Supporting Information

Transfer Learning–Enabled Discovery of MXene Anchors for Advanced Li–S Batteries

Jianqiang, Wang, Haiyuan Chen, Yin Hu, and Xiaobin Niu*.*

School of Materials and Energy, University of Electronic Science and Technology of China, Chengdu 611731, P.R. China

*Corresponding authors: hychen@uestc.edu.cn; xbniu@uestc.edu.cn

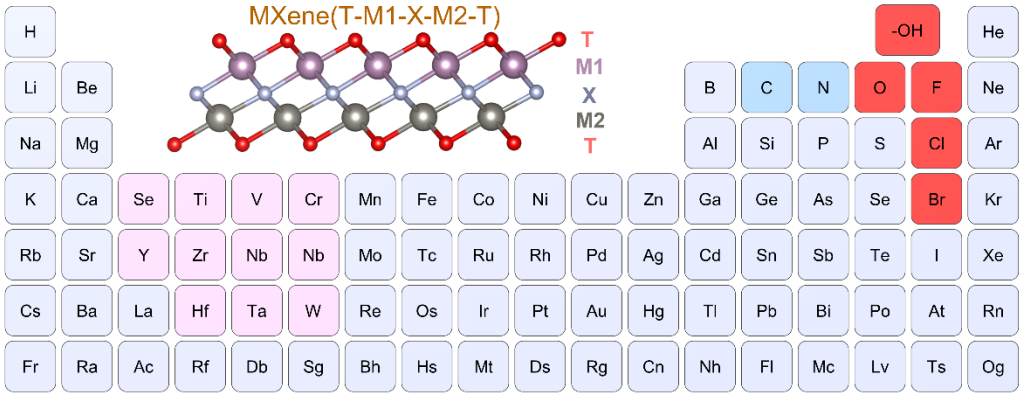

Figure S1. General representation of the MXene structure in this study, along with the constituent elements and functional groups.

