

Supplementary information for the manuscript

**“A new metallic π -conjugated carbon sheet used for the
cathode of Li-S batteries.”**

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1. NVT molecular dynamics simulation at 300K.

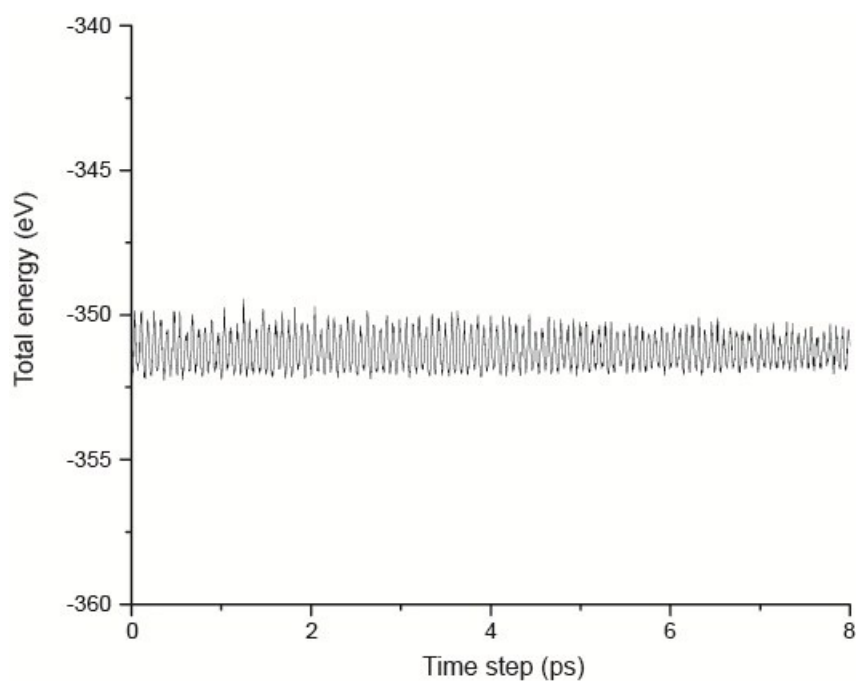


Fig. S1. Total energy change with time step within 8ps for PHE-graphene.

2. The adsorption geometries and energies of Li_2S_n and S_8 on PHE-graphene.

Table. S1. The adsorption energies of Li_2S_n and S_8 clusters on PHE-graphene.

Clusters	Li_2S	Li_2S_2	Li_2S_3	Li_2S_4	Li_2S_5	Li_2S_6	Li_2S_7	Li_2S_8	S_8
Adsorption energy (eV)	1.029	0.611	0.676	0.357	0.199	0.245	0.249	0.231	0.037

