Supporting Information

Pb^{2+} Removal Based on Confinement Effect in Polygonal Carbon Nanotube: A Molecular Dynamics Simulation

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Supporting information includes:

Table S1. Force field parameters of atoms involved in this work.

Table S2. The trajectory of each Pb^{2+} ion (No.1~No.5) in 4N, 5N, 6N, 8N, 4F, 5F, 6F and 8F, respectively.

Table S3. Presentation of hydrogen-bonding network versus the time.

Figure S1. Representative initial configurations of 4F, 5F, 6F and 8F. (a)~(d) represents 4-, 5-, 6-, 8-CNT in the z-direction, and (e)~(h) represents 4-, 5-, 6-, 8-CNT in the y-direction, respectively

Figure S2. Pore size distributions (PSDs) of PCNTs calculated by zeo^{++}.

Figure S3. RDF plots of H_3O^+ in PCNTs/G without Pb^{2+}.

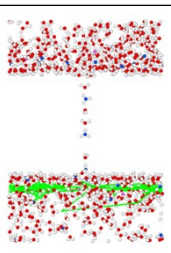
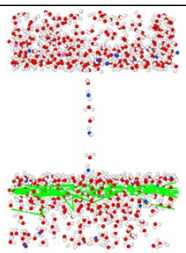
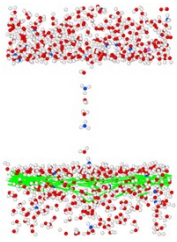
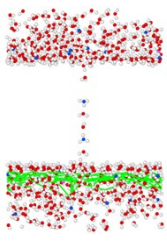
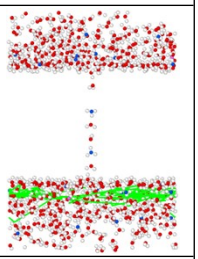
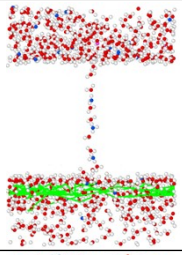
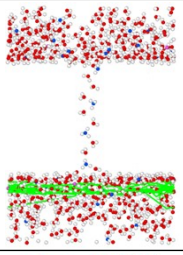
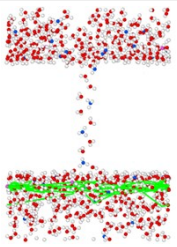
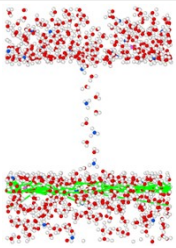
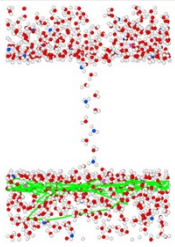
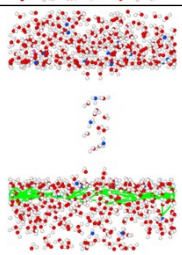
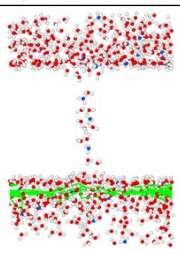
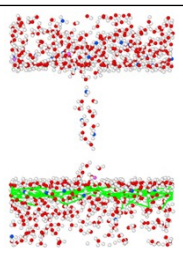
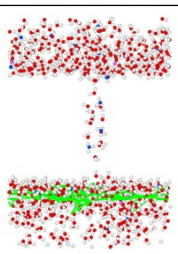
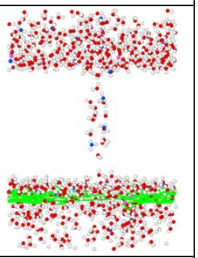
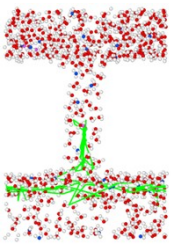
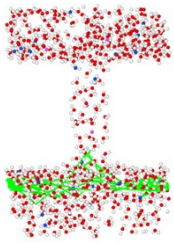
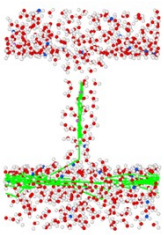
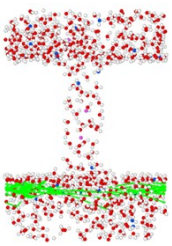
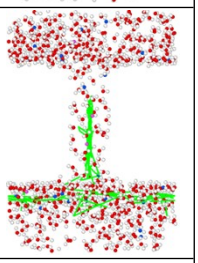
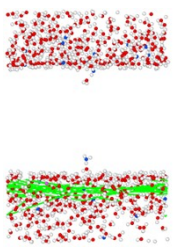
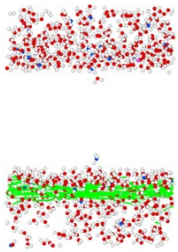
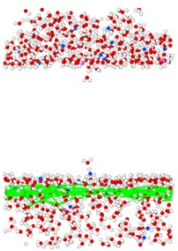
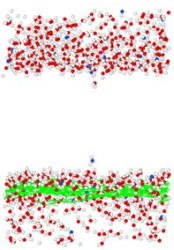
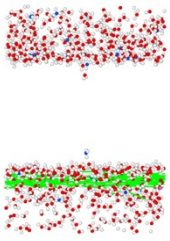
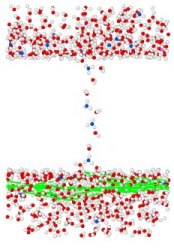
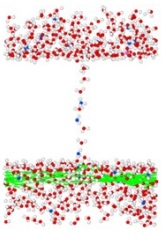
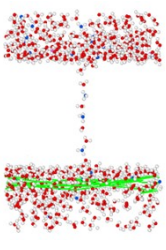
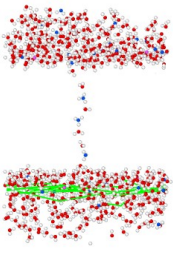
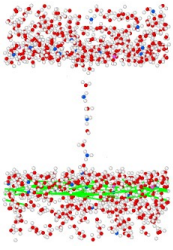
Figure S4. RDF plots of H_3O^+ in fluorinated PCNTs/G without Pb^{2+}.

