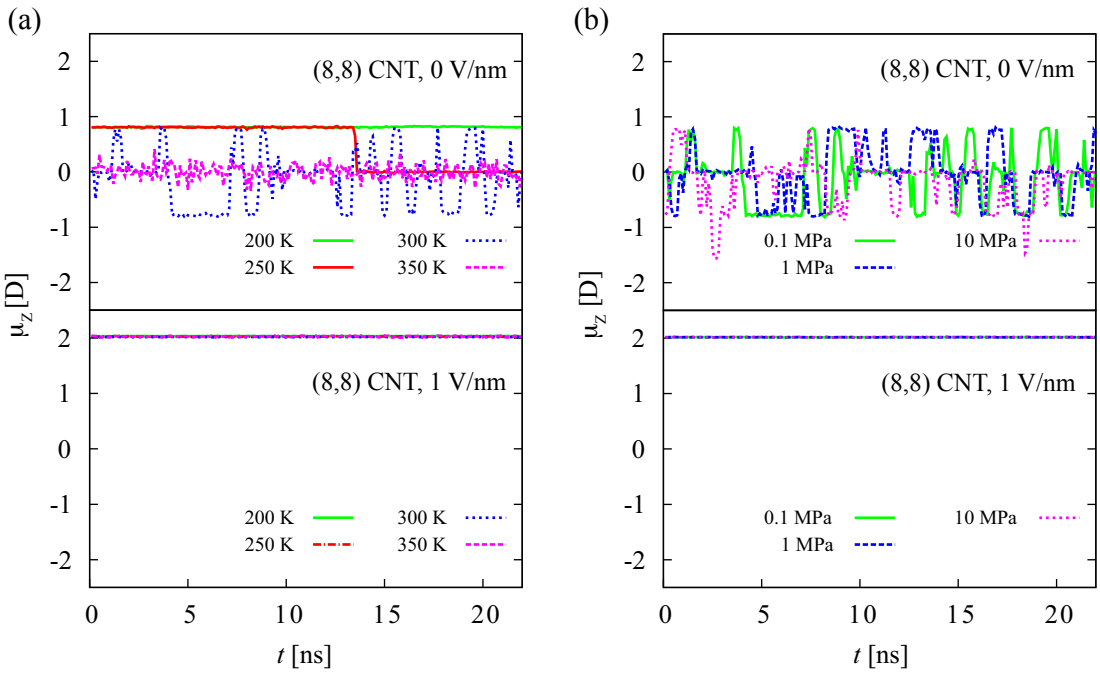

Figure S2. Average z-component of dipole moment (μ_z) of the TIP4P water model in an (8,8) CNT: (**a**) at various temperatures from T = 200 K to 350 K, P = 0.1 MPa, and E = 0 V/nm (top) and 1 V/nm (bottom). (**b**) at P = 0.1 MPa to 10 MPa, T = 300 K, and E = 0 V/nm (top) and 1 V/nm (bottom).