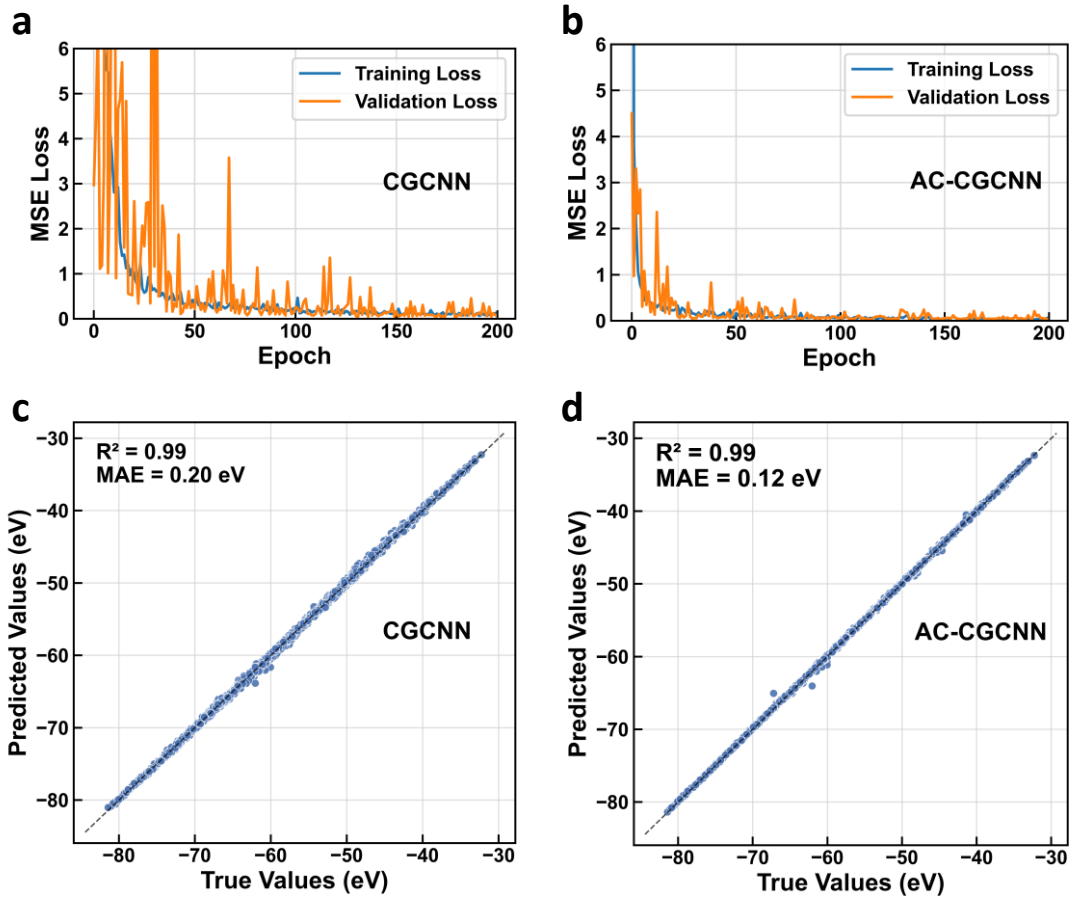

Figure S2. Training/validation MSE of the pretrained (a) CGCNN, (b) AC-CGCNN and the scatter plots of predicted versus true values on the source domain test set: (c) CGCNN, (d) AC-CGCNN.

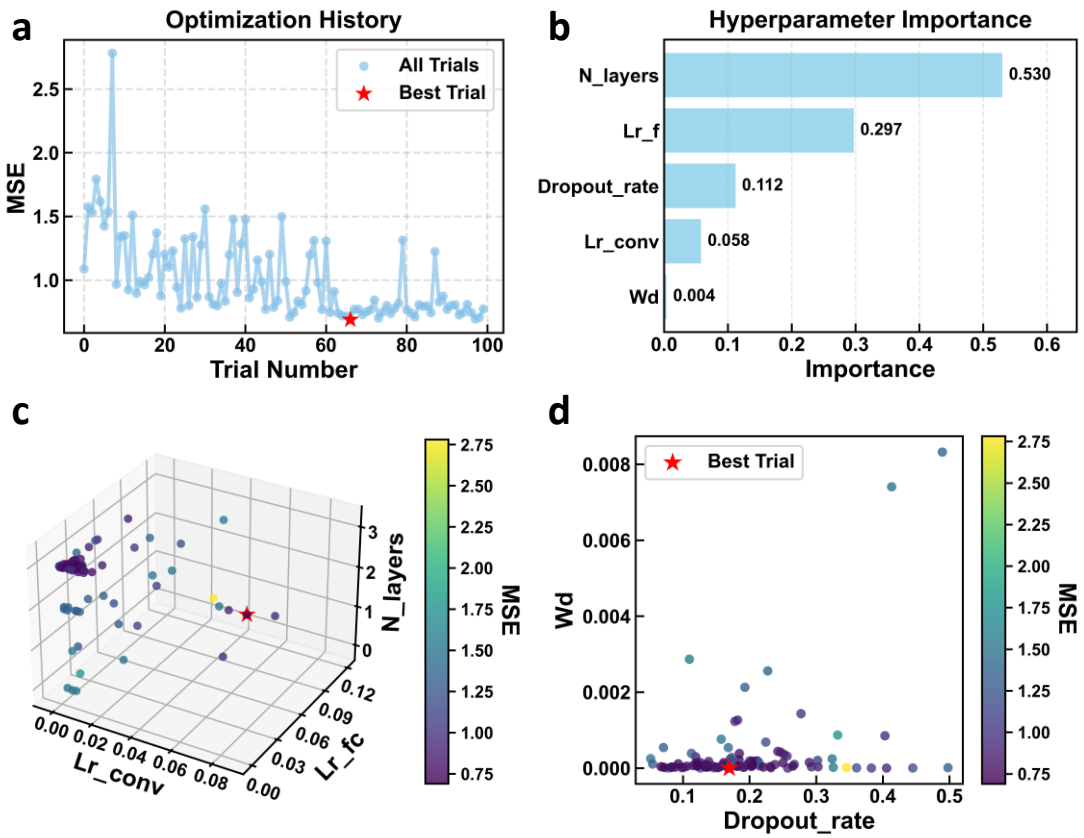

Figure S3. Hyperparameter optimization of CGCNN-TF using Optuna. (a) represent the optimization history, (b) represent the importance of hyperparameters. (c) (d)represent the impact of different hyperparameter combinations on the MSE.

