Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information For

LC_{567}: A new 2D semimetallic carbon allotrope as a promising anode material for lithium-ion batteries

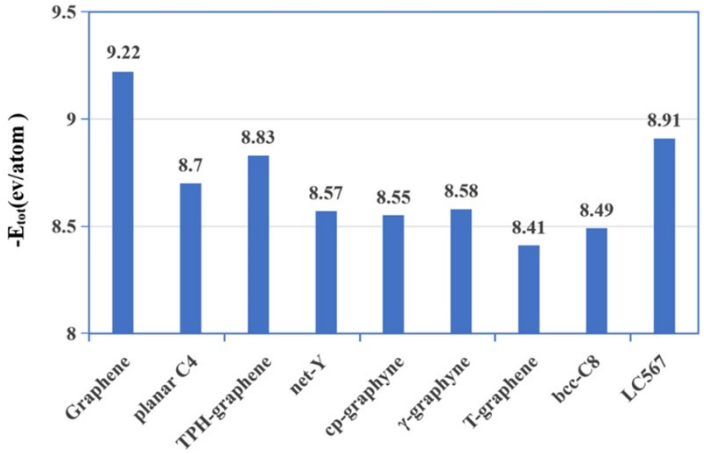


Figure S1. The total energy per atom for graphene allotrope.

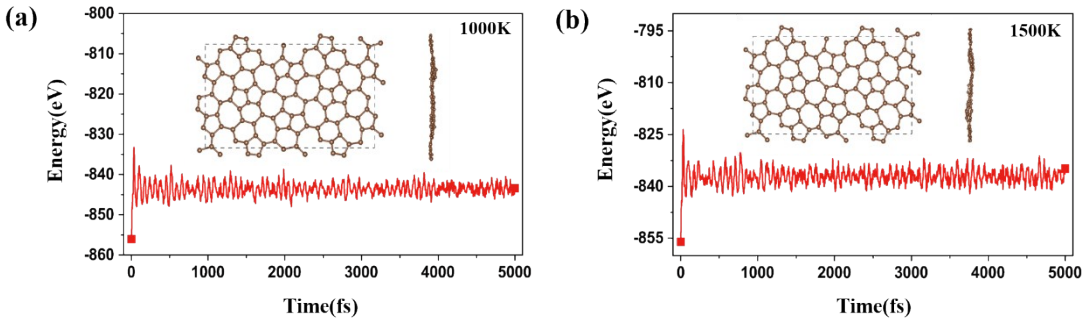


Figure S2. The change of total energy and structure of LC_{567} with time at 1000 K and 1500 K.

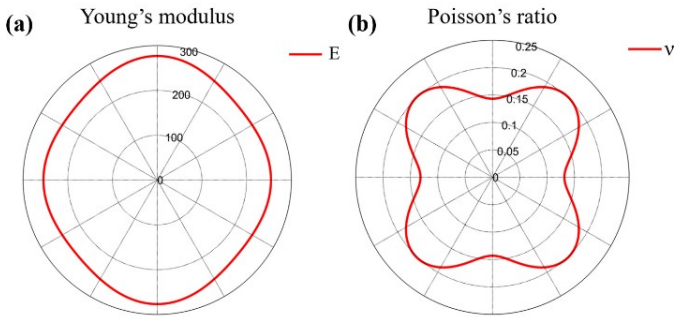


Figure S3. (a) Young's modulus in all directions of LC_{567}; (b) LC_{567} Poisson's ratio in all directions.

