Supporting information

A General Atomic Surface Modification Strategy for Improving Anchoring and Electrocatalysis Behavior of $Ti_3C_2T_2$ MXene in Lithium-Sulfur Batteries

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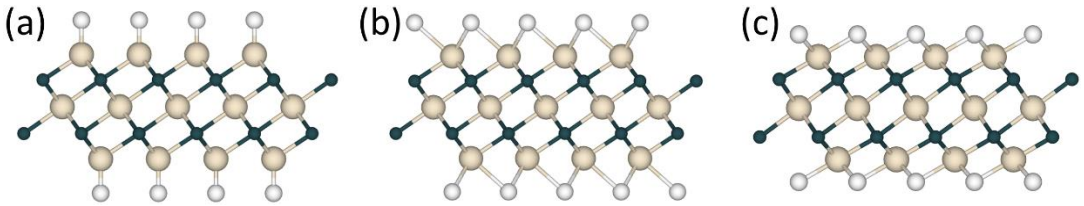

Fig. S1 Three possible configurations for $Ti_3C_2T_2$ (a) Mode I, (b) Mode II, (c) Mode III with different functional group positions. White balls are functional groups T.

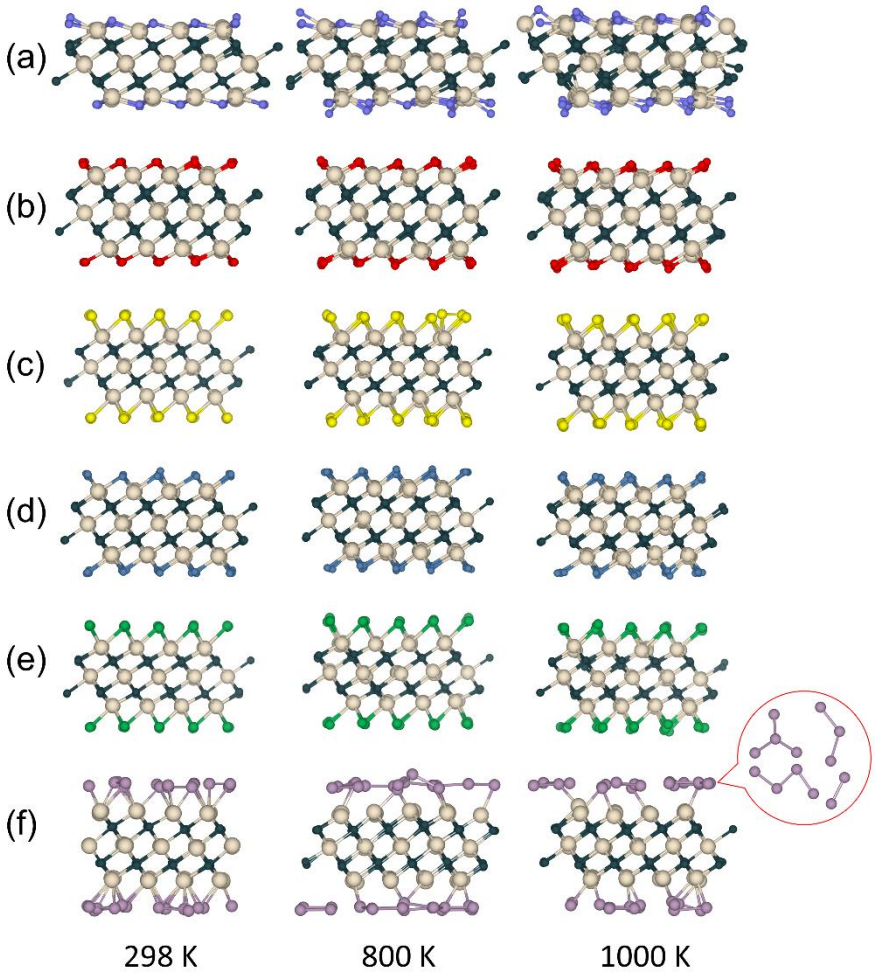

Fig. S2 Snapshots of the equilibrium structure of (a) $Ti_3C_2N_2$, (b) $Ti_3C_2O_2$, (c) $Ti_3C_2S_2$, (d) $Ti_3C_2F_2$, (e) $Ti_3C_2Cl_2$ and (f) $Ti_3C_2P_2$ after 5 ps AIMD simulation.

