

SUPPORTING INFORMATION

Atomic Insights into A Family of Single Transition Metal Atom-Doped MXenes for Catalytic Conversion of Lithium Polysulfide in Lithium-Sulfur Batteries

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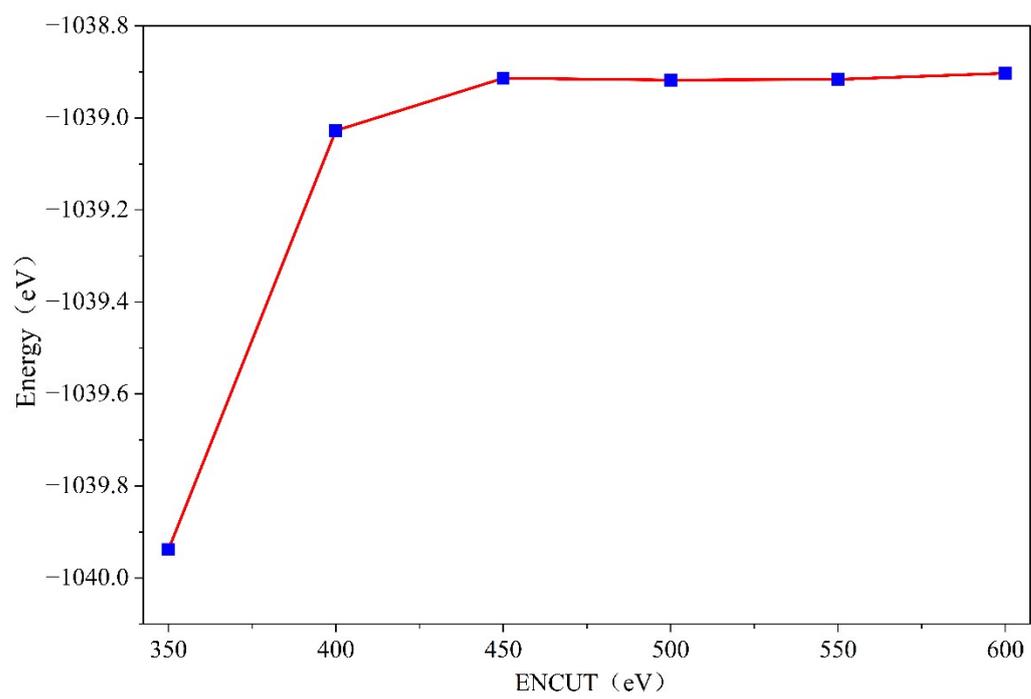


