Electronic supplementary information

Universal Screening Strategy for Accelerated Design of Superior Oxygen Evolution/Reduction Electrocatalysts

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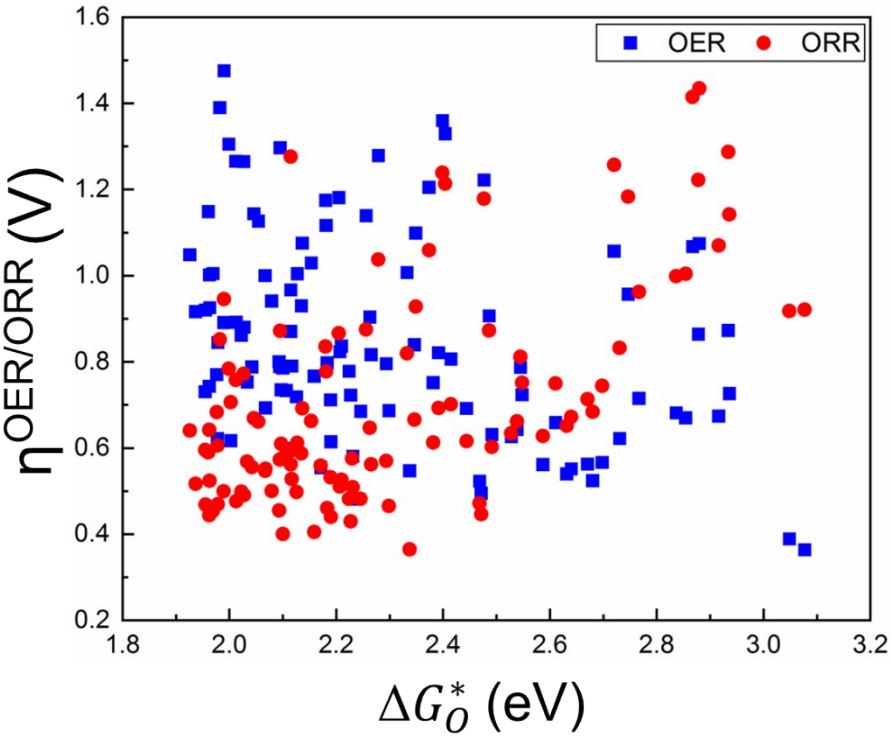

Fig. S1. Correlation between reaction free energy of O* ($^{\Delta G^*_O}$) and theoretical overpotentials (OER and ORR). The data points do not show clear summit of volcano plot between $^{\Delta G^*_O}$ and catalytic activity, forbidding $^{\Delta G_O}$-based prediction. The data points are from **Table S7.**

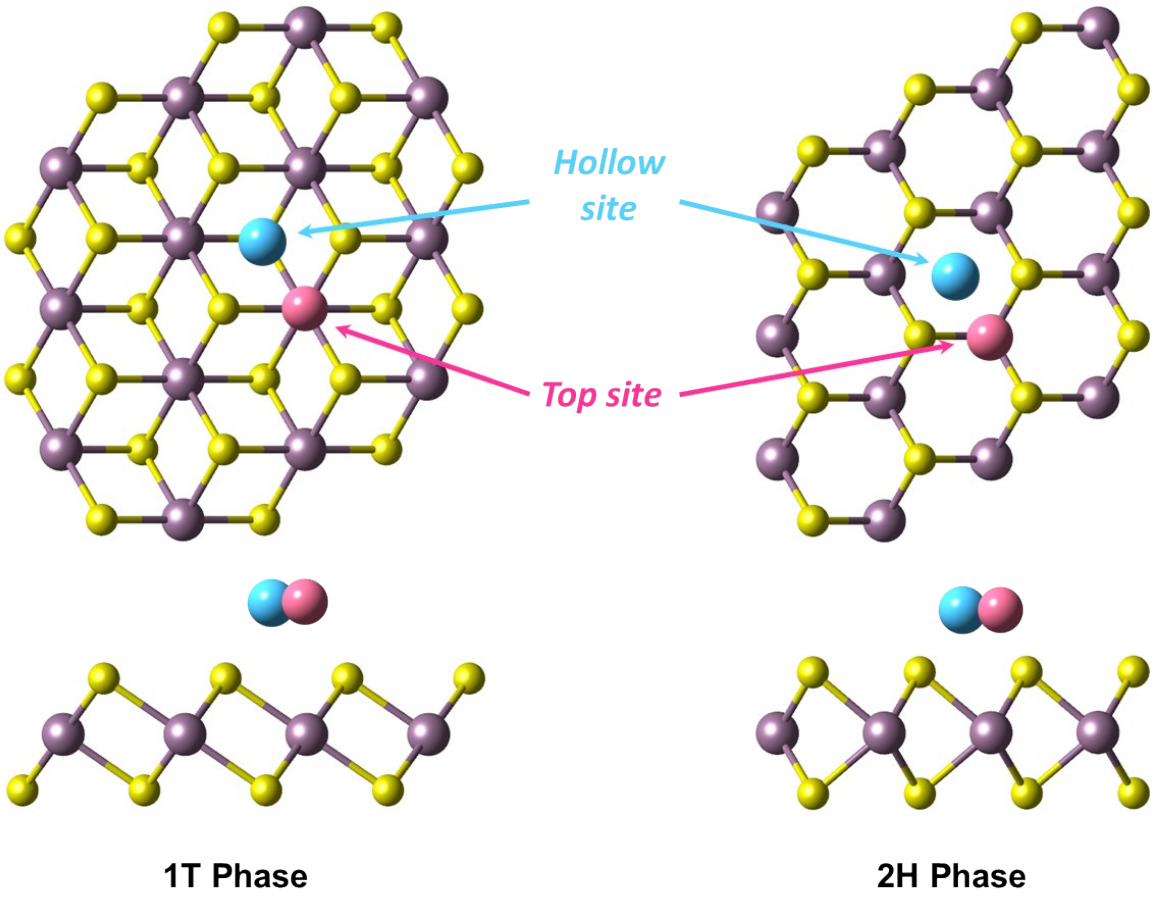

Fig. S2. Top and side views of the single atom anchoring site on the transition metal dichalcogenide (purple: metal, yellow: chalcogen).

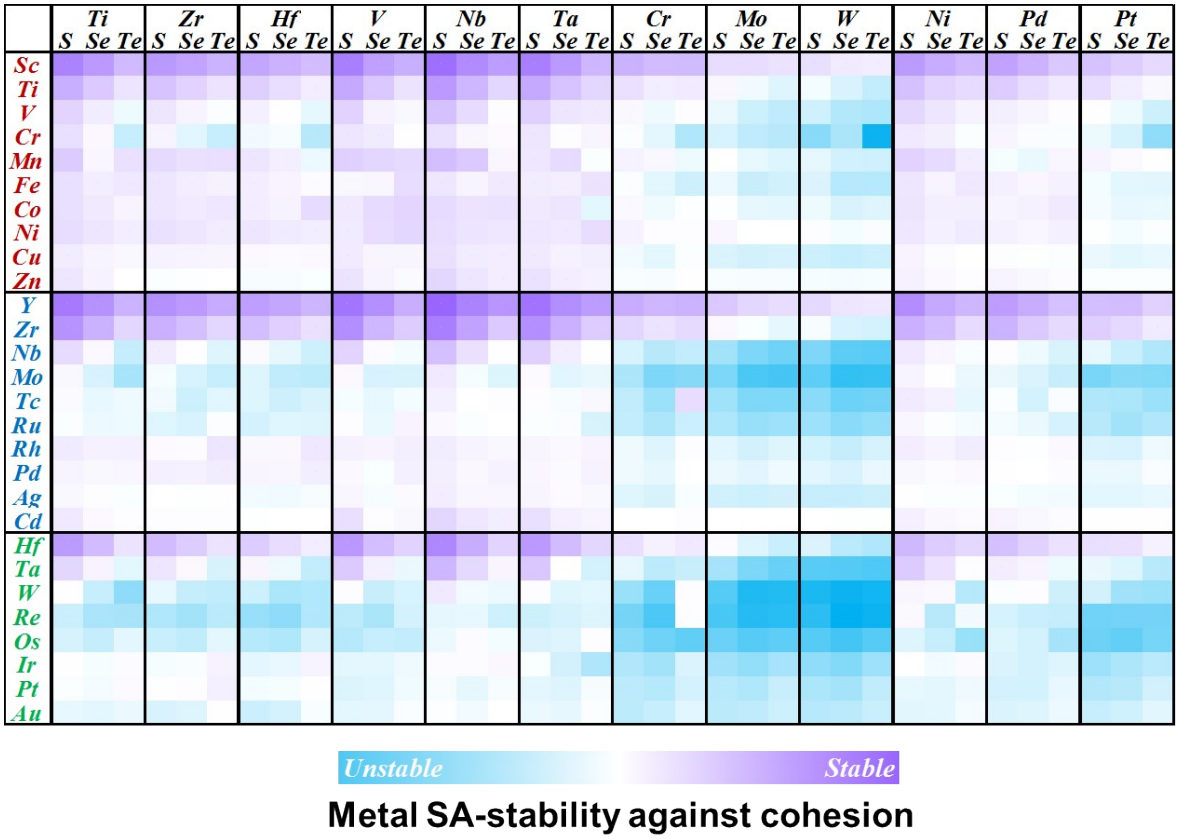

Fig. S3. Color-map for metal SA-stability against cohesion (E_b−E_{coh}) for various SA-anchored transition metal dichalcogenides (SA@MX_2). The metal SA-stability against cohesion is the difference of the binding energy of the SA on MX_2 (E_b) from the cohesive energy of metal (E_{coh}). The stronger purple regions indicate that their SA@MX_2 have higher stability over the metal aggregation.

