Supporting Information

Adsorption and Diffusion of Li with S on Pristine and Double-Vacancy Defected Graphene for Cathodes of Li-S Batteries

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Figure S1

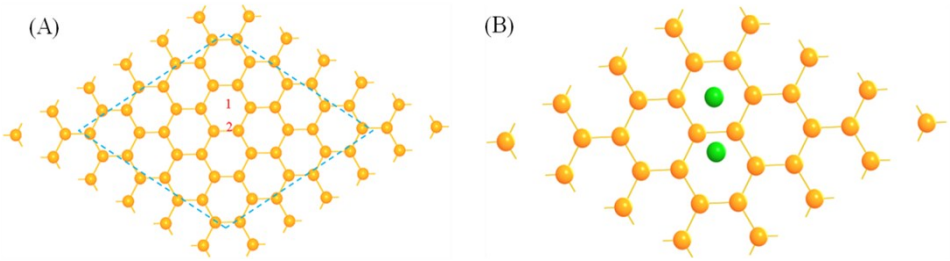

Figure S1. Schematic representation of the possible configurations (A) and the most stable configuration of S_2 absorbed on graphene. Note the numbers in (A) represent the mass center of S_2 for the two possible configurations.

Table S1. Adsorption energies (E_{ad}) for S_2 adsorbed on pristine graphene for the two configurations in Figure S1 (A).

Site	E_{ad}(eV)
1	-0.080
2	-0.094

Figure S2

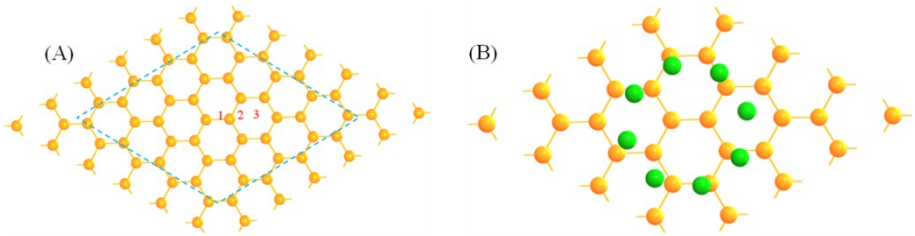

Figure S2. Schematic representation of the possible configurations (A) and the most stable configuration (B) of S_8 absorbed on graphene. Note the numbers in (A) represent the mass center of S_8 for the possible configurations.

Table S2 Adsorption energies (E_{ad}) for S_8 absorbed on pristine graphene with double-vacancy for the possible configurations in Figure S2 (A).

Site	E_{ad}(eV)
1	-0.088
2	-0.085
3	-0.088

Figure S3

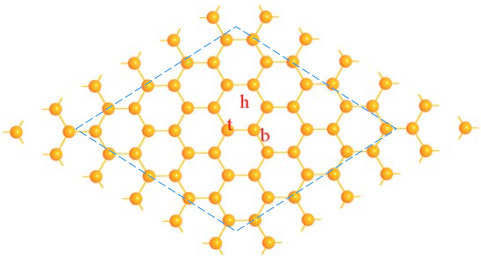

Figure S3. Schematic representation of the possible sites of S absorbed on graphene

Table S3. Average distance between S and carbon (d_{S-C}), angle between S and the near-neighbor C (θ_{C-S-C}), adsorption energy (E_{ad}) for S adsorbed on pristine graphene with the sites shown in Figure S3

Site	ds-c	θ_{C-S-C}	E_{ad}(eV)
t	1.93	--	-0.659
h	3.31	51.1	-0.369
b	1.91	46.0	-0.995

Figure S4

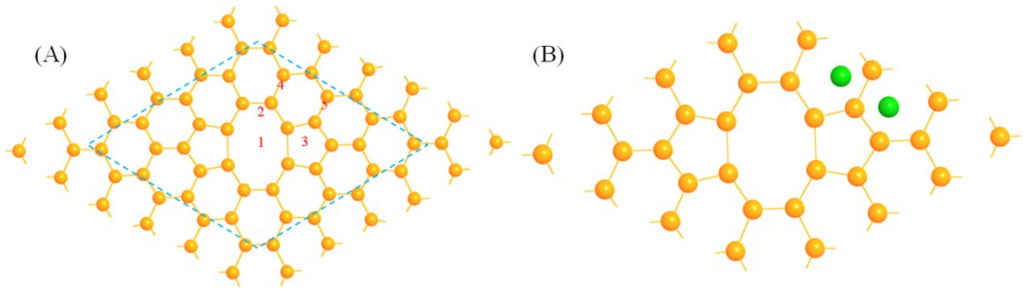

Figure S4. Schematic representation of the possible configurations (A) and the most stable configuration (B) of S_2 absorbed on graphene with double-vacancy. Note the numbers in (A) represent the mass center of S_2 for the possible configurations.

Table S4. Adsorption energies (E_{ad}) for S_2 absorbed on graphene with double-vacancy for the possible configurations in Figure S4 (A).

