Supporting Information

Enhanced separation of tetrafluoropropanol from water via carbon nanotubes membranes: insights from molecular dynamics simulations

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Table S1 The Lennard-Jones parameters and charges of CNTs and function groups.

Interaction		σ (Å)	ε (Kcal/mol)	Charge
CNT	C-C	1.9924	0.0700	0.000
Function group-F	F-F	1.6300	0.1050	-0.250
H_2O	O-O	1.7682	0.1521	-0.834
H_2O	H-H	0.2245	0.0460	0.417
TFP	C_1-C_1	2.0500	0.0420	0.447
TFP	C_2-C_2	2.3000	0.0200	0.500
TFP	C_3-C_3	2.0100	0.0560	0.027
TFP	F-F	1.6300	0.1050	-0.250
TFP	O_F-O_F	1.7650	0.1921	-0.557
TFP	H_{F1}-H_{F1}	1.3000	0.0300	0.053
TFP	H_{F2}-H_{F2}	1.3400	0.0350	0.053
TFP	H_{F3}-H_{F3}	1.3400	0.0350	0.053
TFP	H_{OH}-H_{OH}	0.2245	0.0460	0.424

* The atoms of TFP are shown below.

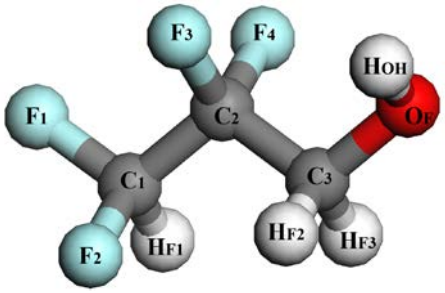

Table S2 The TFP and water flux of CNT membrane with different temperature under 4 atm pressure. All flux calculations are 10ns.

Temperature(K)	Normalized flux(molecule/CNTs·10ns)			α_{TFP}	Mass fraction of TFP（%）
	TFP	water	total		
283.15	7	8	15	2.63	86.52
303.15	24	13	37	5.54	92.96
323.15	29	15	44	5.80	93.41
343.15	32	11	43	8.73	95.52

Table S3 The diffusion coefficient of TFP and water in CNT membrane with different temperature.

Temperature(K)	Diffusion coefficient (10^{-5}Å^2/ns)	
	TFP	water
283.15	17.17	1.980
303.15	33.84	5.512
323.15	47.01	8.222
343.15	59.00	9.009

Table S4 The TFP and water flux of CNT membrane with different pore sizes under 4 atm pressure. All flux calculations are 10ns.

diameter	Normalized flux(molecule/CNTs·10ns)			α_{TFP}	Mass fraction of TFP（%）
	TFP	water	total		
(5,5)	0	6	6	0	0
(6,6)	0	327	327	0	0
(7,7)	16	3	19	16	97.51
(8,8)	32	11	43	8.73	95.52
(9,9)	27	38	65	2.133	83.90
(10,10)	36	44	80	2.453	85.72
(11,11)	39	37	76	3.163	88.55
(12,12)	44	41	85	3.22	88.73
(13,13)	44	60	104	2.2	84.33
(14,14)	47	54	101	2.61	86.46

Table S5 Diameter of CNTs.

Size	Diameter of CNT（Å）	
	C-C	internal
(5,5)	6.78	3.28
(6,6)	8.14	4.64
(7,7)	9.49	5.99
(8,8)	10.85	7.35
(9,9)	12.2	8.7
(10,10)	13.56	10.06
(11,11)	14.92	11.42
(12,12)	16.27	12.77
(13,13)	17.63	14.13
(14,14)	18.98	15.48

Table S6 The TFP and water flux of entrance modified CNT membrane with different pore sizes under 4 atm pressure. All flux calculations are 10ns.

