Supporting information for

Strain and Solvation Effects on Ti_3C_2O-TiN Heterostructure as Bifunctional Electrocatalysts for Li-S Batteries: A First-Principles Study

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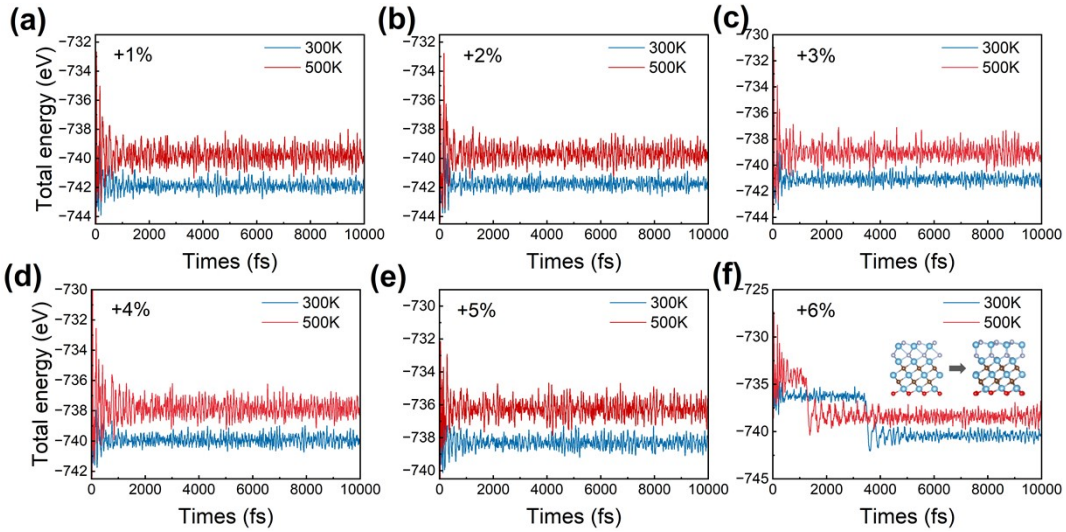

Figure S1. AIMD simulation of TiN/Ti_3C_2O heterostructure under tensile strain conditions at 300 K and 500K, respectively.

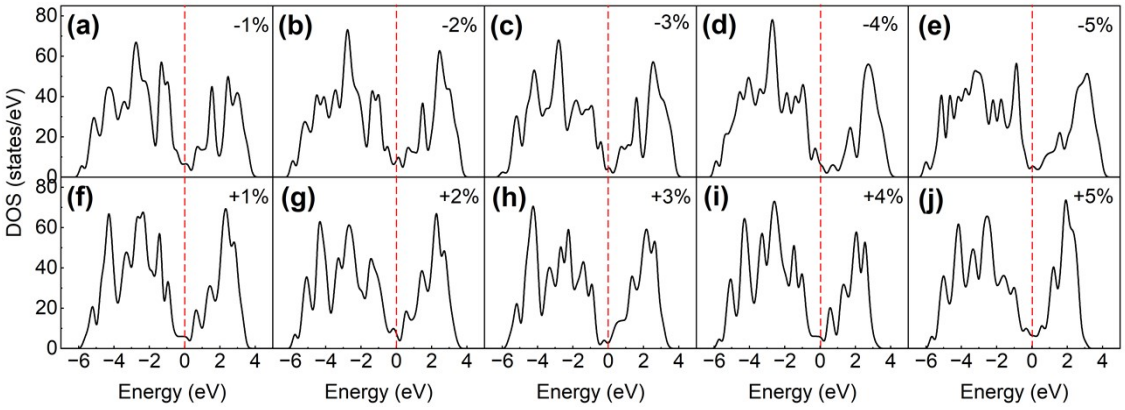

Figure S2. The total density of TiN/Ti_3C_2O heterostructure. (a) -1 %, (b) -2 %, (c) -3 %, (d) -4 %, (e) -5%, (f) +1 %, (g) +2 %, (h) +3 %, (i) +4 %, (j) +5 %.

