

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

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Supporting Information for

Porous phosphorous and nitrogen dual doped graphene blocking layer for high performance Li–S batteries

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Figure S1

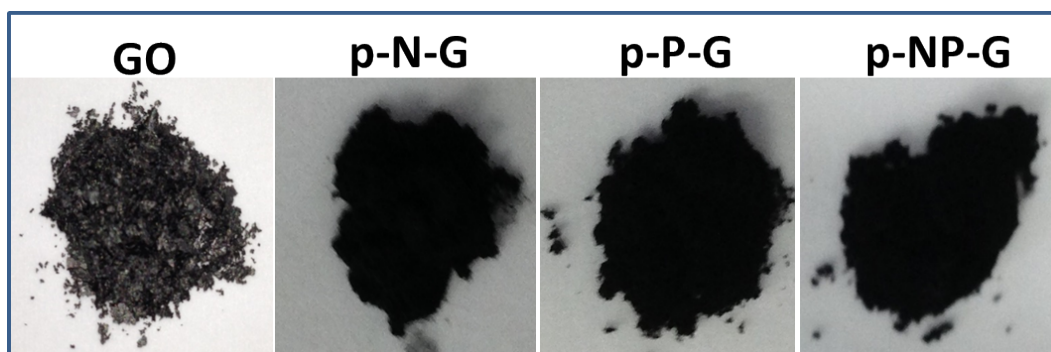


Fig. S1 Digital photographs of GO, p-N-G, p-P-G and p-NP-G

Figure S2

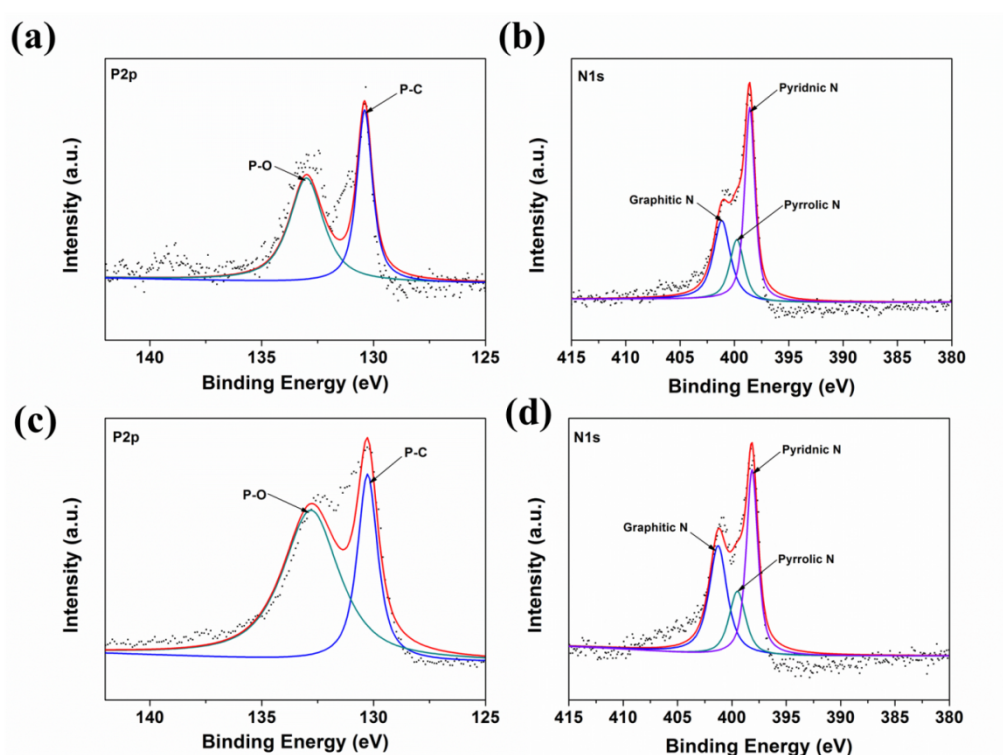


Fig. S2 High resolution P2p XPS spectra of p-P-G (a) and p-NP-G (c); High resolution N1s XPS spectra of p-N-G (b) and p-NP-G (d)

