

## Supporting Information

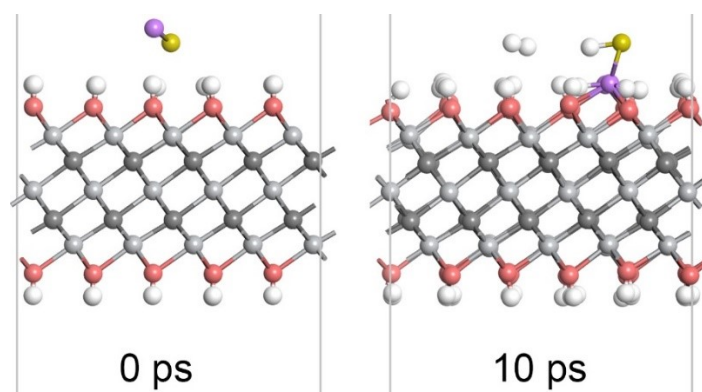
### **S-Doped $\text{Ti}_3\text{C}_2\text{F}_2$ MXene as an Ideal Sulfur Cathode Host for High-Performance Rechargeable Lithium-Sulfur Batteries**

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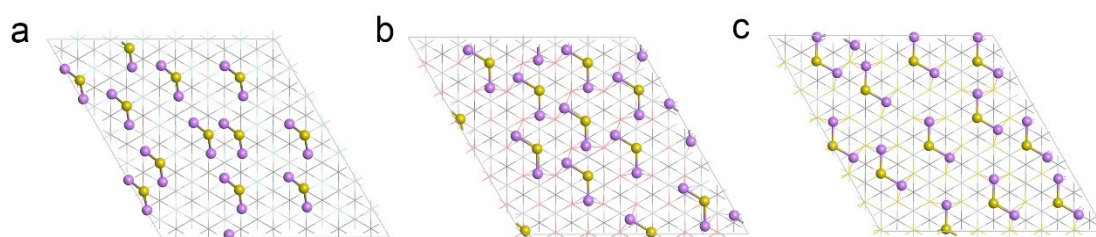
zhangyw@ihpc.a-star.edu.sg



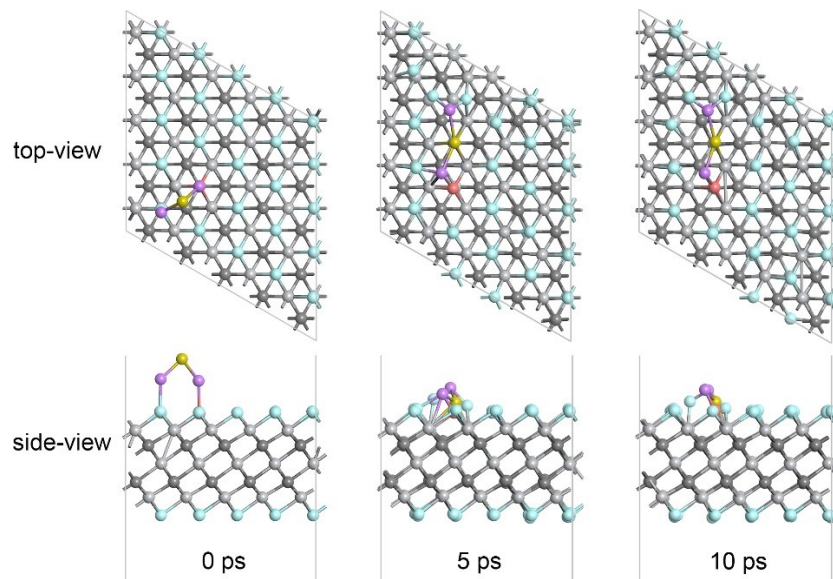
**Fig S1.** AIMD snapshots of  $\text{Li}_2\text{S}$  on  $\text{Ti}_3\text{C}_2(\text{OH})_2$  at 0 and 10 ps.