diameter	Normalized flux(molecule/CNTs·10ns)			α_{water}	Mass fraction of water（%）
	TFP	water	total		
(7,7)	0	41	41	+∞	100
(8,8)	2	110	112	18.333	88.231
(9,9)	1	208	209	69.333	96.593
(10,10)	3	382	385	42.444	94.552
(11,11)	5	431	436	28.733	92.156
(12,12)	9	681	690	25.222	91.161
(13,13)	19	604	623	10.596	81.249
(14,14)	38	661	699	5.798	70.335

Table S7 The TFP and water flux of interior and/or entrance modified CNT membrane with different pore sizes under 4 atm pressure. All flux calculations are 10ns. (9,9)-m represents interior modified of (9,9) CNTs and (9,9)-e-m represents interior and entrance modified of (9,9) CNTs.

diameter	Normalized flux(molecule/CNTs·10ns)			α_{water}	Mass fraction of water（%）
	TFP	water	total		
(9,9)-m	0	135	135	+∞	100
(10,10)-m	1	167	168	18.333	88.231
(10,10)-e-m	0	239	239	69.333	96.593
(11,11)-e-m	0	356	356	42.444	94.552
(12,12)-e-m	2	230	232	28.733	92.156
(13,13)-e-m	2	125	127	25.222	91.161
(14,14)-e-m	18	108	623	10.596	81.249

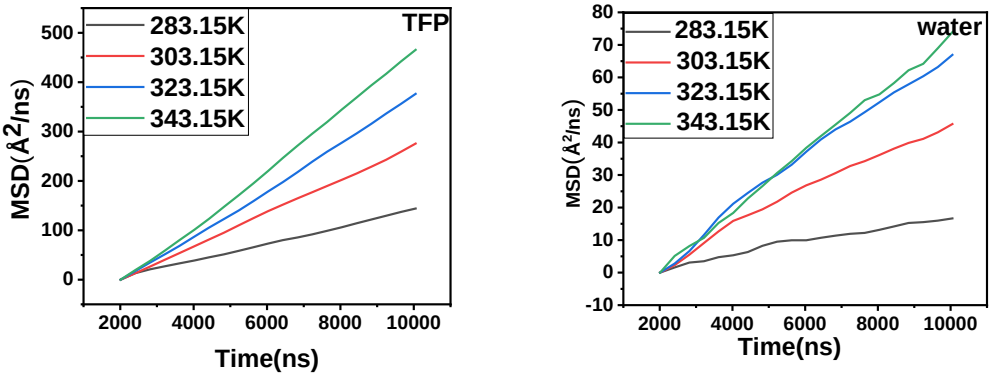

Fig.S1 The MSD of TFP and water in CNT membrane with different temperature.

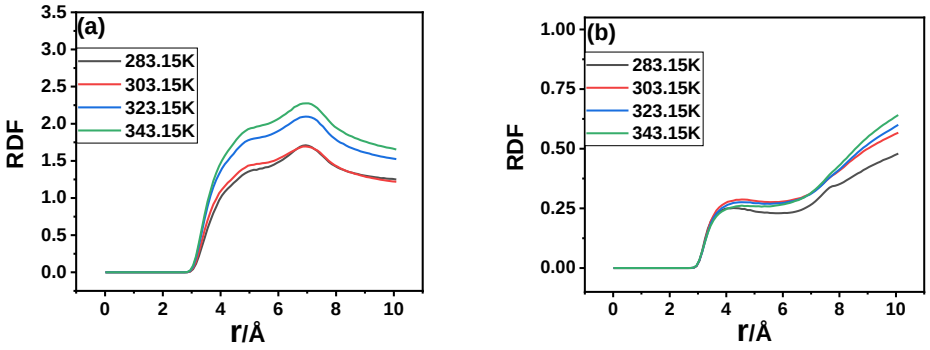

Fig.S2 The RDF profiles of oxygen atom of CNTs(C) and TFP(OT) (a), water (OW) (b).