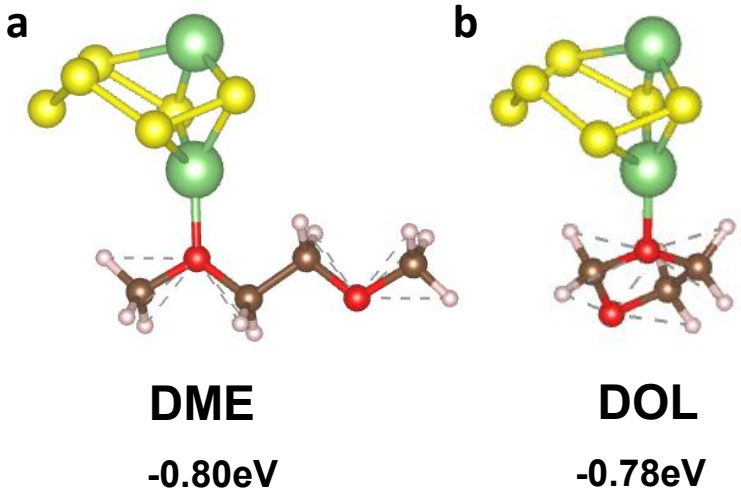

Figure S4. The optimized geometry structures Li_2S_6 attached to (a) DME and (b) DOL.

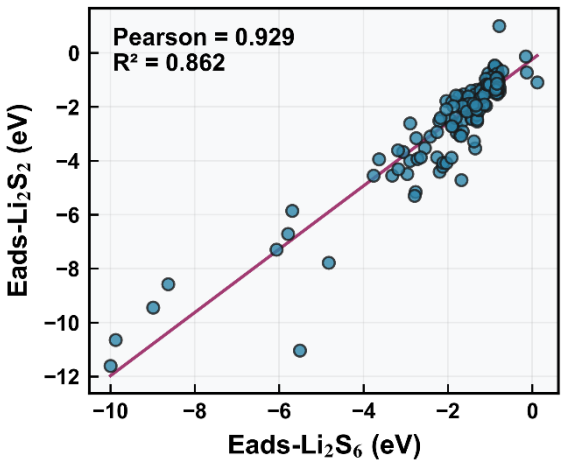

Figure S5. Li_2S_2 vs. Li_2S_6 Adsorption Energy Correlation.

