Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

1. HER pathway

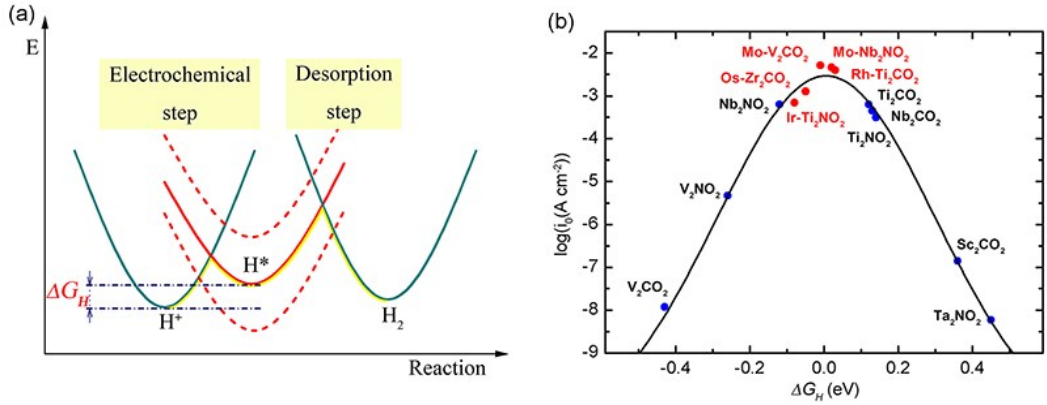

Figure S1. (a) Schematic illustration for reaction pathway in hydrogen evolution reaction. (b) The HER volcano plots of MXenes with 1/9 H coverage following the method by Nørskov *et al*.[1]

2. Scheme to calculate Gibbs free energy for adsorbed hydrogen

We calculate the ΔG_H of oxygen-terminated MXenes (M_2XO_2) at the same hydrogen coverage. The hydrogen stability is depended on the difference of binding energy.[1-3]

$$\Delta E_H = E_{(system+H)} - E_{(system)} - \frac{1}{2}E_{(H_2)} \qquad (1)$$

$E_{(system+H)}$is the energy of the M_2XO_2 with one hydrogen atom adsorbed on it, $E_{(system)}$and $E_{(H_2)}$are the total energies of the M_2XO_2, and the gaseous hydrogen molecule, respectively. The Gibbs free energy for adsorbed hydrogen is according to the following formula.[1-3]

$$\Delta G_H = \Delta E_H + \Delta E_{ZPE} - T\Delta S_H \qquad (2)$$

Here ΔE_{ZPE} is the differential zero-point energy between the adsorbed state and the gas phase state. ΔS_H is approximately equal to the entropy of gas phase H_2 at standard conditions (300K, 1bar).[3,4]

3. HER activities for pristine MXenes

Table S1. The most stable adsorption site of O atom and the charge of it (e_O), the calculation ΔG_H at different hydrogen coverage. The active site is indicated in red.

System	Adsorption site of O atom	Charge of O^- ion (e)	Structure	1/9 H coverage ΔG_H (eV)	1/4 H coverage ΔG_H (eV)
Ti_2CO_2	Fcc	-1.10		0.12	0.22
Nb_2CO_2	Fcc	-1.10		0.13	0.16
Zr_2CO_2	Fcc	-1.25		0.81	0.86
Ta_2CO_2	Fcc	-1.16		0.63	0.72
V_2CO_2	Fcc	-0.97		-0.43	-1.22
Hf_2CO_2	Fcc	-1.24		1.08	1.14
Sc_2CO_2	Fcc+Hcp	-1.29		0.36	0.47
Y_2CO_2	Fcc+Hcp	-1.31		0.87	0.92
Ti_2NO_2	Fcc	-1.10		0.14	0.20
Nb_2NO_2	Hcp	-1.12		-0.12	-0.15
Zr_2NO_2	Fcc	-1.27		0.65	0.80
Ta_2NO_2	Hcp	-1.18		0.45	0.58
V_2NO_2	Fcc	-1.00		-0.26	-1.56
Hf_2NO_2	Fcc	-1.25		0.99	1.19
Sc_2NO_2	Fcc	-1.11		-0.95	-1.49
Y_2NO_2	Fcc	-1.30		-0.70	-1.23

4. The adsorption properties of transition metal atom

Table S2. The adsorption energy between MXenes and single transition metal atom (ΔE_{TM-ads}), the more negative the value, the stronger the interaction. "-" means that it is difficult for cadmium and mercury to be adsorbed on MXenes, the interatomic distances between them and the MXenes layer are too far (>3 Å).