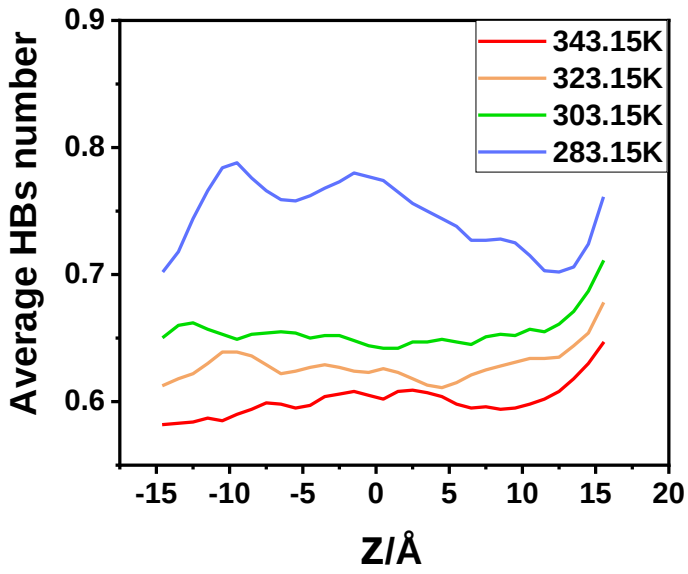

Fig.S3 HBs in CNTs with different temperatures.

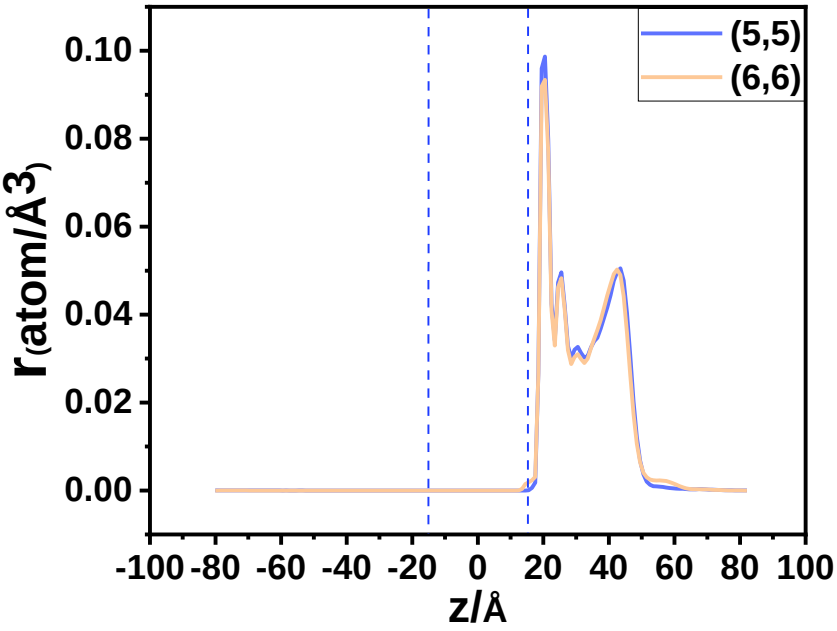

Fig.S4 The z-axis density distribution of TFP in the CNTs membrane, where the CNTs lies from z=-1.4 to z=1.4nm.