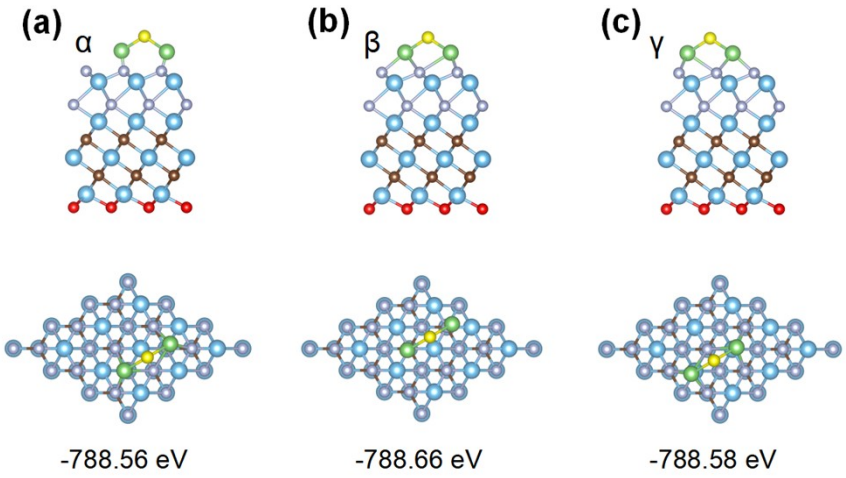

Figure S3. Illustration of the three possible adsorption sites of a Li_2S molecule on the Ti_3C_2O-TiN heterostructure surface.

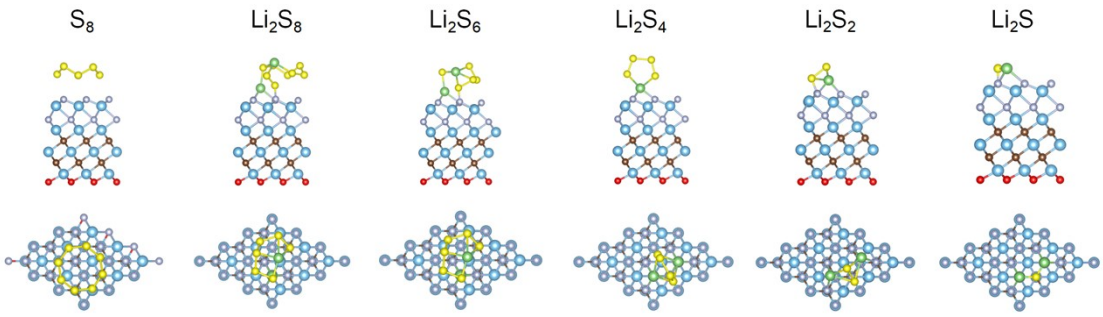

Figure S4. Optimized adsorption configurations of S_8/LiPSs intermediates on the Ti_3C_2O-TiN heterostructure surface.

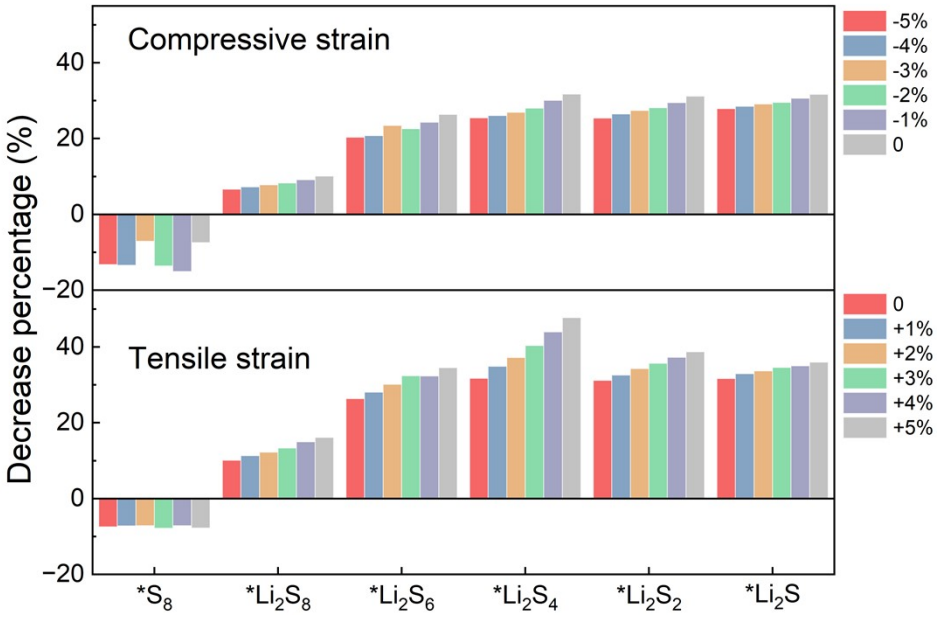

Figure S5. Deduction percentages of adsorption free energies by solvent correction.

