Supplementary Information

Extensive First-Principles Molecular Dynamics Study on the Li Encapsulation into C_{60} and Its Experimental Confirmation

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In this Supplementary information, we present a discussion on a van der Waals interaction between carbon atoms and the detailed results of our first-principles molecular dynamics (MD) simulations.

1. Effect of van der Waals interaction

In our energy scale of the MD simulations, van der Waals (vdW) interaction [S1,S2] is much smaller than the major Coulomb and exchange interactions, and not necessary to be incorporated. This is quite obvious if we compare the incident kinetic energy of several to several tens eV with the order of the vdW interaction ~ 0.1 eV. So, we do not think its necessary to include vdW correction in our MD simulations. Another reason is that local density approximation (LDA) can effectively describe the vdW interaction for carbon systems, although generalized gradient approximation (GGA) cannot. In fact, LDA works good for describing the interlayer C-C interaction of AAA and ABA graphites, and fcc C_{60} crystal as shown in the following Table S1 [S3].

Table S1. Calculated lattice constant, binding energy, and mechanical properties of diamond, graphite, and C_{60}, which are comparable to the experimental values written inside the parentheses.

		Lattice constant(Å)	Binding Energy	Elastic constant (Mbar)		Bulk modulus
				$C_{11}+C_{12}$	C_{33}	
Diamond		3.53 (3.56)				444 (442) GPa
Graphite	AA A	c=3.49	23.0 meV/atom			
	AB A	c=3.24 (3.35[a])	37.6 (35[a]) meV/atom	13.7 (13.3[b])	0.49 (0.41[b])	0.45 (0.41[b]) Mbar
	fcc	13.85 (14.2[c])	1.6 (1.71[d]) eV/C_{60}			15.8 (15.6[e]) GPa

[a] Ref. [S4], [b] Ref. [S5], [c] Ref. [S6], [d] Ref. [S7], [e] Ref. [S8]

2. Detailed result of the first-principles MD simulations

Here we list the results of the first-principles molecular dynamics (MD) simulations for Li/Li^+ with 10 eV, 20 eV, 30 eV, and 40 eV kinetic energies at z = 5 Å from the C_{60} center (0, 0, 0) with the incident angles 0°, 10.5°, 21°, 29.5°, 32°, 38°, and 42° from the normal (z) direction toward the impinging point x = 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0, –0.1, –0.2, –0.3, –0.4, –0.5, –0.6, –0.7, –0.8, –0.9, –1.0 Å from the center of the hexagon (six-membered ring) or the pentagon (five-membered ring) in Tables S2 and S3. In these tables, "E" (marked with yellow colour) indicates the successfully encapsulated cases, while the symbol "(E)D", for example, means almost encapsulated "(E)" but finally destructed "D". Similarly, "B&D" means bounced "B" and destructed "D". In the last two tables for pentagon, "E/B" (marked with grey colour) means "E" for the Li^+ attack to C_{60} and "B" for the Li attack to C_{60}.

Table S2. First-principles molecular dynamics (MD) results for the incident angles 0°, 10.5°, 21°, 29.5°, 32°, 38°, and 42° for 10 eV, 20 eV, 30 eV, and 40 eV for hexagon. Here again “E”, “B”, “G”, and “D” indicate, respectively, encapsulation, bounce, going through, and destruction.

Hexagon							Hexagon						
10 eV	0°	10.5°	21°	29.5°	38°	42°	20 eV	0°	10.5°	21°	29.5°	38°	42°
1 Å	B	B	B	B	B	B	1 Å	B	B	B	B	B	B
0.9 Å							0.9 Å						
0.8 Å							0.8 Å						
0.7 Å							0.7 Å		E	E	E		
0.6 Å							0.6 Å						
0.5 Å							0.5 Å						
0.4 Å	E	E					0.4 Å	G					
0.3 Å							0.3 Å						
0.2 Å							0.2 Å	E	G				
0.1 Å							0.1 Å						
0 Å							0 Å						
-0.1 Å		B					-0.1 Å			B	B	B	B
-0.2 Å							-0.2 Å						
-0.3 Å							-0.3 Å	G	E				
-0.4 Å							-0.4 Å						
-0.5 Å	B						-0.5 Å	B	B				
-0.6 Å							-0.6 Å						
-0.7 Å							-0.7 Å						
-0.8 Å							-0.8 Å						
-0.9 Å							-0.9 Å						
-1 Å							-1 Å						