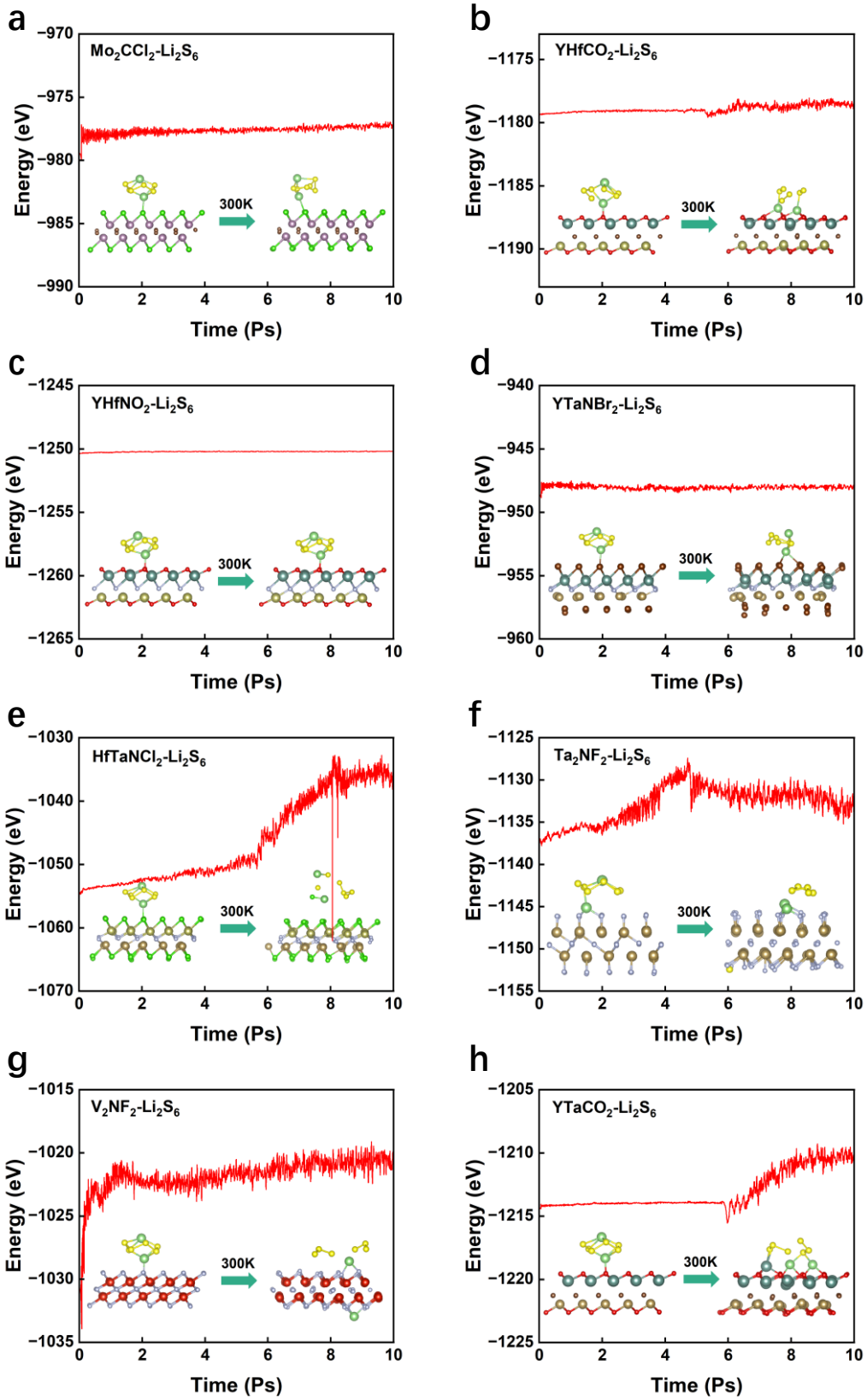

Figure S6. The adsorption energies and the energetic trajectories of (a) Mo_2CCl_2, (b)$YHfCO_2$, (c)$YHfNO_2$, (d)$YTaNBr_2$, (e)$HfTaNCl_2$, (f) Ta_2NF_2, (g)V_2NF_2, (h)$YTaCO_2$ under 300K AIMD simulations.