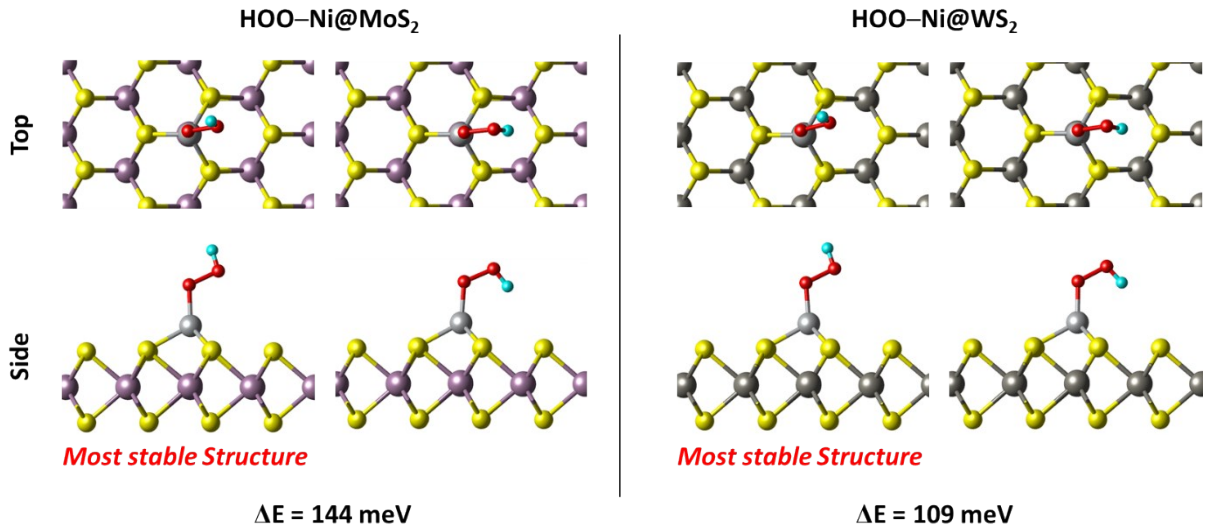

Fig. S4. Adsorption energy change (ΔE) depending on configurations of OOH in Ni@MoS_2/WS_2. These models are chosen not only because they have survived from the 2nd screening but also because they are one of the popular TMDs (Mo: purple, W: dark gray, S: yellow, Ni: silver, O: red, H: cyan).

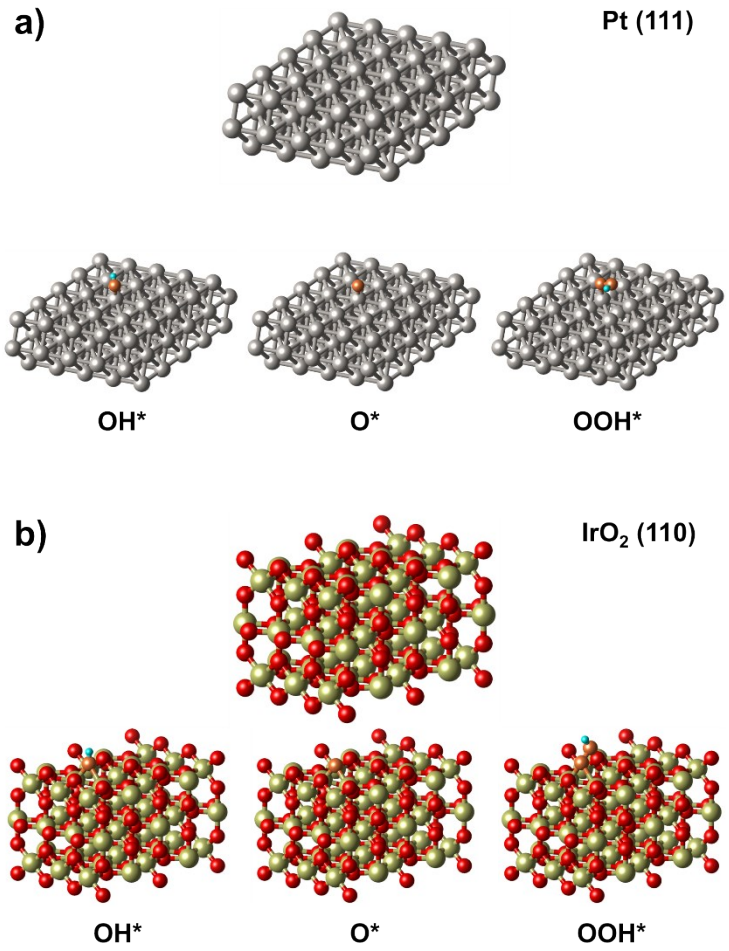

Fig. S5. Optimized geometries of Pt (111) and IrO2 (110) surfaces and their reaction intermediates (Pt: silver, Ir: dark-yellow, O in IrO_2: red, O in H_2O: orange, H: cyan).

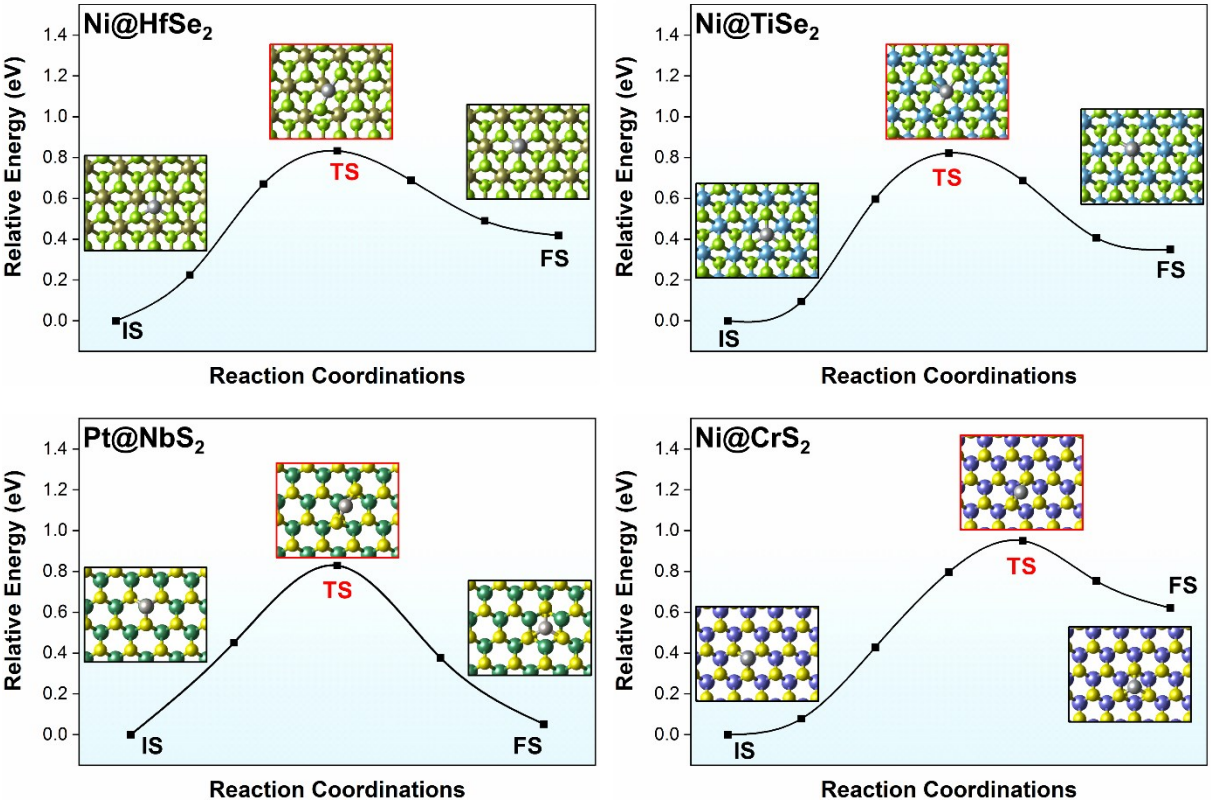

Fig. S6. Reaction pathways for $Ni@HfSe_2$, $Ni@TiSe_2$, $Pt@NbS_2$, and $Ni@CrS_2$, where a metal single atom migrates to a neighboring site [IS: initial state, TS: transition state, FS: final state].

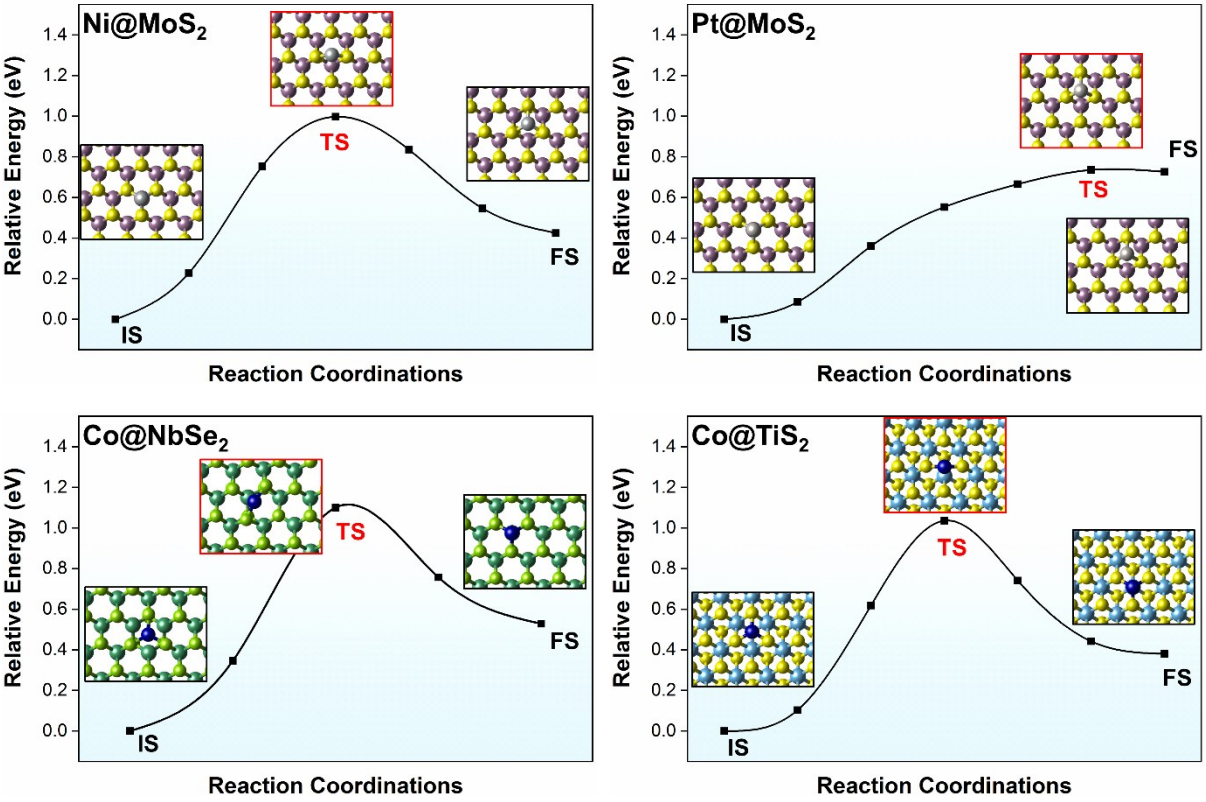

Fig. S7. Reaction pathways for Ni@MoS_2, Pt@MoS_2, Co@$NbSe_2$, and Co@TiS_2, where a metal single atom migrates to a neighboring site [IS: initial state, TS: transition state, FS: final state].

