Electronic Supplementary Material (ESI):

Decoration of defective graphene with MoS_2 enabling enhanced anchoring and catalytic conversion of polysulfides for lithium-sulfur batteries: A first-principles study

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Table S1 The EDFT, ZPE – TΔS and G values of S_8 and Li_2S_n adsorbed on the different heterostructures.

	$Li_2S_8^*$			$Li_2S_6^*$			$Li_2S_4^*$		
	E_{DFT} (eV)	ZPE – TΔS (eV)	*G* (eV)	E_{DFT} (eV)	ZPE – TΔS (eV)	*G* (eV)	E_{DFT} (eV)	ZPE – TΔS (eV)	*G* (eV)
PG/MoS_2	-861.32	-0.06	-861.38	-852.90	-0.07	-852.97	-844.03	-0.05	-844.08
SWG/MoS_2	-856.52	-0.07	-856.59	-848.12	-0.07	-848.19	-839.29	-0.04	-839.33
SVG/MoS_2	-844.59	-0.09	-844.68	-836.22	-0.07	-836.29	-827.46	-0.06	-827.52
DVG/MoS_2	-833.59	-0.07	-833.66	-825.20	-0.08	-825.28	-816.39	-0.07	-816.46
RDVG/MoS_2	-834.37	-0.07	-834.44	-825.93	-0.11	-826.04	-817.18	-0.07	-817.25
PG/MoS_2 (MoS_2 side)	-861.54	-0.05	-861.59	-852.98	-0.05	-853.03	-844.48	-0.01	-844.49
	$Li_2S_2^*$			Li_2S^*			S_8*		
	E_{DFT} (eV)	ZPE – TΔS (eV)	*G* (eV)	E_{DFT} (eV)	ZPE – TΔS (eV)	*G* (eV)	E_{DFT} (eV)	ZPE – TΔS (eV)	*G* (eV)
PG/MoS_2	-834.83	-0.07	-834.90	-829.67	-0.06	-829.73	-884.78	-0.06	-854.84
SWG/MoS_2	-830.30	-0.07	-830.37	-824.96	-0.03	-824.99	-850.01	-0.09	-850.10
SVG/MoS_2	-818.81	0.03	-818.78	-815.01	0.07	-814.94	-837.71	-0.07	-837.78
DVG/MoS_2	-807.78	0.04	-807.74	-802.79	0.04	-802.75	-826.81	-0.06	-826.87
RDVG/MoS_2	-808.54	-0.06	-808.60	-803.37	-0.06	-803.43	-827.72	-0.06	-827.78
PG/MoS_2 (MoS_2 side)	-835.34	-0.02	-835.36	-830.35	-0.05	-830.40	-854.78	-0.06	-854.84

Table S2 Calculated the binding energy E_b (eV) for heterostructures with S_8/Li_2S_n.

	Li_2S	Li_2S_2	Li_2S_4	Li_2S_6	Li_2S_8	S_8
PG/MoS_2	0.73	0.75	0.60	0.82	0.90	0.76
SWG/MoS_2	0.82	1.02	0.62	0.84	0.90	0.79
SVG/MoS_2	3.10	1.76	1.07	1.16	1.20	0.72
DVG/MoS_2	1.76	1.61	0.87	1.02	1.08	0.69
RDVG/MoS_2	1.49	1.52	0.81	0.90	1.00	0.76
PG/MoS_2 (MoS_2 side)	1.41	1.26	1.06	0.89	1.12	0.76

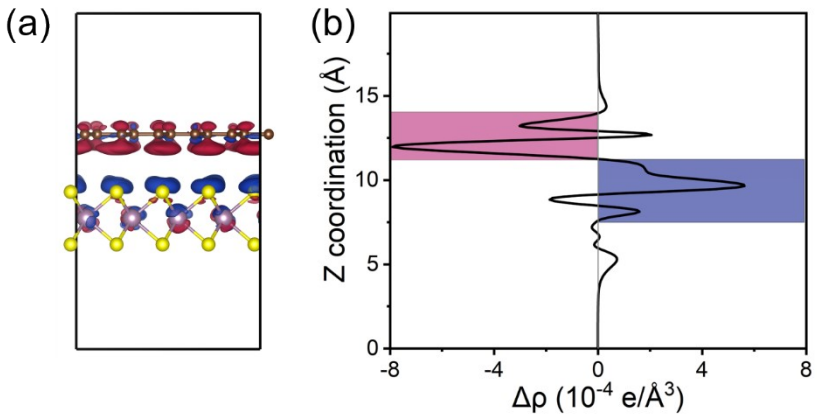

Fig. S1(a) Charge density difference and (b) planar-averaged electron density difference Δρ(z) for PG/MoS_2. The electron accumulation (depletion) region is shown in blue (fuchsia). The value of the isosurface is set to 0.0001 e/Bhhr^3.