Figure S1. Energy varies with the change of ENCUT

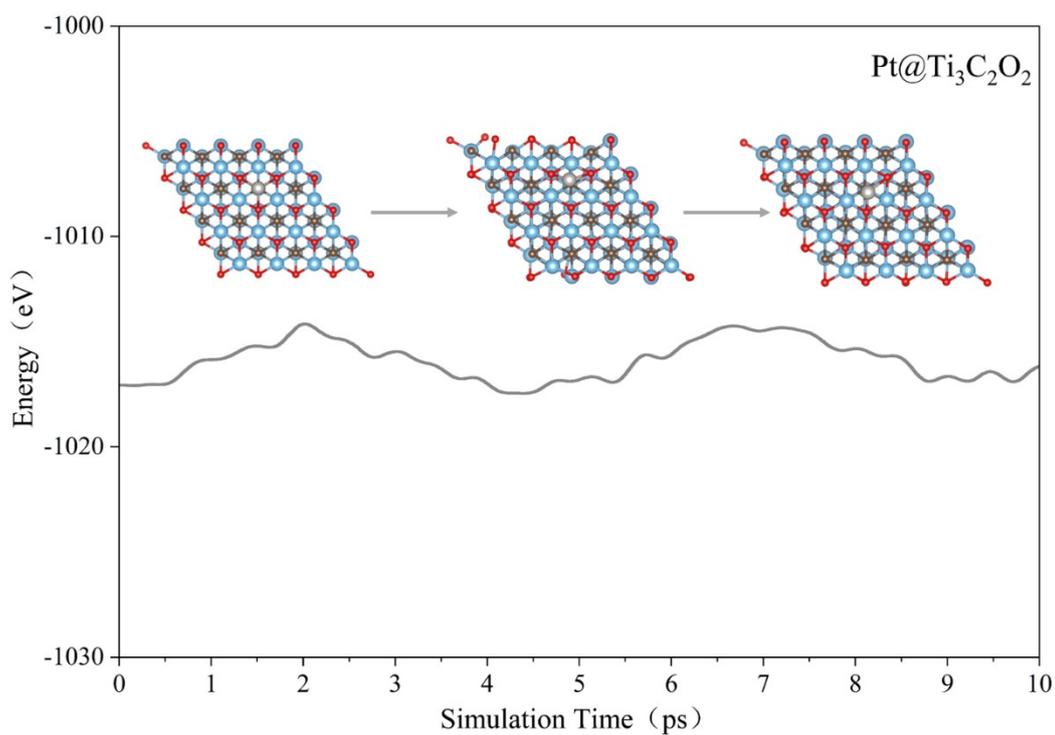
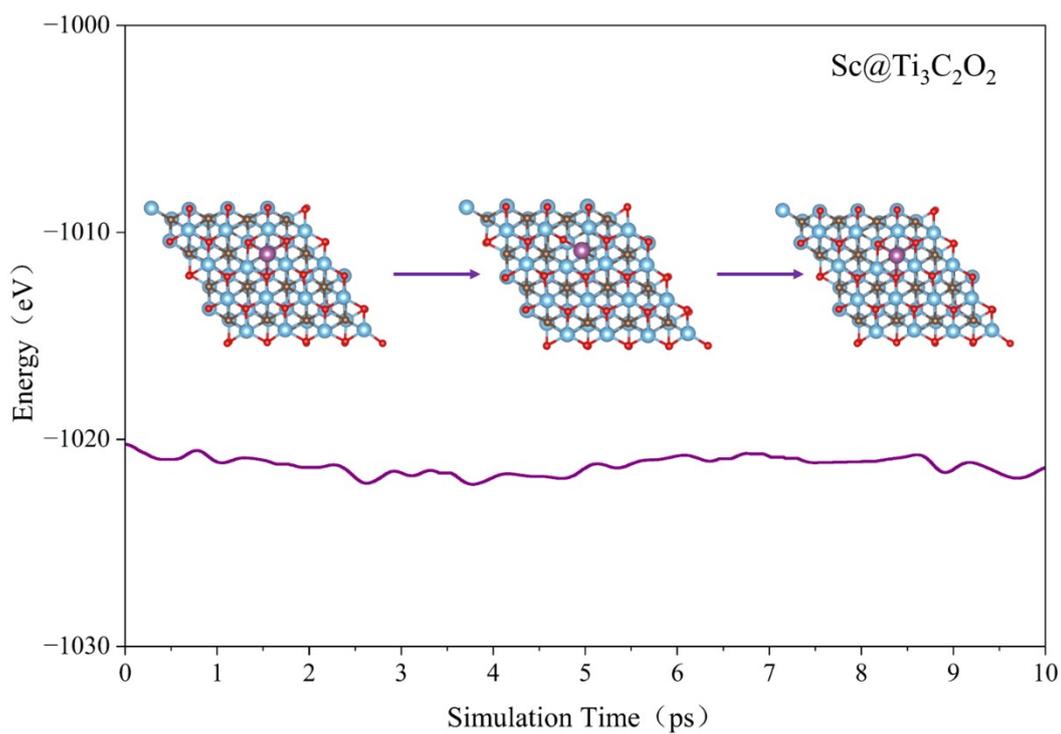
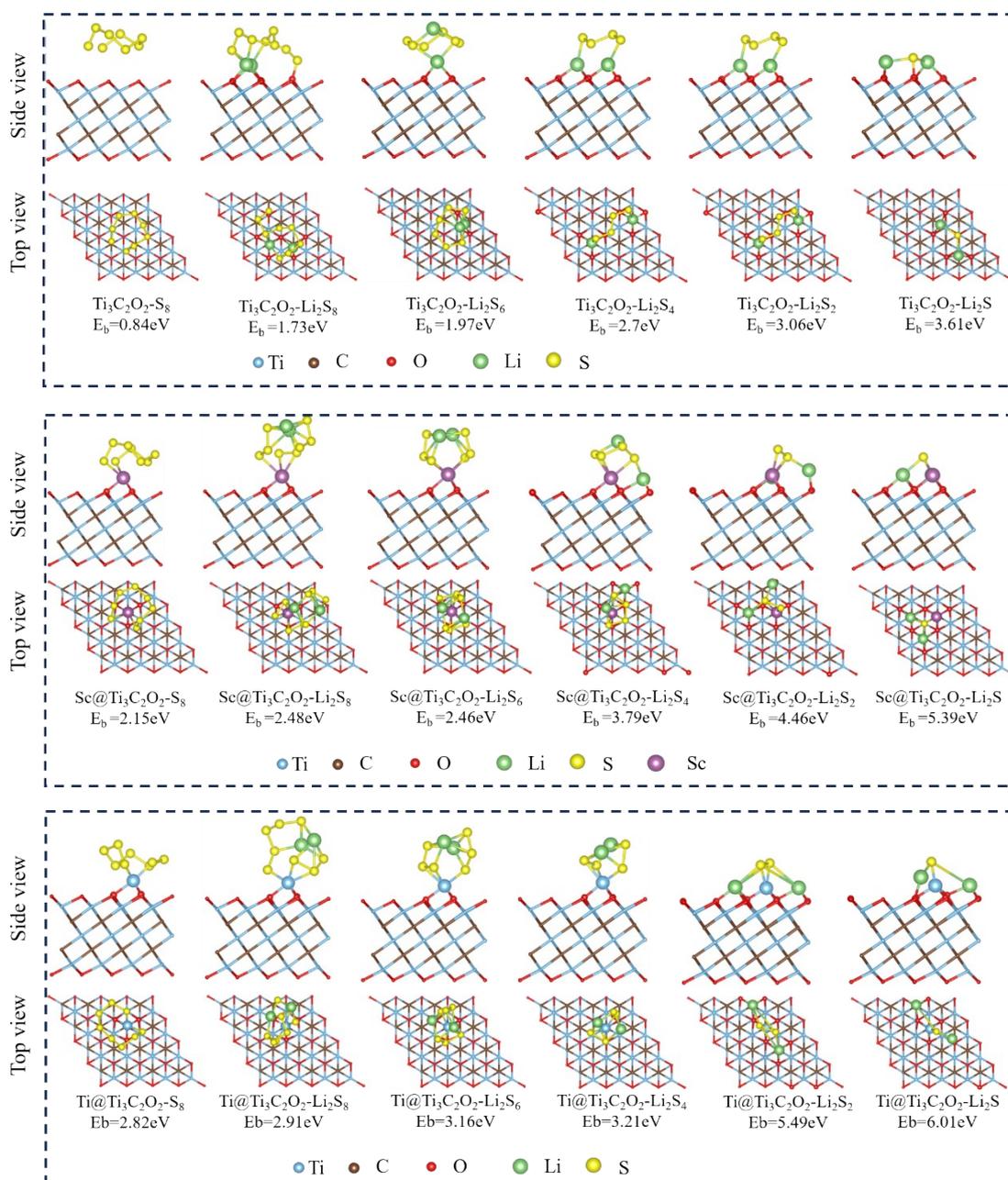
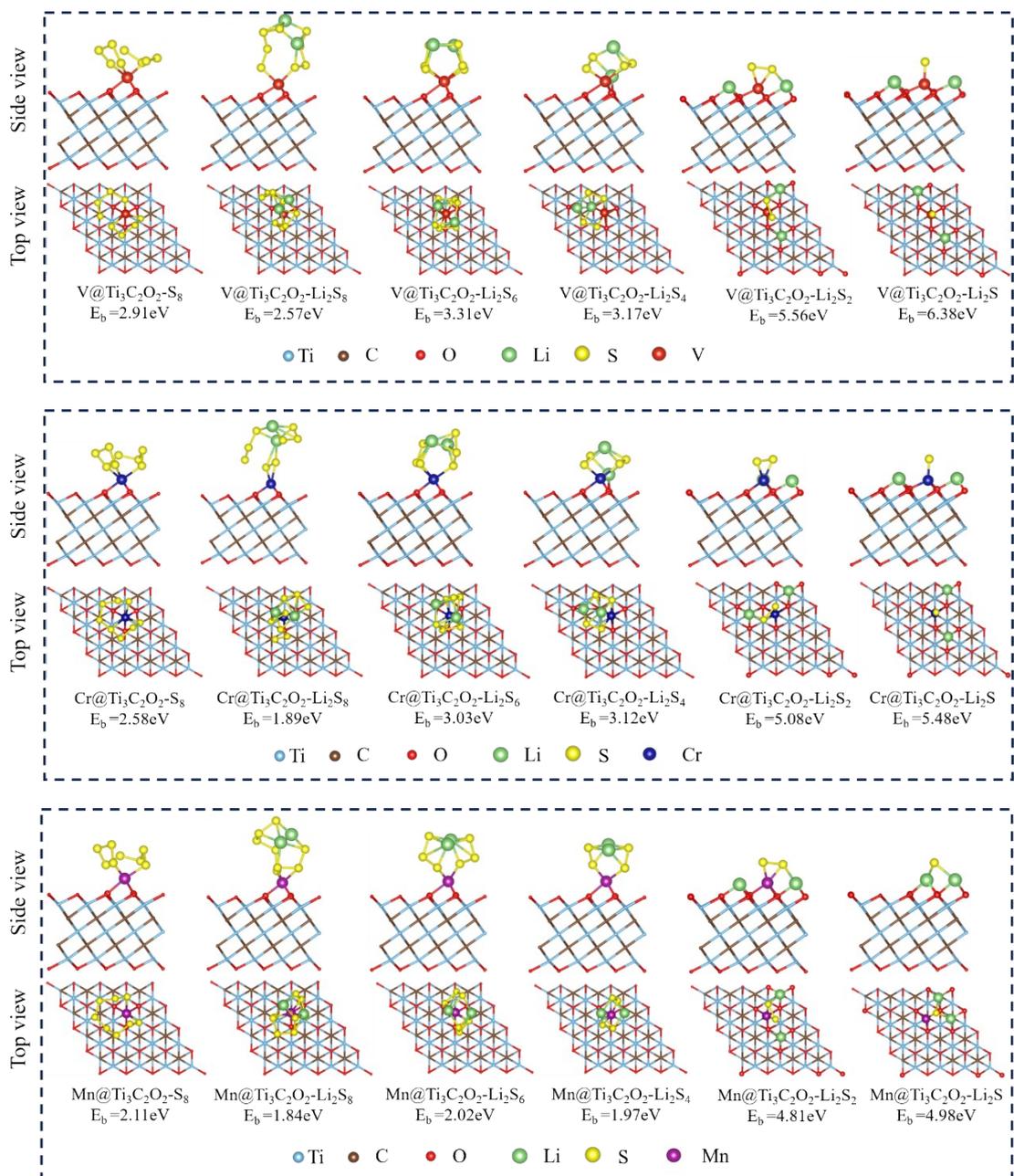