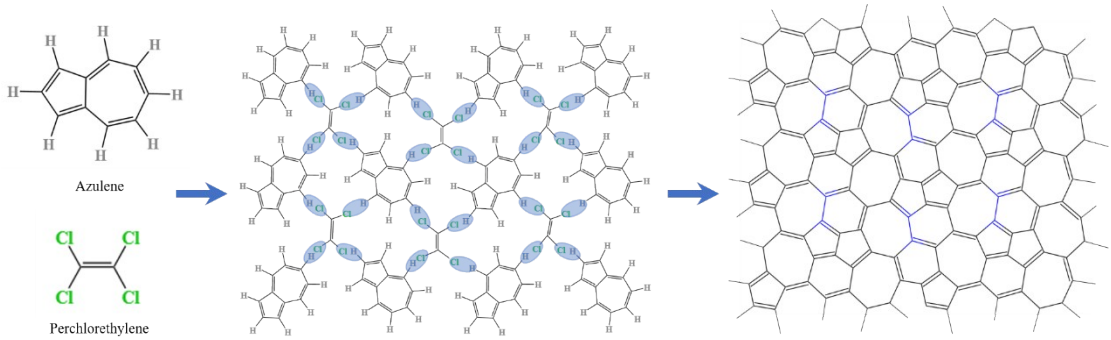


Figure S4. The flowchart of LC_{567} composed of azulene and perchloroethylene.

The LC_{567} can be made up of dehydrogenated azulene molecules and dechlorinated perchloroethylene molecules, here we propose a possible synthesis routine, as shown above. Firstly, azulene molecules and perchloroethylene molecules need to be arranged in an appropriate way; secondly, by fusing well-arranged molecules through H-Cl-zipping, C-C coupling are coupled between C-Cl and C-H moiety which are linked together through a self-assembly process; finally, LC_{567} is obtained. By calculating the energy before and after the reaction, the synthesis process is an exothermic reaction, which proves the feasibility of the reaction.

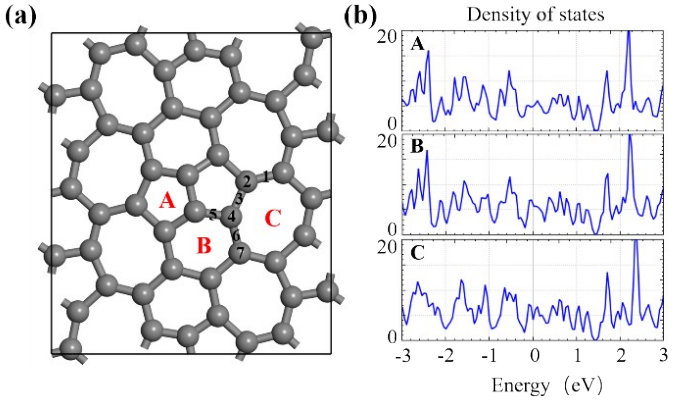


Figure S5. (a) Possible lithium adsorption sites on LC_{567} (top view); (b) Density of states for lithium-ion adsorption at different sites.

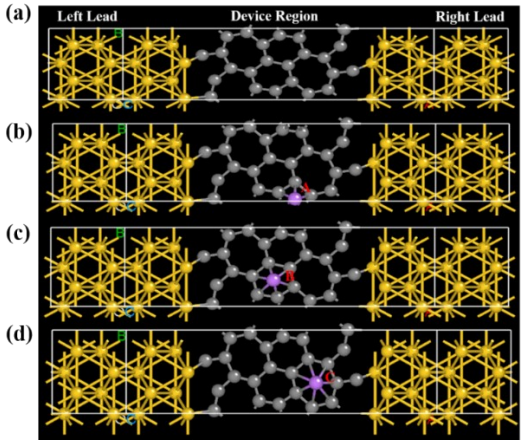


Figure S6. (a)- (d) The structures before and after adsorption are made into devices.

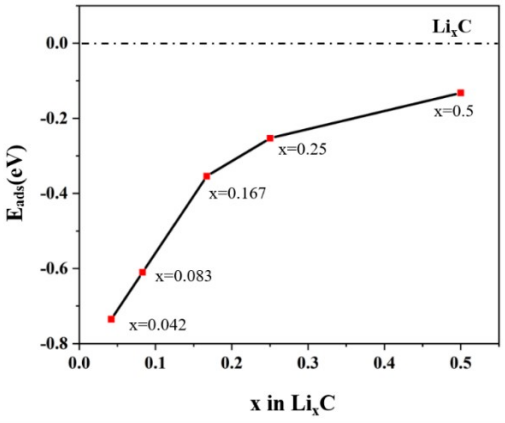


Figure S7 The adsorption energy as a function of Li atoms.