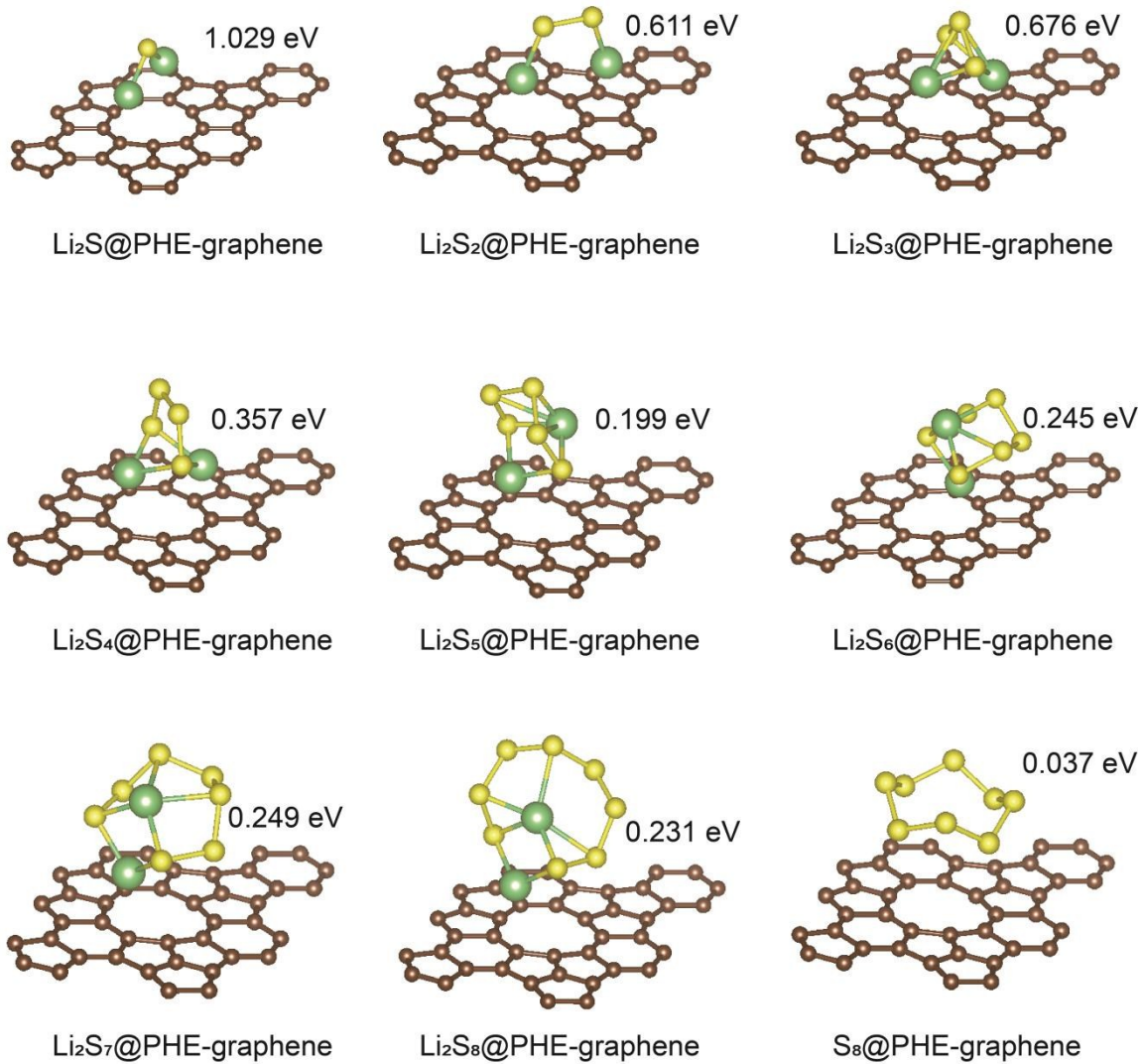


Fig. S2. The adsorption geometries of Li_2S_n and S_8 clusters on PHE-graphene.

3. The POSCAR files of optimized unit-cells for PHE-graphene and other two-dimensional carbon allotropes including hexagonal heackelite, oblique heackelite, rectangular heackelite, pza-C10, biphenylene, pentahexoctite, pentaheptite, OPG-L, phagraphene, planar T-graphene, HOP graphene, THD-graphene, DHP-graphene, graphene, graphdiyne, α -graphyne, β -graphyne, γ -graphyne and 6,6,12-graphyne.

No.1 PHE-graphene

1.000000

2.869056 4.969350 0.000000

-5.738112 0.000001 0.000000

0.000000 0.000000 15.00619

C

10

Direct

0.666667 0.333333 0.500000

0.326256 0.409832 0.500000

0.590167 0.916422 0.500000

0.083577 0.673744 0.500000

0.083578 0.409832 0.500000

0.590169 0.673745 0.500000

0.326255 0.916422 0.500000

0.387856 0.193927 0.500000

0.806072 0.193927 0.500000

0.806073 0.612145 0.500000

No.2 Hexagonal heackelite

1.000000

7.092510	-0.000103	0.000000
-3.546346	6.142241	0.000000
0.000000	0.000000	14.968335

