Electronic Supplementary Information for

Significant curvature effects of partially charged carbon nanotubes on electrolyte behavior using Monte Carlo simulation

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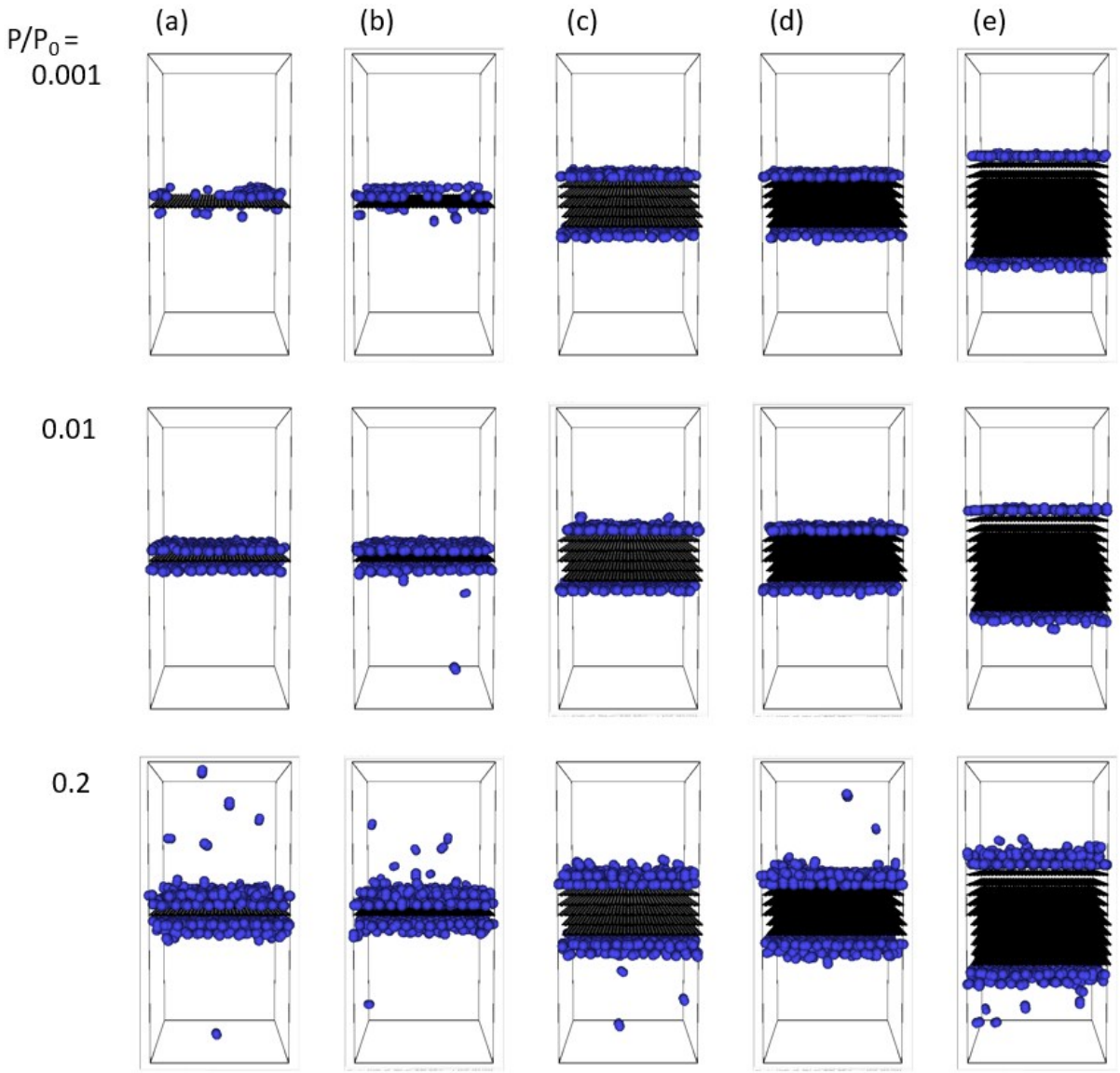

Figure S1. Snapshots of N_2 adsorbed on graphene in the 1-layered partially charged graphene (a), 1-layered non-charged graphene (b), 5-layered partially charged graphene (c), 5-layered non-charged graphene (d), and 10-layered non-charged graphene (e) models. Blue and black spheres represent nitrogen and carbon atoms, respectively.