System	ΔE_{TM-ads}														
	Pt	Pd	W	Mo	Os	Ru	Ir	Rh	Ag	Au	Re	Cu	Zn	Cd	Hg
Ti_2CO_2	-1.74	-1.37	-7.16	-7.47	-4.76	-3.98	-3.29	-2.72	-0.88	-0.35	-6.24	-0.71	-0.03	-	-
Nb_2CO_2	-1.75	-1.34	-7.08	-7.20	-4.63	-4.08	-3.78	-2.73	-0.85	-0.35	-6.07	-0.76	-0.01	-	-
Zr_2CO_2	-1.32	-1.05	-5.39	-5.91	-3.64	-3.44	-2.68	-2.25	-0.62	-0.10	-4.63	-0.40	0.08	-	-
Ta_2CO_2	-1.48	-1.23	-5.67	-6.10	-3.71	-3.59	-3.70	-2.52	-0.63	-0.12	-4.81	-0.31	0.07	-	-
V_2CO_2	-1.84	-1.46	-8.67	-8.36	-5.67	-4.63	-3.43	-2.84	-1.03	-0.70	-7.27	-1.08	-0.09	-	-
Hf_2CO_2	-1.28	-0.96	-4.99	-5.64	-3.53	-3.44	-2.72	-2.36	-0.43	-0.02	-4.32	-0.57	0.12	-	-
Sc_2CO_2	-1.29	-1.20	-4.76	-5.19	-4.10	-2.58	-2.99	-0.96	-0.55	-0.04	-4.4	-0.89	0.04	-	-
Y_2CO_2	-1.26	-1.19	-6.67	-3.56	-4.53	-2.58	-3.33	-1.15	-0.56	-0.03	-4.34	-0.89	0.05	-	-
Ti_2NO_2	-3.05	-1.57	-7.99	-8.34	-5.65	-4.37	-4.31	-2.96	-0.95	-0.52	-6.96	-0.89	-0.38	-	-
Nb_2NO_2	-3.26	-1.47	-7.26	-7.41	-5.20	-4.48	-4.37	-3.08	-0.91	-0.45	-6.34	-0.91	-0.33	-	-
Zr_2NO_2	-2.85	-1.25	-5.83	-6.24	-4.38	-4.23	-4.08	-2.90	-0.75	-0.20	-5.11	-0.62	-0.10	-	-
Ta_2NO_2	-2.77	-1.18	-5.94	-6.31	-4.46	-4.19	-4.18	-2.87	-0.72	-0.23	-5.26	-0.53	-0.17	-	-
V_2NO_2	-3.33	-1.94	-8.19	-8.42	-6.34	-4.78	-4.47	-3.20	-1.16	-0.76	-7.45	-1.26	-0.67	-	-
Hf_2NO_2	-2.10	-1.21	-5.18	-5.72	-3.99	-3.94	-3.98	-2.83	-0.57	-0.14	-4.56	-0.66	-0.05	-	-
Sc_2NO_2	-2.29	-1.72	-8.10	-6.38	-5.83	-4.84	-4.47	-3.49	-1.19	-0.65	-7.21	-1.22	-0.69	-	-
Y_2NO_2	-2.25	-1.69	-5.43	-8.26	-6.68	-5.58	-4.56	-3.52	-1.00	-0.77	-7.29	-1.56	-0.53	-	-

5. HER activities for TM-modified MXenes

Table S3. The ΔG_H of materials after surface modified by single transition metal atom. The S_0, S_1, S_2 represents the different H adsorption sites, as shown in Figure 2.