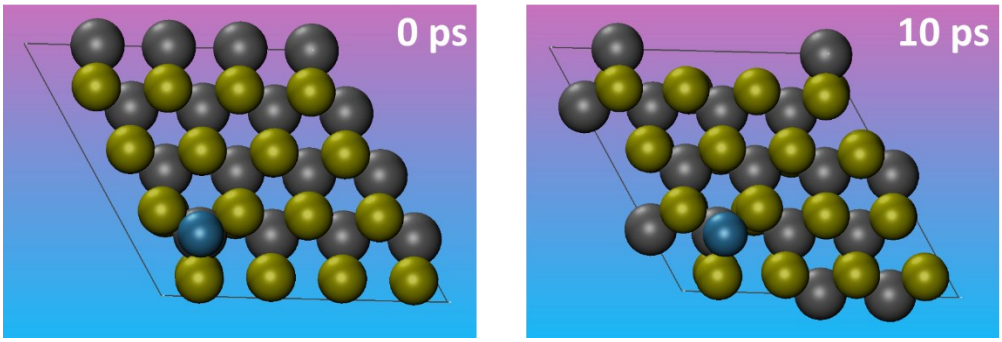

Fig. S8. Snapshot for initial and final configurations of Pt@MoS_2. The a*b-initio* molecular dynamics simulation was performed at 298K for 10 ps with a 2.5fs timestep.

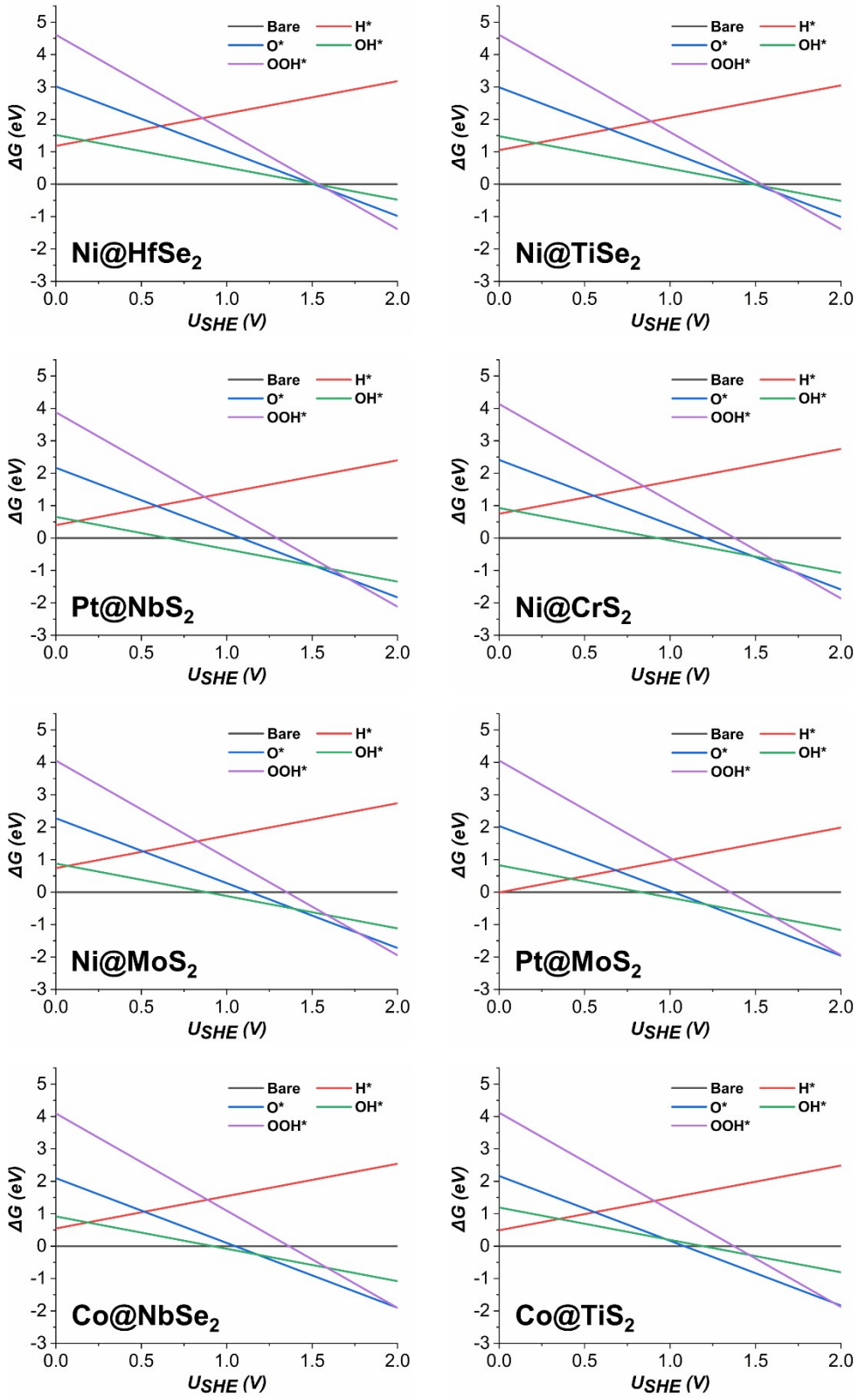

Fig. S9. Plot of reaction free energies for promising SA@MX_2 at pH=0 with respect to the theoretical standard hydrogen electrode potential (U_{SHE}).

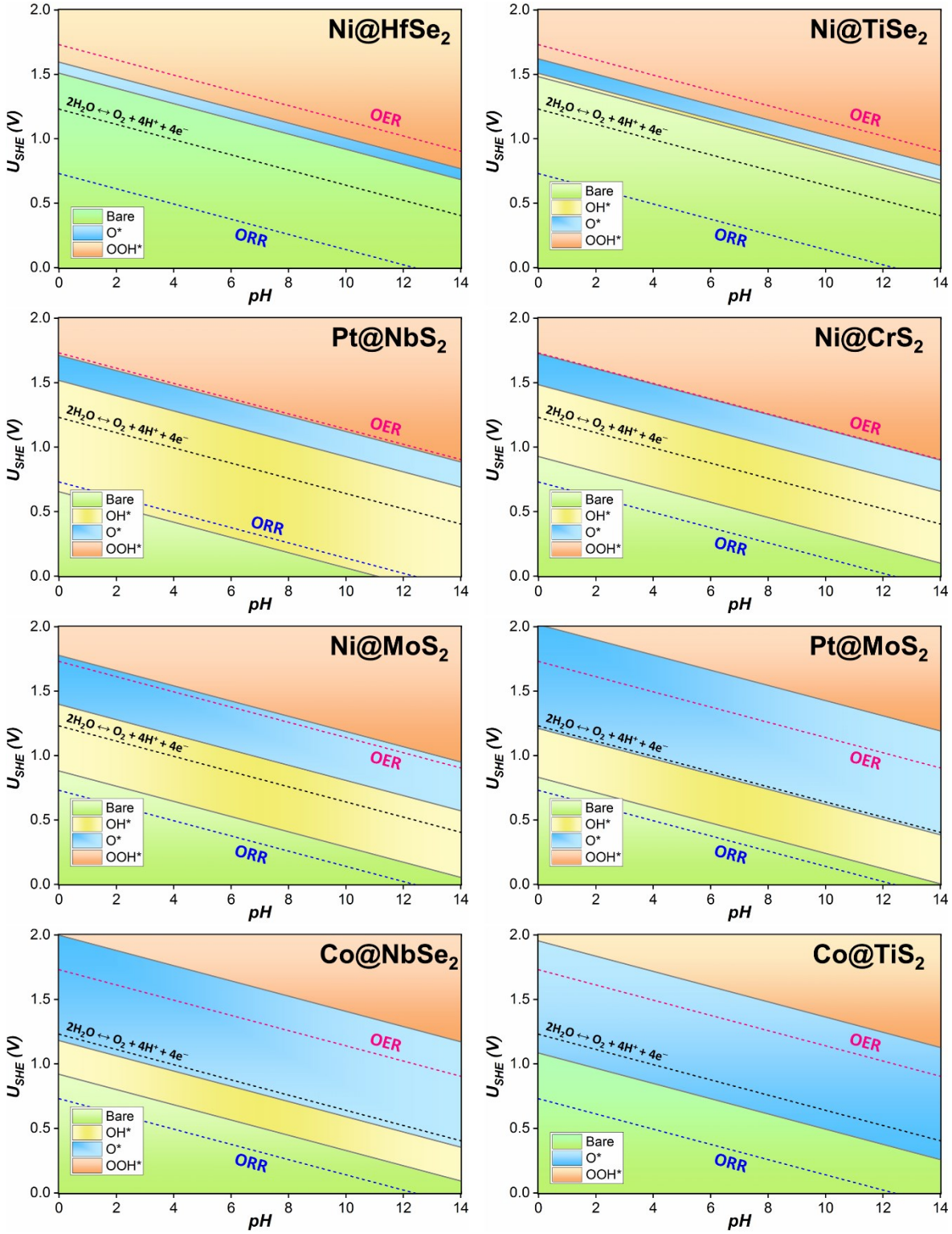

Fig. S10. Surface Pourbaix diagram for promising SA@MX_2. The black dashed line denotes OER/ORR at equilibrium (U_{eq} = 1.23 V – 0.059 pH). The pink and blue dashed lines represent the oxidizing state for OER and ORR, respectively, at an overpotential 0.5 V. Gray solid line denotes the phase boundary of two oxidizing states.

Table S1. Structural phases (*1T* and *2H*) of the various transition metal dichalcogenides studied here.[a]

Group 4			*Group 5*			*Group 6*			*Group 10*		
TiS_2	**$TiSe_2$**	**$TiTe_2$**	**VS_2**	**VSe_2**	**VTe_2**	**CrS_2**	**$CrSe_2$**	**$CrTe_2$**	**NiS_2**	**$NiSe_2$**	**$NiTe_2$**
1T	*1T*	*1T*	*2H*	*1T*	*1T*	*2H*	*2H*	*2H*	*1T*	*1T*	*1T*
ZrS_2	**$ZrSe_2$**	**$ZrTe_2$**	**NbS_2**	**$NbSe_2$**	**$NbTe_2$**	**MoS_2**	**$MoSe_2$**	**$MoTe_2$**	**PdS_2**	**$PdSe_2$**	**$PdTe_2$**
1T	*1T*	*1T*	*2H*	*2H*	*2H*	*2H*	*2H*	*2H*	*1T*	*1T*	*1T*
HfS_2	**$HfSe_2$**	**$HfTe_2$**	**TaS_2**	**$TaSe_2$**	**$TaTe_2$**	**WS_2**	**WSe_2**	**WTe_2**	**PtS_2**	**$PtSe_2$**	**$PtTe_2$**
1T	*1T*	*1T*	*2H*	*2H*	*2H*	*2H*	*2H*	*2H*	*1T*	*1T*	*1T*

[a]Vanadium dichalcogenides (VS_2, VSe_2, and VTe_2) are ferromagnetic, whereas $CrTe_2$ is anti-ferromagnetic.