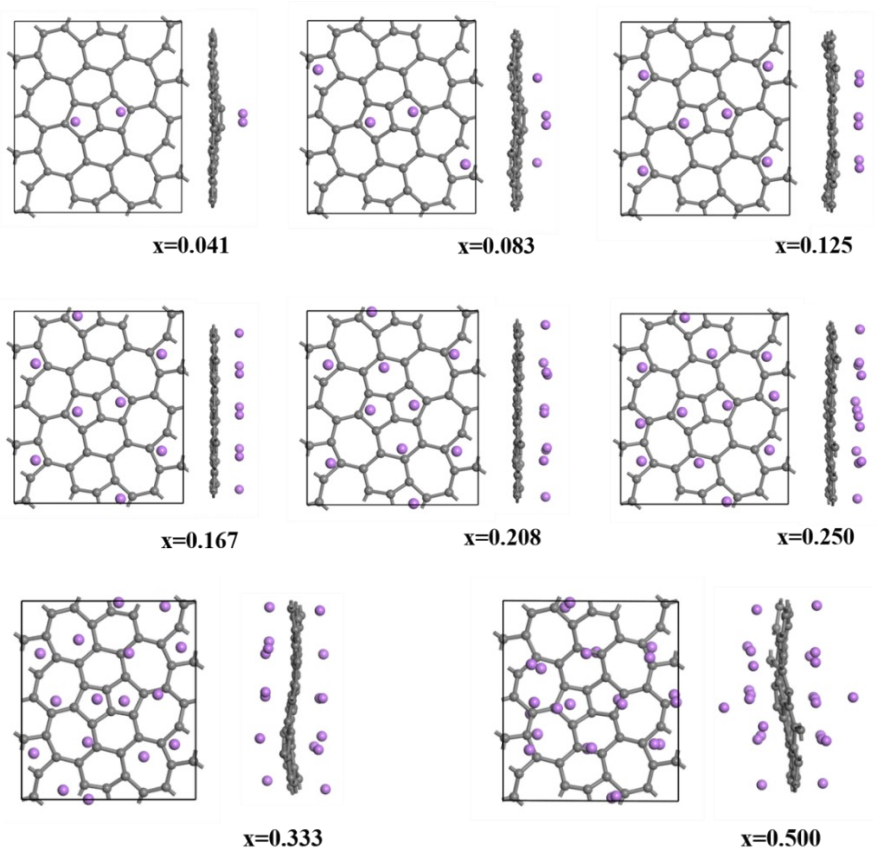


Figure S8. Structures of LC_{567} with various Li concentrations. In each partial, left show the top view and right side view.