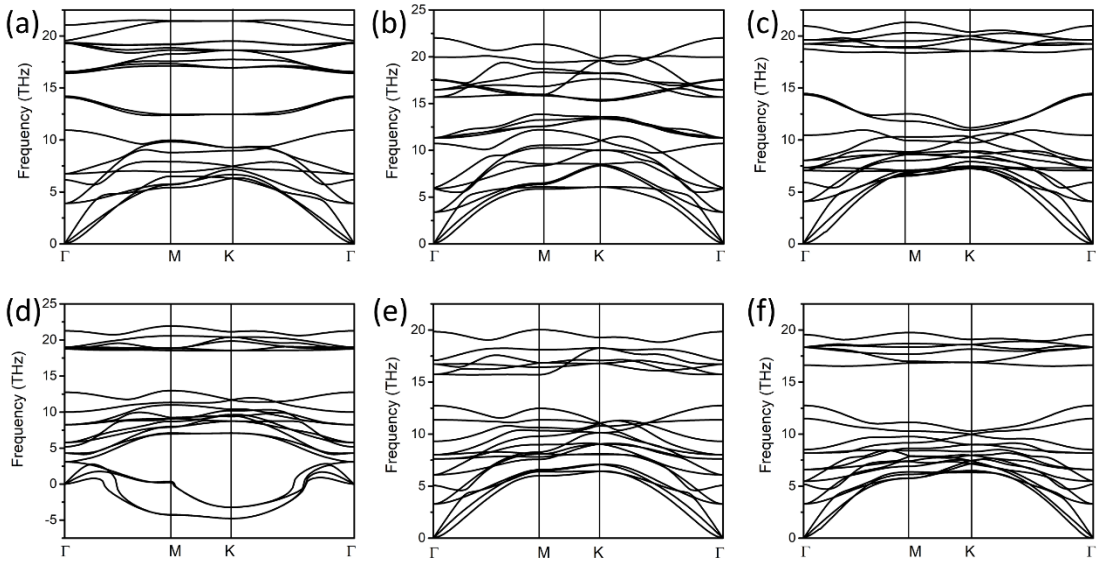

Fig. S3 Calculated phonon dispersions along the high symmetrical directions of the Brillouin zone for (a) $Ti_3C_2N_2$, (b) $Ti_3C_2O_2$, (c) $Ti_3C_2F_2$, (d) $Ti_3C_2P_2$, (e) $Ti_3C_2S_2$, and (f) $Ti_3C_2Cl_2$.

