Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Ab initio Molecular Dynamics Simulations of Water and an Excess Proton in Water Confined in Carbon Nanotubes

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Supplementary Information

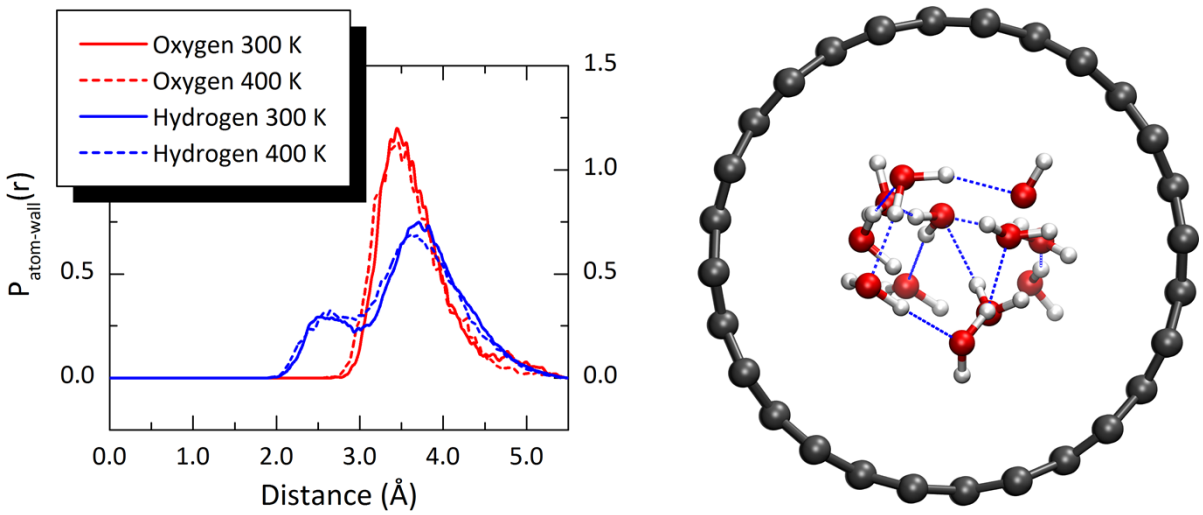


Figure S1. (Left) Distribution function of the axial distance of the oxygen and hydrogen atoms from the inner wall of the CNT for N-14 at 300 and 400 K and (right) snapshot of N-14 at 400 K down the CNT axis. Hydrogen bonds are denoted by dashed lines.

