Electronic Supporting Information for

Energetic Contribution to Hydration Shell in One-Dimensional Aqueous Electrolyte Solution by Anomalous Hydrogen Bonds

Tomonori Ohba[*] *and Hirofumi Kanoh*

*To whom correspondence should be addressed

E-mail: ohba@pchem2.s.chiba-u.ac.jp

This PDF file includes:

Potential Model

<u>TIP5P model</u>: The site–site potential used here is as follows:

$$\Phi_{ij} = \Sigma \; 4 \; \varepsilon_{ij} \left[\; (\sigma_{ij}/r_{ij})^{12} - (\sigma_{ij}/r_{ij})^{6} \; \right] + (1/4\pi\varepsilon_0) \; q_i q_j \; / \; r_{ij} \qquad (1)$$

where ε_{ij} and σ_{ij} are the potential well depth and collision diameter, and r_{ij} is the distance between sites. The coulombic interaction term is described by the point charges at sites.

Table S1 Molecular numbers of Na^+, Cl^-, and water and densities in CNTs of diameter D = 0.7–2.0 nm

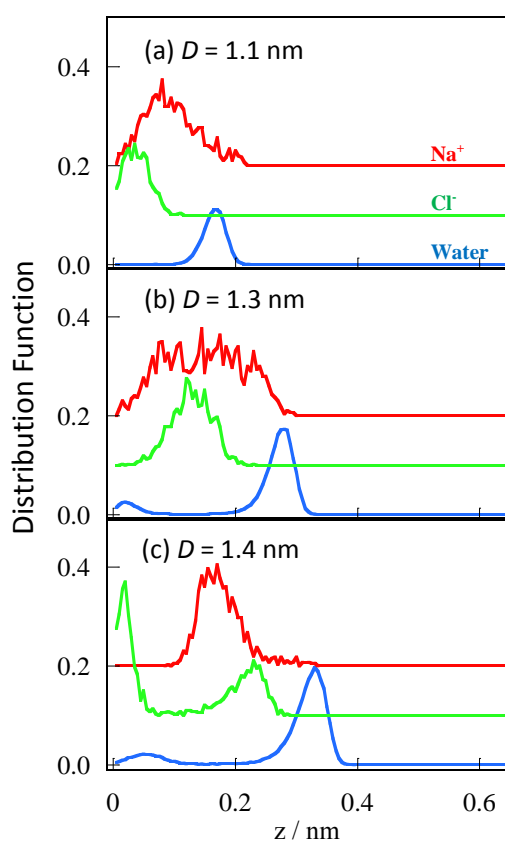| D / nm =	0.7	0.8	0.9	1.0	1.2	1.5	2.0
Na^+	2	2	2	2	4	7	15
Cl^-	2	2	2	2	4	7	15
Water	31	31	31	62	147	326	730
d / kg L^{-1}	-	-	0.37	0.70	0.82	0.93	1.01
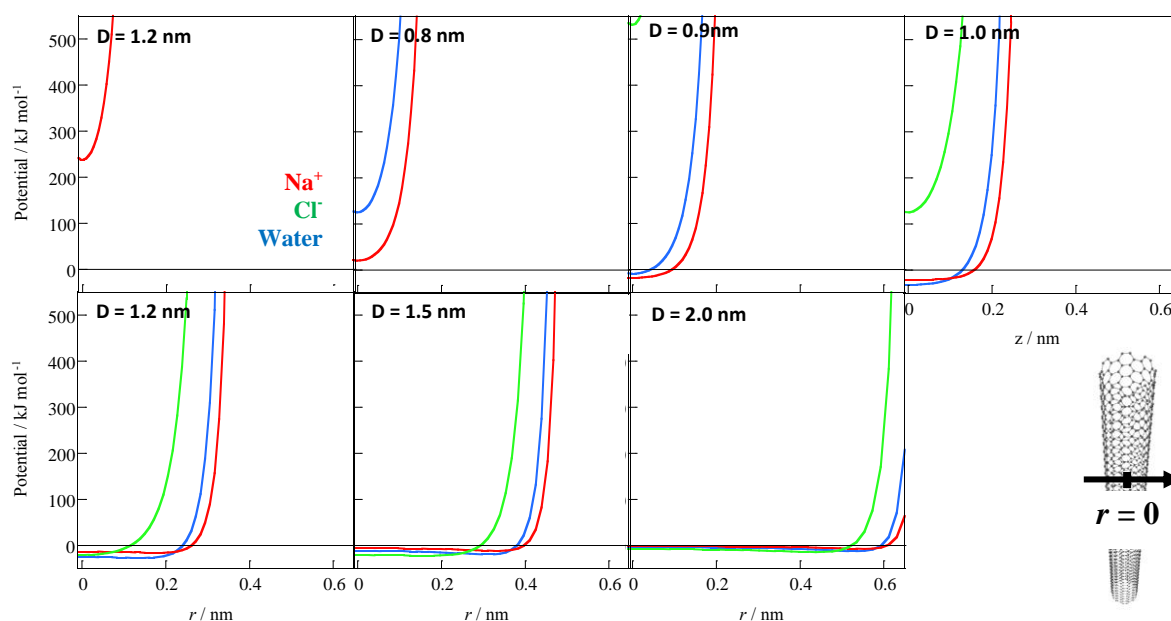
**Figure S1.** Potential profiles of Na^+, Cl^-, and water molecules in CNTs of diameters 0.7–2.0 nm.
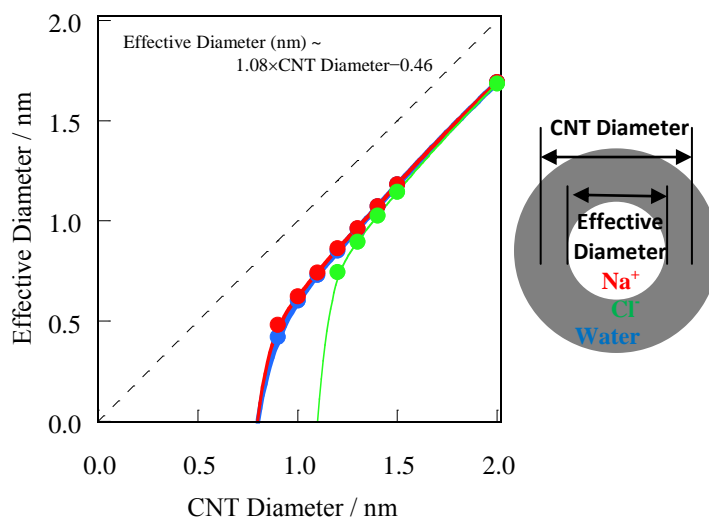
Figure S2. Effective diameters of Na^+, Cl^-, and water molecules as function of CNT diameter.