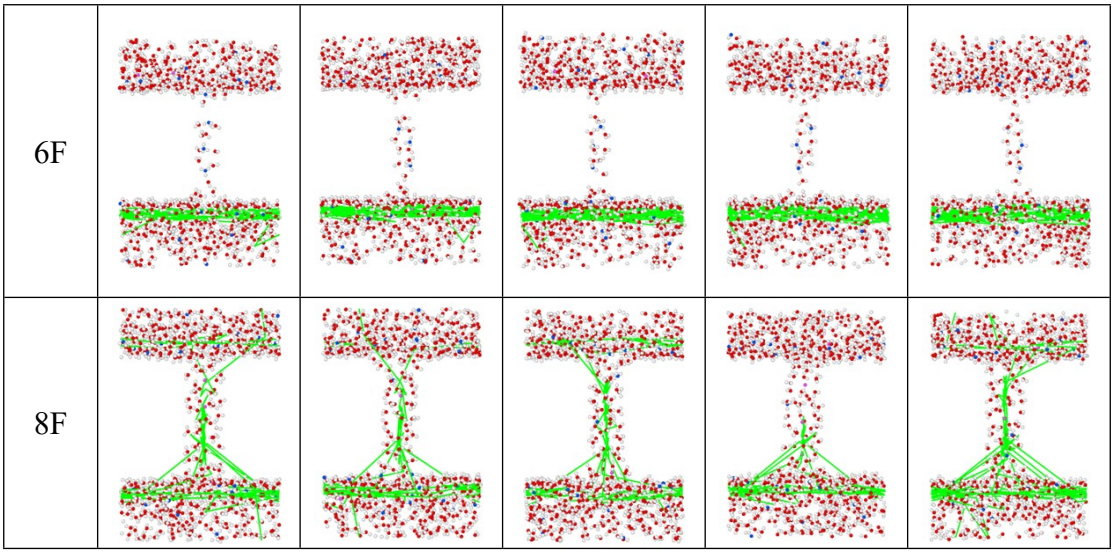
Figure S5. Side (upper) and top (lower) views of hydrogen-bonding representation. (a)~(d) represents 4N, 5N, 6N and 8N, and (e)~(h) represents 4F, 5F, 6F and 8F. (i) and (j) represents the hydrogen-bonding network containing Pb^{2+} in 8N and 8F, respectively. Where grey, red, white, blue, yellow and pink respectively represents carbon, oxygen, hydrogen, O_hydronium, fluorine and Pb^{2+}.