Table S2. The most stable single atom anchoring site on the transition metal dichalcogenides (MX_2) (*h*: hollow site and *t*: top site). The asterisk (*h** or *t**) means that the other anchoring site is not stable.

M	Ti			Zr			Hf			V			Nb			Ta			Cr			Mo			W			Ni			Pd			Pt		
X_2	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te
P[a]	T	T	T	T	T	T	T	T	T	H	T	T	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	T	T	T	T	T	T	T	T	T
Sc	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*t*	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*t*	*h**	*t*	*h*	*h*	*h*	*h*
Ti	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*t**	*h*	*h*	*h*	*t*	*h*	*h*
V	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*t*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*
Cr	*t*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*t*
Mn	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*t*	*h*	*h*	*t*	*t*	*t*	*h*	*t*	*t*	*t*	*t**	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*t*	*h*	*t*	*h*	*h*	*h*	*h*
Fe	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t**	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*t*	*h*	*t*	*h*	*h*	*t*	*t*	*h*
Co	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h**	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*h*	*t*	*t*	*t*
Ni	*h*	*h*	*t*	*h*	*h*	*t**	*h*	*h*	*t**	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t**	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*t*	*t*	*t*
Cu	*h*	*h*	*t**	*h*	*h*	*t**	*h*	*h*	*t**	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h**	*h*	*t*	*t*	*h*	*t*	*t*
Zn	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*
Y	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*t*	*h*	*h*	*t*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*t*	*h**	*t*	*h*	*h*	*t*	*t*
Zr	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*h*	*h**	*h*	*h*	*t*	*h*	*h*
Nb	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*t**	*h**	*h*	*h*	*t*	*h**	*t*
Mo	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t**	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h**	*t*	*t*
Tc	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*t*	*h*	*t*	*h*	*t*	*h*	*t**
Ru	*t*	*h*	*h*	*t*	*t*	*h*	*t*	*h*	*t*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*t*	*t*	*t*	*t*
Rh	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*
Pd	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h**	*t*	*t*	*t*	*t*	*t*	*t*
Ag	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t**	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*
Cd	*h*	*h*	*h*	*h*	*h*	*h*	*t**	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*t*	*t*	*t**	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*h*	*h*	*h**	*h*	*h*	*h*	*h*	*h*	*h*
Hf	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*t**	*t*	*t*	*t**	*t*	*t*	*h*	*h*	*t**	*h**	*h**	*t**	*h*	*h*	*h*
Ta	*t*	*t*	*h*	*h*	*h*	*t*	*h*	*h*	*t*	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*t*	*t*	*t*	*t*	*t**	*t*	*t*	*t*	*t*	*t*	*t*	*t**	*t**	*t**	*h**	*h**	*t**	*h**	*h*	*t**
W	*h*	*h*	*t*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*h*	*t*	*h*	*t*	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t**	*h*	*t**	*h*	*t*	*h*	*t*	*h**	*h*
Re	*h*	*h**	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*h*	*h*	*t*	*h**	*t*	*t*	*h*	*t**	*t*	*t*	*t*	*t*	*t*	*h*	*t**	*h*	*h*	*h*	*h*	*h**	*h*	*h*
Os	*h*	*h**	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t**	*h*	*t*	*h**	*h*	*h*	*h**	*t*	*t*	*h**	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h**	*h*	*h*	*t*	*t*	*t*	*t*
Ir	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t*	*t*	*t*	*h*	*h*	*t*	*h*	*t*	*h**	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*
Pt	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*t**	*t*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*h**	*t*	*t*	*t*	*t*	*t*	*t*

Au	*t*	*t*	*t*	*t**	*t**	*h*	*t*	*h*	*h*	*t*	*t*	*t*	*t*	*t*	*t*	*t*	*t**	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*	*h*

[a]*P* means the structure phase of transition metal dichalcogenides (T : 1T phase and H : 2H phase).

Table S3. Binding energies (E_b in eV) of single atoms (SA) on the transition metal dichalcogenides (MX_2).[a] All values are positive, indicating that metal single atoms can be favorably anchored on the basal plane of transition metal dichalcogenides.

M	Ti			Zr			Hf			V			Nb			Ta			Cr			Mo			W			Ni			Pd			Pt		
X_2	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te	S	Se	Te
Sc	9.4	8.2	6.6	8.2	7.7	6.9	7.5	7.0	6.4	9.5	7.9	7.1	10.	8.8	8.0	9.6	8.2	6.7	7.0	6.4	6.5	4.8	4.8	4.5	4.7	4.1	3.9	8.1	7.2	6.6	7.7	6.8	5.8	6.1	5.6	4.9
Ti	8.1	6.8	5.3	7.0	6.3	5.4	6.4	5.7	4.9	8.4	6.8	5.4	9.2	7.6	6.1	8.4	7.1	6.1	5.5	4.9	5.0	4.4	3.7	3.3	3.7	3.1	2.6	7.1	6.2	5.8	6.6	5.7	5.1	5.7	4.9	4.4
V	6.6	5.5	4.1	5.8	5.1	4.4	5.2	4.5	3.9	6.7	5.1	4.8	7.6	6.3	4.6	6.9	5.8	5.6	4.9	4.1	4.7	4.0	3.3	3.0	3.4	2.7	2.6	6.4	5.7	5.1	5.3	5.0	4.6	4.5	4.1	3.3
Cr	4.9	3.7	2.0	3.9	2.6	1.9	3.0	3.1	1.6	4.5	4.3	3.4	4.8	3.7	3.5	4.6	3.4	3.8	3.2	2.7	1.4	2.3	1.8	1.6	0.5	1.3	-2.5	4.4	4.1	3.2	3.8	3.1	3.1	2.8	2.3	0.7
Mn	4.7	2.5	3.6	4.0	3.6	3.7	3.4	2.9	1.7	4.5	4.1	3.9	5.3	4.8	2.6	3.3	3.9	2.0	2.8	2.4	1.7	2.1	1.5	1.3	1.5	1.0	1.0	4.4	3.9	2.9	1.9	1.6	2.5	2.7	2.4	2.1
Fe	5.1	4.3	4.6	4.8	4.4	4.2	4.4	4.0	3.7	3.8	3.9	5.2	4.7	4.0	4.5	4.4	4.3	4.8	3.4	2.8	2.3	3.0	2.2	2.4	2.6	1.7	1.7	4.7	4.1	4.6	4.2	3.9	4.1	3.2	2.8	2.8
Co	5.2	4.6	4.2	4.8	4.5	4.8	4.5	4.2	5.3	4.6	5.4	5.7	5.4	4.9	5.0	4.6	4.8	2.9	3.9	3.2	3.5	3.5	3.0	2.9	3.2	2.7	2.8	4.9	4.4	4.4	4.2	4.2	4.6	3.3	3.0	3.1
Ni	5.4	5.0	4.5	5.2	5.0	4.6	4.9	4.7	4.5	4.7	5.4	5.7	5.4	5.0	4.9	4.9	4.8	5.4	4.3	3.8	3.8	4.1	3.7	3.7	3.8	3.4	3.5	4.9	4.4	4.7	4.4	4.1	4.4	3.6	3.4	3.6
Cu	3.6	3.3	3.1	3.3	3.3	3.2	3.0	2.9	3.0	3.7	3.2	3.2	4.2	3.6	3.6	3.7	3.4	3.5	2.4	2.0	2.6	1.8	1.6	1.7	1.5	1.3	1.5	3.2	2.9	2.7	2.8	2.6	2.6	2.2	2.0	2.1
Zn	1.8	1.2	0.5	0.5	0.5	0.5	0.4	0.4	0.4	1.9	1.1	0.8	2.5	1.8	1.4	2.0	1.4	1.2	0.4	0.3	0.6	0.4	0.3	0.3	0.3	0.3	0.3	1.2	0.8	0.7	1.1	0.9	0.7	0.4	0.4	0.4
Y	10.	9.0	7.4	9.1	8.6	7.8	8.4	8.0	7.3	10.	9.2	7.6	11.	9.8	8.9	11.	9.2	8.5	7.7	7.2	7.4	6.3	5.6	5.3	5.5	4.8	4.7	9.3	7.9	7.2	8.5	7.7	6.7	6.8	6.8	5.9
Zr	11.	9.3	7.5	9.4	8.6	7.5	8.6	7.8	6.9	11.	9.0	8.0	12.	10	8.1	11.	9.4	8.0	7.5	6.9	7.3	5.7	5.3	4.9	5.3	4.5	4.4	9.4	8.7	7.2	9.2	8.1	7.3	7.8	7.4	6.5
Nb	8.6	7.1	5.4	7.7	6.8	6.0	7.0	6.2	5.6	8.9	7.0	6.5	9.9	8.2	6.8	9.1	7.6	6.8	5.8	5.1	5.3	4.6	3.7	3.3	3.7	2.9	2.8	7.9	7.2	6.6	6.9	6.3	5.9	6.2	5.5	4.9
Mo	6.4	5.1	4.0	5.8	5.0	4.6	5.2	4.5	4.4	6.3	5.1	5.1	7.1	5.8	5.2	6.2	5.3	5.5	4.0	2.9	3.1	2.9	1.7	1.6	2.2	1.1	1.2	6.6	6.0	5.5	5.5	5.1	4.7	2.8	3.2	3.0
Tc	6.3	5.5	5.6	5.7	4.8	5.3	5.2	4.9	5.1	5.8	5.5	5.8	6.8	6.0	6.2	6.2	5.9	6.4	4.6	3.7	7.7	3.8	3.0	3.0	3.2	2.6	2.7	7.0	6.7	5.4	5.9	5.0	5.9	4.2	4.1	3.7
Ru	5.8	5.5	5.5	5.2	5.0	5.8	4.9	5.2	5.2	6.0	5.4	6.5	6.2	5.8	5.9	5.8	5.8	5.0	4.5	4.0	4.7	4.0	3.5	3.6	3.6	3.1	3.4	6.4	5.8	5.7	5.7	5.4	5.0	4.2	3.8	4.1
Rh	5.9	5.6	5.7	5.2	5.1	6.2	5.3	5.3	6.1	5.6	5.5	5.7	5.9	5.5	5.3	5.4	5.2	5.5	4.6	4.2	5.1	4.2	3.9	4.2	3.9	3.5	4.0	5.8	5.5	5.9	5.1	4.9	5.2	4.1	4.0	4.5
Pd	3.7	3.4	3.5	3.8	3.8	4.0	3.6	3.5	3.9	3.4	2.9	3.8	3.9	3.5	3.7	3.5	3.3	3.7	2.7	2.5	3.1	2.6	2.4	2.7	2.4	2.1	2.5	3.5	3.3	3.4	3.2	3.1	3.3	2.6	2.6	2.9
Ag	2.5	2.2	2.0	2.1	2.1	2.2	1.8	1.8	2.0	2.6	1.9	2.4	3.0	2.6	2.6	2.6	2.4	2.5	1.4	1.2	2.0	1.0	0.9	1.1	0.8	0.8	0.9	2.2	2.0	2.0	2.0	1.9	1.8	1.5	1.5	1.6
Cd	1.4	0.6	0.4	0.5	0.5	0.5	0.3	0.3	0.4	1.9	0.4	0.7	2.4	1.5	1.2	2.0	1.1	0.9	0.4	0.3	0.5	0.4	0.3	0.3	0.3	0.3	0.3	1.1	0.7	0.6	0.9	0.7	0.5	0.4	0.4	0.4
Hf	11.	9.0	7.0	9.0	8.1	7.0	8.2	7.4	6.5	11.	8.9	7.9	12.	9.7	7.8	11.	9.0	7.7	7.2	6.3	6.7	5.8	4.9	4.4	4.8	4.0	3.8	9.2	8.2	7.6	8.7	7.9	7.1	7.2	7.1	6.3
Ta	9.3	7.8	6.6	8.5	7.6	6.4	7.8	6.9	5.9	10.	8.0	6.8	11.	9.2	7.8	10.	7.3	6.2	6.7	5.7	6.0	5.2	4.2	3.7	3.4	3.2	3.1	9.9	8.7	7.4	8.2	7.8	6.9	6.8	6.5	5.6
W	8.1	6.7	5.4	7.5	6.7	6.6	6.9	6.1	6.3	8.2	6.8	7.1	9.1	7.8	7.6	8.2	7.3	7.4	5.7	4.5	8.2	4.1	2.8	2.8	2.6	2.3	2.4	8.5	8.4	6.3	8.0	8.2	6.9	7.0	5.8	5.7
Re	6.0	5.2	5.1	5.3	5.0	5.6	4.8	4.5	5.4	5.7	5.2	6.2	6.6	6.6	6.1	6.0	6.2	6.5	4.0	2.9	7.3	2.9	2.1	2.1	2.2	1.2	1.4	7.5	5.5	6.9	6.2	5.9	5.8	3.9	3.9	3.9
Os	6.4	6.0	6.7	6.1	5.9	6.7	5.6	5.5	6.4	5.6	6.0	5.9	6.9	7.5	7.1	6.5	6.6	7.5	4.5	3.9	3.6	3.8	3.3	3.5	3.3	2.9	3.3	6.6	6.0	4.9	6.5	6.3	5.3	3.9	3.7	4.1
Ir	6.2	5.9	6.3	5.9	6.0	6.8	5.5	5.6	6.7	5.5	5.5	5.7	6.3	6.3	6.5	6.0	5.1	4.2	4.3	4.0	5.2	3.9	3.6	4.0	3.5	3.2	3.8	6.1	5.8	6.4	5.3	5.1	5.4	3.8	4.2	4.5
Pt	5.4	5.3	5.7	5.6	5.6	6.2	5.2	5.3	5.5	4.7	4.8	5.2	5.3	4.9	5.3	4.9	4.8	5.3	4.0	3.8	4.5	3.9	3.7	4.2	3.5	3.4	4.0	4.9	4.9	5.1	4.5	4.5	5.0	3.7	3.8	4.4
Au	2.4	2.3	2.5	2.1	2.2	3.1	1.8	2.0	2.8	2.3	2.4	2.8	2.9	2.7	3.0	2.5	2.4	2.9	1.4	1.6	2.3	1.4	1.5	1.8	1.3	1.4	1.7	2.3	2.3	2.8	2.1	2.2	2.5	1.7	1.9	2.3