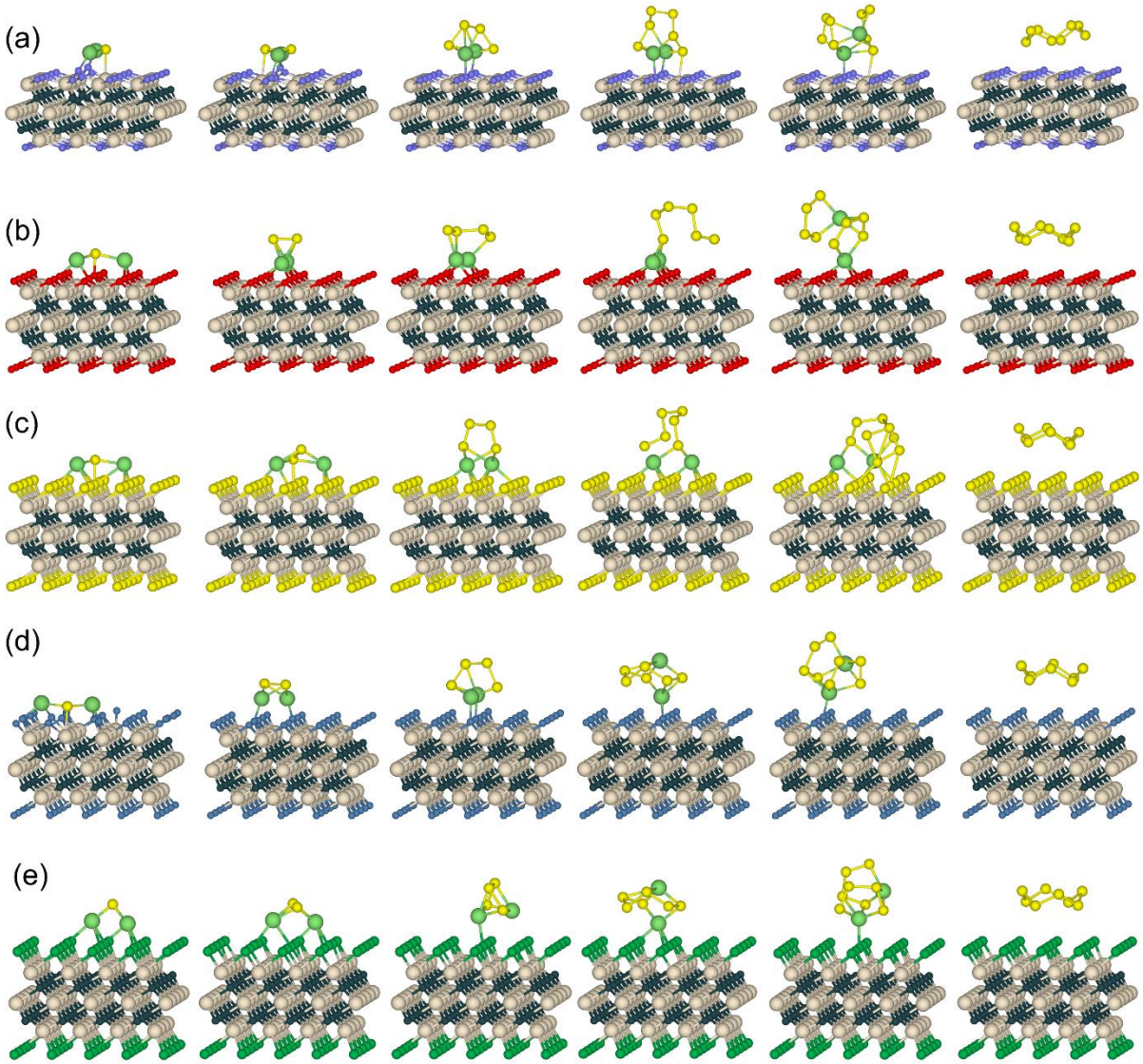

Fig. S4 Adsorption configurations of Li_2S_n and S_8 on the surface of (a) $Ti_3C_2N_2$, (b) $Ti_3C_2O_2$, (c) $Ti_3C_2S_2$, (d) $Ti_3C_2F_2$ and (e) $Ti_3C_2Cl_2$.