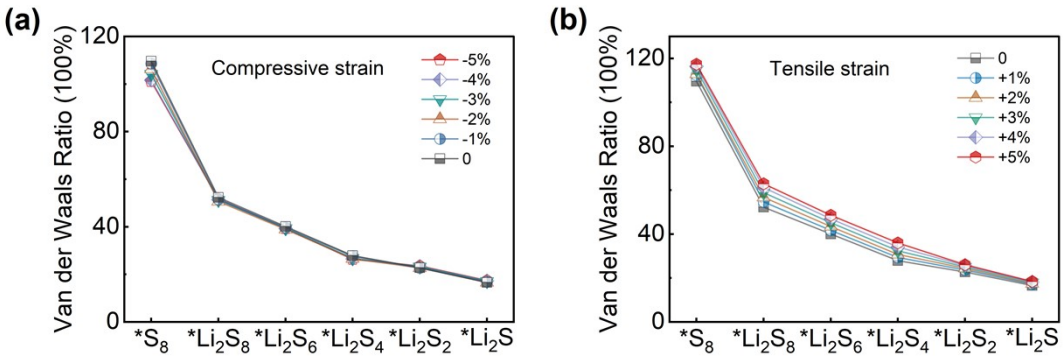

Figure S6. Ratios of vdW interaction to the adsorption energies of S_8/LiPSs on Ti_3C_2O-TiN heterostructure surface under various strain conditions.

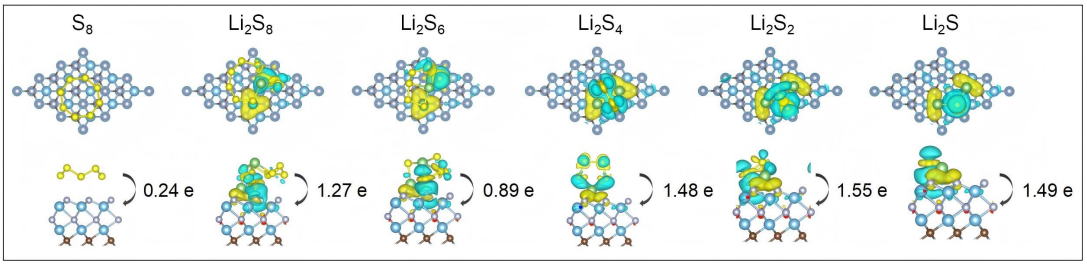

Figure S7. Charge density difference plots of S_8/LiPSs adsorbed on Ti_3C_2O-TiN heterostructure. Yellow and blue regions represent charge accumulation and depletion, respectively. The isosurface value was set to 0.003 e Å-3 for all plots.

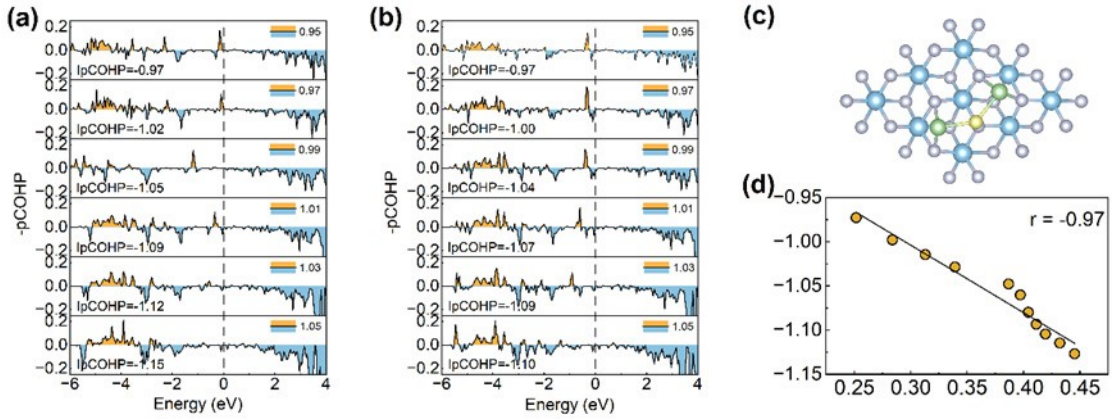

Figure S8. pCOHP and IpCOHP of (a) Li-N_1 bonds and (b) Li-N_2 bonds in Li_2S adsorbed on the Ti_3C_2O-TiN heterostructure under different strain conditions. (c) The optimized adsorption configuration of Li_2S adsorbed on the Ti_3C_2O-TiN heterostructure. (d) Correlation between the total IpCOHP values of Li-N bonds and the decomposition energy barrier of Li_2S.