Site	E_{ad}(eV)
1	-0.001
2	-0.059
3	-0.050
4	-0.088
5	-0.091

Figure S5

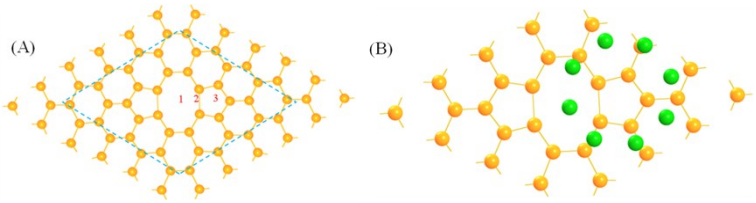

Figure S5. (A) Schematic representation of the possible configurations (A) and the most stable configuration (B) of S_8 absorbed on graphene with double-vacancy. Note the numbers in (A) represent the mass center of S_8 for the possible configurations.

Table S5. Adsorption energies (E_{ad}) for S_8 absorbed on pristine graphene with double-vacancy for the possible configurations in Figure S5 (A).

Site	E_{ad}(eV)
1	-0.083
2	-0.086
3	-0.092

Figure S6

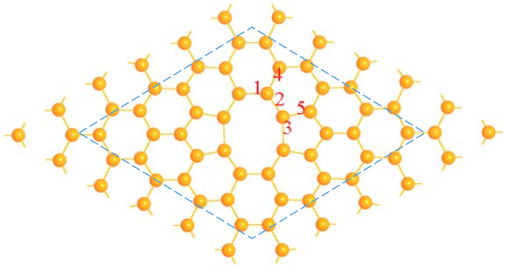

Figure S6. Schematic representation of the possible sites of S absorbed graphene with double-vacancy

Table S6. Average distance between S and carbon (d_{S-C}), angle between S and the near-neighbor C (θ_{C-S-C}), adsorption energy (E_{ad}) for S adsorbed on double vacancy graphene with the sites shown in Figure S6

Site	d_{S-C}	θ_{C-S-C}	E_{ad}(eV)
1	1.90	45.9	-1.018
2	1.85	51.5	-2.166
3	1.73	95.3	-4.224
4	1.86	53.3	-1.623
5	1.88	46.3	-1.851

Figure S7

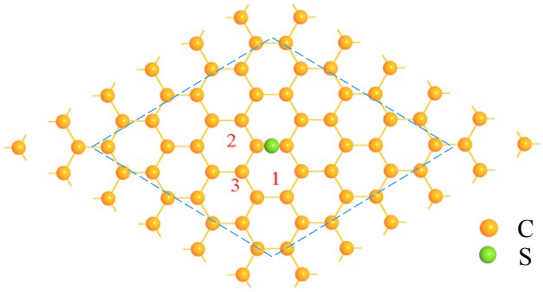

Figure S7. Schematic representation of possible configurations of LiS absorbed on graphene. Note the numbers represent the possible sites of Li ion.

TableS7. Average distance between S and Li (d_{S-Li}), distance between S and the nearest-neighbor C (d_{S-C}), angle between S and the near-neighbor C (θ_{C-S-C}), adsorption energy (E_{ad}) and cohesive Energy (ΔE_c) for the adsorption of LiS cluster on pristine graphene.

Site	d_{S-Li}	d_{S-C}	θ_{C-S-C}	E_{ad}(eV)	ΔE_c(eV)
1	2.15	3.28	25.1	-0.323	-2.646
2	2.20	3.37	24.3	-0.879	-3.203
3	2.23	3.40	23.5	-0.813	-3.136

Figure S8

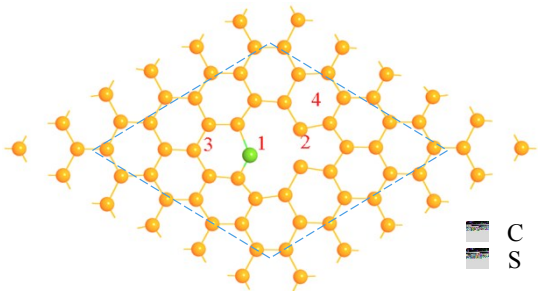

Figure S8. Schematic representation of possible configurations of LiS absorbed on graphene with double-vacancy. Note the numbers represent the possible sites of Li ion.

Table S8. Average distance between S and Li (d_{S-Li}), distance between S and the nearest-neighbor C (d_{S-C}), angle between S and the near-neighbor C (θ_{C-S-C}), adsorption energy (E_{ad}) and cohesive Energy (ΔE_c) for the adsorption of LiS cluster on double-vacancy graphene

Site	d_{S-Li}	d_{S-C}	θ_{C-S-C}	E_{ad}(eV)	ΔE_c(eV)
1	2.27	1.73	97.3	-1.591	-0.687
2	2.57	1.75	94.0	-3.212	-2.307
3	2.36	1.76	93.7	-2.809	-1.904
4	3.65	1.75	94.4	-2.927	-2.022

Figure S9

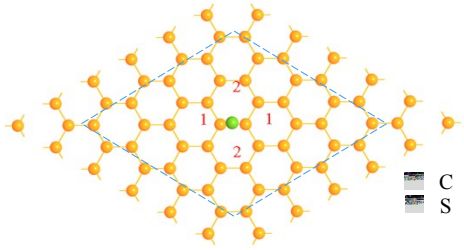

Figure S9. Schematic representation of two possible configurations of Li_2S absorbed on graphene, Note the numbers represent the locations of two Li atoms.