[a]The binding energy is calculated by $E_b = E(MX_2) + E(SA) - E(SA@MX_2)$, where $E(MX_2)$, $E(SA)$ and $E(SA@MX_2)$ are the energies of MX_2, SA, and the SA anchored on MX_2, respectively. The binding energy is given by the negative value of adsorption energy.

Table S4. Reaction free energies of O* (ΔG_O^* in eV) for various single atom anchored transition metal dichalcogenides (SA@MX_2 ; M = Ti, Zr, Hf, V, Nb and Ta). The ΔG_O^* values of the promising candidates for superior OER/ORR electrocatalysts are highlighted in bold.

M	***Ti***			***Zr***			***Hf***			***V***			***Nb***			***Ta***		
X_2	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***
SA	ΔG_O^*																	
Sc	**2.42**	1.65	0.59	1.70	1.41	0.93	1.20	0.88	0.60	**2.34**	1.39	0.96	**2.81**	1.81	1.40	**2.34**	1.38	0.32
Ti	0.92	0.38	0.01	0.69	0.20	-0.31	0.56	0.06	-0.49	1.34	0.53	-0.14	1.42	0.75	-0.02	1.20	0.56	0.14
V	0.15	-0.28	-0.79	0.06	-0.33	-0.73	-0.03	-0.42	-0.89	0.27	-0.43	-0.36	0.32	-0.11	-0.93	0.18	-0.20	0.11
Cr	0.79	0.27	-0.91	0.42	-0.45	-0.92	-0.04	0.48	-0.94	0.53	0.72	-0.31	0.07	-0.18	0.11	0.43	-0.14	0.26
Mn	1.61	0.01	1.63	1.48	1.45	1.71	1.34	1.34	-0.21	1.70	1.20	1.32	1.77	1.77	0.00	0.54	1.45	-0.68
Fe	**2.15**	1.83	**2.10**	**2.19**	**2.03**	1.65	**2.13**	**2.04**	**1.92**	0.96	0.81	**2.12**	1.20	1.02	**2.05**	1.42	1.56	1.77
Co	**2.17**	**1.95**	1.50	**2.08**	**1.97**	**2.06**	**1.99**	**1.90**	**3.05**	**2.88**	**2.78**	**2.87**	**2.56**	**2.10**	**2.20**	1.66	**2.23**	-0.10
Ni	3.16	**2.99**	**2.24**	3.20	**3.06**	**2.43**	3.14	**3.02**	**2.47**	3.26	**2.87**	**2.86**	3.10	**2.99**	**2.83**	3.38	**3.05**	**2.86**
Cu	3.72	3.52	**2.87**	3.53	3.52	**2.96**	3.14	3.30	**2.95**	3.47	**2.30**	**2.58**	3.71	3.19	**2.80**	3.42	**3.06**	**2.83**
Zn	3.13	**2.60**	**2.08**	**2.35**	**2.14**	**2.11**	**2.07**	**2.09**	**1.91**	3.38	**2.48**	1.67	3.54	**2.93**	**2.45**	3.35	**2.72**	**2.22**
Y	**2.75**	**1.92**	0.88	**2.14**	1.79	1.32	1.61	1.36	1.03	**2.68**	**2.12**	1.05	3.17	**2.29**	1.79	**2.83**	**1.94**	1.50
Zr	1.47	0.82	0.03	0.85	0.39	-0.13	0.53	0.05	-0.40	1.65	0.56	0.12	1.81	0.97	-0.16	1.46	0.68	0.05
Nb	0.32	-0.26	-0.86	0.42	-0.08	-0.64	0.30	-0.18	-0.65	0.69	-0.19	-0.16	0.82	0.22	-0.21	0.65	0.08	-0.19
Mo	0.01	-0.43	-0.76	0.01	-0.28	-0.41	-0.04	-0.33	-0.38	0.01	-0.54	-0.15	-0.10	-0.39	-0.34	-0.23	-0.40	-0.07
Tc	0.09	0.01	0.60	0.12	0.22	0.18	0.13	0.14	0.31	0.03	0.03	0.28	0.13	0.16	0.55	0.18	0.40	0.75
Ru	0.74	1.22	1.23	1.35	1.23	1.57	1.41	1.60	1.40	0.68	0.37	**2.06**	1.33	1.48	1.49	1.62	1.68	0.18
Rh	**2.78**	**2.62**	**2.32**	**2.49**	**2.48**	**2.64**	**2.67**	**2.71**	**2.57**	1.69	1.38	**1.90**	**2.53**	1.51	0.97	**2.58**	1.59	1.41
Pd	3.81	3.72	3.56	4.01	3.90	3.86	3.98	3.90	3.88	**2.94**	**2.53**	**2.76**	3.25	**2.86**	**2.61**	3.20	**2.95**	**2.75**
Ag	4.12	3.77	3.59	3.82	3.99	3.64	3.62	3.54	3.65	4.58	3.38	3.35	4.47	4.00	3.51	4.43	3.95	3.41
Cd	1.66	**1.87**	**2.02**	1.73	**2.21**	**2.07**	**2.07**	**2.57**	**2.29**	4.17	**2.43**	**2.42**	4.24	3.62	3.17	4.18	3.14	**2.62**
Hf	1.53	0.82	-0.03	0.68	0.17	-0.39	0.35	-0.15	-0.67	1.74	0.65	0.19	1.84	0.88	-0.23	1.47	0.63	-0.12
Ta	0.18	-0.24	-0.70	0.15	-0.42	-0.80	0.04	-0.49	-0.94	0.57	-0.39	-1.05	0.68	0.02	-0.38	0.51	-0.66	-1.38
W	-0.44	-0.92	-1.03	-0.38	-0.71	-0.67	-0.43	-0.78	-0.75	-0.42	-1.27	-0.48	-0.43	0.55	1.24	-0.59	1.84	-0.42
Re	-0.46	-0.39	-0.28	-0.47	-0.38	0.09	-0.47	-0.34	0.08	-0.49	-0.47	0.19	-0.46	**2.74**	0.04	-0.32	1.46	0.37
Os	0.53	0.74	1.31	0.85	0.84	1.34	0.91	0.95	1.09	0.35	-0.17	-0.01	0.87	1.64	1.36	1.20	1.42	1.27
Ir	**2.07**	**2.02**	**1.91**	**2.36**	**2.12**	**2.21**	**2.33**	**2.43**	**2.16**	0.54	0.42	0.35	**2.15**	**2.38**	1.25	**2.48**	0.58	0.41
Pt	3.23	3.21	**3.06**	3.54	3.48	3.31	3.51	3.51	**2.79**	1.82	**2.68**	1.66	**2.17**	**1.90**	1.70	**2.06**	**1.97**	**1.93**
Au	3.09	**3.01**	**2.95**	**2.71**	**2.92**	3.88	**2.50**	**2.79**	3.87	3.09	**2.66**	**2.72**	3.25	**3.01**	**2.81**	3.16	**2.89**	**2.76**

Table S5. Adsorption free energies of O* (ΔG_O^* in eV) for various single atom anchored transition metal dichalcogenides (SA@MX_2 ; M = Cr, Mo, W, Ni, Pd and Pt). The ΔG_O^* values of the promising candidates for superior OER/ORR electrocatalysts are highlighted in bold.

