

## Electronic supplementary information

### Density functional theory study of Li binding to graphene

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We have provided the distribution of charge density and density of states (DOS) of individual lithium clusters ( $\text{Li}_2$ ,  $\text{Li}_3$ ,  $\text{Li}_4$ ), and the detailed atomic coordinates of the adsorbed geometries in Figure 1.

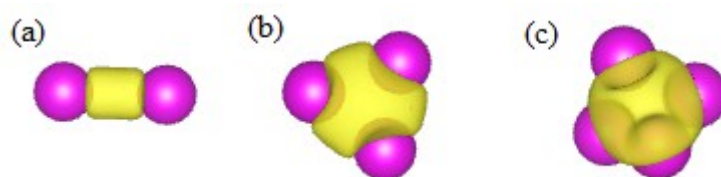


Fig.S1 The distribution of charge densities for individual lithium clusters including (a)  $\text{Li}_2$ , (b)  $\text{Li}_3$  and (c)  $\text{Li}_4$ .

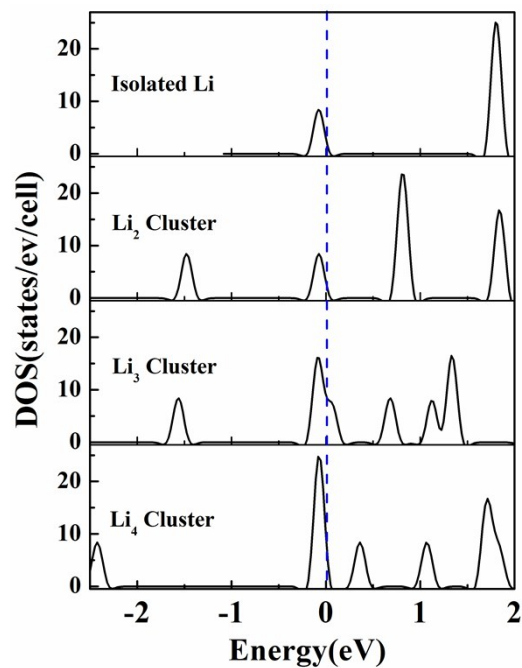


Fig.S2 The density of states (DOS) of  $\text{Li}_2$ ,  $\text{Li}_3$  and  $\text{Li}_4$  clusters, corresponding to Fig. S1(a)-(c), respectively. Note that the DOS is the sum of spin-up and spin-down bands.

The xyz coordinates of the adsorbed geometries in Figure1. Note that the formation is with the POSCAR of VASP.

#### POSCAR of $\text{LiC}_6$

1.0

4.2677998543	0.0000000000	0.0000000000
2.1338999271	3.6960230921	0.0000000000
0.0000000000	0.0000000000	18.0000000000

C Li

6 1

Direct

0.472550005	0.872940004	0.489300013
0.805890024	0.206269994	0.489300013
0.139219999	0.539610028	0.489300013
0.472550005	0.206269994	0.489300013
0.805890024	0.539610028	0.489300013
0.139219999	0.872940004	0.489300013
0.472550005	0.539610028	0.592630029

## POSCAR of Li<sub>2</sub>C<sub>12</sub>

1.0

4.9279999733000004	0.0000000000000000	0.0000000000000000
3.6960000991999999	6.4016599565999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

C Li  
12 2

Direct

0.8401687313235513	0.1846184246966160	0.5499516918271468
0.1724397848171151	0.4073659054290175	0.5496698618692619
0.3389214614034444	0.1848933585778880	0.5493912466246940
0.6732682067712474	0.4072336366826619	0.5502969997308824
0.8394809586868348	0.5188614103060090	0.5498468039528390
0.1717577165214550	0.7415200613583011	0.5498560945560769
0.3388075064681644	0.5187689860776388	0.5499836058653003
0.6729669808512000	0.7412379587731479	0.5489227715479430
0.8396380138226363	0.8519547146212929	0.5498021895677496
0.1722751901170483	0.0741875030168018	0.5499135513694213
0.3386370393102851	0.8525705451318899	0.5489884256240387
0.6731716135949100	0.0736213281888780	0.5493390822969531
0.5094959025847317	0.6716242497039531	0.6560926088856434
0.4974309027273662	0.2742019534359059	0.6537448122820493

## POSCAR of Li<sub>3</sub>C<sub>18</sub>

1.0

7.3920001983999999	0.0000000000000000	0.0000000000000000
3.6960000991999999	6.4016599565999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

C Li  
18 3

Direct

0.9070438657435957	0.1259980851836389	0.5904310261814203
0.1286761358927109	0.3482126471627822	0.5912732143799246
0.2394877152749544	0.1266588981445622	0.5910487234392434
0.4614951530733649	0.3486025580330789	0.5898482583630766
0.5726178823434154	0.1261081546156007	0.5903437636754632
0.7956980639148767	0.3485553681838169	0.5897384167202659
0.9070445806066516	0.4598279733621453	0.5904990460830675
0.1278961348195509	0.6824753424590142	0.5898344459411433
0.2389150192000358	0.4597571162718452	0.5904112178238208
0.4615847368005745	0.6827658648181867	0.5898797207985496
0.5730397074340416	0.4599318270889441	0.5883007203884247
0.7953328357203944	0.6825302762015255	0.5898014762534913
0.9061631740735407	0.7933689396974160	0.5905509416356622