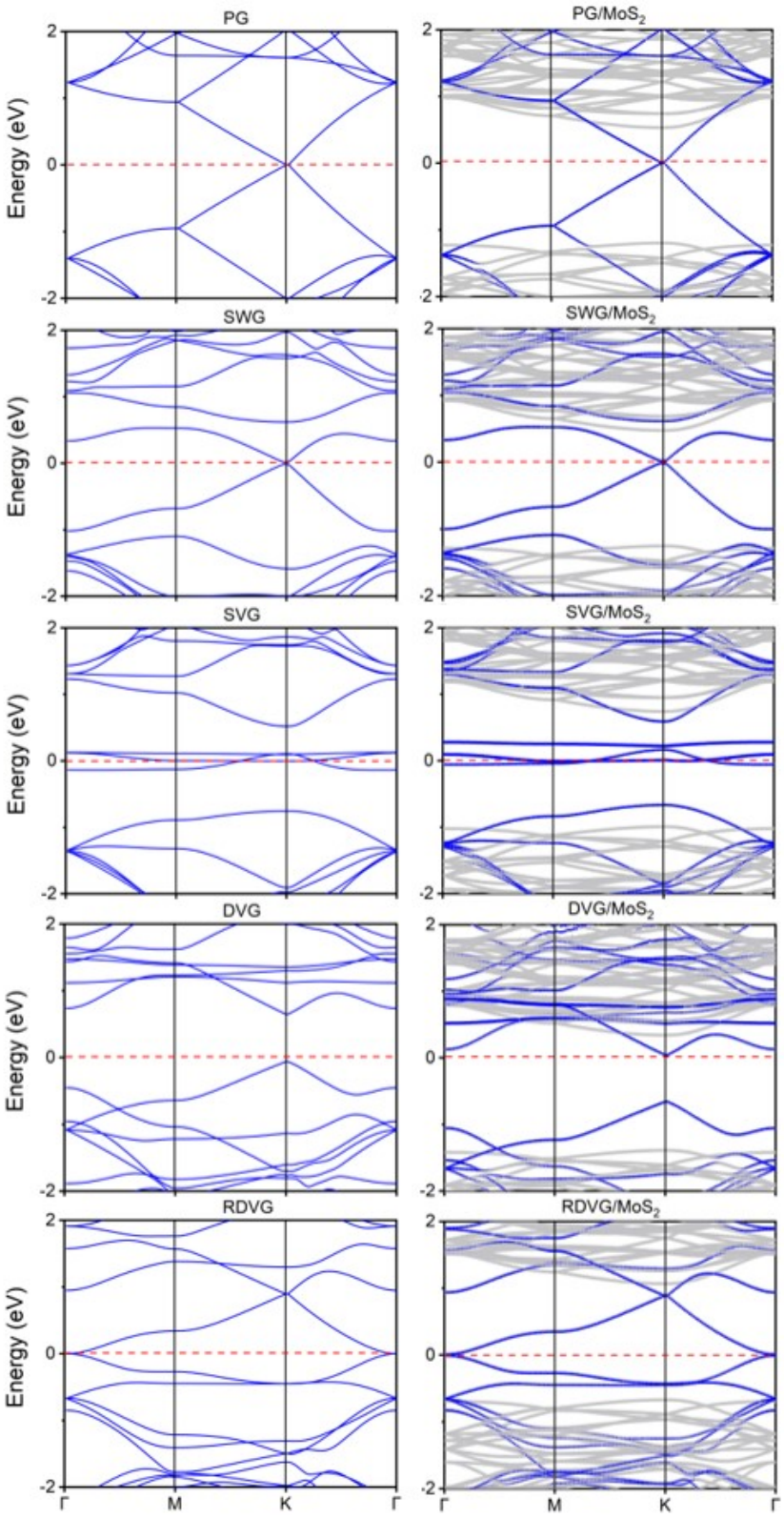

Fig. S2 Band structures of the free-standing PG, SWG, SVG, DVG, RDVG, and heterostructures of PG/MoS_2, SWG/MoS_2, SVG/MoS_2, DVG/MoS_2, and RDVG/MoS_2, respectively. Gray and blue lines represent the band structure of the heterostructures systems and projected to the PG/DG, respectively. The Fermi level is set at zero represented by the red dashed lines.