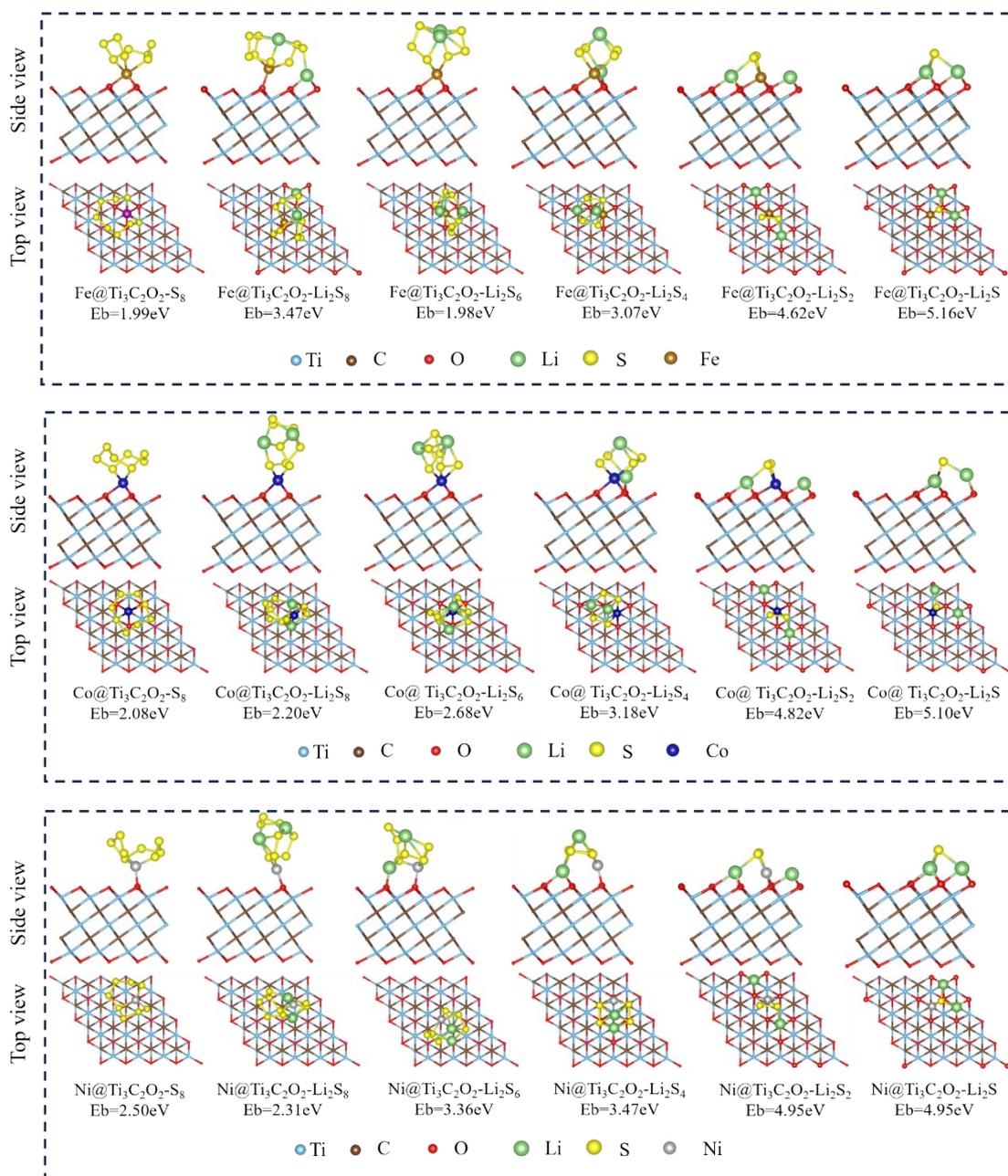
Figure S2. Energy evolutions of transition metal atoms (Sc and Pt) on pristine Ti₃C₂O₂ nanosheet during 10 ps AIMD simulations at 350 K. The figure also shows the corresponding structure's changes during the simulation process.



