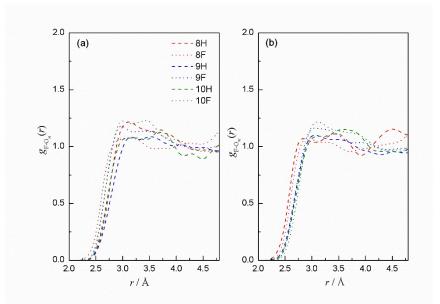
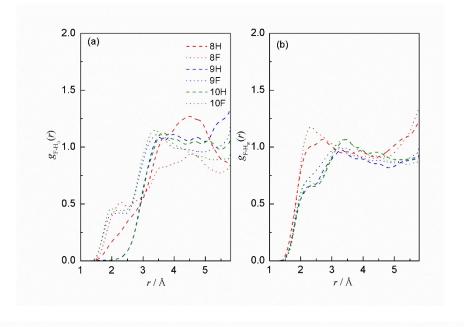
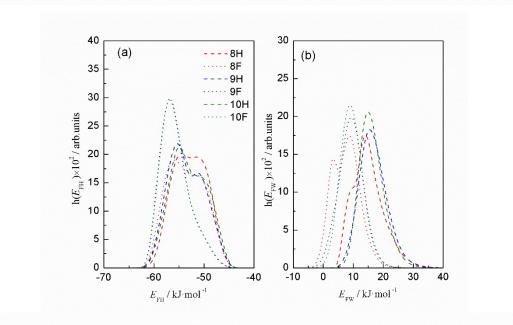
## **Supplementary information**



**Fig. S1** Radial distribution functions for the F-O pairs confined in the different CNTs: (a)  $F-O_H$ , (b)  $F-O_W$ . The capital letter F represents fluorine, O corresponds to oxygen and the subscripts W and H represent water and hydronium.



**Fig. S2** Radial distribution functions for the F-H pairs confined in the different CNTs: (a)  $F-H_{H}$ , (b)  $F-H_{W}$ . The capital H corresponds to hydrogen.



**Fig. S3** Normalized statistical distributions of the pair-potential energy  $E_{ij}$  for the fluorine-hydronium (a) and fluorine-water (b) pairs that classified as hydrogen bonded by the geometric criterion.  $h(^{E_{ij}})$  denotes the probability of molecular pairs of pair-potential energy  $E_{ij}$ .