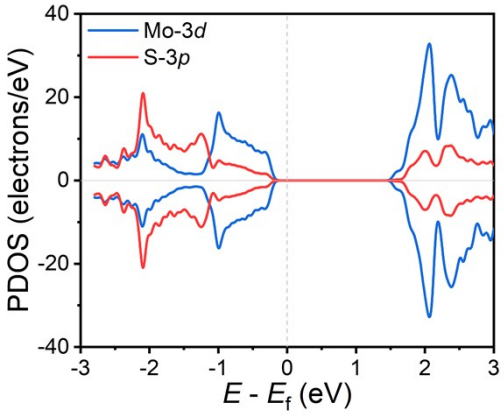

Fig. S3 Partial density of states (PDOS) of the free-standing MoS_2 molecular layer.

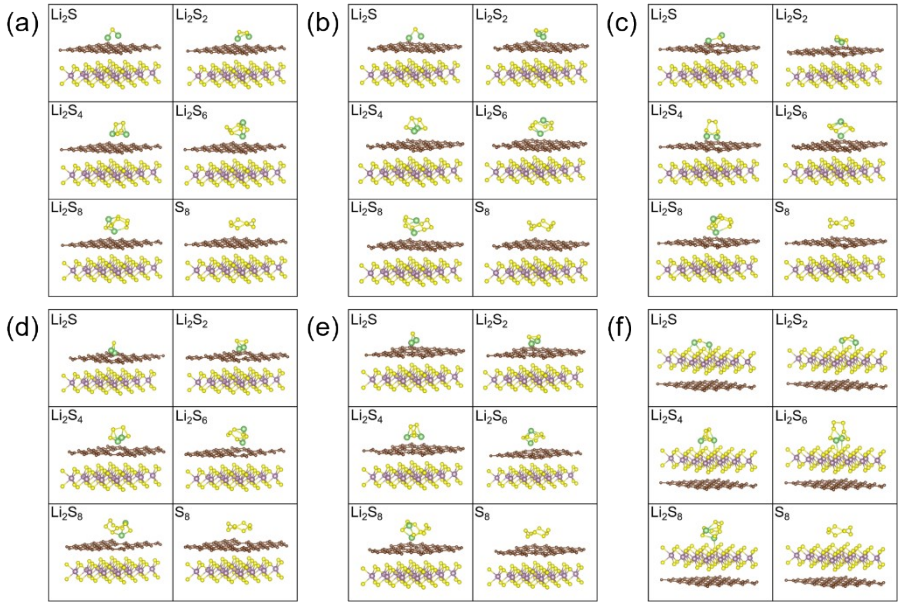

Fig. S4 Optimized structures of Li_2S_n/S_8 adsorbed on (a) the graphene side and (f) the MoS_2 side of the PG/MoS_2 eterostructure, (b) the SWG/MoS_2, (c) the SVG/MoS_2, (d) the DVG/MoS_2, and (e) the RDVG/MoS_2 heterostructures.

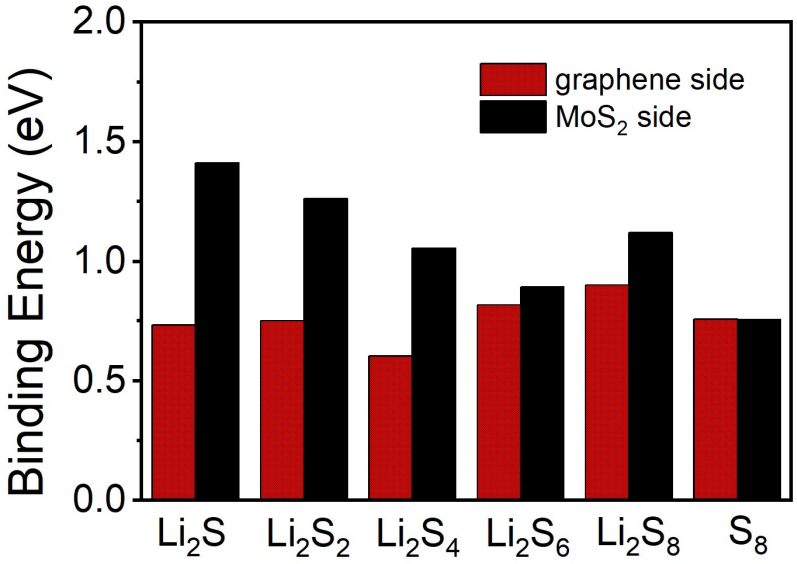

Fig. S5 The comparison of the binding energy on primitive graphene side and MoS_2 sides of the PG/MoS_2 heterostructure.