0.1287669602396164	0.0157932598784001	0.5910975879782470
0.2389304465989071	0.7941153982910194	0.5904167500773099
0.4609513721061447	0.0160219029062958	0.5909944980261770
0.5726430026287446	0.7941951358287369	0.5901046766270213
0.7953038758914985	0.0150551073773286	0.5900160645641819
0.3038172493472047	0.5903009753226272	0.7003683337787905
0.7056044517727571	0.1990438271310282	0.6994419156506595
0.6958276615174270	0.5999813770420275	0.6995188316140357

POSCAR of \*Li<sub>3</sub>C<sub>18</sub>

1.0

7.3920001983999999	0.0000000000000000	0.0000000000000000
3.6960000991999999	6.4016599565999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

C Li

18 3

Direct

0.9079068376926216	0.1260353480914915	0.5909205868303644
0.1280290449536423	0.3481683311453665	0.5909898301055705
0.2398644200027533	0.1264405976513885	0.5908327579240762
0.4616407734667831	0.3482549875378851	0.5906514606140760
0.5730013344546379	0.1248911992876884	0.5909222867476913
0.7970355518640488	0.3489265243070960	0.5909213904252866
0.9073120282352178	0.4603617289759043	0.5909874997550659
0.1274314529899883	0.6824807557151757	0.5909232054326097
0.2383098066131879	0.4596049412778669	0.5909204100001872
0.4623266484379229	0.6836231530823866	0.5909186858923405
0.5736838885300273	0.4603025383402723	0.5906450164912513
0.7954869664931863	0.6820695098719298	0.5908360340668750
0.9058105629795605	0.7924131710252311	0.5911125154444505
0.1295328574369847	0.0161236281722736	0.5911155433766808
0.2394578570437389	0.7945034095124939	0.5909199591400238
0.4615720525893039	0.0146286459186342	0.5909894064489976
0.5737533882738219	0.7939154349845481	0.5909877437436108
0.7959051619369291	0.0140246604966734	0.5909240106300473
0.3485392463691710	0.5734631039416556	0.6961709114488102
0.6868335872806526	0.2351731437684279	0.6961746430876303
0.5176665253558568	0.4043352908956308	0.8398957343943323

POSCAR of Li<sub>4</sub>C<sub>24</sub>

1.0

9.8559999466	0.0000000000	0.0000000000
3.6960000992	6.4016599566	0.0000000000
0.0000000000	0.0000000000	18.0000000000

C	Li		
24	4		
Direct			
0.909579992	0.276019990	0.364140004	
0.075819999	0.497689992	0.364050001	
0.158889994	0.276360005	0.364179999	
0.325819999	0.497759998	0.364600003	
0.409359992	0.275209993	0.364100009	
0.576900005	0.497599989	0.365009993	
0.660570025	0.274830014	0.364450008	
0.827040017	0.497520000	0.364109993	
0.909510016	0.609109998	0.363739997	
0.075220004	0.832159996	0.363649994	
0.158450007	0.609489977	0.364219993	
0.325670004	0.832509995	0.364560008	
0.409520000	0.609319985	0.364289999	
0.576889992	0.831480026	0.363539994	
0.660390019	0.609120011	0.364309996	
0.826590002	0.831139982	0.363750011	
0.908879995	0.943109989	0.363950014	
0.075599998	0.165849999	0.364179999	
0.158419997	0.943979979	0.364289999	
0.325659990	0.165079996	0.364430010	
0.409280002	0.943729997	0.364109993	
0.576900005	0.163760006	0.363599986	
0.660380006	0.942059994	0.363799989	
0.826799989	0.164389998	0.364360005	
0.216250002	0.738089979	0.467850000	
0.505129993	0.740869999	0.468400002	
0.504320025	0.350309998	0.468360007	
0.410239995	0.608500004	0.610430002	

POSCAR of Li<sub>5</sub>C<sub>30</sub>

1.0

7.3920001984	0.0000000000	0.0000000000
6.1599998474	10.6694327103	0.0000000000
0.0000000000	0.0000000000	18.0000000000

C	Li		
30	5		
Direct			
0.399450004	0.864510000	0.346769989	
0.621860027	0.997070014	0.346340001	
0.732949972	0.864269972	0.346729994	
0.955429971	0.997150004	0.346049994	

0.065669999	0.864340007	0.346089989
0.288470000	0.997470021	0.346500009
0.399859995	0.063579999	0.346210003
0.622309983	0.196640000	0.344060004
0.733420014	0.063450001	0.345820010
0.956080019	0.196640000	0.345169991
0.066560000	0.063730001	0.345770001
0.288850009	0.196740001	0.345649987
0.399879992	0.263330013	0.343930006
0.622229993	0.397350013	0.340559989
0.733349979	0.263790011	0.343809992
0.955540001	0.397280008	0.344370008
0.067010000	0.263489991	0.345429987
0.288480014	0.397460014	0.343459994
0.399419993	0.464289993	0.340680003
0.621519983	0.598010004	0.342489988
0.733099997	0.463970006	0.342139989
0.954879999	0.597809970	0.345910013
0.066100001	0.464150012	0.344689995
0.288199991	0.597670019	0.342689991
0.399370015	0.664680004	0.342729986
0.621540010	0.798020005	0.346879989
0.732580006	0.664529979	0.345849991
0.954710007	0.797930002	0.345950007
0.065629996	0.664810002	0.345259994
0.288010001	0.797850013	0.345829993
0.226630002	0.518639982	0.450459987
0.510569990	0.434549987	0.579200029
0.790530026	0.357230008	0.450830013
0.517000020	0.671159983	0.457800001
0.507499993	0.235440001	0.464370012