M	***Cr***			***Mo***			***W***			***Ni***			***Pd***			***Pt***		
X_2	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***	***S***	***Se***	***Te***
SA	ΔG_O^*																	
Sc	0.76	0.65	0.46	-0.68	-0.31	-0.49	-0.47	-0.74	-0.82	1.73	1.27	0.97	1.59	1.31	0.50	0.52	0.26	0.60
Ti	0.13	-0.05	-0.21	0.05	-0.30	-0.62	-0.24	-0.63	-1.07	1.07	0.37	0.37	0.78	-0.07	-0.45	0.50	0.06	-0.63
V	0.24	-0.23	0.09	-0.11	-0.56	-0.79	-0.44	-0.87	-1.00	0.27	-0.04	-0.45	-0.40	-0.49	-0.57	-0.05	-0.35	-1.20
Cr	0.88	0.51	-0.68	0.60	0.21	0.13	-1.12	-0.17	-3.93	0.55	0.46	-0.17	0.73	-0.01	0.40	0.26	0.18	-1.62
Mn	0.81	1.02	-0.07	0.58	0.38	0.18	0.84	0.09	0.52	0.63	1.23	-0.28	-0.51	-0.96	0.40	**2.02**	0.85	0.59
Fe	1.10	0.87	-0.13	1.23	0.19	0.73	1.03	0.63	0.45	**1.95**	0.52	1.36	1.34	1.40	1.43	1.10	0.82	0.73
Co	1.31	0.88	0.91	1.13	0.77	0.61	0.97	0.63	0.55	1.53	1.06	0.87	**2.01**	**2.09**	**1.99**	1.09	0.73	0.46
Ni	**2.41**	**2.01**	**1.94**	**2.28**	**1.89**	1.79	**2.13**	1.76	1.72	**2.41**	**1.92**	1.41	**2.48**	**2.64**	1.70	**2.17**	1.80	1.58
Cu	**2.60**	**2.33**	**2.78**	**2.04**	**1.88**	1.83	1.82	1.71	1.68	**3.03**	**2.59**	**2.13**	3.09	**2.67**	**2.24**	**2.42**	**2.33**	**2.05**
Zn	**2.04**	**2.03**	**2.14**	**2.27**	**2.04**	**1.97**	**2.31**	**2.22**	**1.93**	**2.82**	**2.24**	0.81	**2.86**	**2.51**	1.13	**2.07**	**2.19**	1.45
Y	1.01	0.84	0.86	0.30	-0.03	-0.21	-0.21	-0.53	-0.60	**2.20**	1.45	1.06	1.82	1.82	0.94	0.68	0.90	0.29
Zr	-0.46	-0.52	-0.16	0.00	-0.58	-0.70	-0.47	-0.74	-0.76	1.01	1.16	-0.11	1.48	0.80	0.15	0.76	0.84	0.13
Nb	0.05	-0.15	-0.68	-0.58	-1.05	-1.32	-1.05	-1.49	-1.64	0.21	-0.24	-0.18	-0.45	-0.65	-0.91	0.21	-0.80	-0.81
Mo	-0.46	-0.96	-0.95	-1.15	-1.84	-1.94	-1.49	-2.13	-2.15	0.49	0.16	-0.17	0.14	-0.04	-0.72	-1.03	-1.27	-1.47
Tc	-0.43	-0.83	**2.94**	-0.65	-1.02	-1.11	-0.84	-1.18	-1.21	0.82	0.98	-0.84	0.61	-0.70	0.65	-0.87	-0.14	-1.25
Ru	0.50	0.34	0.23	0.57	0.44	0.32	0.51	0.32	0.33	0.67	0.35	0.15	**1.90**	1.08	-0.06	0.37	0.03	-0.11
Rh	1.68	1.48	1.62	1.63	1.39	1.37	1.53	1.29	1.31	1.62	1.31	1.36	1.70	1.45	1.21	1.57	1.31	1.25
Pd	3.22	**2.95**	**2.89**	3.18	**2.92**	**2.87**	3.07	**2.81**	**2.80**	3.13	**2.70**	**2.48**	3.28	**2.98**	**2.55**	3.07	**2.90**	**2.68**
Ag	**3.04**	**2.98**	3.58	**2.71**	**2.73**	**2.68**	**2.54**	**2.59**	**2.54**	3.81	3.64	3.08	3.72	3.68	3.36	3.16	3.20	3.13
Cd	**2.85**	**2.78**	**2.81**	**2.88**	**2.82**	**2.69**	**2.87**	**2.82**	**2.66**	3.39	**2.98**	**2.50**	3.37	3.10	1.45	**2.85**	**2.94**	1.76
Hf	-0.10	-0.17	-0.13	-0.17	-0.74	-0.91	-0.71	-0.86	-1.05	1.06	0.69	0.66	1.12	0.63	0.42	0.23	0.60	-0.36
Ta	0.22	-0.38	-0.36	-0.78	-1.43	-1.78	-2.19	-2.05	-2.21	0.68	0.03	-0.43	-0.69	-0.83	-0.57	-0.81	-1.11	-0.96
W	-0.64	-1.16	**1.88**	-1.57	-2.47	-2.34	-2.56	-2.54	-2.52	-0.48	-0.04	-1.52	-0.19	0.28	-0.91	0.07	-0.69	-0.85
Re	-0.90	-1.39	**2.94**	-1.47	-1.87	-1.91	-1.76	-2.45	-2.41	0.96	-1.20	0.87	0.54	0.49	0.39	-0.50	-0.44	-0.84
Os	-0.31	-0.40	-0.02	-0.59	-0.87	-0.83	-0.73	-0.99	-0.86	-0.38	-0.60	-0.46	1.45	1.24	-0.72	-1.39	-0.94	-0.99
Ir	0.65	0.58	0.87	0.75	0.49	0.55	0.63	0.40	0.51	1.02	0.56	0.79	0.81	0.66	0.35	0.57	0.68	0.38
Pt	**2.03**	1.80	1.64	**2.04**	1.81	**1.90**	**1.92**	1.70	1.85	**1.98**	1.63	1.50	**2.25**	**1.96**	1.69	**2.11**	**1.88**	1.79
Au	**1.90**	**2.19**	**2.67**	**1.91**	**2.09**	**2.16**	1.86	**2.05**	**2.05**	**2.62**	**2.74**	**2.46**	**2.54**	**2.74**	**2.61**	**2.11**	**2.35**	**2.57**

Table S6. Reaction free energies of OH* (ΔG_{OH}^{*} in eV) for the SA@MX_2 survived from 1st screening.

TiS_2		$TiSe_2$		$TiTe_2$		ZrS_2		$ZrSe_2$		$ZrTe_2$		HfS_2		$HfSe_2$		$HfTe_2$	
Co	1.19	***Au***	0.94	***Au***	0.99	***Au***	0.53	***Au***	0.78	***Cd***	0.75	***Au***	0.32	***Au***	0.63	***Cd***	0.80
Fe	0.96	***Cd***	0.59	***Cd***	1.80	***Co***	0.76	***Cd***	0.66	***Co***	1.04	***Cd***	0.64	***Cd***	0.71	***Co***	1.72
Ir	0.73	***Co***	0.75	***Cu***	0.78	***Fe***	0.75	***Co***	0.74	***Cu***	0.86	***Co***	1.12	***Co***	0.71	***Cu***	0.81
Rh	1.13	***Ir***	0.90	***Fe***	1.57	***Ir***	1.10	***Fe***	0.66	***Ir***	0.91	***Fe***	0.70	***Fe***	0.62	***Fe***	1.29
Sc	1.06	***Ni***	1.48	***Ir***	0.80	***Rh***	1.15	***Ir***	0.89	***Ni***	1.08	***Ir***	1.08	***Ir***	1.24	***Ir***	0.82
Y	1.03	***Rh***	1.18	***Ni***	0.90	***Y***	0.71	***Ni***	1.55	***Rh***	1.17	***Rh***	1.32	***Ni***	1.52	***Ni***	1.11
		Y	0.72	***Pt***	1.66	***Zn***	-0.07	***Rh***	1.20	***Zn***	0.17	***Zn***	0.05	***Rh***	1.42	***Pt***	1.44
		Zn	0.25	***Rh***	1.02			***Zn***	0.02					***Zn***	0.14	***Rh***	1.07
				Zn	0.18											***Zn***	0.22

VS_2		VSe_2		VTe_2		NbS_2		$NbSe_2$		$NbTe_2$		TaS_2		$TaSe_2$		$TaTe_2$	
Co	0.80	***Au***	0.88	***Au***	0.79	***Co***	0.87	***Au***	1.04	***Au***	0.97	***Ir***	1.15	***Au***	0.92	***Au***	0.90
Pd	1.34	***Cd***	0.09	***Cd***	0.27	***Ir***	1.01	***Co***	0.92	***Co***	1.17	***Pt***	0.64	***Co***	1.12	***Cd***	0.55
Sc	1.17	***Co***	1.45	***Co***	1.68	***Pt***	0.65	***Ir***	1.07	***Cu***	0.86	***Rh***	1.30	***Cu***	0.96	***Cu***	0.77
Y	0.99	***Cu***	2.24	***Cu***	0.57	***Rh***	1.23	***Ni***	1.44	***Fe***	0.64	***Sc***	1.07	***Ni***	1.37	***Ni***	1.50
		Ni	1.92	***Fe***	1.34	***Sc***	1.30	***Pd***	1.19	***Ni***	1.10	***Y***	1.09	***Pd***	1.28	***Pd***	1.15
		Pd	0.83	***Ni***	1.81			***Pt***	0.59	***Pd***	1.09			***Pt***	0.66	***Pt***	0.73
		Pt	0.93	***Pd***	1.13			***Re***	1.57	***Zn***	0.24			***Y***	0.64	***Zn***	0.10
		Y	0.69	***Rh***	0.84			***Y***	0.79					***Zn***	0.35		
		Zn	0.23	***Ru***	1.36			***Zn***	0.46								

