Supporting Information

Pb²⁺ 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 Pb²⁺ 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 ydirection, respectively

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

Figure S3. RDF plots of H₃O⁺ in PCNTs/G without Pb²⁺.

Figure S4. RDF plots of H₃O⁺ in fluorinated PCNTs/G without Pb²⁺.

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+} .

Atom	ε _{ij} (kcal/mol)	σ (Å)	Charge(e)	Ref.	
С	0.105	3.851	0.00	1, 2	
C _{C-F}	0.105	3.851	+0.109	1, 2	
F	0.069	3.08	-0.109	3	
O _{tip} _H ₂ O	0.184	3.553	-0.82	4, 5	
H _{tip} _H ₂ O	0.010	0.900	+0.41	4, 5	
O*_H ₃ O ⁺	0.184	3.553	-0.38	4, 5	
H*_H ₃ O ⁺	0.010	0.900	+0.46	4, 5	
Pb ²⁺	0.663	4.297	+2.00	6	

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

Pb²⁺-No.1 Pb²⁺-No.3 Pb²⁺-No.4 Pb²⁺-No.5 $Pb^{2+}-No.2$ 4N 5N 6N 8N Constant State 4F 5F 1.

Table S2. The trajectory of each Pb²⁺ ion (No.1~No.5) in 4N, 5N, 6N, 8N, 4F, 5F, 6F and 8F, respectively.





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 H₃O⁺ in PCNTs/G without Pb²⁺.



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+} .

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

References

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