System	Site	$\Delta G_{H/\mathrm{eV}}$												
		Pt	Pd	W	Mo	Os	Ru	Ir	Rh	Ag	Au	Re	Cu	Zn
Ti_2CO_2	S_0	-0.13	0.21	0.23	1.09	0.36	-0.34	-0.09	0.43	0.31	-0.64	0.10	0.46	-0.22
	S_1	-0.19	0.14	0.20	0.21	0.14	0.36	-0.33	0.03	0.24	0.11	0.25	0.24	-0.18
	S_2	-0.21	0.17	0.30	0.30	0.21	0.27	-0.24	0.11	0.25	0.07	0.29	0.22	-0.18
Nb_2CO_2	S_0	-0.24	0.19	-0.37	0.78	0.12	0.44	0.26	0.33	0.33	-0.21	-0.24	0.35	0.11
	S_1	-0.30	0.24	0.22	0.27	0.15	0.17	0.04	0.16	0.26	0.13	0.20	0.30	0.20
	S_2	-0.19	0.26	0.27	0.37	0.25	0.25	0.12	0.19	0.28	0.12	0.28	0.24	0.14
Zr_2CO_2	S_0	0.54	1.00	1.55	1.55	-0.05	0.53	0.15	0.68	0.85	-0.66	0.18	1.06	0.86
	S_1	0.49	0.79	0.79	0.83	0.68	0.65	0.18	0.49	0.84	0.65	0.81	0.82	0.95
	S_2	0.46	0.81	0.85	0.88	0.34	0.71	0.11	0.55	0.82	0.46	0.83	0.82	0.87
Ta_2CO_2	S_0	0.32	0.73	-0.48	0.98	0.05	0.70	0.69	0.67	0.78	0.36	0.78	0.80	0.48
	S_1	0.58	0.80	0.72	0.77	-0.38	0.68	0.61	0.63	0.73	0.60	0.65	0.69	0.57
	S_2	0.27	0.81	0.82	0.87	-0.03	0.70	0.60	0.54	0.74	0.66	0.75	0.72	0.56
V_2CO_2	S_0	-0.89	-0.54	-0.22	-0.31	0.45	0.34	-0.29	-0.51	-0.17	-0.31	-0.69	-0.70	-0.27
	S_1	-0.88	-0.56	-0.10	-0.09	-0.33	-0.26	-0.53	-0.28	-0.20	-0.29	-1.40	-0.36	-0.34
	S_2	-0.85	-0.36	-0.52	-0.01	-0.09	-0.16	-0.46	-0.30	-0.17	-0.29	-1.32	-0.44	-0.31
Hf_2CO_2	S_0	-0.60	1.23	-0.22	1.01	0.35	0.44	0.22	0.83	0.84	0.31	0.98	1.33	0.99
	S_1	0.73	1.06	1.07	1.11	0.91	0.88	0.31	0.67	1.07	0.86	1.07	1.10	1.04
	S_2	0.69	1.09	1.14	1.16	0.42	0.93	0.21	0.72	1.05	0.44	1.14	1.11	1.04
Sc_2CO_2	S_0	0.97	0.32	0.71	1.17	0.12	-0.36	-0.27	-0.97	-0.38	-0.34	0.44	0.78	0.26
	S_1	1.31	0.25	0.26	0.99	0.40	-0.14	0.07	-0.75	-0.58	-0.07	0.21	1.02	0.34
	S_2	0.56	0.10	0.32	-0.33	0.34	0.21	-0.02	-0.73	-0.76	-0.07	-0.63	0.90	0.39
Y_2CO_2	S_0	0.17	0.22	0.53	0.60	0.39	-0.19	0.03	-0.85	0.22	-0.35	-0.58	0.88	0.28
	S_1	0.51	0.30	0.53	-0.53	0.61	0.39	0.25	-0.66	-0.04	-0.14	-0.79	1.01	0.39
	S_2	0.61	0.18	0.67	-0.39	0.67	0.37	0.44	-0.22	-0.29	-0.09	-0.97	0.75	0.30
Ti_2NO_2	S_0	0.35	0.12	0.10	1.21	0.46	0.72	0.09	0.63	0.42	-1.19	0.32	0.48	-0.13
	S_1	0.20	0.28	0.46	0.48	0.32	0.33	-0.08	0.31	0.38	0.22	0.37	0.35	-0.11
	S_2	0.26	0.30	0.49	0.50	0.37	0.35	-0.27	0.31	0.40	0.21	0.45	0.38	-0.16
Nb_2NO_2	S_0	0.70	-0.22	-0.16	0.74	0.50	0.41	0.82	-0.32	0.07	0.33	0.10	-0.17	0.21
	S_1	0.46	-0.05	-0.06	-0.02	0.32	0.25	0.49	-0.68	-0.03	0.28	-0.05	-0.28	0.25
	S_2	0.63	-0.23	0.02	0.02	0.43	0.31	0.85	-0.24	0.04	0.38	0.07	-0.23	0.25
Zr_2NO_2	S_0	1.01	0.78	1.46	1.40	0.35	0.87	1.00	0.80	0.58	-0.33	0.74	0.96	0.59
	S_1	0.64	0.67	0.87	0.87	0.25	0.82	0.83	0.66	0.85	0.57	0.82	0.87	0.64
	S_2	1.08	0.78	0.94	0.91	0.30	0.79	0.82	0.77	0.74	0.69	0.86	0.92	0.63
Ta_2NO_2	S_0	-0.28	0.38	-0.95	-0.12	-1.21	-0.35	-0.30	-0.16	0.60	-0.71	-0.04	1.06	0.29
	S_1	0.59	0.38	0.39	0.52	-1.52	-0.84	0.29	-0.59	0.54	0.79	-0.82	0.85	0.38
	S_2	0.62	0.31	0.53	0.62	-1.11	-0.38	0.63	-0.25	0.57	0.82	-0.73	0.84	0.37