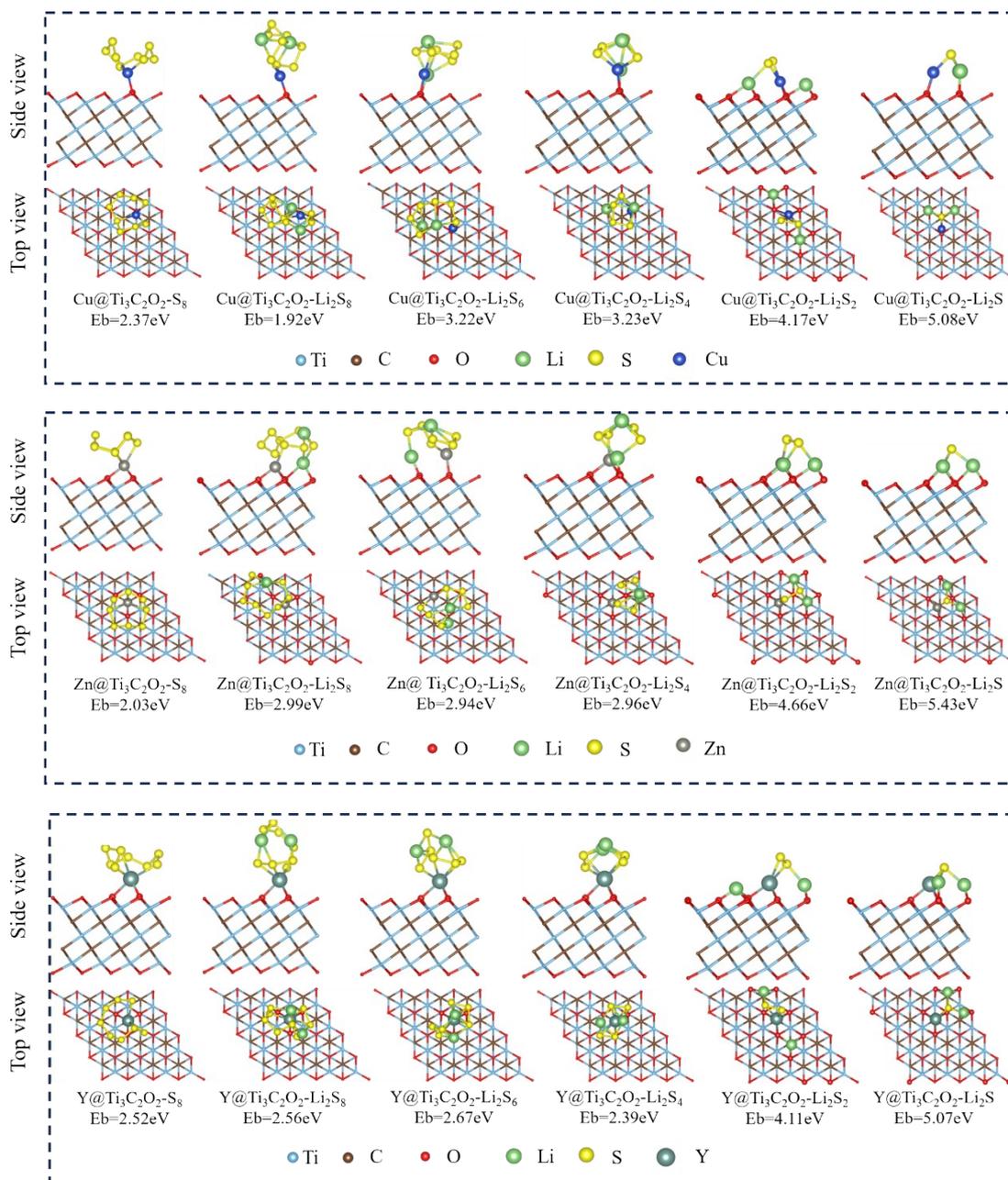
FigureS3. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Ti}_3\text{C}_2\text{O}_2$, $\text{Sc@Ti}_3\text{C}_2\text{O}_2$ and $\text{Ti@Ti}_3\text{C}_2\text{O}_2$ nanosheets.