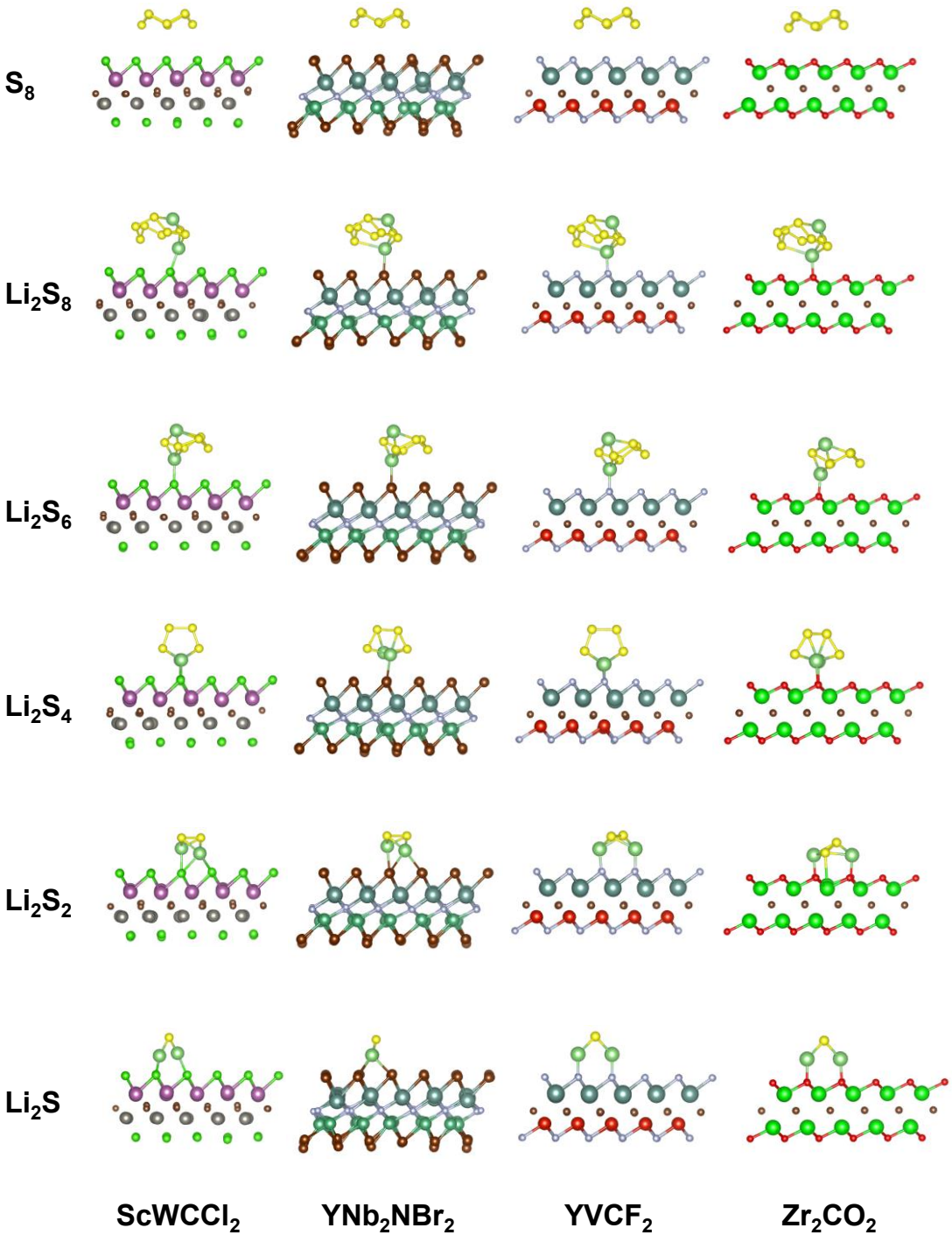

Figure S7. The optimized adsorption configurations for each stage of the sulfur reduction process.

Table S1. The atomic features of AC-CGCNN. The first nine features are the original features of CGCNN, and the last are additional features added in this work.

Features	Properties
Group number	Group in the periodic table
Period	Period in the periodic table
Electron negativity	Tendency of an atom to attract a shared pair of electrons
Covalent radius	Covalent radius by Cerdero et al
Num valence	Total valance electron
First ionization energy	First ionization energy
Electron affinity	Electron affinity
Block	Orbital type of valence electrons
Atomic volume	Atomic volume
Atomic number	Number of elements in the periodic table
Atomic radius	Atomic radius
Atomic radius rahm	Atomic radius by Rahm et al.
Atomic weight	The mass of an atom
Covalent radius pyykko	Single bond covalent radius by Pyykko et al
Covalent radius pyykko double	Double bond covalent radius by Pyykko et al
Covalent radius pyykko triple	Triple bond covalent radius by Pyykko et al
Covalent radius slater	Covalent radius by Slater
c6 gb	C_6 dispersion coefficient in a.u
Dipole polarizability	Dipole polarizability
En allen	Allen's scale of electronegativity
En ghosh	Ghosh's scale of electronegativity
En pauling	Pauling's scale of elect
Gs energy	DFT energy per atom of T=0K ground state
Gs mag moment	DFT magnetic moment of T=0K ground stat
Lattice constant	Geometric parameters describing the size of crystal cells
Mendeleev number	Atom number in mendeleev's periodic table
Num d unfilled	Unfilled electron in d shell
Num d valence	Valance electron in d shell

Num f unfilled	Unfilled electron in f shell
Num f valence	Valance electron in f shell
Num p unfilled	Unfilled electron in p shell
Num p valence	Valance electron in p shell
Num s unfilled	Unfilled electron in s shell
Num s valence	Valance electron in s shell
Num unfilled	Total unfilled electron
Polarizability	Ability to form instantaneous dipoles
Vdw radius	Van der Waals radius
Vdw radius alvarez	Van der Waals radius according to Alvarez
Vdw radius mm3	Van der Waals radius from the MM3 FF
Vdw radius uff	Van der Waals radius from the UFF

Table S2. The final hyperparameters of all models.