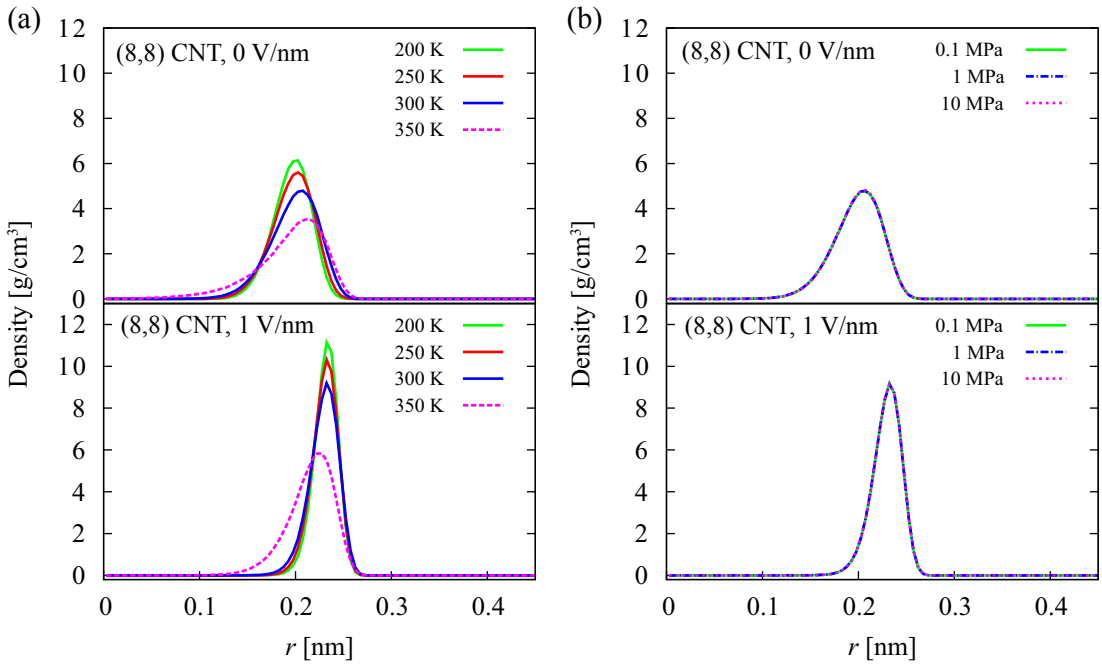

Figure S3. Distribution of radial density of oxygen atoms in an (8,8) CNT: (**a**) at various temperatures of 200 K to 350 K and constant pressure at 0.1 MPa. The electric field are 0 V/nm (top) and 1 V/nm (bottom). (**b**) at various pressures of 0.1 MPa to 10 MPa, constant temperature of 300 K, and E = 0 V/nm (top) and 1 V/nm (bottom). r = 0 indicates position of the CNT axis.

Table S1. Structures of the TIP4P water model in an (8,8) CNT at various temperatures from 200 K to 350 K, at a constant pressure at 0.1 MPa, and under the electric fields of 0 V/nm and 1 V/nm.

Temperature [K]	Structure at 0 V/nm	Structure at 1 V/nm
200	(4,0)	(5,2)
250	(4,0)	(5,2)
300	(4,0)	(5,2)
350	disorder	(4,2)

Table S2. Structures of the TIP4P water model in an (8,8) CNT at various pressures from 0.1 MPa to 10 MPa, at constant temperature of 300 K, and the electric fields are 0 V/nm and 1 V/nm.

Pressure [MPa]	Structure at 0 V/nm	Structure at 1 V/nm
0.1	(4,0)	(5,2)
1	(4,0)	(5,2)
10	(4,0)	(5,2)