CrS_2		$CrSe_2$		$CrTe_2$		MoS_2		$MoSe_2$		$MoTe_2$		WS_2		WSe_2		WTe_2	
Ag	0.68	***Ag***	0.66	***Au***	0.66	***Ag***	0.35	***Ag***	0.41	***Ag***	0.40	***Ag***	0.19	***Ag***	0.28	***Ag***	0.27
Au	-0.30	***Au***	0.05	***Cd***	0.64	***Au***	-0.28	***Au***	-0.04	***Au***	0.11	***Cd***	1.46	***Au***	-0.05	***Au***	0.04
Cd	1.00	***Cd***	1.03	***Cu***	0.69	***Cd***	1.39	***Cd***	1.41	***Cd***	1.36	***Ni***	0.79	***Cd***	1.53	***Cd***	1.47
Cu	0.41	***Cu***	0.23	***Ni***	0.52	***Cu***	-0.14	***Cu***	-0.22	***Pd***	1.27	***Pt***	0.76	***Pd***	1.26	***Pd***	1.24
Ni	0.93	***Ni***	0.68	***Pd***	1.21	***Ni***	0.88	***Ni***	0.63	***Pt***	0.76	***Zn***	1.07	***Zn***	1.06	***Zn***	0.99
Pt	0.77	***Pd***	1.28	***Re***	3.57	***Pt***	0.83	***Pd***	1.32	***Zn***	0.86						
Zn	0.37	***Zn***	0.43	***Tc***	2.89	***Zn***	0.83	***Zn***	0.89								
				W	1.96												
				Zn	0.17												

NiS_2		$NiSe_2$		$NiTe_2$		PdS_2		$PdSe_2$		$PdTe_2$		PtS_2		$PtSe_2$		$PtTe_2$	
Au	0.45	***Au***	0.67	***Au***	0.77	***Au***	0.38	***Au***	0.65	***Au***	0.88	***Au***	-0.06	***Au***	0.24	***Au***	0.60
Cu	0.87	***Cd***	0.76	***Cd***	0.62	***Co***	0.95	***Co***	1.21	***Co***	1.01	***Cd***	0.91	***Cd***	0.90	***Cu***	0.10
Fe	0.99	***Cu***	0.64	***Cu***	0.41	***Ni***	0.95	***Cu***	0.62	***Cu***	0.43	***Cu***	0.19	***Cu***	0.26	***Pd***	1.13
Ni	0.88	***Ni***	0.55	***Pd***	0.89	***Pt***	0.80	***Ni***	0.79	***Pd***	1.06	***Mn***	2.56	***Pd***	1.30		
Pt	0.67	***Pd***	1.13			***Ru***	1.15	***Pd***	1.38			***Ni***	0.72	***Pt***	0.71		
Y	0.79	***Zn***	0.34			***Zn***	0.54	***Pt***	0.73			***Pt***	0.67	***Zn***	0.39		
Zn	0.48							***Zn***	0.43			***Zn***	0.35				

Table S7. Reaction free energies of intermediates (ΔG_X^*; X:O, OH, and OOH in eV), Gibbs free energy changes (ΔG_N; *N*=1-8) of each elementary reaction step and theoretical overpotentials (η_{OER} and η_{ORR} in V) for the SA@MX_2 survived from 1st/2nd screenings. The results for IrO_2 (110) and Pt (111) surfaces are also reported for comparison.

System	ΔG_{OH}^*	ΔG_O^*	ΔG_{OOH}^*	G1	G2	G3	G4	η^{OER}	G5	G6	G7	G8	η^{ORR}
IrO2(110)	1.52	2.89	4.60	1.52	1.37	1.71	0.32	**0.479**	-0.32	-1.71	-1.37	-1.52	0.906
Pt(111)	1.08	2.62	4.24	1.08	1.53	1.62	0.68	0.388	-0.68	-1.62	-1.53	-1.08	**0.546**
Co@TiS_2	1.19	2.17	4.12	1.19	0.97	1.95	0.80	0.723	-0.80	-1.95	-0.97	-1.19	0.430
Ir@TiS_2	0.73	2.07	4.01	0.73	1.33	1.95	0.91	0.719	-0.91	-1.95	-1.33	-0.73	0.498
Fe@TiS_2	0.96	2.15	4.20	0.96	1.19	2.05	0.72	0.823	-0.72	-2.05	-1.19	-0.96	0.510
Sc@TiS_2	1.06	2.42	4.87	1.06	1.35	2.45	0.05	1.222	-0.05	-2.45	-1.35	-1.06	1.179
Co@$TiSe_2$	0.75	1.95	4.07	0.75	1.20	2.12	0.85	0.892	-0.85	-2.12	-1.20	-0.75	0.476
Ir@$TiSe_2$	0.90	2.02	4.19	0.90	1.12	2.17	0.73	0.941	-0.73	-2.17	-1.12	-0.90	0.500
Cd@$TiSe_2$	0.59	1.87	4.14	0.59	1.28	2.28	0.78	1.049	-0.78	-2.28	-1.28	-0.59	0.640
Rh@$TiSe_2$	1.18	2.62	4.37	1.18	1.44	1.75	0.55	0.524	-0.55	-1.75	-1.44	-1.18	0.684
Y@$TiSe_2$	0.72	1.92	4.54	0.72	1.20	2.62	0.38	1.390	-0.38	-2.62	-1.20	-0.72	0.852
Ni@$TiSe_2$	1.48	2.99	4.61	1.48	1.51	1.62	0.31	0.389	-0.31	-1.62	-1.51	-1.48	0.917
Ir@$TiTe_2$	0.80	1.91	4.14	0.80	1.10	2.23	0.78	1.005	-0.78	-2.23	-1.10	-0.80	0.454
Ni@$TiTe_2$	0.90	2.24	4.16	0.90	1.34	1.92	0.76	0.686	-0.76	-1.92	-1.34	-0.90	0.466
Rh@$TiTe_2$	1.02	2.32	4.30	1.02	1.30	1.98	0.62	0.752	-0.62	-1.98	-1.30	-1.02	0.613
Fe@ZrS_2	0.75	2.19	4.10	0.75	1.44	1.92	0.82	0.685	-0.82	-1.92	-1.44	-0.75	0.482
Co@ZrS_2	0.76	2.08	4.38	0.76	1.31	2.31	0.54	1.075	-0.54	-2.31	-1.31	-0.76	0.692
Ir@ZrS_2	1.10	2.36	4.39	1.10	1.26	2.04	0.53	0.806	-0.53	-2.04	-1.26	-1.10	0.701
Rh@ZrS_2	1.15	2.49	4.44	1.15	1.34	1.95	0.48	0.723	-0.48	-1.95	-1.34	-1.15	0.751
Y@ZrS_2	0.71	2.14	4.56	0.71	1.43	2.41	0.36	1.181	-0.36	-2.41	-1.43	-0.71	0.866
Ir@$ZrSe_2$	0.89	2.12	4.15	0.89	1.23	2.03	0.77	0.798	-0.77	-2.03	-1.23	-0.89	0.461
Co@$ZrSe_2$	0.74	1.97	4.08	0.74	1.23	2.11	0.84	0.880	-0.84	-2.11	-1.23	-0.74	0.491
Fe@$ZrSe_2$	0.66	2.03	4.05	0.66	1.38	2.02	0.87	0.789	-0.87	-2.02	-1.38	-0.66	0.573
Rh@$ZrSe_2$	1.20	2.48	4.50	1.20	1.28	2.02	0.42	0.787	-0.42	-2.02	-1.28	-1.20	0.812
Ir@$ZrTe_2$	0.91	2.21	4.25	0.91	1.30	2.05	0.67	0.817	-0.67	-2.05	-1.30	-0.91	0.562
Co@$ZrTe_2$	1.04	2.06	4.25	1.04	1.02	2.20	0.67	0.967	-0.67	-2.20	-1.02	-1.04	0.562
Ni@$ZrTe_2$	1.08	2.43	4.29	1.08	1.35	1.86	0.63	0.631	-0.63	-1.86	-1.35	-1.08	0.603
Cd@$ZrTe_2$	0.75	2.07	4.30	0.75	1.32	2.23	0.62	1.004	-0.62	-2.23	-1.32	-0.75	0.612
Rh@$ZrTe_2$	1.17	2.64	4.43	1.17	1.47	1.80	0.49	0.567	-0.49	-1.80	-1.47	-1.17	0.745
Fe@HfS_2	0.70	2.13	4.07	0.70	1.43	1.94	0.85	0.712	-0.85	-1.94	-1.43	-0.70	0.532
Cd@HfS_2	0.64	2.07	4.23	0.64	1.43	2.16	0.69	0.930	-0.69	-2.16	-1.43	-0.64	0.588
Co@HfS_2	1.12	1.99	4.35	1.12	0.87	2.36	0.57	1.126	-0.57	-2.36	-0.87	-1.12	0.661
Ir@HfS_2	1.08	2.33	4.38	1.08	1.25	2.05	0.54	0.821	-0.54	-2.05	-1.25	-1.08	0.693
Rh@HfS_2	1.32	2.67	4.52	1.32	1.35	1.85	0.40	0.622	-0.40	-1.85	-1.35	-1.32	0.833
Co@$HfSe_2$	0.71	1.90	4.06	0.71	1.20	2.16	0.86	0.925	-0.86	-2.16	-1.20	-0.71	0.524
Fe@$HfSe_2$	0.62	2.04	4.00	0.62	1.42	1.97	0.92	0.735	-0.92	-1.97	-1.42	-0.62	0.610
Ir@$HfSe_2$	1.24	2.43	4.56	1.24	1.18	2.14	0.36	0.906	-0.36	-2.14	-1.18	-1.24	0.873
Ni@$HfSe_2$	1.52	3.02	4.61	1.52	1.50	1.59	0.31	0.364	-0.31	-1.59	-1.50	-1.52	0.921
Rh@$HfSe_2$	1.42	2.71	4.65	1.42	1.29	1.95	0.27	0.715	-0.27	-1.95	-1.29	-1.42	0.962
Ir@$HfTe_2$	0.82	2.16	4.17	0.82	1.34	2.01	0.75	0.778	-0.75	-2.01	-1.34	-0.82	0.482
Fe@$HfTe_2$	1.29	1.92	3.77	1.29	0.62	1.85	1.15	0.622	-1.15	-1.85	-0.62	-1.29	0.606
Ni@$HfTe_2$	1.11	2.47	4.32	1.11	1.36	1.86	0.60	0.626	-0.60	-1.86	-1.36	-1.11	0.634
Rh@$HfTe_2$	1.07	2.57	4.34	1.07	1.50	1.77	0.58	0.540	-0.58	-1.77	-1.50	-1.07	0.652
Cd@$HfTe_2$	0.80	2.29	4.36	0.80	1.49	2.07	0.56	0.840	-0.56	-2.07	-1.49	-0.80	0.666
Pt@$HfTe_2$	1.44	2.79	4.69	1.44	1.36	1.90	0.23	0.670	-0.23	-1.90	-1.36	-1.44	1.004
Sc@VS_2	1.17	2.34	4.93	1.17	1.17	2.59	-0.01	1.360	0.01	-2.59	-1.17	-1.17	1.239
Y@VSe_2	0.69	2.12	4.47	0.69	1.43	2.35	0.45	1.117	-0.45	-2.35	-1.43	-0.69	0.778