C

16

Direct

0.434153	0.248309	0.500000
0.751686	0.185842	0.500000
0.814159	0.565848	0.500000
0.565846	0.814157	0.500000
0.185841	0.751685	0.500000
0.248310	0.434154	0.500000
0.789914	-0.000008	0.500000
-0.000008	0.789914	0.500000
0.210069	0.210069	0.500000
0.589585	0.476927	0.500000
0.523081	0.112668	0.500000
0.887349	0.410422	0.500000
0.410421	0.887348	0.500000
0.112667	0.523080	0.500000

0.476927 0.589585 0.500000

0.000000 0.000000 0.500000

No.3 Oblique heackelite

1.000000

6.096465 0.0144806 0.000000

1.228688 5.3890705 0.000000

0.000000 0.0000000 14.961644

C

12

Direct

0.643691 0.438966 0.500000

0.645281 0.679694 0.500000

0.086875 0.696455 0.500000

0.202096 0.422205 0.500000

0.203185 0.915211 0.500000

0.085786 0.203449 0.500000

0.440219 0.879872 0.500000

0.848753 0.238788 0.500000

0.850048 0.777556 0.500000

0.438924 0.341104 0.500000

0.762351 0.030106 0.500000

0.526620 0.088554 0.500000

No.4 Rectangular heackelite

1.000000

4.748935 -0.178167 0.000000

1.304090 4.569844 0.000000

0.000000 0.000000 14.964649

C

8

Direct

0.116653 0.565888 0.500000

0.883347 0.434112 0.500000

0.434112 0.883347 0.500000

0.565888 0.116653 0.500000

0.879441 0.120559 0.500000

0.120559 0.879441 0.500000

0.407002 0.407002 0.500000

0.592998 0.592998 0.500000

No.5 Pza-C₁₀

1.000000

5.993472 0.636234 0.000000

0.504692 4.600517 0.000000

0.000000 0.000000 14.952497

C

10

Direct

0.261657 0.259272 0.500000

0.632072 0.336987 0.500000

0.863105 0.367252 0.500000

0.852479 0.686130 0.500000

0.482065 0.608425 0.500000

0.251028 0.578153 0.500000

0.062593 0.135914 0.500000

0.051541 0.809491 0.500000

0.505551 0.119420 0.500000

0.608596 0.825985 0.500000

No.6 Biphenylene

1.000000

4.528746 0.000000 0.000000

0.000000 3.760073 0.000000

0.000000 0.000000 14.991926

C

6

Direct

0.660568 0.000000 0.500000

0.161119 0.306387 0.500000

0.339432 0.000000 0.500000

0.838881 0.306387 0.500000

0.161119 0.693613 0.500000

0.838881 0.693613 0.500000

No.7 Pentahexoctite

1.000000

5.780754 0.155517 0.000000

-0.103028 3.831546 0.000000

0.000000 0.000000 14.962354

C

8

Direct

0.747477 0.595497 0.500000

0.203707 0.223643 0.500000

0.356056 0.909565 0.500000

0.595128 0.909576 0.500000

0.975591 0.091107 0.500000

0.975593 0.728033 0.500000

0.747474 0.223655 0.500000

0.203710 0.595486 0.500000

No.8 Pentaheptite

1.000000

4.718015 0.569199 0.000000

0.570808 4.717825 0.000000

0.000000 0.000000 14.956813

C

8

Direct

0.554239	0.440541	0.500000
0.787545	0.572318	0.500000
0.236773	0.123091	0.500000
0.550325	0.126993	0.500000
0.791448	0.885870	0.500000
0.263892	0.599436	0.500000
0.104997	0.889783	0.500000
0.077893	0.413439	0.500000

No.9 OPG-L

1.000000		
4.909786	0.045627	0.000000
2.097072	6.863017	0.000000
0.000000	0.000000	14.972698