Table S1. The lattice constant of TM-TiN/$Ti_3C_2Br_2$ heterostructure and the bonds information under different strain conditions.

Strain	Lattice constant (Å)	Surface Ti-N bond length (Å)	Subsurface Ti-N bond length (Å)	Third-layer Ti-N bond length (Å)	Ti-C bond length (Å)	Ti-O bond length (Å)
-5%	8.61	1.86	2.28	2.06	2.10	1.93
-4%	8.70	1.87	2.30	2.07	2.11	1.94
-3%	8.79	1.87	2.31	2.08	2.12	1.95
-2%	8.88	1.88	2.33	2.09	2.13	1.96
-1%	8.97	1.89	2.34	2.10	2.14	1.96
0%	9.06	1.89	2.36	2.11	2.15	1.97
+1%	9.16	1.90	2.38	2.12	2.17	1.98
+2%	9.25	1.91	2.40	2.13	2.17	1.99
+3%	9.34	1.91	2.42	2.14	2.18	1.20
+4%	9.43	1.92	2.43	2.15	2.19	2.01
+5%	9.52	1.93	2.45	2.16	2.20	2.02

Table S2. Adsorption free energies of S_8/LiPSs on the TiN/Ti_3C_2O heterostructure surface under varying strain conditions in both vacuum and solvent environments.

Strain		*S_8	*Li_2S_8	*Li_2S_6	*Li_2S_4	*Li_2S_2	*Li_2S
-5%	ΔG_{vac}	-1.11	-3.90	-3.87	-4.39	-5.10	-5.66
	ΔG_{sol}	-1.26	-3.64	-3.06	-3.27	-3.80	-4.08
-4%	ΔG_{vac}	-1.03	-3.81	-3.80	-4.28	-5.03	-5.60
	ΔG_{sol}	-1.17	-3.53	-2.98	-3.17	-3.70	-4.00
-3%	ΔG_{vac}	-0.96	-3.78	-3.65	-4.15	-4.95	-5.52
	ΔG_{sol}	-1.02	-3.49	-2.82	-3.03	-3.60	-3.92
-2%	ΔG_{vac}	-0.91	-3.66	-3.60	-3.99	-4.86	-5.43
	ΔG_{sol}	-1.03	-3.36	-2.76	-2.87	-3.49	-3.83
-1%	ΔG_{vac}	-0.83	-3.42	-3.45	-3.75	-4.70	-5.30
	ΔG_{sol}	-0.95	-3.11	-2.59	-2.62	-3.31	-3.67
0%	ΔG_{vac}	-0.82	-3.22	-3.25	-3.58	-4.49	-5.12
	ΔG_{sol}	-0.89	-2.89	-2.38	-2.44	-3.09	-3.50
+1%	ΔG_{vac}	-0.77	-3.00	-3.07	-3.28	-4.29	-4.94
	ΔG_{sol}	-0.83	-2.66	-2.18	-2.13	-2.90	-3.32
+2%	ΔG_{vac}	-0.74	-2.86	-2.88	-3.11	-4.11	-4.77
	ΔG_{sol}	-0.79	-2.51	-1.99	-1.95	-2.70	-3.16
+3%	ΔG_{vac}	-0.71	-2.69	-2.71	-2.89	-3.96	-4.62
	ΔG_{sol}	-0.76	-2.33	-1.82	-1.72	-2.54	-3.02
+4%	ΔG_{vac}	-0.70	-2.53	-2.61	-2.67	-3.82	-4.48
	ΔG_{sol}	-0.75	-2.15	-1.70	-1.50	-2.39	-2.91
+5%	ΔG_{vac}	-0.69	-2.39	-2.47	-2.47	-3.70	-4.37
	ΔG_{sol}	-0.74	-2.00	-1.56	-1.29	-2.27	-2.80

Table S3. The Li-S bond length of adsorbed Li_2S under different strain conditions.

Compressive Strain	Li-S bond length (Å)	Tensile Strain	Li-S bond length (Å)
-5%	2.331	0	2.330
-4%	2.331	+1%	2.332
-3%	2.330	+2%	2.333
-2%	2.329	+3%	2.332
-1%	2.328	+4%	2.331
0	2.330	+5%	2.330