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Molecular Simulation Study of Temperature Effect on Ionic Hydration in Carbon Nanotubes

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Table S1. The details of simulated systems

case	*T*/ K	*D*/nm	Nw	cation/anion	case	*T*/ K	*D*/nm	Nw	cation/anion
1	298	1.00	328	K^+/Cl^-	22	298	1.00	466	Na^+/Cl^-
2	298	1.00	466	K^+/Cl^-	23	373	1.00	328	Na^+/Cl^-
3	373	1.00	328	K^+/Cl^-	24	373	1.00	466	Na^+/Cl^-
4	373	1.00	466	K^+/Cl^-	25	493	1.00	164	Na^+/Cl^-
5	493	1.00	164	K^+/Cl^-	26	493	1.00	328	Na^+/Cl^-
6	493	1.00	328	K^+/Cl^-	27	493	1.00	466	Na^+/Cl^-
7	493	1.00	466	K^+/Cl^-	28	683	1.00	164	Na^+/Cl^-
8	683	1.00	164	K^+/Cl^-	29	683	1.00	328	Na^+/Cl^-
9	683	1.00	328	K^+/Cl^-	30	683	1.00	466	Na^+/Cl^-
10	683	1.00	466	K^+/Cl^-	31	298	0.87	328	Li^+/Cl^-
11	298	1.00	328	Li^+/F^-	32	683	0.87	328	Li^+/Cl^-
12	298	1.00	466	Li^+/F^-	33	298	0.87	328	Na^+/Cl^-
13	373	1.00	328	Li^+/F^-	34	683	0.87	328	Na^+/Cl^-
14	373	1.00	466	Li^+/F^-	35	298	0.87	328	K^+/Cl^-
15	493	1.00	164	Li^+/F^-	36	683	0.87	328	K^+/Cl^-
16	493	1.00	328	Li^+/F^-	37	298	0.73	328	Li^+/Cl^-
17	493	1.00	466	Li^+/F^-	38	683	0.73	328	Li^+/Cl^-
18	683	1.00	164	Li^+/F^-	39	298	0.73	328	Na^+/Cl^-
19	683	1.00	328	Li^+/F^-	40	683	0.73	328	Na^+/Cl^-
20	683	1.00	466	Li^+/F^-	41	298	0.73	328	K^+/Cl^-
21	298	1.00	328	Na^+/Cl^-	42	683	0.73	328	K^+/Cl^-

Nw: the number of water molecules inside the carbon nanotube. The MD simulations of the bulk electrolyte solutions at ambient condition (298 K and 101 KPa) and supercritical condition (683 K and 30 MPa) were also carried out for comparison.