Figure S3. Distributions of Na^+, Cl^-, and water molecules against a CNT axis for CNT diameters of $D = 1.1$ (a), 1.3 (b), and 1.4 nm (c).
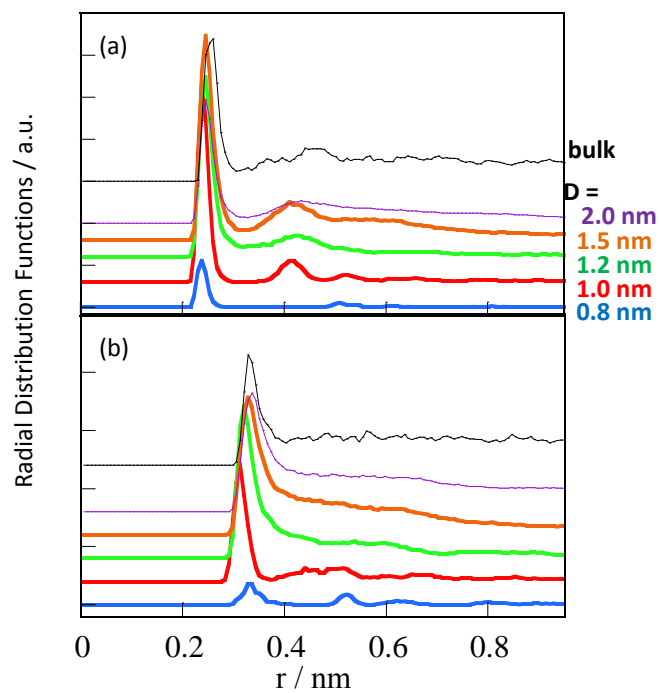
Figure S4. Radial distribution functions of water from (a) Na^+ and (b) Cl^- ions for CNTs of diameter 0.8–2.0 nm.
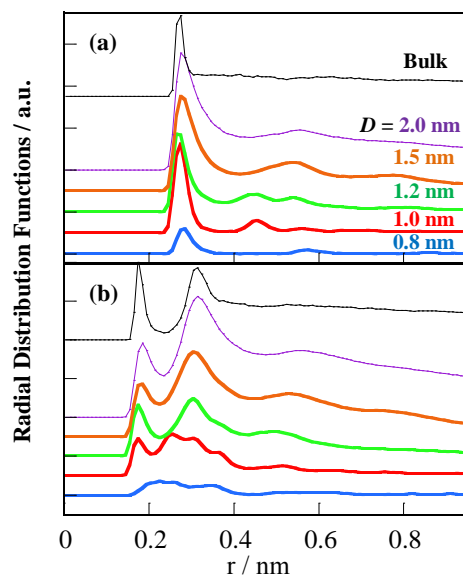
Figure S5. Radial distribution functions between (a) O–O and (b) O–H of water molecules in CNTs of diameters D = 0.8–2.0 nm.