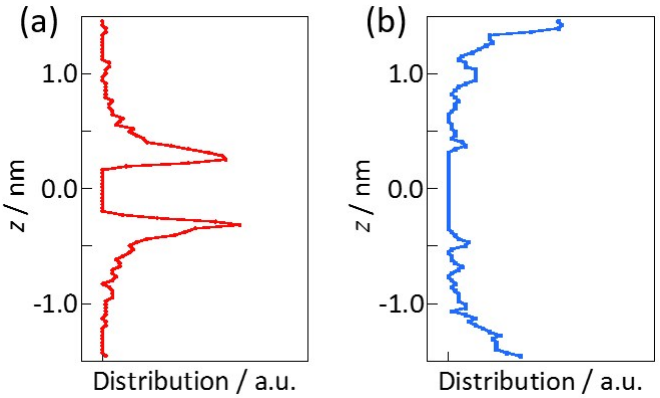

Figure S2. Number distribution of Na (a) and Cl ions (b) on graphene in the partially charged graphene model using canonical MC simulations of each single ion. Graphene is located in the center of the unit cell at $z = 0$.

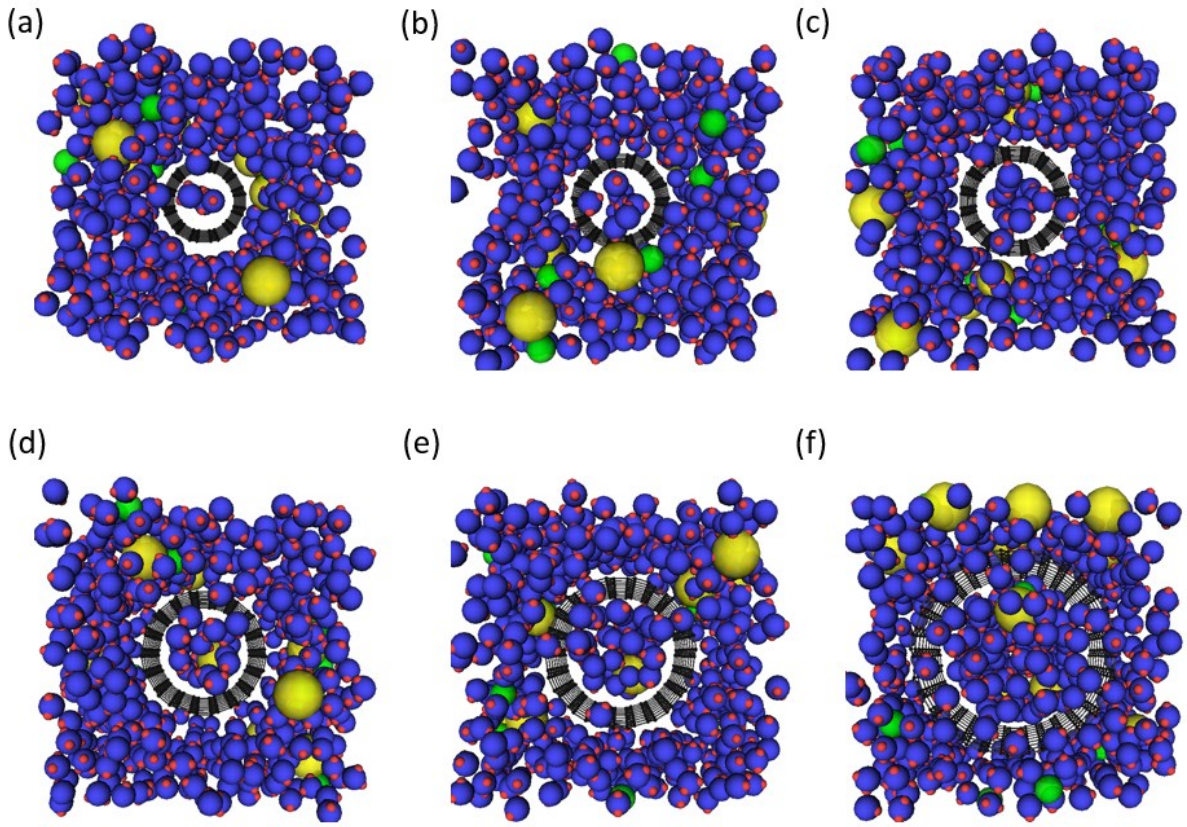

Figure S3. Snapshots of electrolyte adsorbed in the non-charged CNTs with a diameter of 0.8 (a), 1.0 (b), 1.1 (c), 1.2 (d), 1.5 (e), and 2.0 nm (f). Green and yellow spheres represent Na and Cl ions, respectively. A water molecule is depicted by a blue sphere (oxygen) associated with two red spheres (hydrogen). The black cylinder in the center of each snapshot represents a CNT.