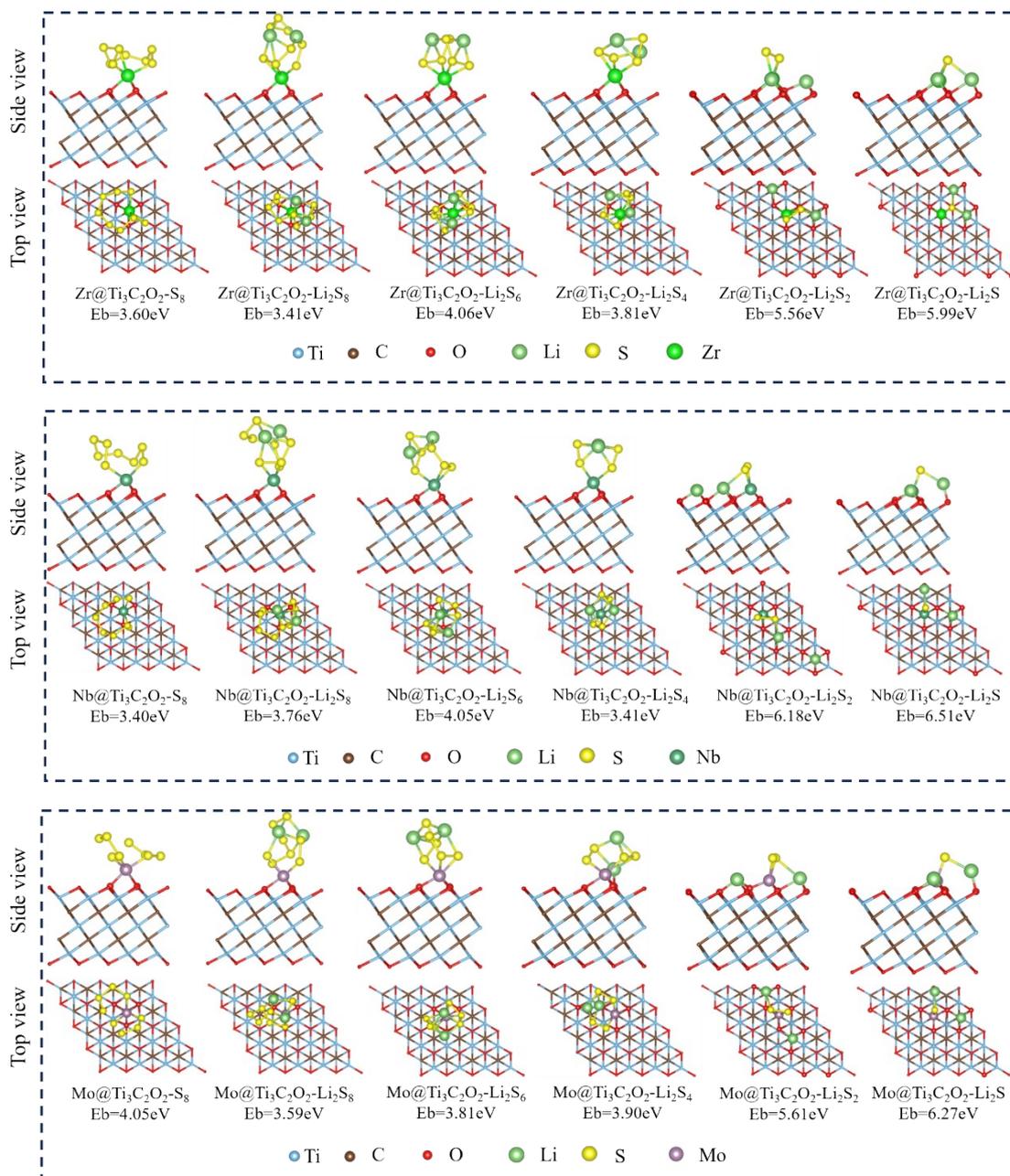
FigureS4. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{V@Ti}_3\text{C}_2\text{O}_2$, $\text{Cr@Ti}_3\text{C}_2\text{O}_2$ and $\text{Mn@Ti}_3\text{C}_2\text{O}_2$ nanosheets.