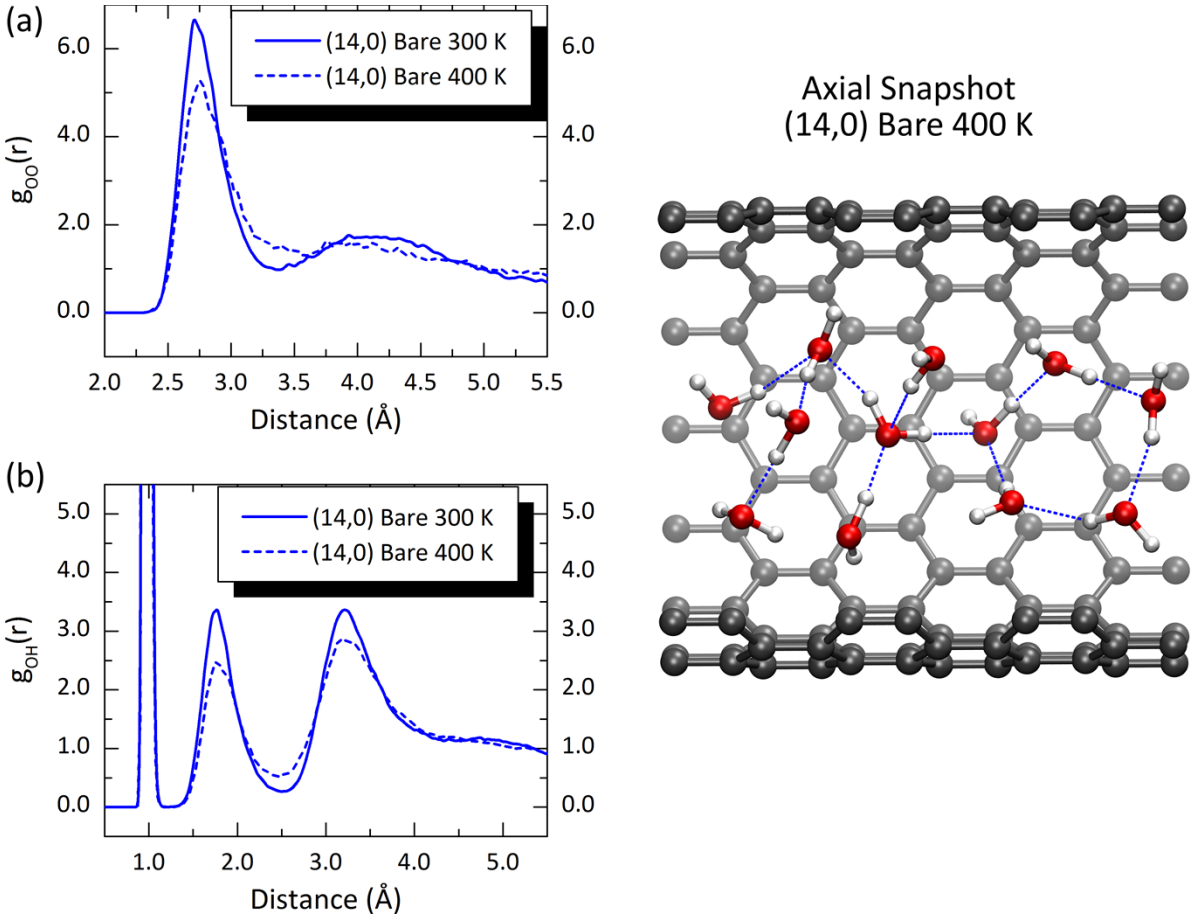
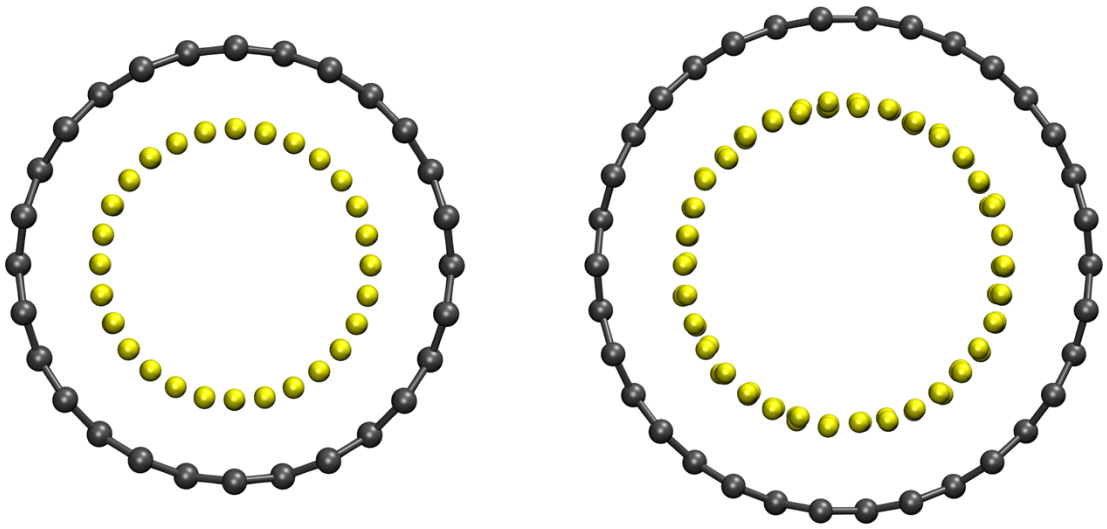


Figure S2. (a) Oxygen–oxygen and (b) oxygen–hydrogen radial distribution functions for N-14 at 300 and 400 K with a representative axial snapshot at 400 K shown in the right panel.



(a) (b)

Figure S3. Relaxed structures under loose convergence criteria of the fluorinated CNTs for (a) F-14 and (b) F-17.