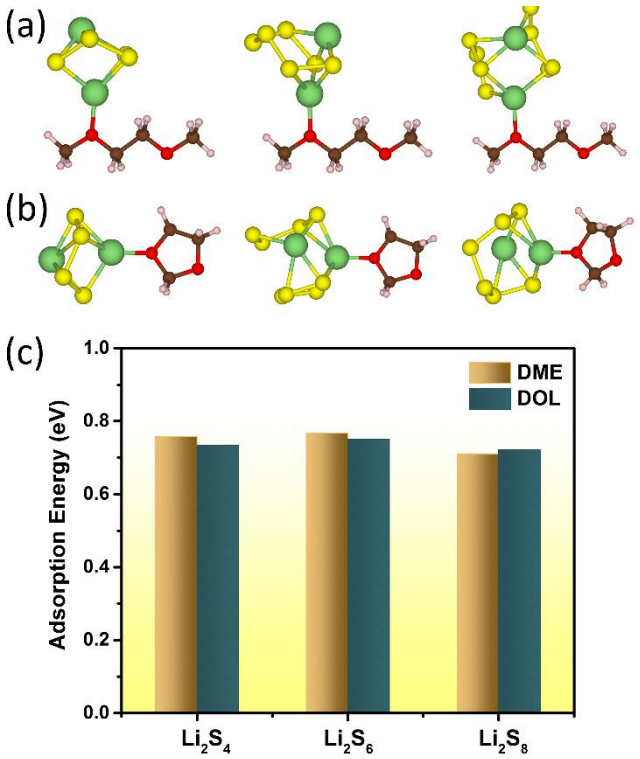

Fig. S5 Configurations of Li_2S_n (n =4, 6, 8) bound with (a) DME and (b) DOL; (c) binding energies of Li_2S_n (n =4, 6, 8) with DME and DOL.

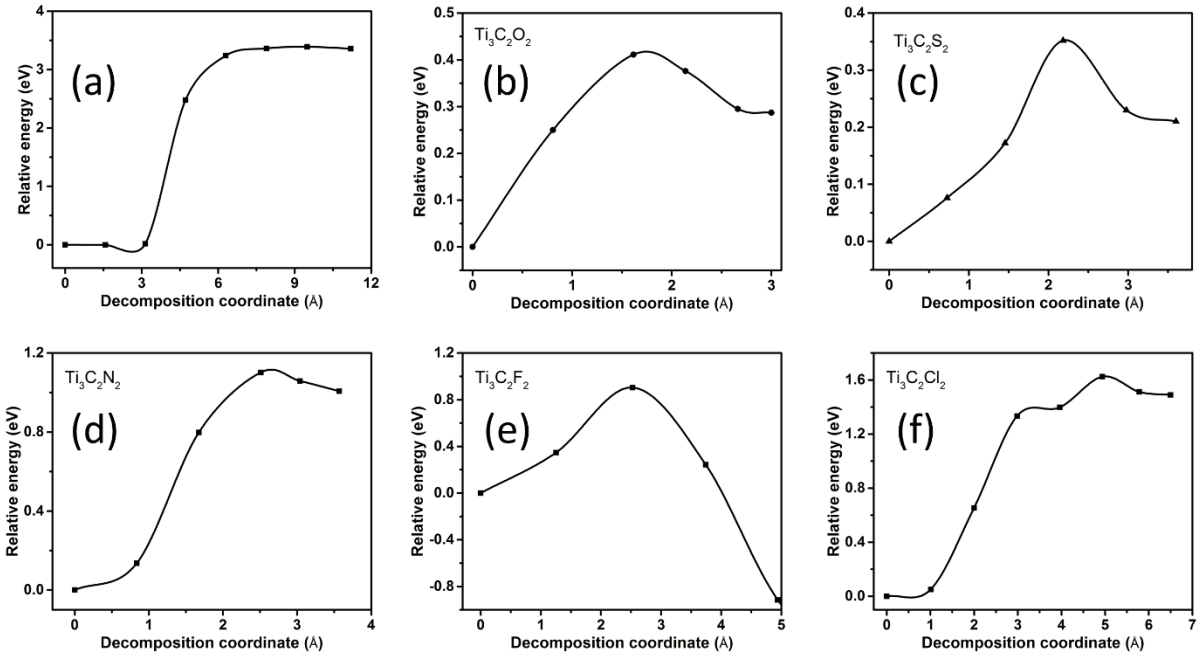

Fig. S6 Energy profiles for the decomposition of Li_2S in (a) vacuum and on (b-f) $Ti_3C_2T_2$ (T= O, S, N, F, Cl),

respectively.