	Hyperparameters	Value
AC-CGCNN-TL	Random State	52
	Hidden layers	2
	Reduction (CAM)	8
	Neighbor cutoff radius	8
	Hidden dim	64
	Optimizer for loss function	Adam
	Learning rate of convolutional layers	0.0012474106337272935
	Learning rate of fully connectional layers	0.00010419095601850053
	Weight decay of convolutional layers	0.000003181884094823365
	Weight decay of fully connectional layers	0.00012592886717206712
CGCNN-TL	Random State	52
	Hidden layers	2
	Neighbor cutoff radius	8
	Hidden dim	64
	Optimizer for loss function Adam	Adam
	Dropout rate	0.169487963059955
	Learning rate of convolutional layers	0.08861266707265483
	Learning rate of fully connectional layers	0.007313400053340794
	Weight decay of all layers	2.722900198584351e-06
AC-CGCNN	Random State	52
	Hidden layers	2
	Reduction (CAM)	8

	Neighbor cutoff radius	8
	Hidden dim	64
	Optimizer for loss function	Adam
	Learning rate	0.001
CGCNN	Random State	52
	Hidden layers	1
	Neighbor cutoff radius	8
	Hidden dim	64
	Optimizer for loss function Adam	Adam
	Learning rate	0.001

Table S3. Feature Grouping Scheme.

Group	Features	Description
Periodic Position	Atomic_number, Group number, Period, Block, Mendeleev_number	Basic positioning of elements in the periodic table
Electronic Configuration	Num_valence, Num_unfilled, Num_s_valence, Num_p_valence, Num_d_valence, Num_f_valence, Num_s_unfilled, Num_p_unfilled, Num_d_unfilled, Num_f_unfilled	Distribution and filling state of electrons in atomic orbitals
Electronic Energy	Electron_negativity, En_allen, En_ghosh, En_pauling, First_ion_en, Electron_affinity, Gs_energy	Energy changes during electron transfer, removal, or addition
Atomic Size	Atomic_radius, Atomic_radius_rahm, Atomic_volume, Lattice_constant	Geometric dimensions of atoms
Radius	covalent_radius_cordero, covalent_radius_pyykko, covalent_radius_pyykko_double, covalent_radius_pyykko_triple, covalent_radius_slater, vdw_radius, vdw_radius_alvarez, vdw_radius_mm3, vdw_radius_uff	Effective interaction distances for chemical bonding or physical adsorption
Physical Properties	dipole_polarizability, Polarizability, atomic_weight, c6_gb, gs_mag_moment	Response characteristics to external fields and intrinsic physical attributes

Table S4. The 8 random state used to evaluate the robustness of the model.

cases	Random state
1	2
2	12
3	31
4	39
5	52
6	56
7	128
8	161

Table S5. Comparison of Key Descriptors for MXene and Related Catalysts.

MXene	E_{ads}-Li_2S_6 (eV)	RDS	RDS Barrier(eV)	Reference
$YNbNBr_2$	-1.89	$Li_2S_4 \rightarrow Li_2S_2$	0.65	This work
$ScWCCl_2$	-2.41	$Li_2S_2 \rightarrow Li_2S$	0.84	This work
Mo_2CF_2	-1.06	$Li_2S_4 \rightarrow Li_2S_2$	0.55	Zhu et al.[22]
V_2CF_2	-0.91	$Li_2S_4 \rightarrow Li_2S_2$	0.44	Zhu et al.[22]
V_2CO_2	-2.02	$Li_2S_2 \rightarrow Li_2S$	0.89	Wu et al.[54]
Mo_2CO_2	-3.13	$Li_2S_2 \rightarrow Li_2S$	1.25	Niu et al.[54]
δ-B-Mo_2C	-4.395	$Li_2S_2 \rightarrow Li_2S$	0.587	Chen et al.[55]