**Table S1.**  $\text{Li}_2\text{S}$  diffusion and decomposition barriers (units: eV) on MXenes.

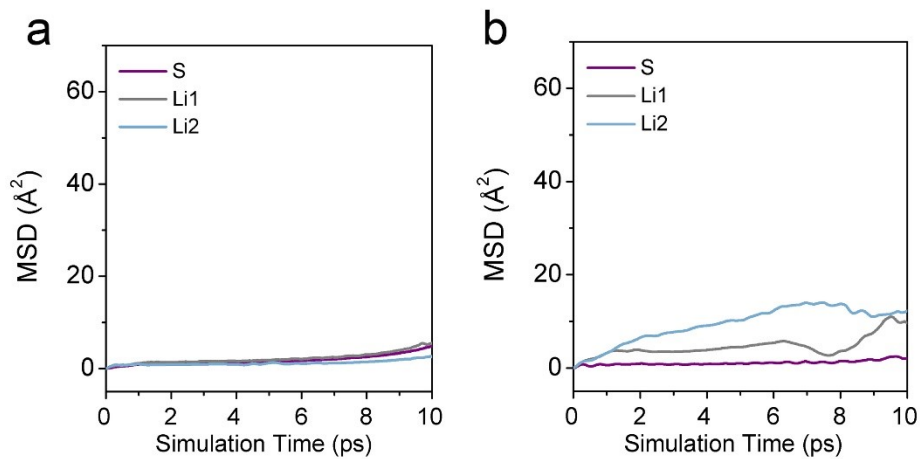
	$\text{Ti}_3\text{C}_2\text{F}_2$	$\text{Ti}_3\text{C}_2\text{O}_2$	$\text{Ti}_3\text{C}_2\text{S}_2$
$\text{Li}_2\text{S}$ diffusion	0.1	1.15	1.38
$\text{Li}_2\text{S}$ decomposition	1.35	0.47	0.34



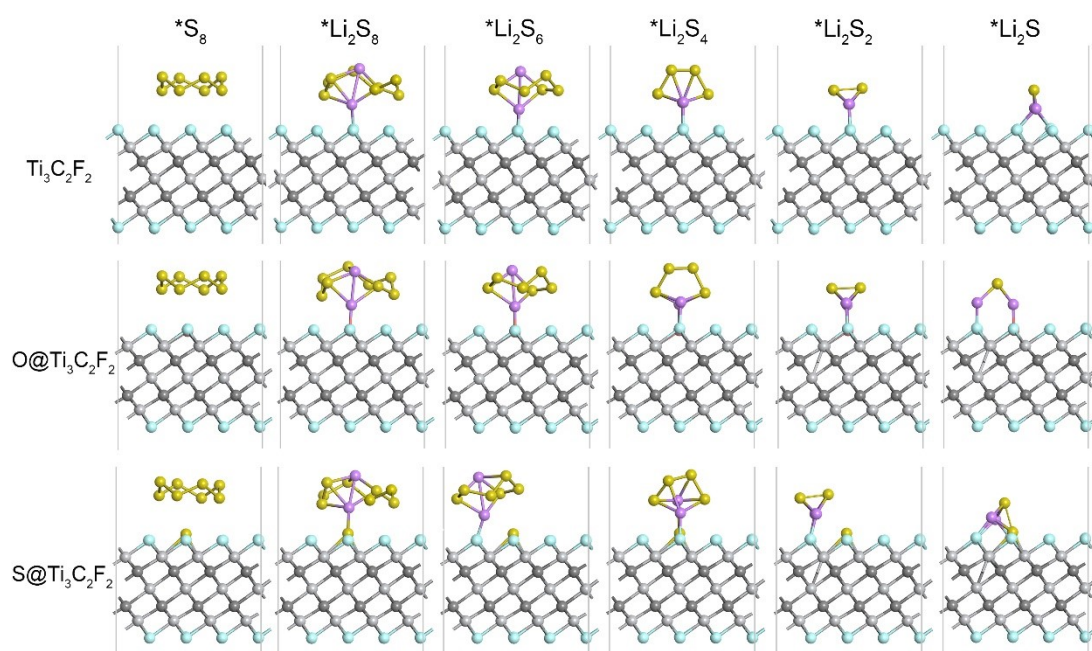
**Fig S2.** Initial structures with a high concentration  $\text{Li}_2\text{S}$  on a)  $\text{Ti}_3\text{C}_2\text{F}_2$ , b)  $\text{Ti}_3\text{C}_2\text{O}_2$  and c)  $\text{Ti}_3\text{C}_2\text{S}_2$ .



**Fig S3.** Snapshots of  $\text{Li}_2\text{S}$  on  $\text{O@Ti}_3\text{C}_2\text{F}_2$ .



**Fig S4.** Calculated MSD of Li and S on a)  $\text{O@Ti}_3\text{C}_2\text{F}_2$  and b)  $\text{S@Ti}_3\text{C}_2\text{F}_2$  as a function of simulation time.