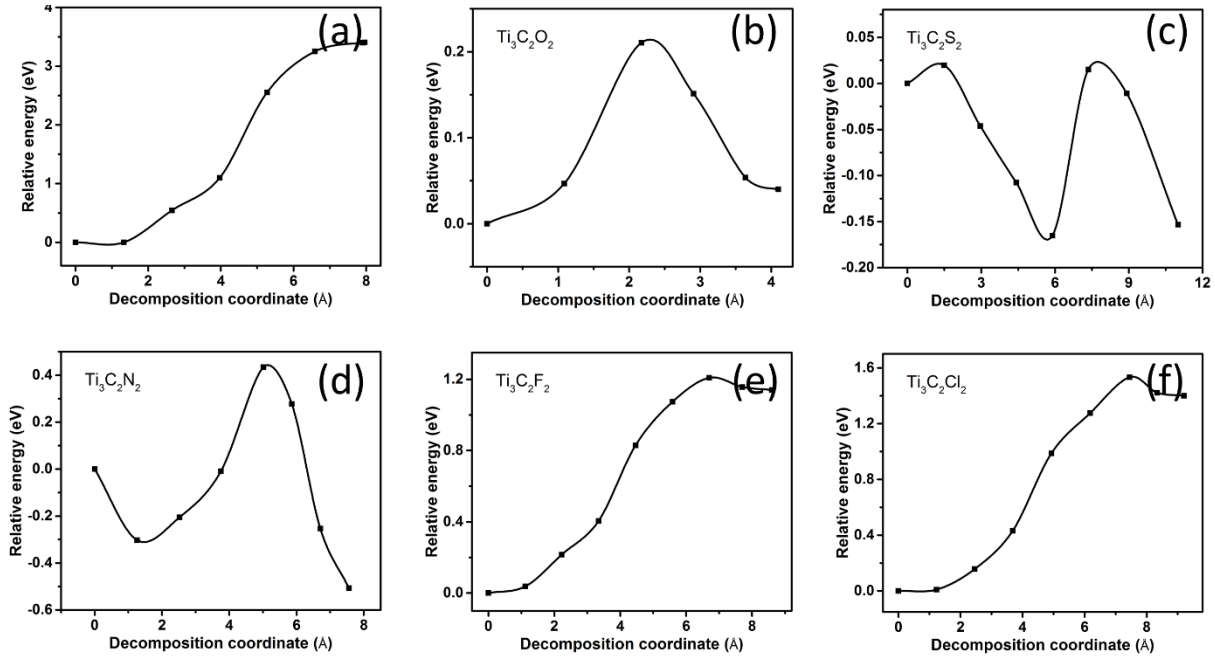

Fig. S7 Energy profiles for the decomposition of Li_2S_6 in (a) vacuum and on (b-f) $Ti_3C_2T_2$ (T= O, S, N, F, Cl), respectively.