Figure S3

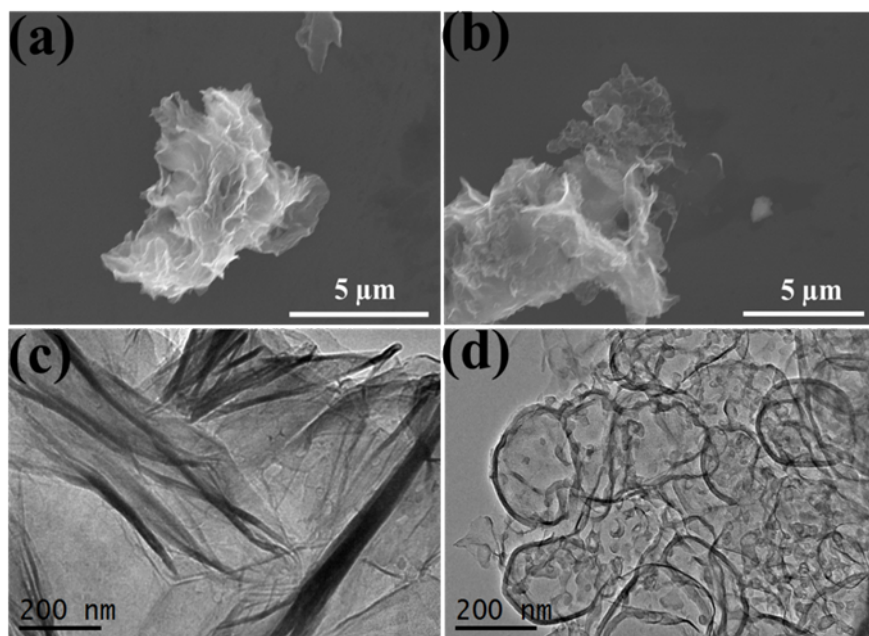


Fig. S3 SEM images of p-N-G (a) and p-P-G (b); TEM images of p-N-G (c) and p-P-G (d)

Figure S4

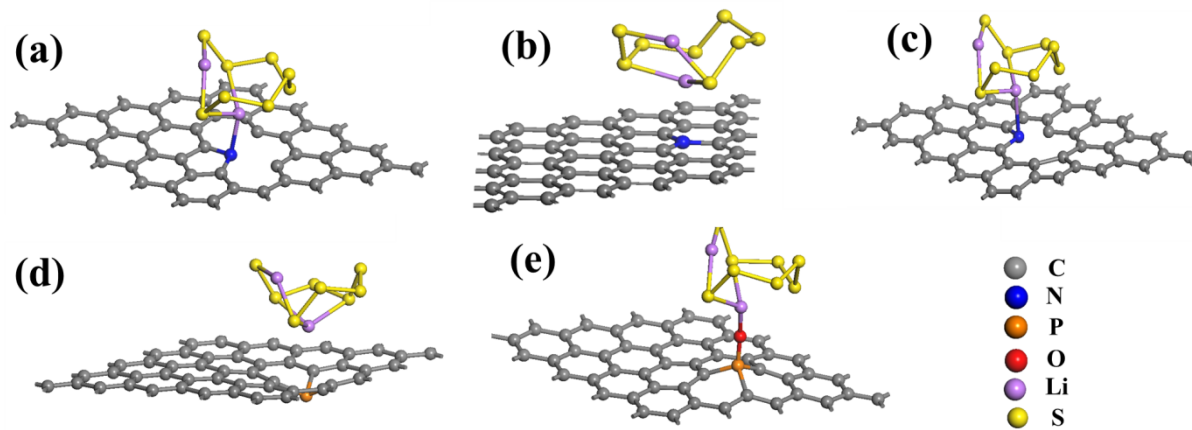


Fig. S4 The most preferential adsorption structures of Li_2S_8 on the different active sites: Pyrrolic N (a), Graphitic N (b), Pyridinic N (c), P (d), -P-O (e). All the models are shown in the most stable configuration

Table S1

Table S1 The contents N, P, O atoms in GO and doped graphene calculated from XPS analysis

Samples	N%	P%	O%	C%
p-NP-G	4.38	1.93	4.43	89.26%
p-P-G	—	1.85	3.73	92.42%
p-N-G	4.54	—	5.38	90.08%
GO	—	—	69.68	30.42

Table S2

Table S2 Physical characteristics of p-NP-G, p-P-G, p-N-G and GO

Sample	BET surface area (m ² /g)	Total pore volume (cm ³ /g)
p-NP-G	573.7	0.28
p-P-G	565.6	0.27
p-N-G	601.80	0.32
GO	198.37	0.016

Table S3

Table S3 Electrochemical performance of Li-S cells basing on different graphene interlayer

graphene type	Initial capacity (mAh/g)	Reversible capacity (mAh/g)	Cycle number	Rate (mA/g)	Ref.
p-NP-G	1158.3	638.0	500th	1675	This work
Graphene	1265	680	300th	1500	21
N doped graphene	~570	~550	100th	1675	35
2rGO-CB	1260	894	100th	200	56
TiO ₂ /Graphene	1050	1048	300th	837.5	57
TiO ₂ nanowire-graphene	1270	1053	200th	335	58
Graphene oxide	1040	~750	100th	167.5	59

Table S4

Table S4 Impedance parameters calculated according to the equivalent circuits

Sample name	Cycle number	Resistance		
		R_e (Ω)	R_s (Ω)	R_{ct} (Ω)
With p-NP-G interlayer	Before cycling	3.04	—	24.87
	100 th cycles	5.52	7.53	7.09
With p-P-G interlayer	Before cycling	3.46	—	44.24
	100 th cycles	8.37	23.92	16.03
With p-N-G interlayer	Before cycling	4.37	—	160.7
	100 th cycles	8.11	28.51	44.46