Molecular Simulation of Ion-Specific Effects in Confined Electrolyte Solutions Using Polarizable Forcefields

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Supporting Information
Figure S1 – (color online) Radial density profiles for water (black line), sodium ions (blue line) and halide ions (green line) for confined electrolyte solutions NaX (X = F, Cl, Br, I), in the 3 nm carbon nanotube. R = 0 and 15 Å correspond to the center of the nanotube and the wall of the nanotube, respectively. For each confined electrolyte solution, a typical configuration is shown to illustrate a structure of the system. Grey segments are bonds between the carbon atoms of the nanotube while the white and red segments are the water molecules. Blue, yellow, green, brass and pink spheres are the Na, F, Cl, Br and I ions, respectively.
Figure S2 – (color online) Radial density profiles for water (black line), sodium ions (blue line) and halide ions (green line) for confined electrolyte solutions NaX (X = F, Cl, Br, I), in the 1 nm carbon nanotube. \( R = 0 \) and 15 Å correspond to the center of the nanotube and the wall of the nanotube, respectively. For each confined electrolyte solution, a typical configuration is shown to illustrate a structure of the system. Grey segments are bonds between the carbon atoms of the nanotube while the white and red segments are the water molecules. Blue, yellow, green, brass and pink spheres are the Na, F, Cl, Br and I ions, respectively.