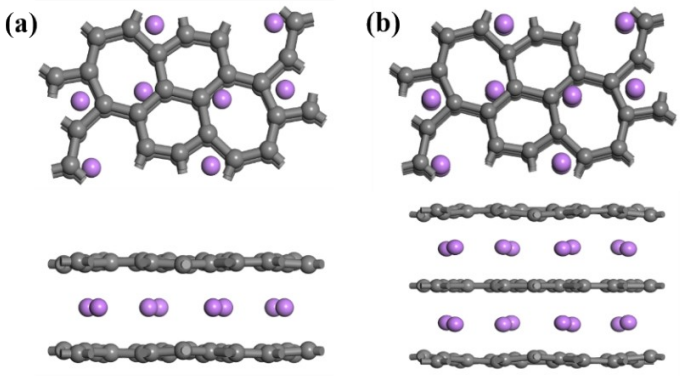
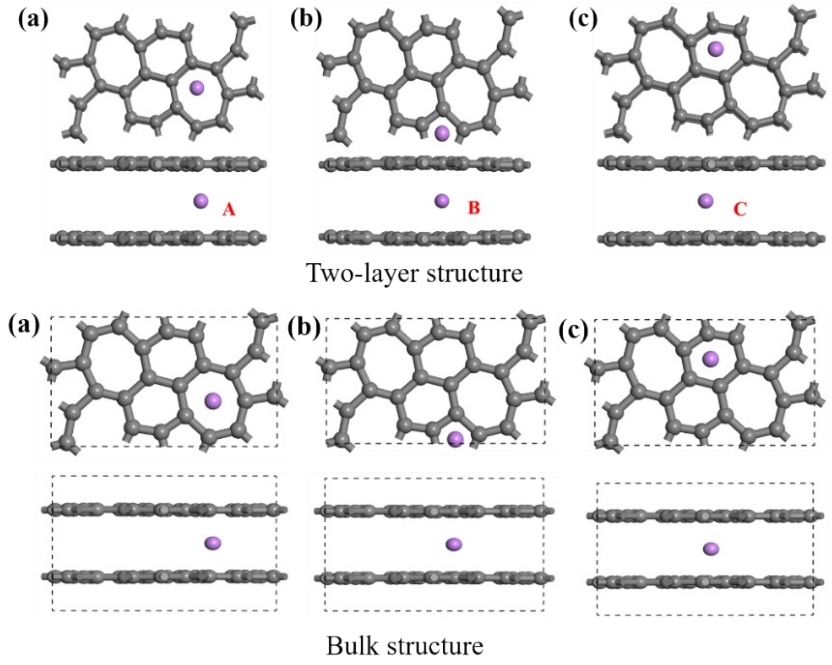


Figure S9. Structures of two- and three-layer LC_{567} with Li concentrations.

We calculate the adsorption energy of the maximum concentration for Li ions in two- and three-layer LC_{567}, and the energy are separately -0.885eV and -1.338eV, indicating the feasibility of Li ions adsorption for two-layer and three-layer LC_{567}. For a three-layer structure, the

maximum theoretical capacity is calculated as 496.9 $mAhg^{-1}$, which is slightly fewer than the single-sided lithium storage in monolayers (558 $mAhg^{-1}$).

Type 1：



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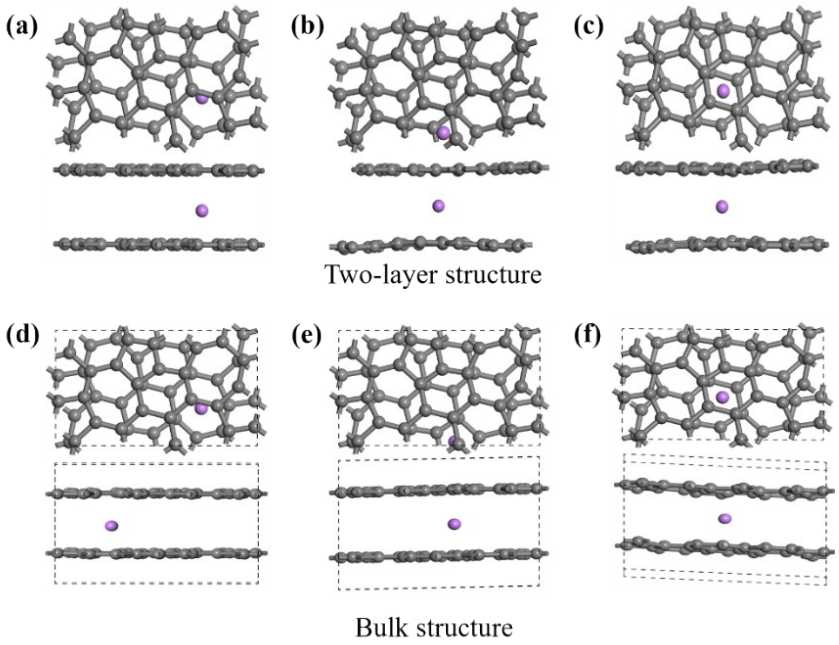