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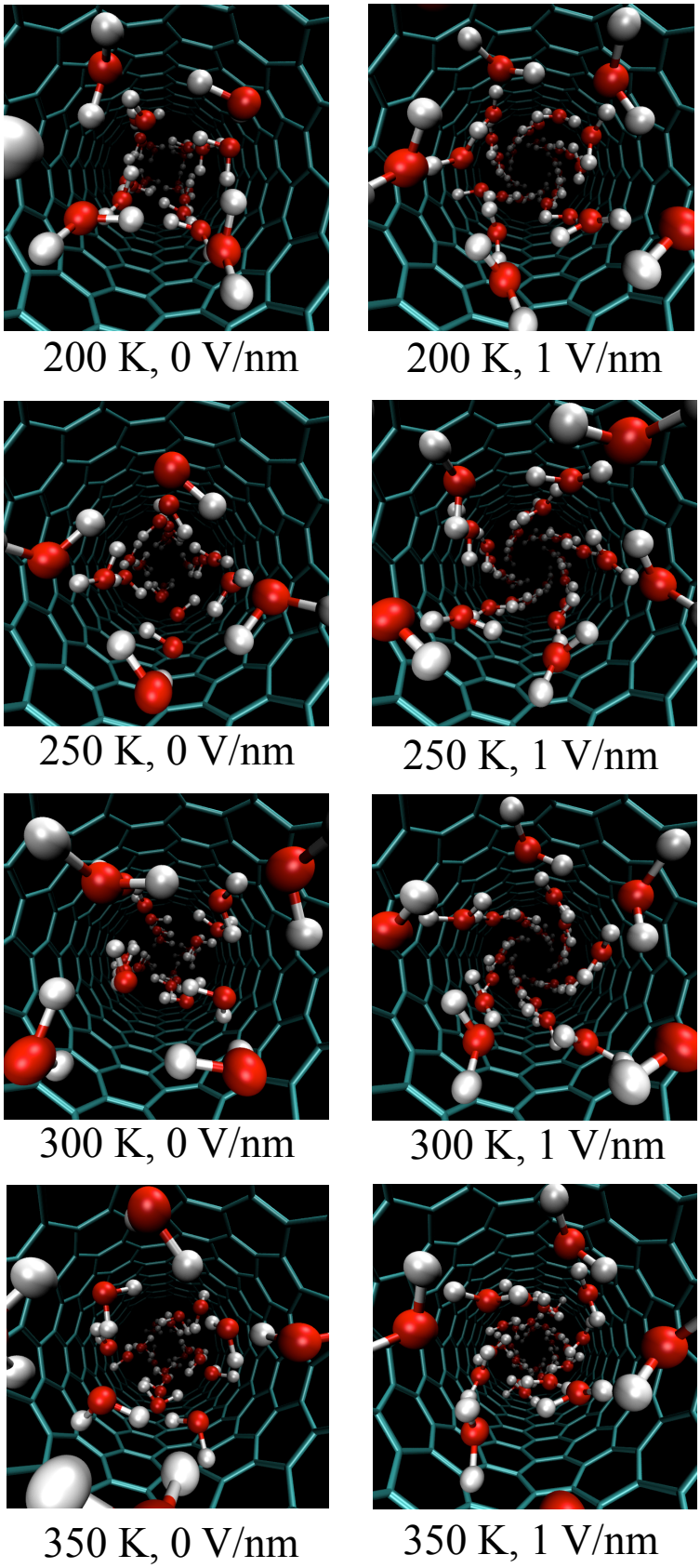

Figure S4. Snapshots of the TIP4P water structures in an (8,8) CNT at various temperatures of 200 K to 350 K, constant pressure at 0.1 MPa, and with E = 0 V/nm and 1 V/nm.