Table S1. Force field parameters for atoms involved in this work.

Atom	ε_{ij} (kcal/mol)	σ (Å)	Charge(|e|)	Ref.
C	0.105	3.851	0.00	1, 2
$C_{C\text{-}F}$	0.105	3.851	+0.109	1, 2
F	0.069	3.08	-0.109	3
$O_{tip}\_H_2O$	0.184	3.553	-0.82	4, 5
$H_{tip}\_H_2O$	0.010	0.900	+0.41	4, 5
$O^*\_H_3O^+$	0.184	3.553	-0.38	4, 5
$H^*\_H_3O^+$	0.010	0.900	+0.46	4, 5
Pb^{2+}	0.663	4.297	+2.00	6

Table S2. The trajectory of each Pb^{2+} ion (No.1~No.5) in 4N, 5N, 6N, 8N, 4F, 5F, 6F and 8F, respectively.

	Pb^{2+}-No.1	Pb^{2+}-No.2	Pb^{2+}-No.3	Pb^{2+}-No.4	Pb^{2+}-No.5
4N					
5N					
6N					
8N					
4F					
5F					



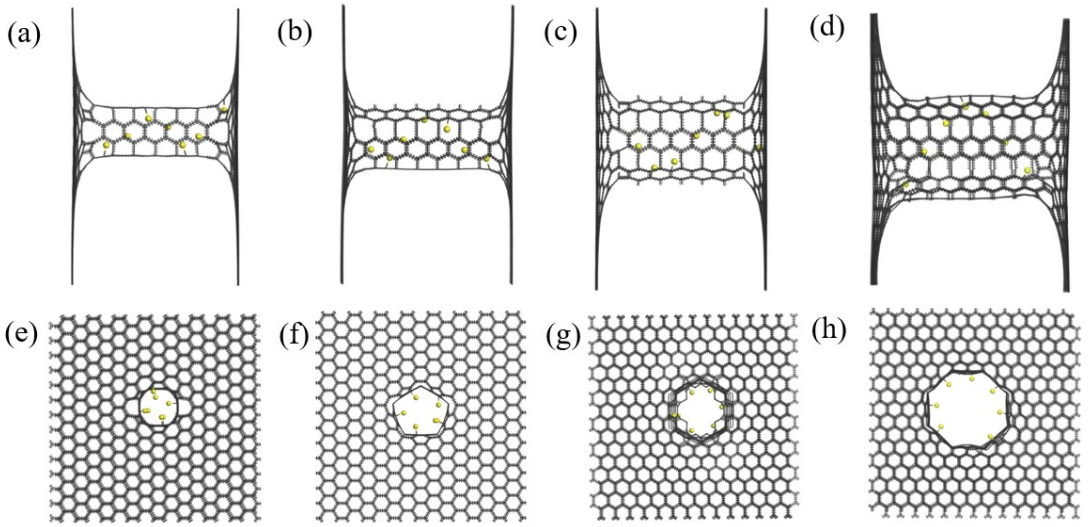


Figure S1. Representative initial configurations of 4F, 5F, 6F and 8F. (a)~(d) represents 4-, 5-, 6-, 8-CNT in the z-direction, and (e)~(h) represents 4-, 5-, 6-, 8-CNT in the y-direction, respectively.