V_2NO_2	S_0	-0.49	-0.68	-0.98	0.84	-0.98	0.21	-0.19	-0.02	0.57	-0.68	-0.77	-0.43	-0.22
	S_1	-0.83	-0.58	-1.13	0.05	-0.54	-0.12	-1.45	-0.28	-0.43	-0.73	-0.23	-0.43	-0.29
	S_2	-0.75	-0.58	-0.08	0.21	-0.70	-0.03	-1.41	-0.28	-0.33	-0.66	-0.68	-0.35	-0.21
Hf_2NO_2	S_0	-0.63	1.07	1.04	1.21	0.44	1.09	1.20	1.05	1.02	-0.31	0.81	1.27	0.90
	S_1	0.95	1.02	1.22	1.21	0.39	1.09	1.16	0.91	1.13	0.90	0.77	1.25	0.97
	S_2	1.00	1.15	1.30	1.27	0.40	1.03	1.16	0.85	1.10	1.04	0.38	1.27	0.97
Sc_2NO_2	S_0	-1.30	-1.02	1.19	0.25	-0.39	-0.73	-0.55	-0.47	-1.39	-1.15	0.74	-0.90	-0.59
	S_1	-1.15	-1.20	-0.58	0.21	-0.44	-0.88	-0.63	-0.93	-1.20	-1.27	-0.07	-1.21	-1.15
	S_2	-1.14	-1.18	-0.66	0.18	-0.43	-0.88	-0.63	-0.92	-1.21	-1.24	-0.08	-1.20	-1.14
Y_2NO_2	S_0	-0.82	-0.95	-0.65	-1.32	-0.57	-0.57	-0.45	-0.40	-0.69	-0.88	-1.32	-0.87	-0.70
	S_1	-1.40	-1.06	0.77	-1.24	-0.42	-0.73	-0.52	-0.86	-1.02	-1.12	-0.60	-1.04	-0.97
	S_2	-1.40	-1.03	0.33	-1.32	-0.37	-0.67	-0.48	-0.80	-1.04	-1.12	-1.11	-1.02	-0.93