Co@VSe_2	1.45	2.78	4.69	1.45	1.32	1.91	0.23	0.682	-0.23	-1.91	-1.32	-1.45	0.998
Rh@VTe_2	0.84	1.90	4.22	0.84	1.06	2.31	0.70	1.084	-0.70	-2.31	-1.06	-0.84	0.526
Ru@VTe_2	1.36	2.06	4.08	1.36	0.70	2.02	0.84	0.790	-0.84	-2.02	-0.70	-1.36	0.528
Fe@VTe_2	1.34	2.12	4.53	1.34	0.78	2.40	0.39	1.175	-0.39	-2.40	-0.78	-1.34	0.835
Ir@NbS_2	1.01	2.15	4.22	1.01	1.14	2.07	0.70	0.836	-0.70	-2.07	-1.14	-1.01	0.526
Pt@NbS_2	0.65	2.17	3.88	0.65	1.52	1.71	1.04	0.481	-1.04	-1.71	-1.52	-0.65	0.576
Rh@NbS_2	1.23	2.53	4.32	1.23	1.30	1.79	0.60	0.561	-0.60	-1.79	-1.30	-1.23	0.628
Sc@NbS_2	1.30	2.81	5.10	1.30	1.50	2.30	-0.18	1.068	0.18	-2.30	-1.50	-1.30	1.415
Co@$NbSe_2$	0.92	2.10	4.10	0.92	1.18	2.00	0.82	0.767	-0.82	-2.00	-1.18	-0.92	0.405
Ir@$NbSe_2$	1.07	2.38	4.31	1.07	1.32	1.92	0.61	0.692	-0.61	-1.92	-1.32	-1.07	0.616
Pt@$NbSe_2$	0.59	1.90	3.88	0.59	1.31	1.97	1.04	0.743	-1.04	-1.97	-1.31	-0.59	0.642
Y@$NbSe_2$	0.79	2.29	4.62	0.79	1.50	2.33	0.30	1.099	-0.30	-2.33	-1.50	-0.79	0.928
Fe@$NbTe_2$	0.64	2.05	4.01	0.64	1.41	1.96	0.91	0.733	-0.91	-1.96	-1.41	-0.64	0.590
Co@$NbTe_2$	1.17	2.20	4.34	1.17	1.03	2.13	0.58	0.904	-0.58	-2.13	-1.03	-1.17	0.647
Pd@$NbTe_2$	1.09	2.61	4.40	1.09	1.52	1.79	0.52	0.563	-0.52	-1.79	-1.52	-1.09	0.713
Pt@TaS_2	0.64	2.06	3.89	0.64	1.42	1.83	1.03	0.599	-1.03	-1.83	-1.42	-0.64	0.594
Ir@TaS_2	1.15	2.48	4.35	1.15	1.33	1.87	0.57	0.643	-0.57	-1.87	-1.33	-1.15	0.662
Rh@TaS_2	1.30	2.58	4.36	1.30	1.28	1.78	0.56	0.552	-0.56	-1.78	-1.28	-1.30	0.672
Sc@TaS_2	1.07	2.34	4.90	1.07	1.27	2.56	0.02	1.329	-0.02	-2.56	-1.27	-1.07	1.214
Pt@$TaSe_2$	0.66	1.97	3.96	0.66	1.31	1.98	0.96	0.753	-0.96	-1.98	-1.31	-0.66	0.568
Co@$TaSe_2$	1.12	2.23	4.26	1.12	1.12	2.03	0.66	0.796	-0.66	-2.03	-1.12	-1.12	0.570
Y@$TaSe_2$	0.64	1.94	4.47	0.64	1.30	2.54	0.45	1.305	-0.45	-2.54	-1.30	-0.64	0.784
Pt@$TaTe_2$	0.73	1.93	4.05	0.73	1.20	2.12	0.87	0.891	-0.87	-2.12	-1.20	-0.73	0.500
Ni@$TaTe_2$	1.50	2.86	4.76	1.50	1.36	1.90	0.16	0.674	-0.16	-1.90	-1.36	-1.50	1.070
Ni@CrS_2	0.93	2.41	4.14	0.93	1.48	1.72	0.78	0.495	-0.78	-1.72	-1.48	-0.93	0.446
Pt@CrS_2	0.77	2.03	4.06	0.77	1.26	2.03	0.86	0.800	-0.86	-2.03	-1.26	-0.77	0.455
Ni@$CrSe_2$	0.68	2.01	3.93	0.68	1.33	1.92	0.99	0.693	-0.99	-1.92	-1.33	-0.68	0.552
Ni@$CrTe_2$	0.52	1.94	3.79	0.52	1.42	1.85	1.13	0.617	-1.13	-1.85	-1.42	-0.52	0.706
Ni@MoS_2	0.88	2.28	4.05	0.88	1.40	1.78	0.87	0.547	-0.87	-1.78	-1.40	-0.88	0.365
Pt@MoS_2	0.83	2.04	4.06	0.83	1.21	2.02	0.86	0.786	-0.86	-2.02	-1.21	-0.83	0.400
Zn@MoS_2	0.83	2.27	4.51	0.83	1.45	2.24	0.41	1.007	-0.41	-2.24	-1.45	-0.83	0.820
Cd@MoS_2	1.39	2.88	4.83	1.39	1.48	1.96	0.09	0.726	-0.09	-1.96	-1.48	-1.39	1.142
Ni@$MoSe_2$	0.63	1.89	3.86	0.63	1.26	1.96	1.06	0.731	-1.06	-1.96	-1.26	-0.63	0.595
Zn@$MoSe_2$	0.89	2.04	4.56	0.89	1.14	2.53	0.36	1.297	-0.36	-2.53	-1.14	-0.89	0.872
Cd@$MoSe_2$	1.41	2.82	4.91	1.41	1.41	2.09	0.01	0.864	-0.01	-2.09	-1.41	-1.41	1.222
Pt@$MoTe_2$	0.76	1.90	4.05	0.76	1.13	2.15	0.87	0.920	-0.87	-2.15	-1.13	-0.76	0.469
Zn@$MoTe_2$	0.86	1.97	4.46	0.86	1.11	2.49	0.46	1.265	-0.46	-2.49	-1.11	-0.86	0.772
Cd@$MoTe_2$	1.36	2.69	4.87	1.36	1.32	2.19	0.05	0.957	-0.05	-2.19	-1.32	-1.36	1.183
Ni@WS_2	0.79	2.13	3.97	0.79	1.34	1.84	0.95	0.615	-0.95	-1.84	-1.34	-0.79	0.440
Pt@WS_2	0.76	1.92	3.99	0.76	1.16	2.07	0.93	0.845	-0.93	-2.07	-1.16	-0.76	0.469
Zn@WS_2	1.07	2.31	4.75	1.07	1.25	2.43	0.17	1.205	-0.17	-2.43	-1.25	-1.07	1.059
Cd@WS_2	1.46	2.87	4.98	1.46	1.41	2.10	-0.06	0.873	0.06	-2.10	-1.41	-1.46	1.287
Zn@WSe_2	1.06	2.22	4.73	1.06	1.16	2.51	0.19	1.279	-0.19	-2.51	-1.16	-1.06	1.038
Au@WSe_2	-0.05	2.05	3.49	-0.05	2.10	1.43	1.43	0.871	-1.43	-1.43	-2.10	0.05	1.276
Cd@WSe_2	1.53	2.82	5.12	1.53	1.29	2.30	-0.20	1.075	0.20	-2.30	-1.29	-1.53	1.435
Zn@WTe_2	0.99	1.93	4.64	0.99	0.94	2.71	0.28	1.475	-0.28	-2.71	-0.94	-0.99	0.945
Cd@WTe_2	1.47	2.66	4.95	1.47	1.20	2.29	-0.03	1.057	0.03	-2.29	-1.20	-1.47	1.257
Ni@NiS_2	0.88	2.41	4.16	0.88	1.53	1.75	0.76	0.523	-0.76	-1.75	-1.53	-0.88	0.472
Pt@NiS_2	0.67	1.98	4.00	0.67	1.31	2.02	0.92	0.788	-0.92	-2.02	-1.31	-0.67	0.555
Fe@NiS_2	0.99	1.95	4.45	0.99	0.96	2.50	0.47	1.266	-0.47	-2.50	-0.96	-0.99	0.758
Y@NiS_2	0.79	2.20	4.57	0.79	1.41	2.37	0.35	1.139	-0.35	-2.37	-1.41	-0.79	0.875
Ni@$NiSe_2$	0.55	1.92	3.92	0.55	1.37	2.00	1.00	0.770	-1.00	-2.00	-1.37	-0.55	0.683
Co@PdS_2	0.95	2.01	4.24	0.95	1.06	2.23	0.68	1.000	-0.68	-2.23	-1.06	-0.95	0.547

Ru@PdS_2	1.15	1.90	4.28	1.15	0.75	2.38	0.64	1.149	-0.64	-2.38	-0.75	-1.15	0.590
Pt@$PdSe_2$	0.73	1.96	4.05	0.73	1.23	2.09	0.87	0.862	-0.87	-2.09	-1.23	-0.73	0.499
Co@$PdSe_2$	1.21	2.09	4.35	1.21	0.89	2.26	0.57	1.030	-0.57	-2.26	-0.89	-1.21	0.663
Co@$PdTe_2$	1.01	1.99	4.36	1.01	0.98	2.37	0.56	1.143	-0.56	-2.37	-0.98	-1.01	0.669
Pd@$PdTe_2$	1.06	2.55	4.44	1.06	1.49	1.89	0.48	0.659	-0.48	-1.89	-1.49	-1.06	0.750
Ni@PtS_2	0.72	2.17	3.98	0.72	1.45	1.81	0.94	0.581	-0.94	-1.81	-1.45	-0.72	0.509
Pt@PtS_2	0.67	2.11	3.90	0.67	1.44	1.78	1.02	0.554	-1.02	-1.78	-1.44	-0.67	0.559
Pt@$PtSe_2$	0.71	1.88	4.02	0.71	1.16	2.15	0.90	0.916	-0.90	-2.15	-1.16	-0.71	0.517