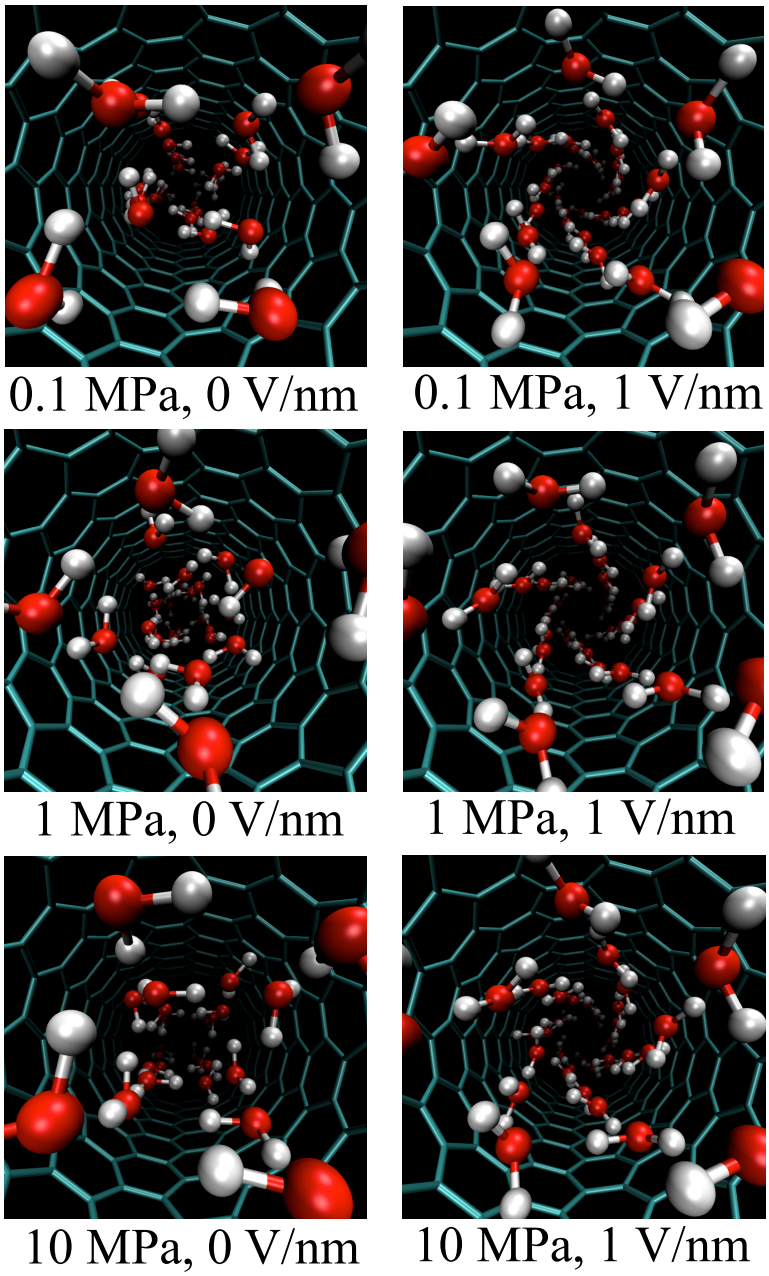

Figure S5. Snapshots of the TIP4P water structures in an (8,8) CNT at various pressure of 0.1 MPa to 10 MPa, constant temperature of 300, and with E = 0 V/nm and 1 V/nm.

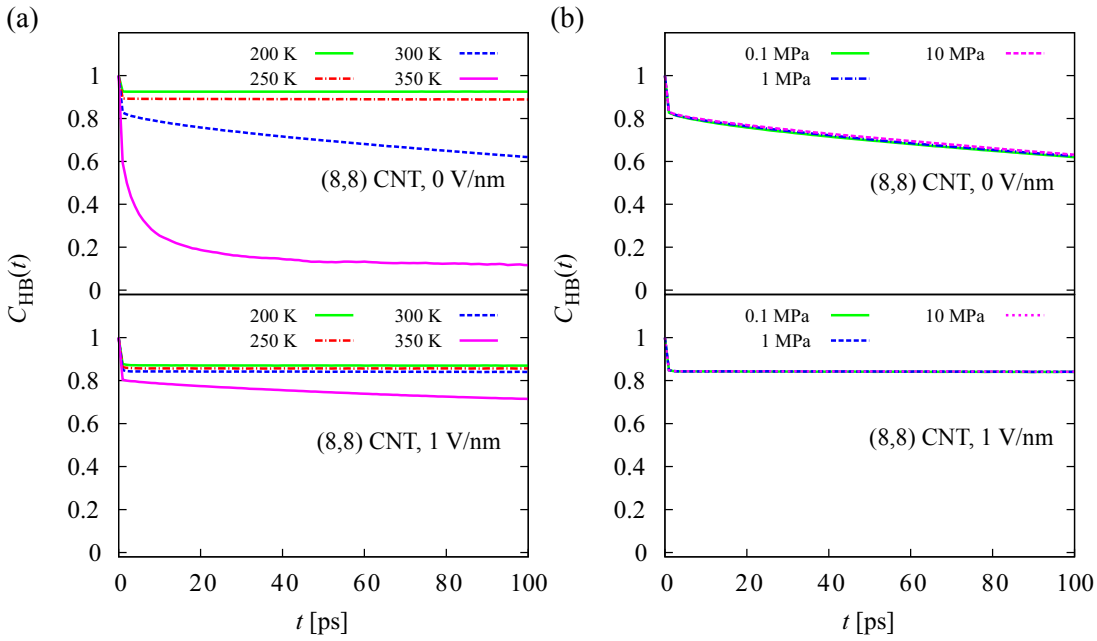

Figure S6. Hydrogen bond autocorrelation functions (C_{HB}) of the TIP4P water model in an (8,8) CNT: (**a**) at temperatures from 200 K to 350 K, constant pressure of 0.1 MPa, and the electric fields of 0 V/nm (top) and 1 V/nm (bottom). (**b**) at various pressures from 0.1 MPa to 10 MPa, constant temperature of 300 K, and the electric fields of 0 V/nm (top) and 1 V/nm (bottom).