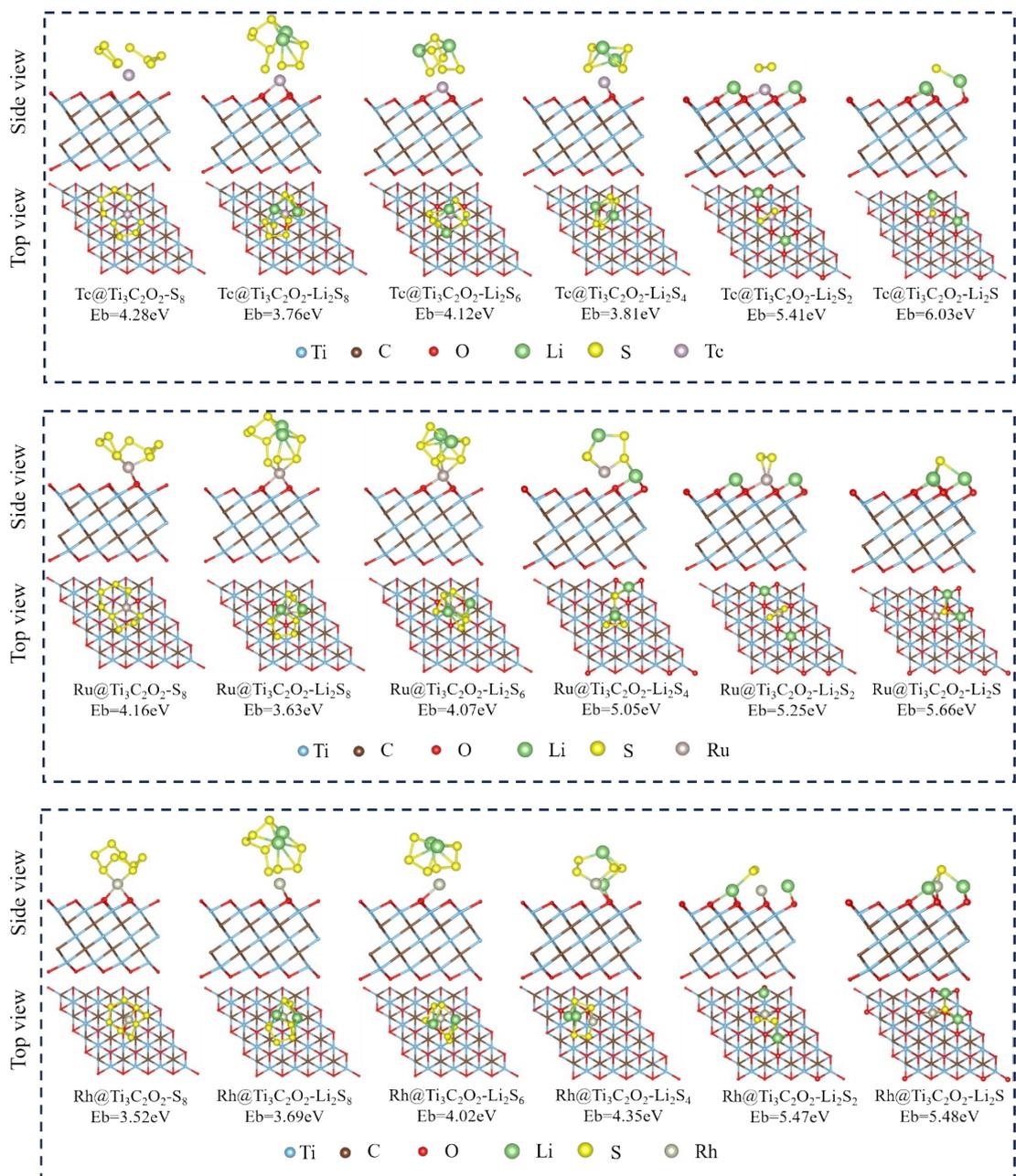
FigureS5. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Fe}@\text{Ti}_3\text{C}_2\text{O}_2$, $\text{Co}@\text{Ti}_3\text{C}_2\text{O}_2$ and $\text{Ni}@\text{Ti}_3\text{C}_2\text{O}_2$ nanosheets.