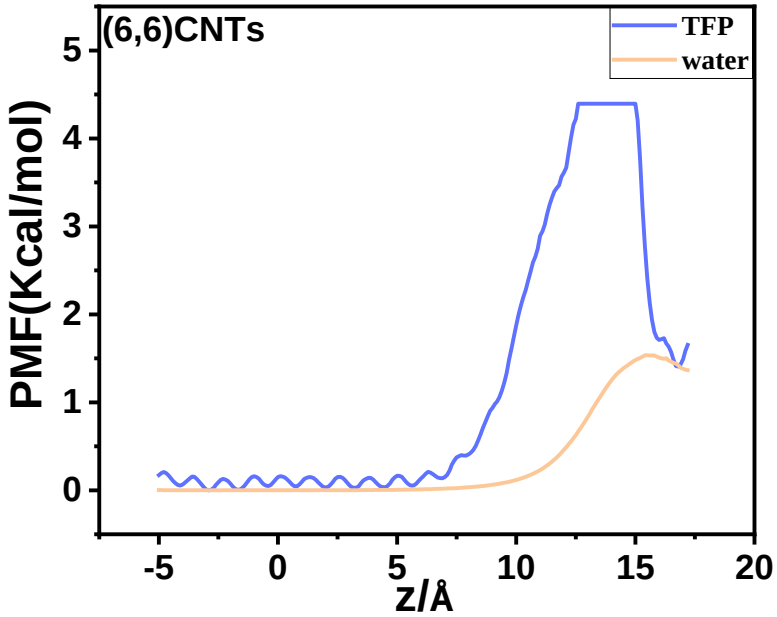

Fig.S5 PMF (potential of mean force) for TFP and water molecules across the (6,6) CNTs membrane (from bulk to the center of CNTs, CNTs locate at z=-14 Å to 14Å).

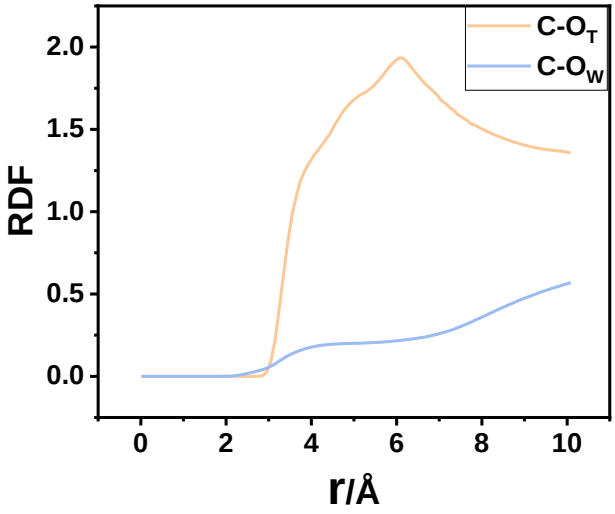

Fig.S6 The RDF profiles of oxygen atom of TFP(O_T), water (O_W) and CNTs(C).

