Supporting Information

Heterostructures of doped graphene and MoX_2 (X = S and Se) as promising anchoring materials for lithium-sulfur batteries: a first-principles study

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Table S1. The charge transfer (ΔQ, e) and shortest distances (Δd, Å) for the adsorption of Li_2S_4, Li_2S_6, and Li_2S_8 clusters on various anchoring materials.

	E_b (Li_2S_4)	E_b (Li_2S_6)	E_b (Li_2S_8)	ΔQ (Li_2S_4)	ΔQ (Li_2S_6)	ΔQ (Li_2S_8)	Δd (Li_2S_4)	Δd (Li_2S_6)	Δd (Li_2S_8)
NG-MoS_2	1.50	1.25	1.69	0.14	0.10	0.10	3.26	3.76	3.86
BG-MoS_2	1.46	1.20	1.72	0.23	0.26	0.26	3.26	3.72	3.60
NG-$MoSe_2$	1.53	1.47	1.79	0.10	0.10	0.10	3.17	3.71	3.63
BG-$MoSe_2$	1.59	1.60	2.05	0.19	0.22	0.41	3.13	3.63	3.62

Table S2. The variance of charge for B (Δe_B, $|e|$) or N atom (Δe_N, $|e|$) of MoX_2/DG materials after adsorption of soluble Li_2S_n species.

	Δe_B			Δe_N		
	Li_2S_4	Li_2S_6	Li_2S_8	Li_2S_4	Li_2S_6	Li_2S_8
NG/MoS_2	/	/	/	0.02	0.06	0.01
NG/$MoSe_2$	/	/	/	0.02	0.07	0.08
BG/MoS_2	-0.08	-0.07	-0.08	/	/	/
BG/$MoSe_2$	-0.06	-0.02	-0.07	/	/	/

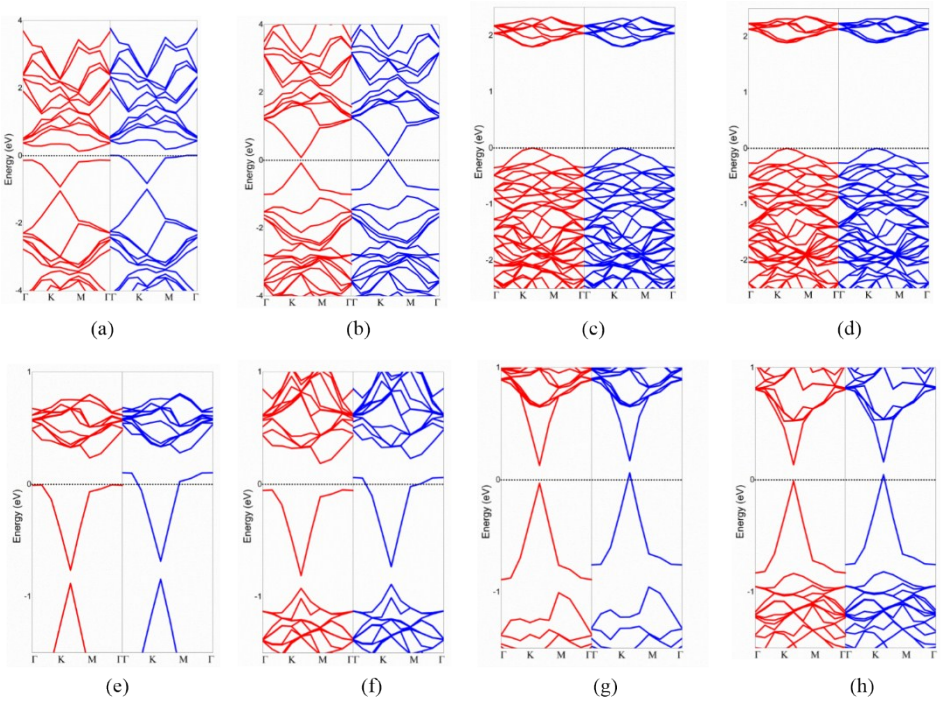

Figure S1. The computed band structures of (a) N-doped graphene (BG), (b) B-doped graphene (NG), (c) MoS_2, (d) $MoSe_2$, (e) NG/MoS_2, (f) NG/$MoSe_2$, (g) BG/MoS_2, and (h) BG/$MoSe_2$. The Fermi level was set as zero in dotted lines.