C

12

Direct

0.914991	0.931806	0.500000
0.085009	0.068194	0.500000
0.585008	0.568194	0.500000

0.414992	0.431806	0.500000
0.605802	0.241715	0.500000
0.394198	0.758285	0.500000
0.894198	0.258285	0.500000
0.105802	0.741715	0.500000
0.384258	0.961413	0.500000
0.615742	0.038587	0.500000
0.884258	0.461413	0.500000
0.115742	0.538587	0.500000

No.10 Phagraphene

1.000000

8.116902	-0.000000	0.000000
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-0.000000	6.643094	0.000000
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0.000000	0.000000	14.978273
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C

20

Direct

0.923852	0.934608	0.500000
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0.076148	0.065392	0.500000
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0.576148	0.934608	0.500000
0.423852	0.065392	0.500000
0.250000	0.979506	0.500000
0.750000	0.020494	0.500000
0.389038	0.645688	0.500000
0.610962	0.354312	0.500000
0.110962	0.645688	0.500000
0.889038	0.354312	0.500000
0.163277	0.440168	0.500000
0.836723	0.559832	0.500000
0.336723	0.440168	0.500000
0.663277	0.559832	0.500000
0.250000	0.770918	0.500000
0.750000	0.229082	0.500000
0.950547	0.719960	0.500000
0.049453	0.280040	0.500000
0.549453	0.719960	0.500000
0.450547	0.280040	0.500000

No.11 Planar T-graphene

1.000000

4.877148 -0.000000 0.000000

0.000000 4.877696 0.000000

0.000000 0.000000 14.987877

C

8

Direct

0.150553 0.349471 0.500000

0.849447 0.650529 0.500000

0.349447 0.849471 0.500000

0.650553 0.150529 0.500000

0.150534 0.650546 0.500000

0.849466 0.349454 0.500000

0.349466 0.150546 0.500000

0.650534 0.849454 0.500000

No.12 HOP graphene

1.000000

5.491138 -2.644441 0.000000

3.760779 3.183190 0.000000

0.000000 0.000000 14.964989

C

10

Direct

0.645551 0.177631 0.500000

0.354449 0.822369 0.500000

-0.000592 0.647812 0.500000

0.000592 0.352188 0.500000

0.243076 0.618464 0.500000

0.756924 0.381536 0.500000

0.758249 0.860893 0.500000

0.241751 0.139107 0.500000

0.390563 0.305581 0.500000

0.609437 0.694419 0.500000

No.13 THD-graphene

1.000000

5.864007 -3.385586 -0.000000

-0.000000 6.771172 0.000000

0.000000 -0.000000 14.998930

C

12

Direct

0.792929 0.787746 0.500000

0.994816 0.787745 0.500000

0.212255 0.005184 0.500000

0.212254 0.207071 0.500000

0.994816 0.207073 0.500000

0.792928 0.005185 0.500000

0.540404 0.878921 0.500000

0.540406 0.661482 0.500000

0.121078 0.661483 0.500000

0.338517 0.878922 0.500000

0.338518 0.459594 0.500000

0.121079 0.459596 0.500000

No.14 DHP-graphene

1.000000

7.063079 0.000000 0.000000

-0.000000 9.959695 0.000000

0.000000 0.000000 14.996807

C

24

Direct

0.692328 0.312887 0.500000

0.307672 0.687113 0.500000

0.307672 0.312887 0.500000

0.692328 0.687113 0.500000

0.192328 0.812887 0.500000

0.807672 0.187113 0.500000

0.807672 0.812887 0.500000

0.192328 0.187113 0.500000

0.317710 0.071568 0.500000

0.682290 0.928432 0.500000

0.682290 0.071568 0.500000

0.317710 0.928432 0.500000

0.817710 0.571568 0.500000

0.182290 0.428432 0.500000

0.182290 0.571568 0.500000

0.817710 0.428432 0.500000

0.500000	0.128523	0.500000
0.500000	0.871477	0.500000
0.000000	0.628523	0.500000
0.000000	0.371477	0.500000
0.500000	0.275954	0.500000
0.500000	0.724046	0.500000
0.000000	0.775954	0.500000
0.000000	0.224046	0.500000