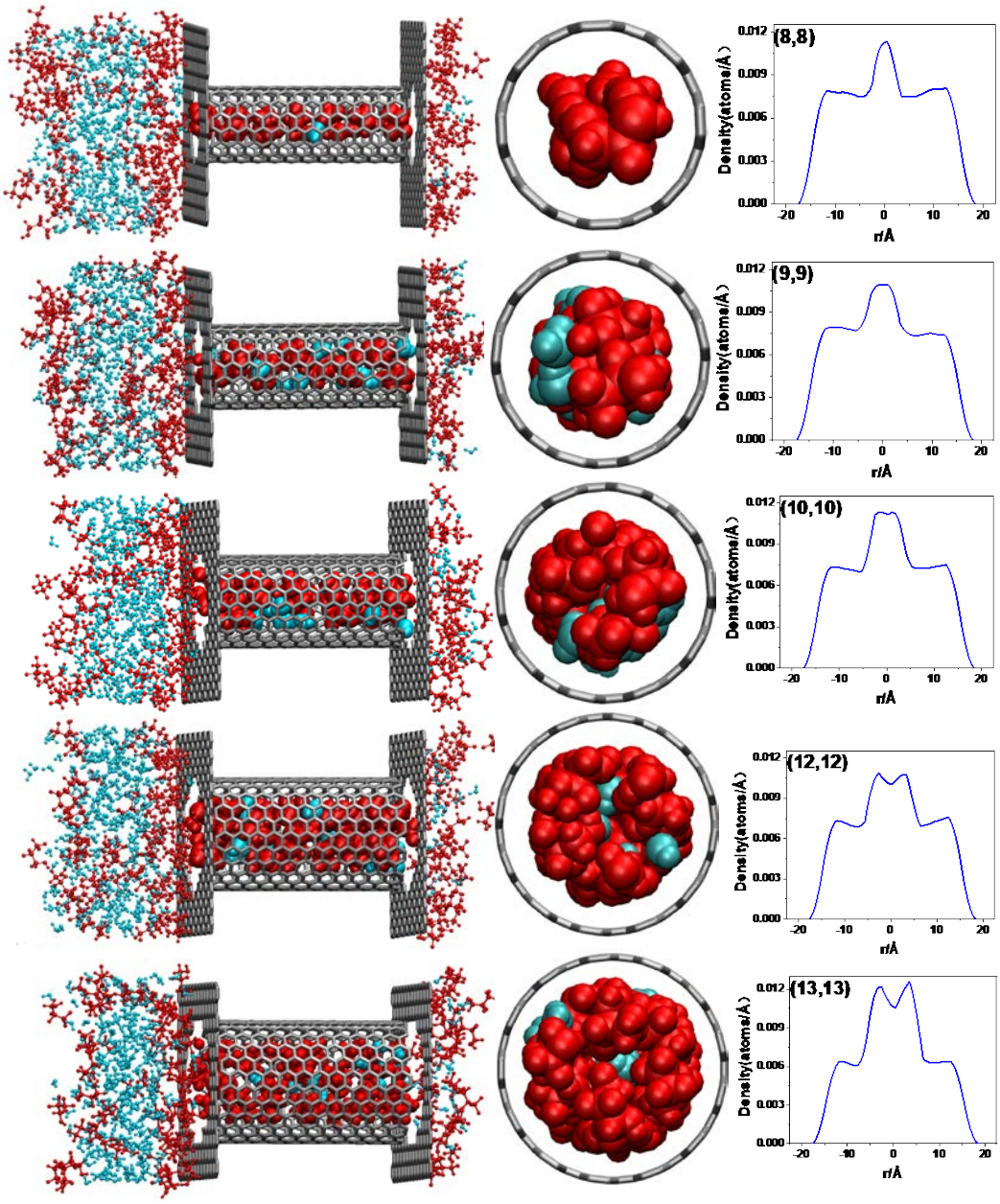

Fig.S7 TFP/water structures inside (8,8), (9,9), (10,10), (12,12) and (13,13) CNTs (red: TFP molecules; blue: water molecules) (a); Density distribution profiles of TFP molecules in the CNTs, and y=0 corresponds to the middle position of CNTs(b).

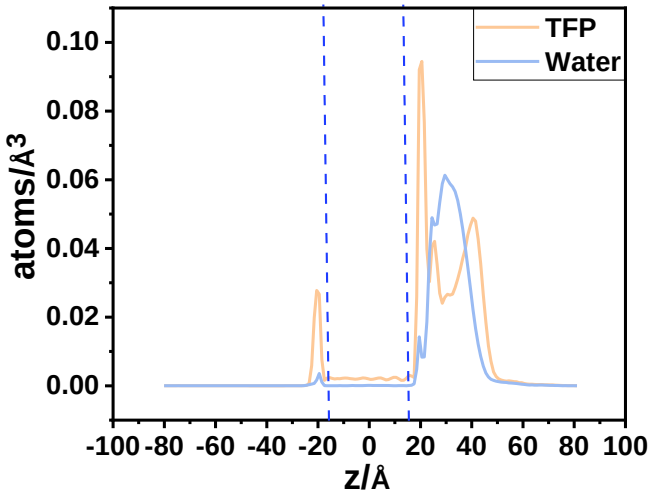

Fig.S8 The z-axis density distribution of TFP and water in CNTs membranes. where the CNTs lies from z=-14 to z=14 Å (dotted line areas).