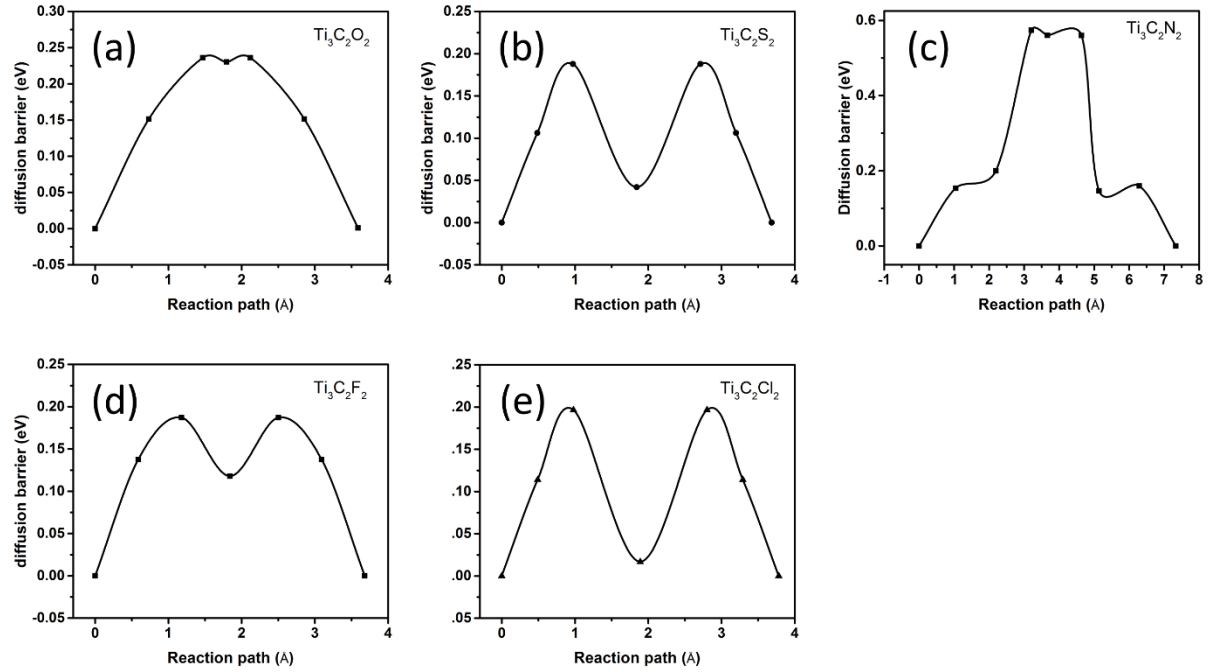

Fig. S8 Energy profiles for Li^+ diffusion on $Ti_3C_2T_2$ (T= O, S, N, F, Cl), respectively.

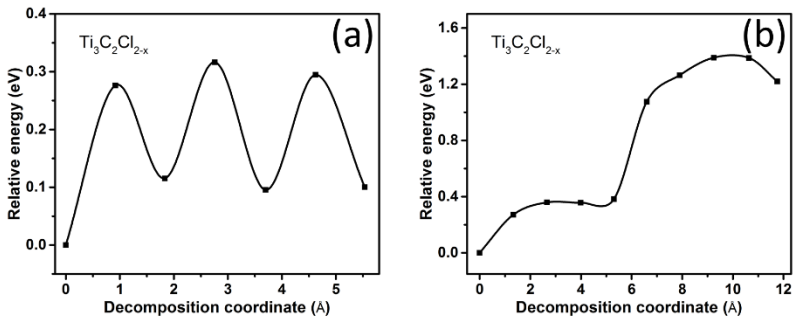

Fig. S9 Energy profiles for the decomposition of (a) Li_2S and (b) Li_2S_6 on $Ti_3C_2Cl_{2-x}$, respectively.

Table S1 Total energies of the three modes $Ti_3C_2T_2$ phases. (eV)

	$Ti_3C_2O_2$	$Ti_3C_2S_2$	$Ti_3C_2N_2$	$Ti_3C_2F_2$	$Ti_3C_2Cl_2$	$Ti_3C_2P_2$
Mode I	-58.730	-50.148	-56.364	-55.428	-43.923	-54.002
Mode II	-62.418	-57.077	-63.860	-58.387	-54.683	-57.660
Mode III	-64.198	-58.007	-62.521	-59.079	-55.202	-58.263

Table S2 Binding energies of function groups on Ti_3C_2. (eV)

$Ti_3C_2O_2$	$Ti_3C_2S_2$	$Ti_3C_2N_2$	$Ti_3C_2F_2$	$Ti_3C_2Cl_2$	$Ti_3C_2P_2$
−15.345	−9.345	−11.086	−12.861	−8.980	−8.263

Table S3 The lattice constants (Å) of $Ti_3C_2T_2$. The *c* constant of $Ti_3C_2T_2$ are all > 20 Å.

Lattice constant (Å)	Ti_3C_2	$Ti_3C_2F_2$	$Ti_3C_2Cl_2$	$Ti_3C_2O_2$	$Ti_3C_2S_2$	$Ti_3C_2N_2$
$a = b$	3.083	3.059	3.173	3.026	3.123	3.284