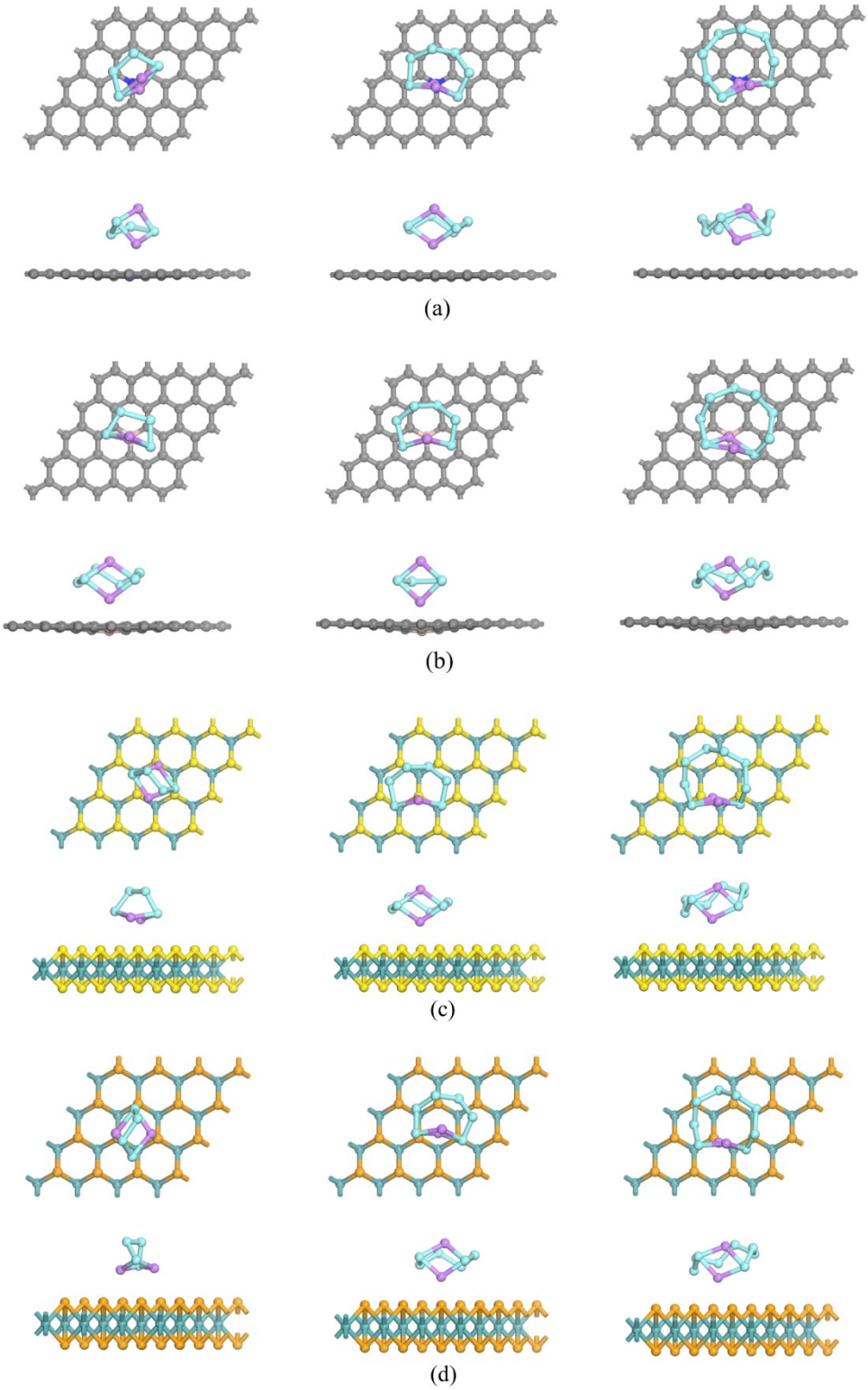

Figure S2. The optimized configurations for Li_2S_4, Li_2S_6, and Li_2S_8 species adsorption on (a) NG, (b) BG, (c) MoS_2, and (d) $MoSe_2$ monolayers.

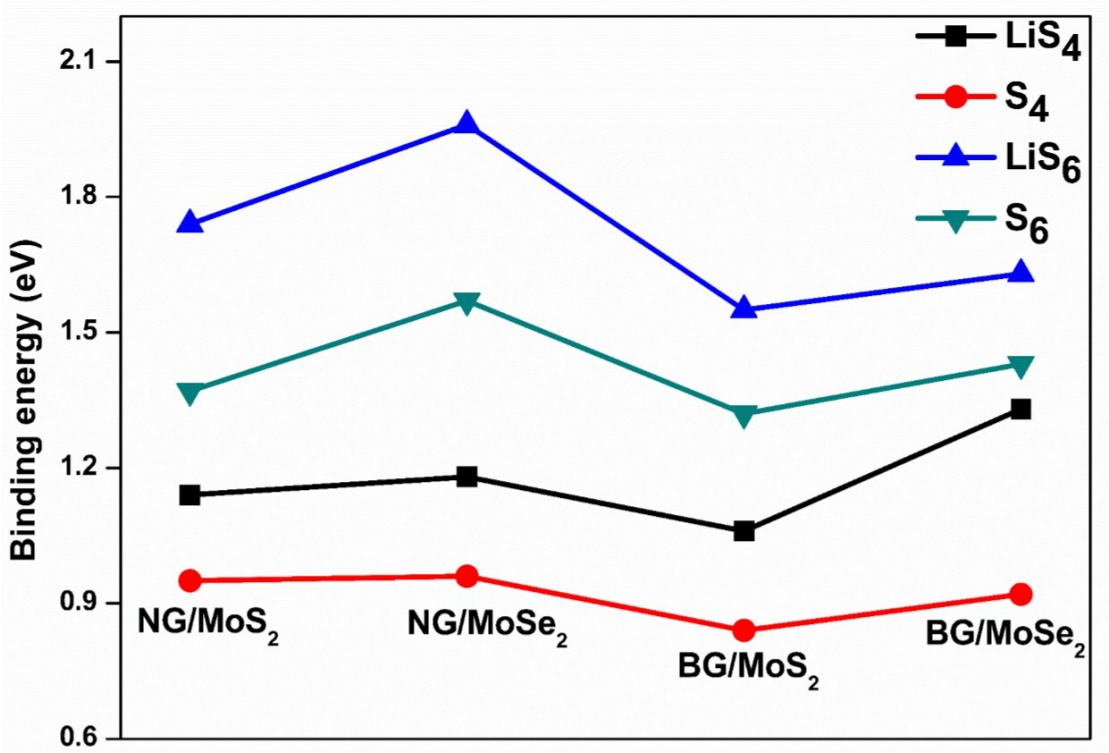

Figure S3. The computed binding energies for LiS_4, S_4, Li_2S_6, and S_6 species adsorption on various heterostructures.