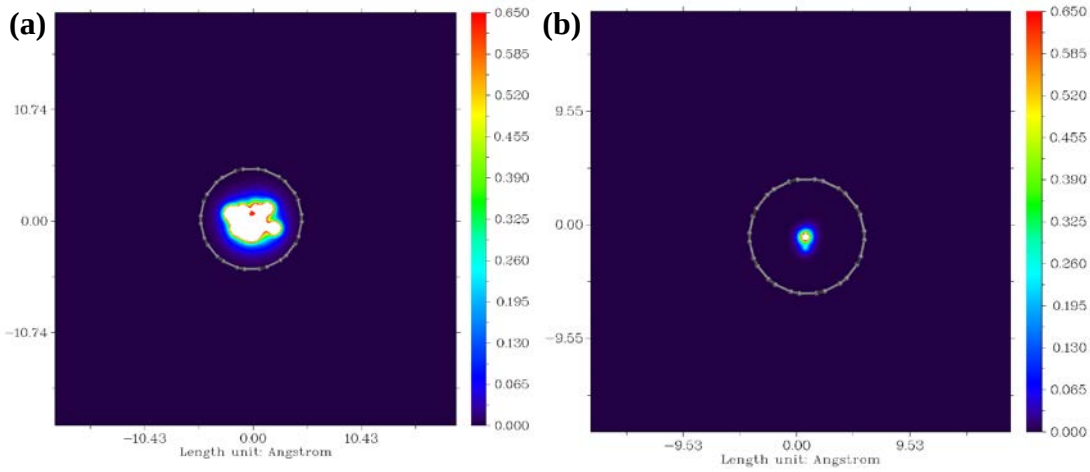

Fig.S9 The x-y plane average density distribution of TFP(a) and water(b) molecules inside CNTs pores.

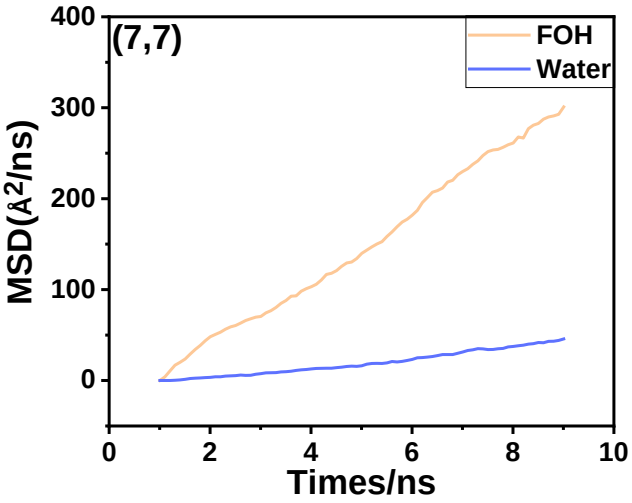

Fig.S10 MSD of TFP and water molecules in (7,7) CNTs.

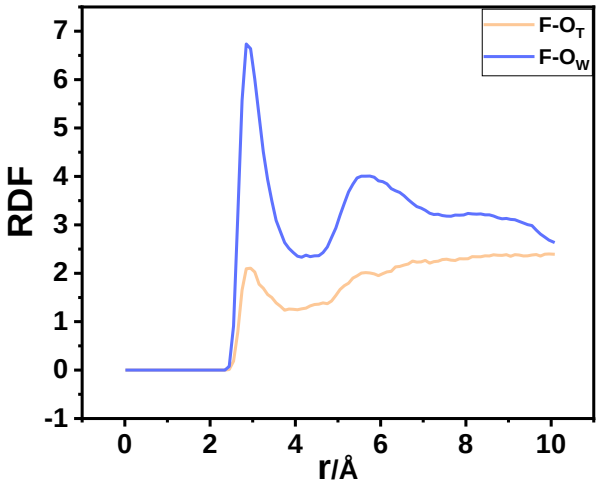

Fig.S11 The RDF profiles of oxygen atom of TFP(O_T), water (O_W) and functional groups(F).