**Fig S5.** Adsorption configurations of polysulfides on  $Ti_3C_2F_2$ ,  $O@Ti_3C_2F_2$  and  $S@Ti_3C_2F_2$ .

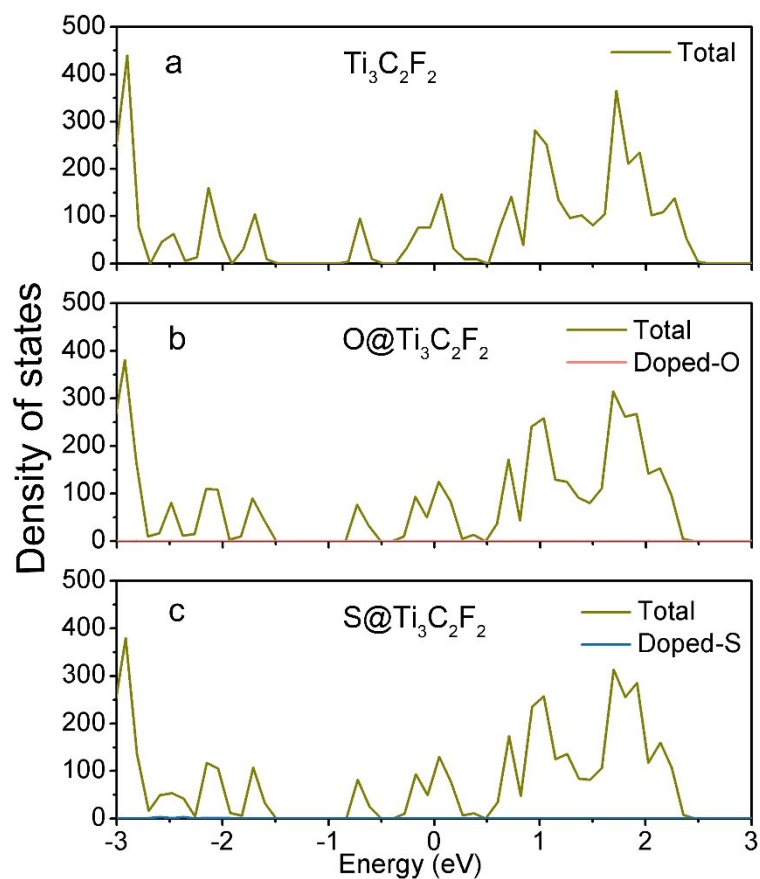


Fig S6. Density of states of a)  $\text{Ti}_3\text{C}_2\text{F}_2$ , b)  $\text{O}@\text{Ti}_3\text{C}_2\text{F}_2$  and c)  $\text{S}@\text{Ti}_3\text{C}_2\text{F}_2$ .

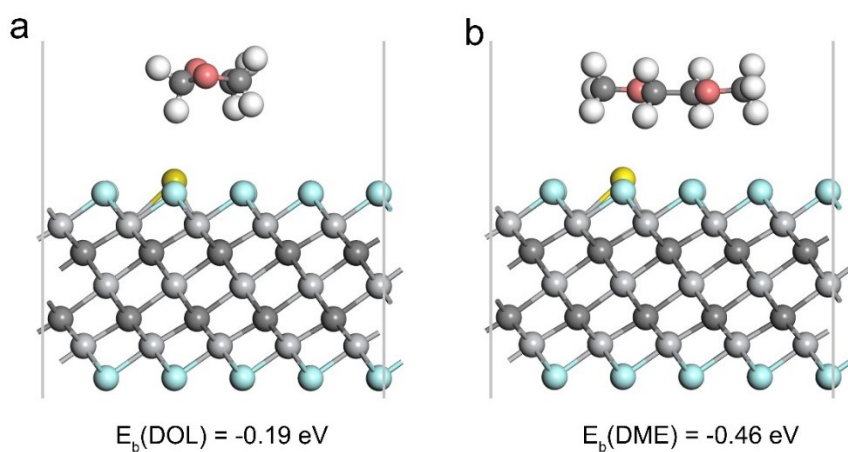


Fig S7. The adsorption configurations and adsorption energies of DOL and DME on  $\text{S}@\text{Ti}_3\text{C}_2\text{F}_2$  are shown in a) and b), respectively.