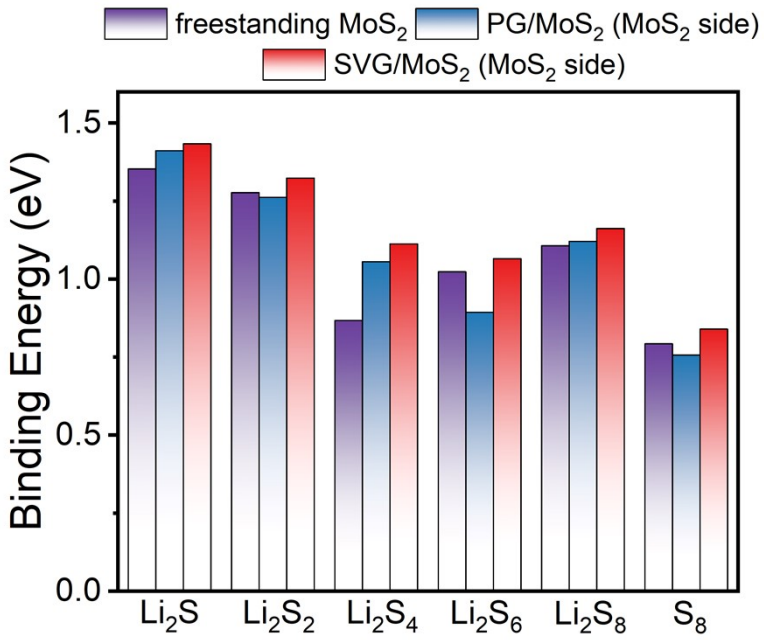

Fig. S6 The comparison of the binding energy on freestanding MoS_2 monolayer, MoS_2 sides of the PG/MoS_2 heterostructure, and MoS_2 sides of the SVG/MoS_2 heterostructure.

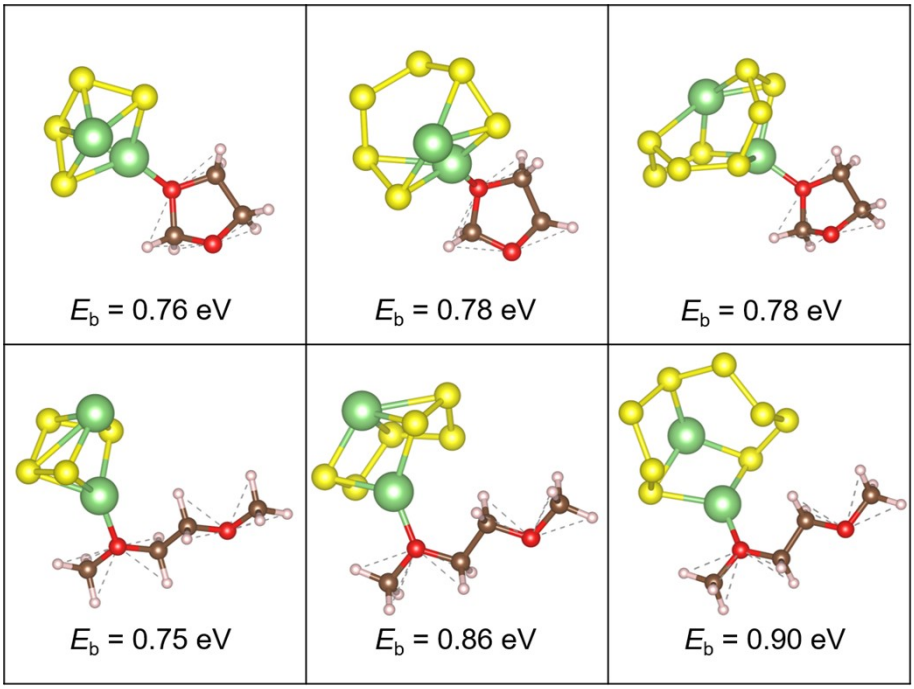

Fig. S7 Configuration of Li_2S_n (n = 4, 6, and 8) anchored on DOL and DME.