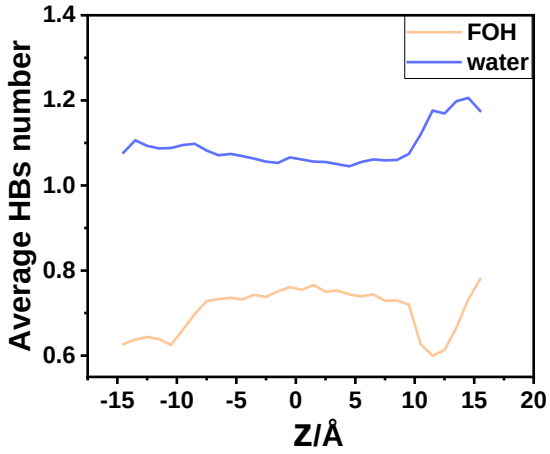

Fig.S12 HBs of TFP and water molecules in fluorine modification CNTs (including the intermolecular hydrogen bonds of water or TFP molecules), where the CNTs lies from z=-14 to z=14Å.

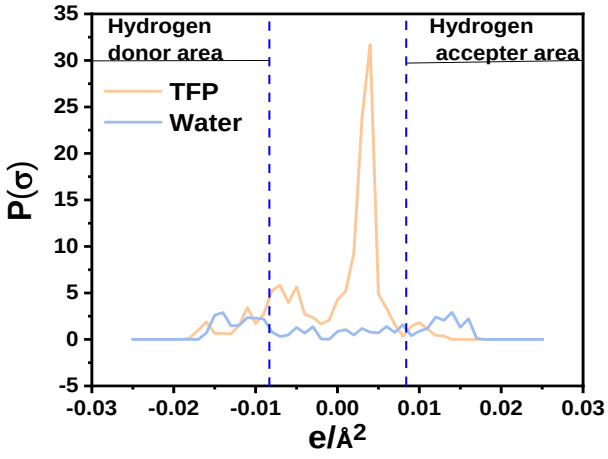

Fig.S13 σ-profile comparison of TFP and water.

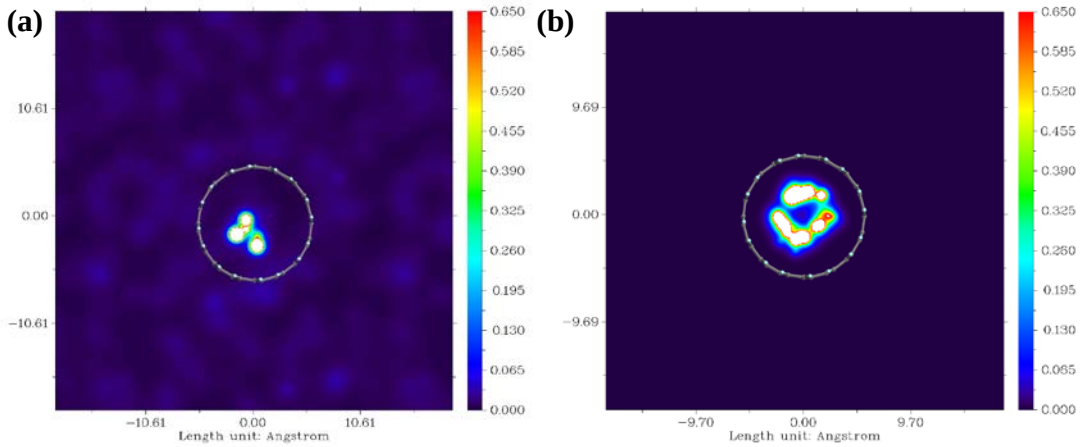

Fig.S14 The x-y plane average density distribution of TFP(a) and water(b) molecules inside fluorine modified CNTs pores.