No.15 Graphene

1.000000		
2.138312	-1.234555	-0.000000
-0.000000	2.469110	-0.000000
-0.000000	-0.000000	14.993051

C

2

Direct

0.000000	0.100000	0.500000
0.666667	0.333333	0.500000

No.16 Graphdiyne

1.000000

8.201007 -4.734854 0.000000

-0.000000 9.469707 -0.000000

0.000000 -0.000000 14.998852

C

18

Direct

0.151136 0.100000 0.500000

0.299073 0.000000 0.500000

0.429120 0.000000 0.500000

0.570880 0.100000 0.500000

0.700927 0.100000 0.500000

0.848864 0.000000 0.500000

0.000000 0.151136 0.500000

0.151136 0.151136 0.500000

0.100000 0.299073 0.500000

0.299073 0.299073 0.500000

0.100000 0.429120 0.500000

0.429120 0.429120 0.500000

0.000000	0.570880	0.500000
0.570880	0.570880	0.500000
0.000000	0.700927	0.500000
0.700927	0.700927	0.500000
0.100000	0.848864	0.500000
0.848864	0.848864	0.500000

No.17 α -graphyne

1.000000		
-3.483779	6.035372	0.000000
-6.968674	-0.000644	0.000000
0.000000	0.000000	14.986003

C

8

Direct

0.666684	0.666684	0.500000
0.333316	0.333316	0.500000
0.449023	0.449022	0.500000
0.550983	0.898063	0.500000
0.101937	0.449017	0.500000

0.550977 0.550978 0.500000

0.449017 0.101937 0.500000

0.898063 0.550983 0.500000

No.18 β -graphyne

1.000000

4.743340 8.215704 -0.000000

-4.743340 8.215704 -0.000000

-0.000000 0.000000 14.975595

C

18

Direct

0.724160 0.854518 0.500000

0.145482 0.578676 0.500000

0.421324 0.724160 0.500000

0.275840 0.145482 0.500000

0.854518 0.421324 0.500000

0.578676 0.275840 0.500000

0.854518 0.724160 0.500000

0.275840 0.578676 0.500000

0.421324	0.854518	0.500000
0.145482	0.275840	0.500000
0.724160	0.421324	0.500000
0.578676	0.145482	0.500000
0.421641	0.578359	0.500000
0.421641	-0.000000	0.500000
-0.000000	0.421641	0.500000
0.578359	0.421641	0.500000
0.578359	0.000000	0.500000
0.000000	0.578359	0.500000

No.19 γ -graphyne

1.000000		
3.446800	5.970034	0.000000
-6.893611	0.000006	0.000000
0.000000	0.000000	14.958788

C

12

Direct

0.793230	0.000003	0.500000
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0.000002	0.793229	0.500000
0.206776	0.206777	0.500000
0.793226	0.793229	0.500000
0.206773	0.000003	0.500000
0.000001	0.206777	0.500000
0.411338	0.000003	0.500000
0.999998	0.411336	0.500000
0.588665	0.588669	0.500000
0.411338	0.411336	0.500000
0.588665	0.000003	0.500000
0.000005	0.588669	0.500000

No.20 6,6,12-graphyne

1.000000		
9.433827	0.000000	0.000000
0.000000	6.906897	0.000000
0.000000	0.000000	14.954921

C

18

Direct

0.868739	0.895467	0.500000
0.131261	0.104533	0.500000
0.131261	0.895467	0.500000
0.868739	0.104533	0.500000
0.259084	0.205291	0.500000
0.740916	0.794709	0.500000
0.740916	0.205291	0.500000
0.259084	0.794709	0.500000
0.500000	0.605123	0.500000
0.500000	0.394877	0.500000
0.627533	0.293373	0.500000
0.372467	0.706627	0.500000
0.372467	0.293373	0.500000
0.627533	0.706627	0.500000
0.000000	0.207823	0.500000
0.000000	0.792177	0.500000
0.000000	0.411286	0.500000
0.000000	0.588714	0.500000