

Supporting Information

Two-dimensional C₅₆₇₈: a promising carbon-based high-performance lithium-ion battery anode

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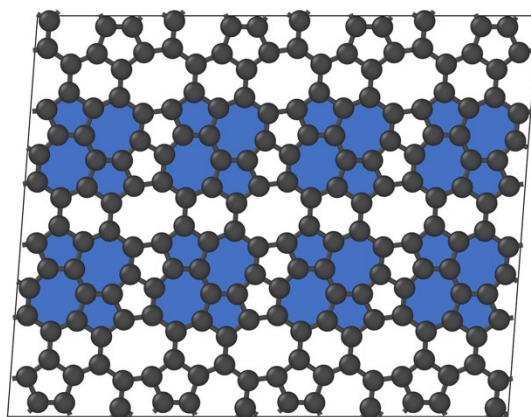


Figure S1. The crystal structure of C₅₆₇₈. The basic unit double inversed pentagon-heptagon alignments are highlighted by blue.

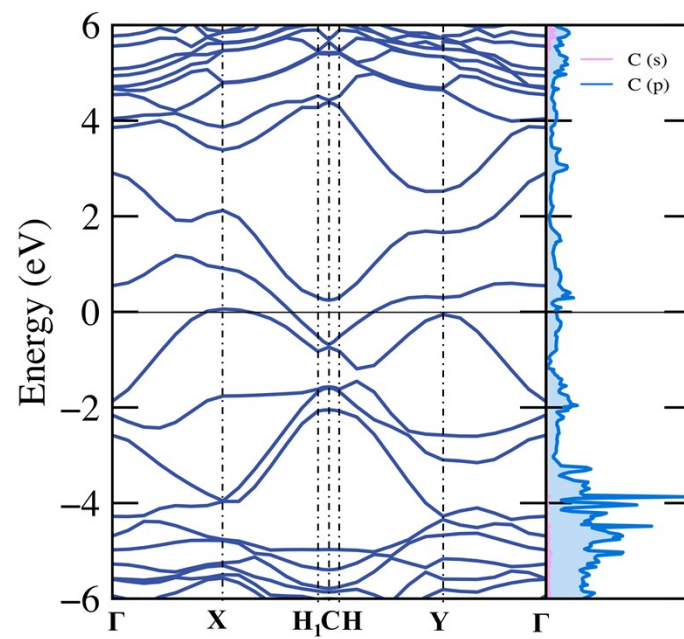


Figure S2. Band structure of C5678 calculated by using HSE06 hybrid functional.

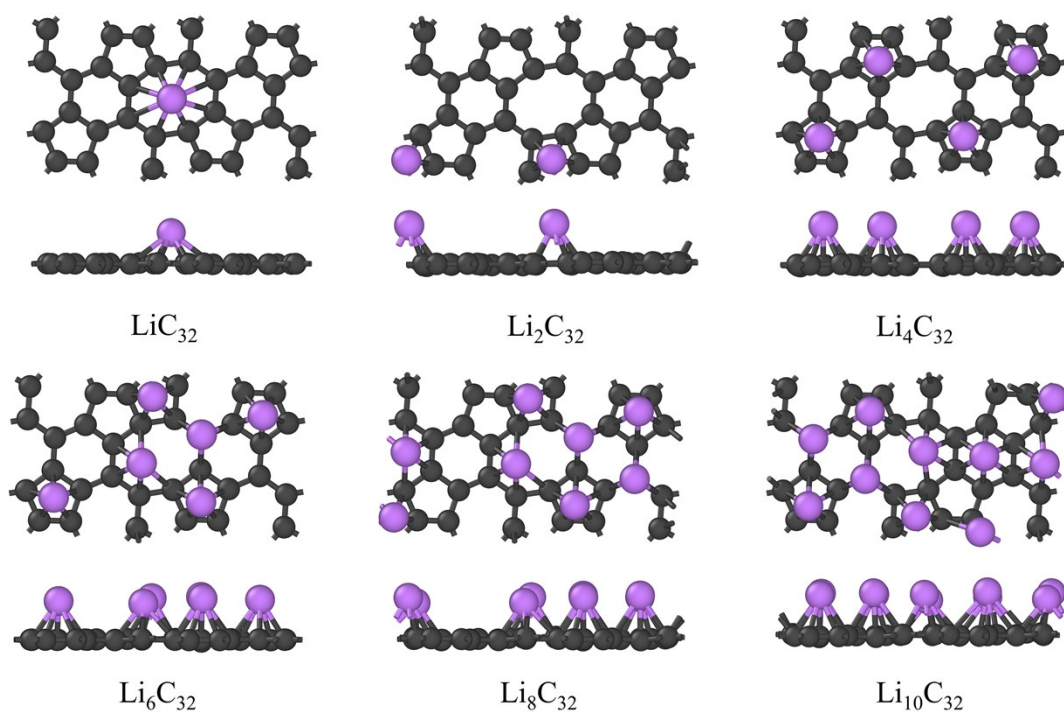


Figure S3. The lowest energy adsorption configurations of Li on the surface of C_{5678} under different lithium adsorbed concentrations.

Table S1 structure information of C₅₆₇₈.

C₅₆₇₈

1.0

6.4060688645682822	0.0003487045504835	0.0014781937690597
0.5132319058387287	6.8418540765823925	0.0902691753230504
0.0129281651156428	0.4619641857049830	35.7877966145544022

C

16

Direct

0.7037245808951959	0.5858405346464390	0.1843746530096274
0.2984485214431356	0.4139845201399481	0.1851572230368069
0.8727205493387098	0.7125328132212024	0.1841085327118625
0.1298211376474959	0.2865955720297051	0.1852548942612242
0.2962136289012811	0.6250490864667049	0.1853047233059954
0.7046529745803235	0.3762960837555394	0.1851543914379835
0.9031127635974792	0.2568843097344364	0.1841963820501394
0.0975164642606874	0.7443910474167680	0.1839080513165084
0.2346943112028912	0.0948962392421259	0.1843030816763631
0.7644150155267299	0.9038848269809087	0.1838973933712006
0.5023748575722832	0.2964093821284174	0.1844846072470584
0.4983725353045078	0.7036778378803284	0.1843912276617999
0.5532542741687312	0.9073242615131636	0.1848307726743377
0.4469983875929232	0.0913392207305349	0.1850315600942678
0.8955512243017708	0.0518888532482422	0.1842344492993470
0.0981791412689423	0.9490560566086491	0.1844326755883426