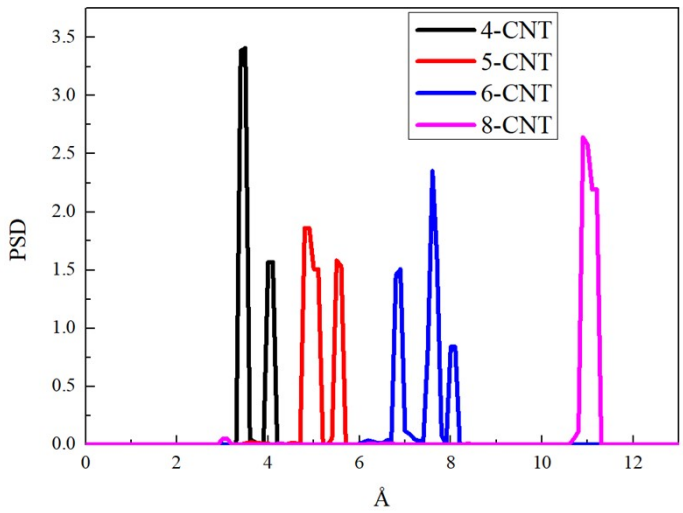


Figure S2. Pore size distributions (PSDs) of PCNTs calculated by zeo^{++}.[7]

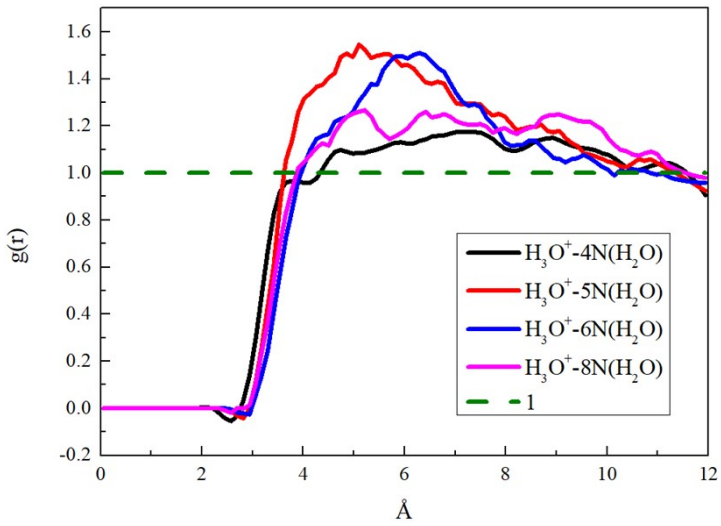


Figure S3. RDF plots of H_3O^+ in PCNTs/G without Pb^{2+}.

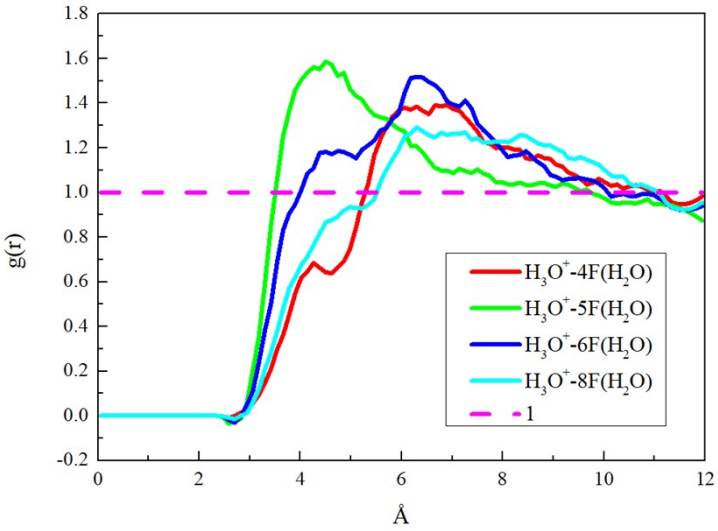


Figure S4. RDF plots of H_3O^+ in fluorinated PCNTs/G without Pb^{2+}.