Hexagon							Hexagon						
30 eV	0°	10.5°	21°	29.5°	38°	42°	40 eV	0°	10.5°	21°	29.5°	38°	42°
1 Å	B	B	B	B	B	B	1 Å	B&D	B	G	E	E	E
0.9 Å				E			0.9 Å	E	G				
0.8 Å	E	E	E		E		0.8 Å			E			
0.7 Å			G	G			0.7 Å	G	E		G		
0.6 Å		G					0.6 Å	(E)D		G			
0.5 Å	G		G	G			0.5 Å	E		(G)D	(E)D	G	
0.4 Å	E		E				0.4 Å	(E)D		E			
0.3 Å		E					0.3 Å				G		
0.2 Å		G	G	E			0.2 Å	E		G		E	
0.1 Å	G				B		0.1 Å	G	G		G		B
0 Å			E	G		B	0 Å			E		B	
-0.1 Å		D	G	E			-0.1 Å		E		E		
-0.2 Å	E	E	E				-0.2 Å	(G)D		E			
-0.3 Å			G	B			-0.3 Å	(E)D	G				
-0.4 Å			E				-0.4 Å						
-0.5 Å	G	G	B				-0.5 Å	E	E	B	B	B	
-0.6 Å	E	E					-0.6 Å	(E)D					
-0.7 Å							-0.7 Å	G					
-0.8 Å		B					-0.8 Å	E		B			
-0.9 Å	B						-0.9 Å		B				
-1 Å							-1 Å	B&D					

Table S3. First-principles molecular dynamics (MD) results for the incident angles 0°, 10.5°, 21°, 29.5°, 32°, 38°, and 42° for 10 eV, 20 eV, 30 eV, and 40 eV for pentagon. Here again “E”, “B”, “G”, and “D” indicate, respectively, encapsulation, bounce, going through, and destruction.

Pentagon					
0 eV	0°	10.5°	21°	29.5°	32°
1 Å	B	B	B	B	B
0.9 Å					
0.8 Å					
0.7 Å					
0.6 Å					
0.5 Å					
0.4 Å					
0.3 Å					
0.2 Å					
0.1 Å					
0 Å					
-0.1 Å					
-0.2 Å					
-0.3 Å					
-0.4 Å					
-0.5 Å					
-0.6 Å					
-0.7 Å					
-0.8 Å					
-0.9 Å					
-1 Å					

Pentagon					
20 eV	0°	10.5°	21°	29.5°	32°
1 Å	B	B	B	B	B
0.9 Å					
0.8 Å					
0.7 Å					
0.6 Å					
0.5 Å					
0.4 Å					
0.3 Å					
0.2 Å					
0.1 Å	E/B				
0 Å					
-0.1 Å					
-0.2 Å	B				
-0.3 Å					
-0.4 Å					
-0.5 Å					
-0.6 Å					
-0.7 Å					
-0.8 Å					
-0.9 Å					
-1 Å					

Pentagon					
30 eV	0°	10.5°	21°	29.5°	32°
1 Å	B&D	B	B	B	B
0.9 Å	B				
0.8 Å					
0.7 Å					
0.6 Å		D	E/B		
0.5 Å					
0.4 Å	E	E	E		
0.3 Å					
0.2 Å					
0.1 Å					
0 Å			B		
-0.1 Å					
-0.2 Å					
-0.3 Å					
-0.4 Å		B			
-0.5 Å	B				
-0.6 Å					
-0.7 Å					
-0.8 Å					
-0.9 Å					
-1 Å	B&D				

Pentagon					
40 eV	0°	10.5°	21°	29.5°	32°
1 Å	B&D	B	B	B	B
0.9 Å	B				
0.8 Å			D		
0.7 Å					
0.6 Å	(E)D	E	E	E	E
0.5 Å	E				
0.4 Å	(E)D	(E)D	G		
0.3 Å					
0.2 Å	(G)D		E		D
0.1 Å	G		D		B
0 Å		G	E	B	
-0.1 Å					
-0.2 Å	(G)D	(D)E	B		
-0.3 Å	(E)D				
-0.4 Å		E			
-0.5 Å	E				
-0.6 Å	(E)D	B			
-0.7 Å	B				
-0.8 Å					
-0.9 Å					
-1 Å	B&D				

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