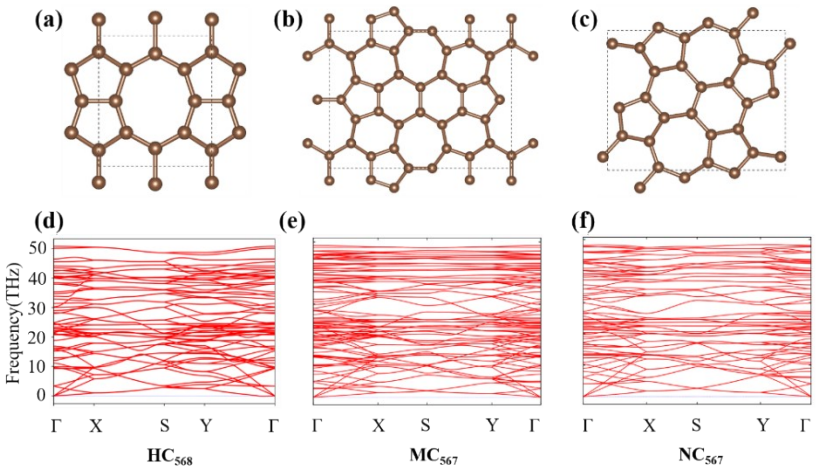
Figure S10. Adsorption of lithium atoms by two types of two-layer stacking structures and their bulk structures.

Table S1. The calculated lattice constant (*a*, *b*, in Å), lattice change of LC_{567} monolayer without and with adsorbed Li atoms.

	a (Å)	*b* (Å)	Lattice variation (%)		Area variation (%)
C	10.658	12.211			
$Li_{0.041}C$	10.661	12.211	0.028	-	0.028
$Li_{0.083}C$	10.665	12.213	0.065	0.016	0.082
$Li_{0.125}C$	10.684	12.213	0.244	0.016	0.260
$Li_{0.167}C$	10.732	12.214	0.694	0.025	0.719
$Li_{0.208}C$	10.733	12.224	0.704	0.106	0.811
$Li_{0.250}C$	10.750	12.224	0.863	0.106	0.971

Table S2. Structural information of various carbon allotropes and diffusion barriers of lithium ions on their surfaces.

Name	**Composition**	**NEB (eV)**				
		5-5	**5-6(6-5)**	**5-7(7-5)**	**7-7**	**6-7(7-6)**
LC_{567}	5-6-7 membered rings	0.18	0.22	0.28	0.31	
MC_{567}	5-6-7 membered rings		0.26	0.31		0.33
NC_{567}	5-6-7 membered rings		0.26	0.29		0.32
ψ-graphene [1]	5-6-7 membered rings		0.26	0.28	0.30	0.31
		5-5	**5-8(8-5)**	**5-6(6-5)**	**6-8(8-6)**	
HC_{568}	5-6-8 membered rings	0.19	0.24		0.32	
		5-5	**5-8(8-5)**	**8-8**		
Popgraphene [2]	5-8 membered rings	0.24	0.36	0.31		
OPG_L [3]	5-8 membered rings	0.22	0.27	0.29		
OPG_Z [3]	5-8 membered rings	0.14	0.26	0.26		



[1] Li, Xiaoyin, Qian Wang, and Puru Jena. ψ-Graphene: a new metallic allotrope of planar carbon with potential applications as anode materials for lithium-ion batteries. The journal of physical chemistry letters 8.14 (2017): 3234-3241.

[2] Wang, Shuai wei, et al. Popgraphene: a new 2D planar carbon allotrope composed of 5–8–5 carbon rings for high-performance lithium-ion battery anodes from bottom-up programming. Journal of Materials Chemistry A 6.16 (2018): 6815-6821.

[3] Gao, Peng fei, et al. OPGs: promising anode materials with high specific capacity and rate capability for Li/Na ion batteries. Nanoscale 10.37 (2018): 17942-17948.