Table S3. Average potential energy per TIP4P water molecule in the reservoirs and in the (8,8) CNT. ΔU is the difference between the potential energies in the CNT (U_{CNT}) and in the reservoirs ($U_{Res.}$), $\Delta U = U_{CNT} - U_{Res}$. The simulation conditions are T = 200 K and 250 K, P = 0.1 MPa, with E = 0 V/nm and 1 V/nm.

***T* [K]**	***E* [V/nm]**	**Energy (*U*)**	**In Reservoir [kJ/mol]**	**In CNT [kJ/mol]**	**ΔU [kJ/mol]**
200	0	LJ	22.61	8.35	–14.26
		Coulomb	–120.60	–104.52	16.08
	1	LJ	22.70	18.23	–4.47
		Coulomb	–119.83	–120.26	–0.43
		Dipole	–1.11	–4.09	–2.98
250	0	LJ	17.81	6.62	–11.19
		Coulomb	–107.10	–100.40	6.70
	1	LJ	17.83	16.72	–1.11
		Coulomb	–106.87	–118.66	–11.79
		Dipole	–1.05	–4.08	–3.03

Table S4. Average Lennard-Johnes (LJ) potential energy for water–water interaction (LJ_{W-W}) and water–CNT interaction (LJ_{W-CNT}) per TIP4P water molecule, in the reservoirs and in the (8,8) CNT. ΔU is the difference between the potential energies in the CNT (U_{CNT}) and in the reservoirs (U_{Res}), $\Delta U = U_{CNT} - U_{Res}$.

***T* [K]**	***E* [V/nm]**	**Energy (*U*)**	**In Reservoir [kJ/mol]**	**In CNT [kJ/mol]**	**ΔU [kJ/mol]**
200	0	LJ_{W-W}	22.61	21.33	–1.28
		LJ_{W-CNT}	0	–12.75	–12.75
	1	LJ_{W-W}	22.70	29.67	6.97
		LJ_{W-CNT}	0	–11.18	–11.18
250	0	LJ_{W-W}	17.81	19.98	2.17
		LJ_{W-CNT}	0	–13.12	–13.12
	1	LJ_{W-W}	17.83	28.65	10.82
		LJ_{W-CNT}	0	–11.66	–11.66

Table S5. Average potential energy per molecule of the TIP4P water and the SPC water in the reservoirs and in the (8,8) CNT at condition of 300 K, 0 V/nm. ΔU is the difference between the potential energies in the CNT (U_{CNT}) and in the reservoirs (U_{Res}), $\Delta U = U_{CNT} - U_{Res}$.

Model	**Energy (*U*)**	**In Reservoir [kJ/kmol]**	**In CNT [kJ/kmol]**	**ΔU [kJ/mol]**
TIP4P	LJ	14.80	5.42	–9.38
	Coulomb	–97.43	–93.47	3.96
			Total:	–5.42
SPC	LJ	14.08	3.71	–10.37
	Coulomb	–97.20	–85.07	12.13
			Total:	1.76

Table S6. Average potential energy per molecule of the TIP4P water and the SPC water in the reservoirs and in the (8,8) CNT at condition of 350 K, 1 V/nm. ΔU is the difference between the potential energies in the CNT (U_{CNT}) and in the reservoirs (U_{Res}), $\Delta U = U_{CNT} - U_{Res}$.

Model	**Energy (*U*)**	**In Reservoir [kJ/kmol]**	**In CNT [kJ/kmol]**	**ΔU [kJ/mol]**
TIP4P	LJ	12.73	10.09	–2.64
	Coulomb	–89.40	–103.58	–14.18
	Dipole	–1.04	–4.08	–3.04
			Total:	–19.86
SPC	LJ	12.40	13.38	0.98
	Coulomb	–89.99	–109.51	–19.52
	Dipole	–1.11	–4.21	–3.10
			Total:	–21.64