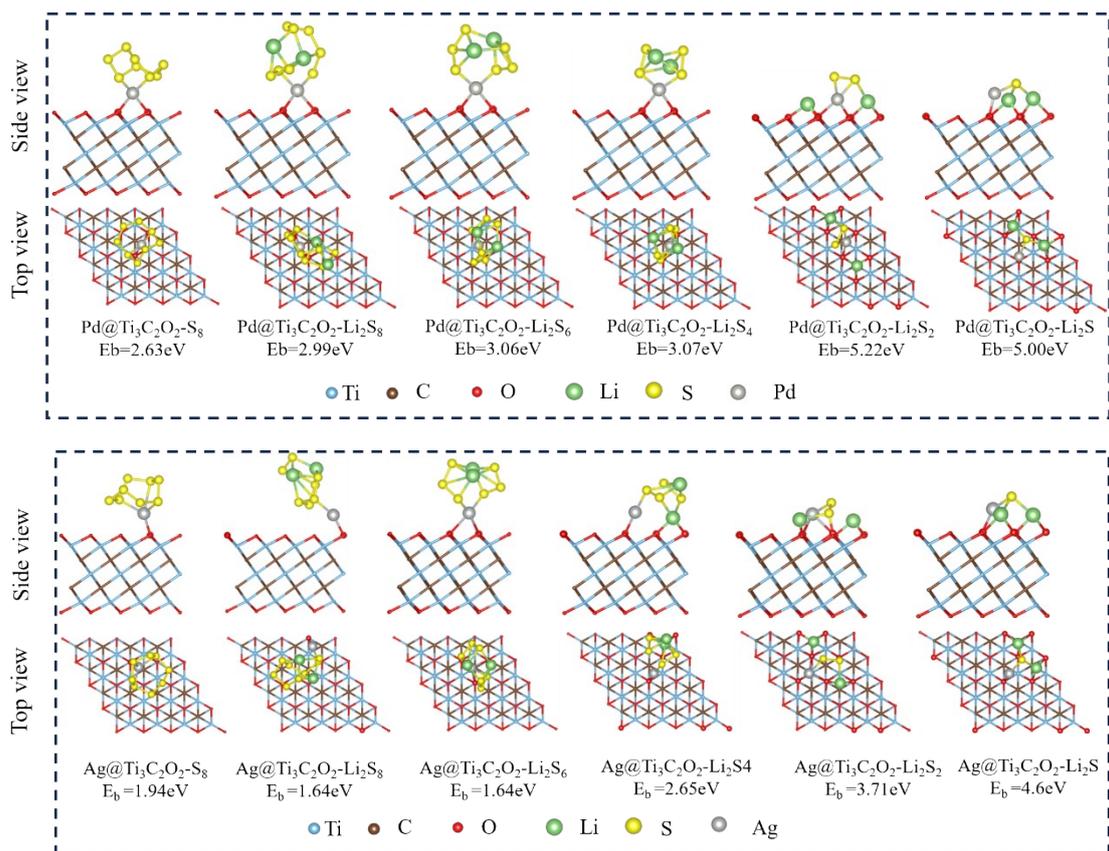
FigureS6. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Cu}@\text{Ti}_3\text{C}_2\text{O}_2$, $\text{Zn}@\text{Ti}_3\text{C}_2\text{O}_2$ and $\text{Y}@\text{Ti}_3\text{C}_2\text{O}_2$ nanosheets.