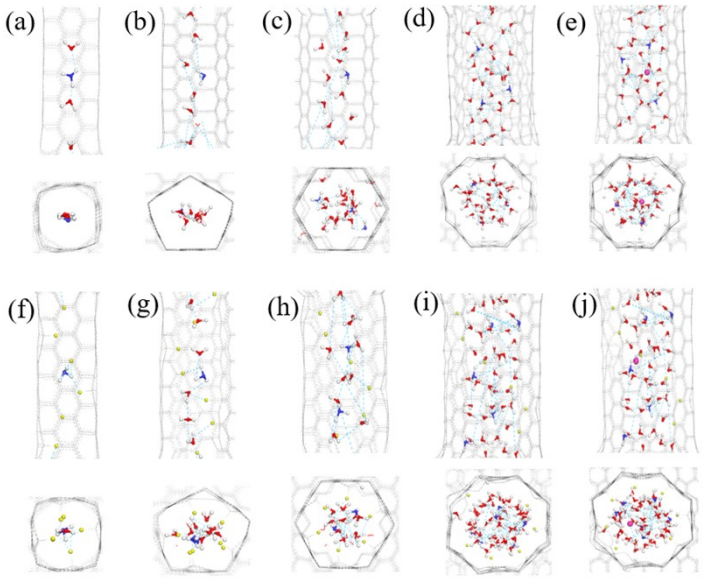
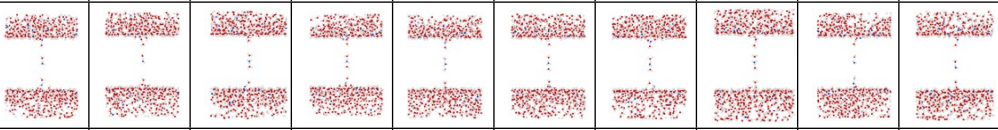
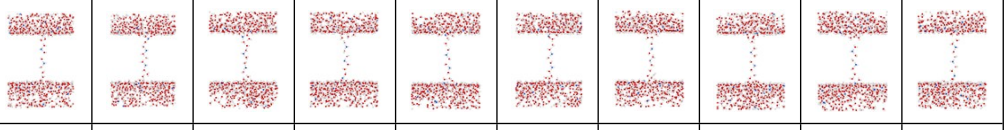
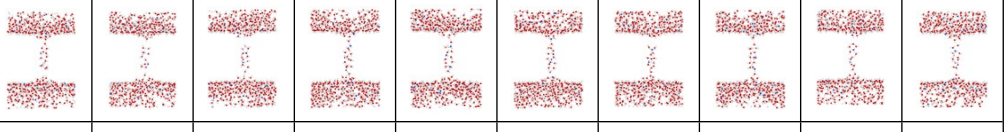
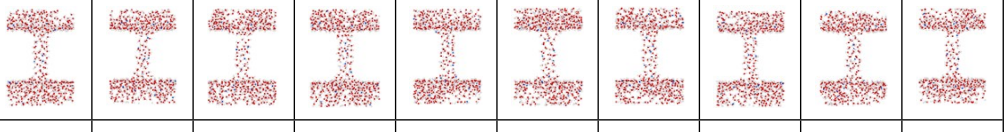
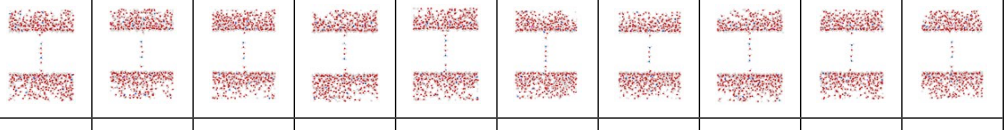
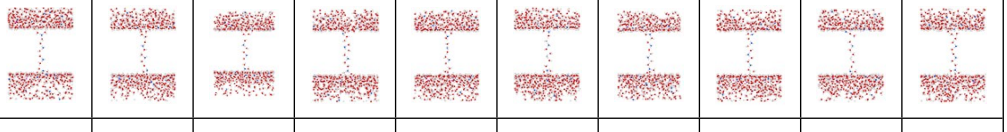
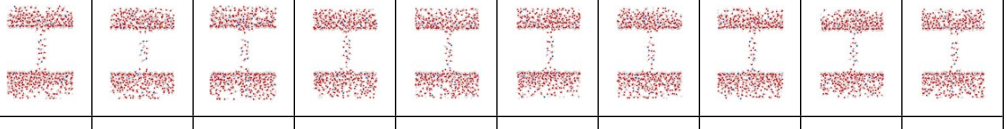
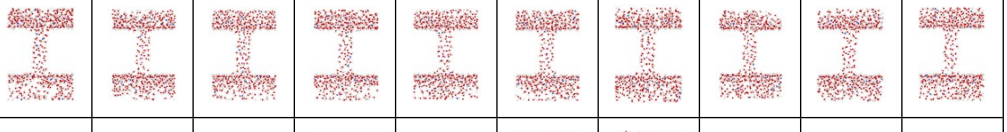
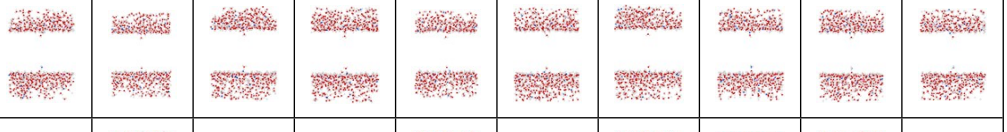
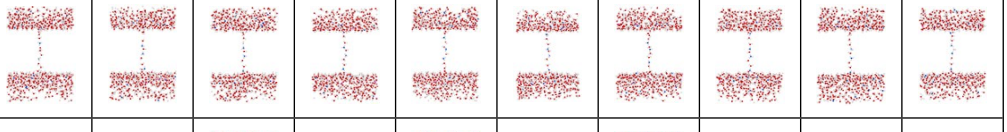
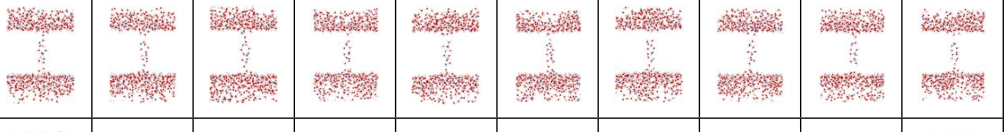
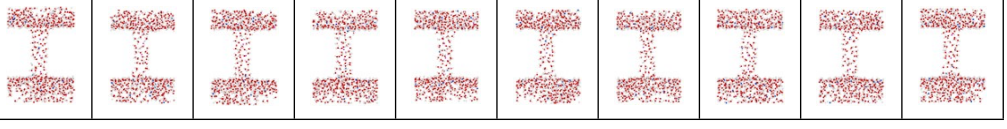


Figure S5. Side (upper) and top (lower) views of hydrogen-bonding representation. (a)~(d) represents 4N, 5N, 6N and 8N, and (e)~(h) represents 4F, 5F, 6F and 8F. (i) and (j) represents the hydrogen-bonding network containing Pb^{2+} in 8N and 8F, respectively. Where grey, red, white, blue, yellow and pink respectively represents carbon, oxygen, hydrogen, O_hydronium, fluorine and Pb^{2+}.

Table S3. Presentation of hydrogen-bonding network versus the time.

	2 ns	4 ns	6 ns	8 ns	10 ns	12 ns	14 ns	16 ns	18 ns	20 ns
4N										
5N										
6N										
8N										
4N-Pb										
5N-Pb										
6N-Pb										
8N-Pb										
4F-Pb										
5F-Pb										
6F-Pb										
8F-Pb										

References

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