Table S9. Average distance between S and Li (d_{S-Li}), angle between S and Li ($\theta_{Li-S-Li}$), distance between S and the nearest-neighbor C (d_{S-C}), angle between S and the near-neighbor C (θ_{C-S-C}), adsorption energy (E_{ad}) and cohesive Energy (ΔE_c) for the adsorption of Li_2S cluster on pristine graphene.

Site	d_{S-Li}	$\theta_{Li-S-Li}$	d_{S-C}	θ_{C-S-C}	E_{ad}(eV)	ΔE_c(eV)
1	2.20	105.4	3.51	23.4	-1.086	-3.326
2	2.19	81.2	3.76	21.9	-1.095	-3.331

Figure S10

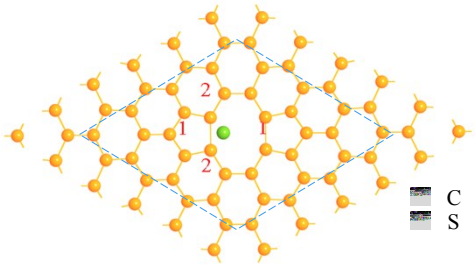

Figure S10. Schematic representation of proposed two possible configurations of Li_2S absorbed on graphene with double-vacancy, Note the numbers represent the locations of two Li atoms.

TableS10. Average distance between S and Li ($d_{S\text{-}Li}$), angle between S and Li ($\theta_{Li\text{-}S\text{-}Li}$), distance between S and the nearest-neighbor C ($d_{S\text{-}C}$), angle between S and the near-neighbor C ($\theta_{C\text{-}S\text{-}C}$), adsorption energy ($E_{ad}$) and cohesive Energy ($\Delta E_c$) for the adsorption of Li_2S cluster on double-vacancy graphene.

Site	$d_{S\text{-}Li}$	$\theta_{Li\text{-}S\text{-}Li}$	$d_{S\text{-}C}$	$\theta_{C\text{-}S\text{-}C}$	E_{ad}(eV)	ΔE_c(eV)
1	2.17	133.4	2.94	34.5	-1.501	-1.919
2	2.25	123.8	2.72	36.9	-1.661	-1.999

Figure S11

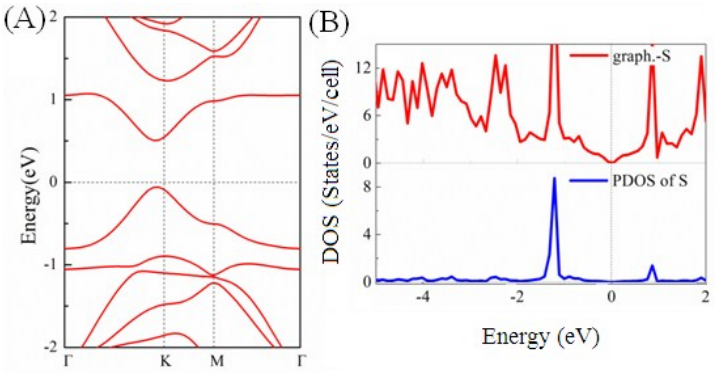

Figure S11. Band structure, density of states (DOS) and partial density of states (PDOS) of S-adsorbed graphene.

Figure S12

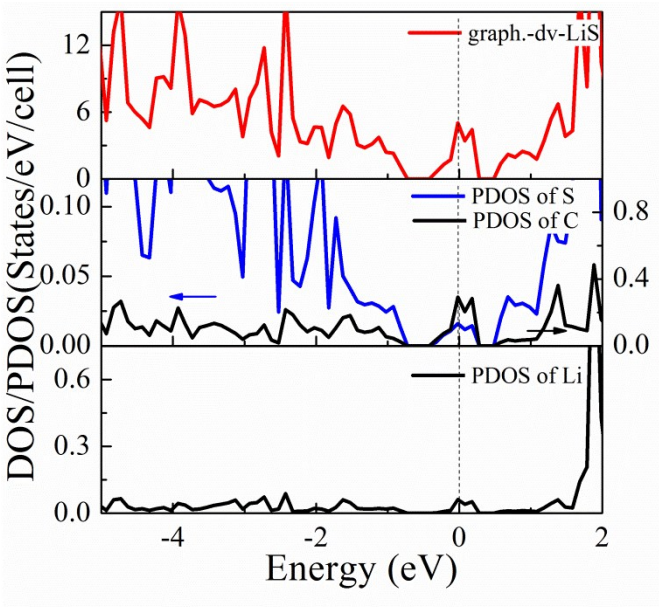

Figure S12, The density of states (DOS) and partial density of states (PDOS) of two-vacancy graphene with one S adsorbed at the edge of vacancy and one Li adsorbed near the vacancy.