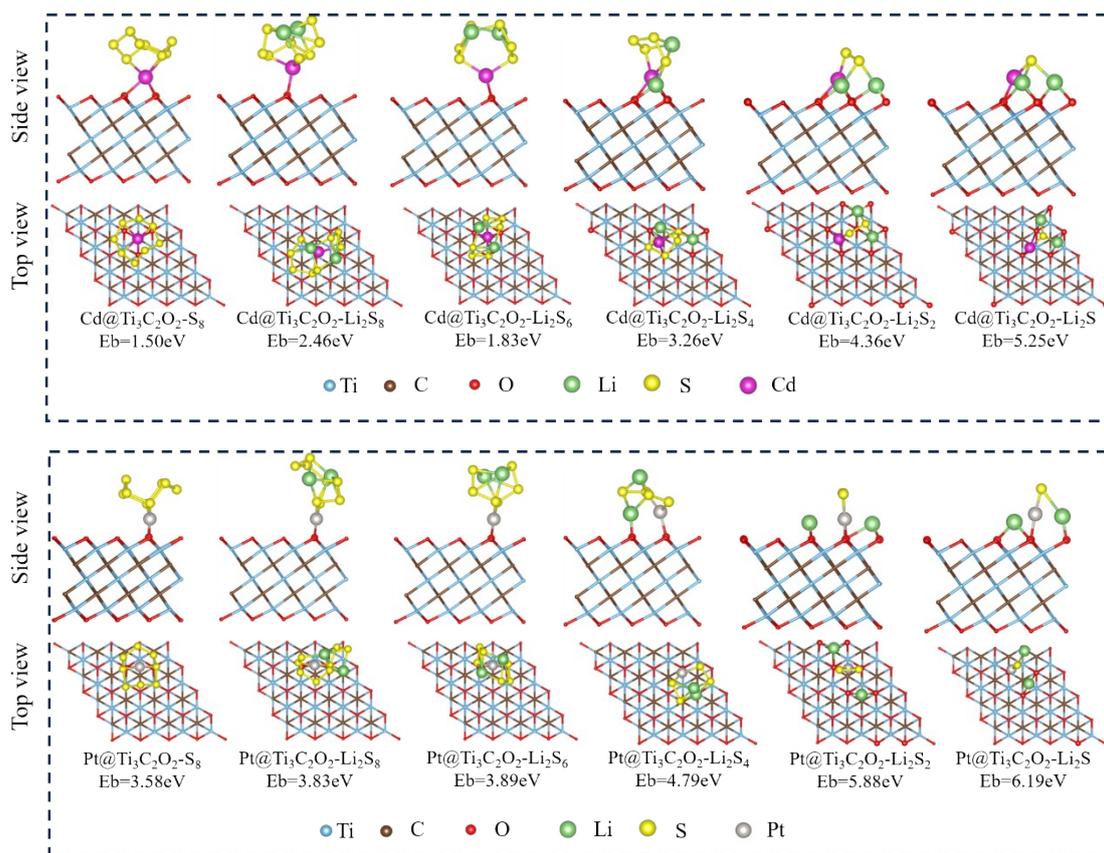
FigureS7. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Zr@Ti}_3\text{C}_2\text{O}_2$, $\text{Nb@Ti}_3\text{C}_2\text{O}_2$ and $\text{Mo@Ti}_3\text{C}_2\text{O}_2$ nanosheets.



FigureS8. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Tc@Ti}_3\text{C}_2\text{O}_2$, $\text{Ru@Ti}_3\text{C}_2\text{O}_2$ and $\text{Rh@Ti}_3\text{C}_2\text{O}_2$ nanosheets.



FigureS9. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Pd@Ti}_3\text{C}_2\text{O}_2$ and $\text{Ag@Ti}_3\text{C}_2\text{O}_2$ nanosheets.



FigureS10. Binding structures and E_b values of $\text{Li}_2\text{S}_n/\text{S}_8$ species on $\text{Cd@Ti}_3\text{C}_2\text{O}_2$ and $\text{Pt@Ti}_3\text{C}_2\text{O}_2$ nanosheets.

Table S1 Relative energies of the three sites Ti₃C₂O₂ phases (eV)

Site	α	β	γ
Energy	0.88	1.33	0

TableS2. Performance comparison between SM@Mxene catalyst and the catalysts mentioned in the literature

Catalyst	Binding energy (Li ₂ Sn)	ΔG_{PDS}	Year	Ref
Sc@Ti ₃ C ₂ O ₂	2.46-3.79eV	0.53	-	This Work
V ₂ NS ₂	5.05-6.8eV	0.49eV	2021	1
S@F-MXene	1.1-1.3eV	0.65eV	2023	2
SA-Zn-MXene	1.2-1.5eV	0.71eV	2020	3
HE-MXene	14.04-20.82eV	6.94eV	2024	4
VO ₂ -V ₂ CO ₂	-	0.69eV	2019	5
CoNPs@MXene	4.5eV	9.65eV	2022	6

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