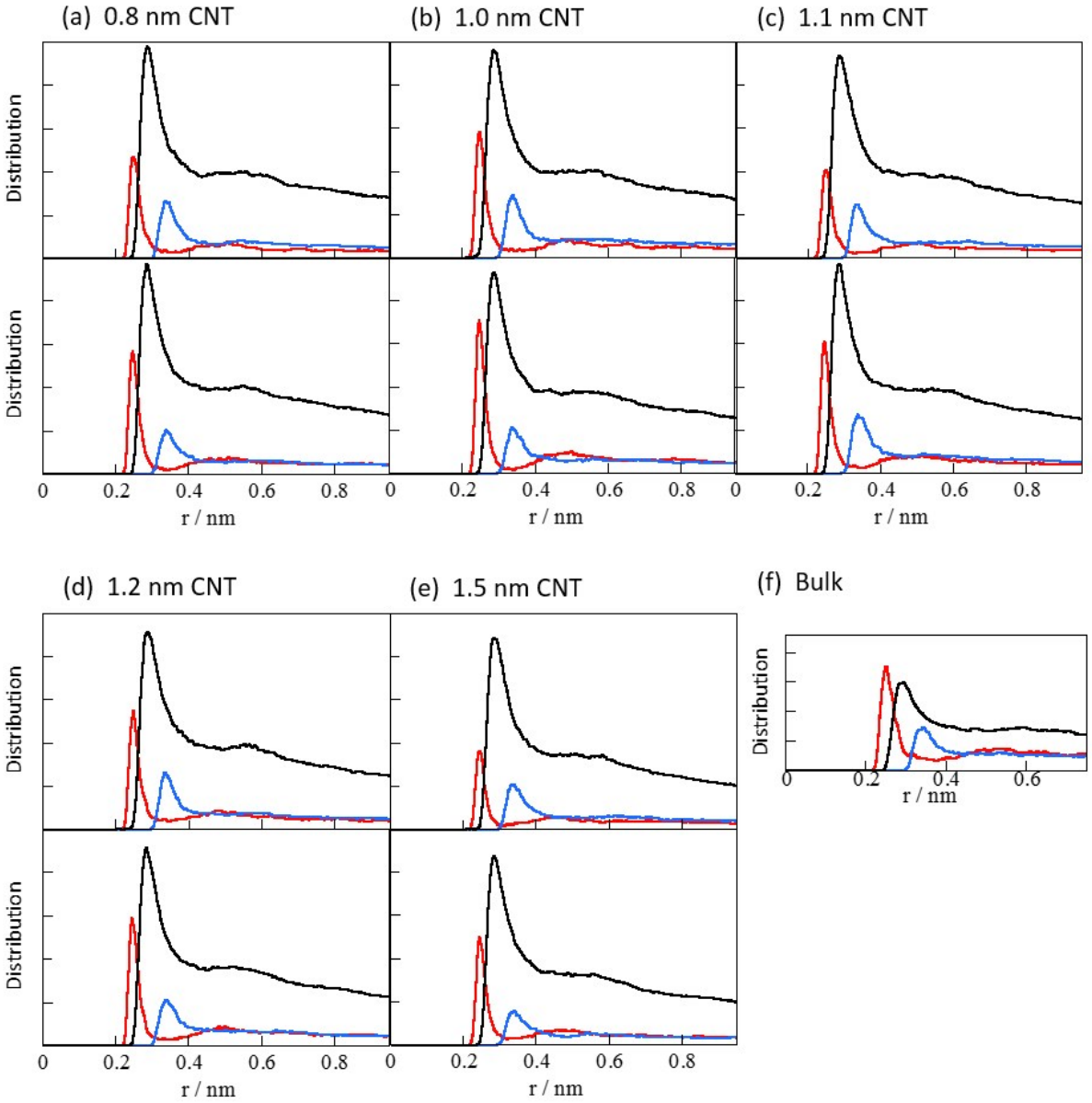

Figure S4. Radial distribution functions of Na−water (red curves), Cl−water (blue curves), and water−water (black curves) in the external sites of partially charged CNTs (top) and non-charged CNTs (bottom).