

Supplementary Information

**Confinement and surface effects of aqueous solutions within
charged carbon nanotubes**

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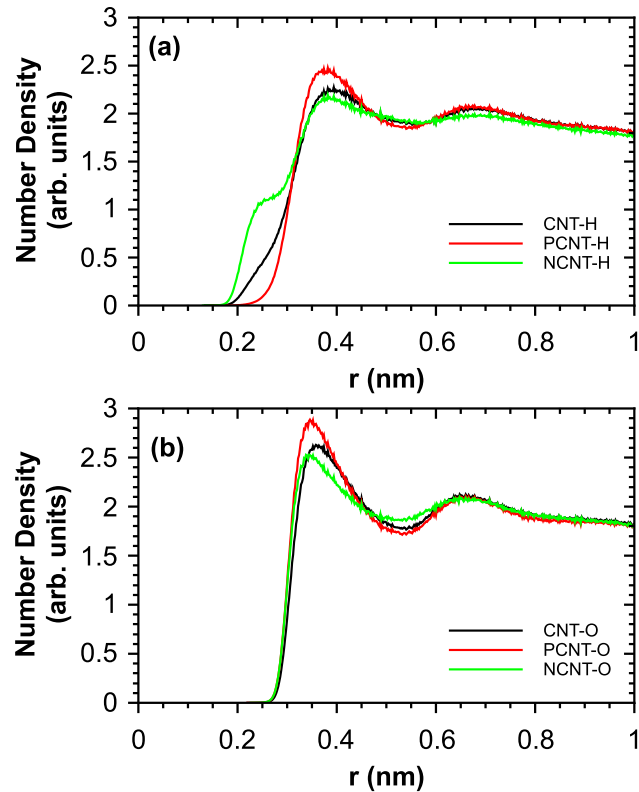


Fig. S1: (a) Hydrogen and (b) Oxygen radial distribution profiles of 1 M NaCl solution in neutral and charged tubes (PCNT, NCNT) of diameter 2.167 nm (16,16 CNT). Distance is taken from the surface out to 1nm, which corresponds to approximately the center of the tube.

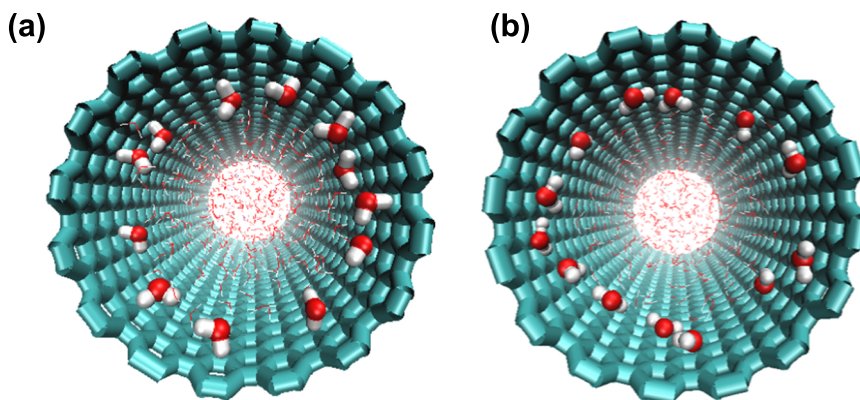


Fig. S2: A representative snapshot of the water orientation at the CNT surface of (a) negatively and (b) positively charged 2.167 nm tubes containing 1M NaCl. One ring of water molecules nearest to the CNT surface has been highlighted (other water and ions are not magnified for clarity). In negative tubes, the water is oriented with a hydrogen atom pointing toward the wall, while in positive tubes the oxygen is tilted slightly toward the wall.

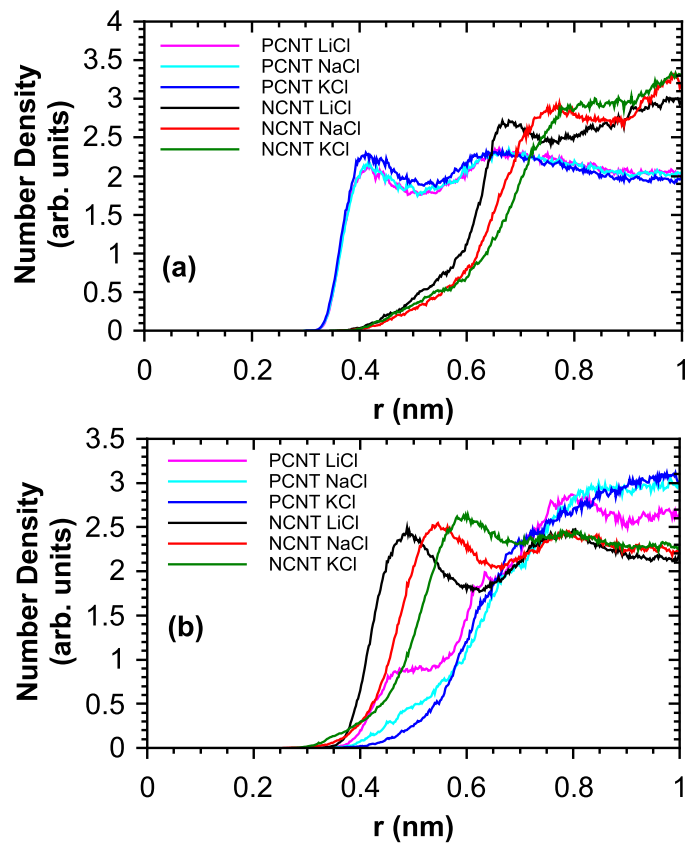


Fig. S3: (a) Chloride and (b) Cation radial distribution profiles of 1 M solutions in positively (PCNT) and negatively (NCNT) charged tubes of diameter 2.167 nm (16,16 CNT). Distance is taken from the surface out to 1nm, which corresponds to approximately the center of the tube.