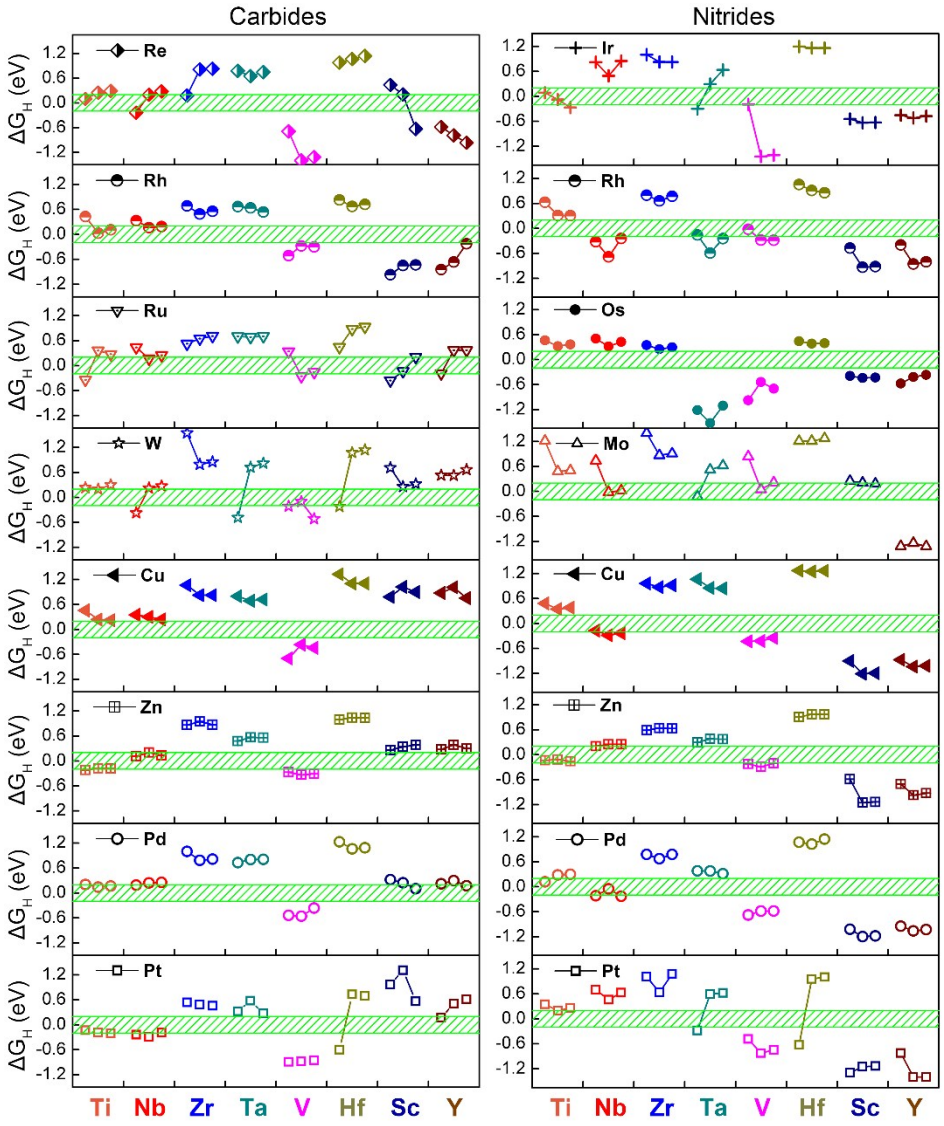

Figure S2. The $^{\Delta G_H}$ of various metal modified MXenes. The left and right panels exhibit carbides and nitrides respectively. The green shaded area marks the HER active energy range with the $^{\Delta G_H}$ in the region between -0.2 and 0.2 eV. Furthermore, the $^{\Delta G_H}$ values for the three H adsorption sites (S_0, S_1, S_2) of each material are plotted in the order of S_0-S_1-S_2.

6. Activation energy barrier for HER on MXenes

Here, we show the activation barriers for the TM-M_2XO_2 combination beyond the ones shown in the main text.

It has been demonstrated that the simulation on H-reaction can be influenced by the water environment.[5,6] Therefore, for rationally simulating the activation energy barrier of H-reaction, we add the H_2O molecules on the surface of MXenes one side with one H_3O^+ ion, according to the ordinary distance between water and the length of hydrogen bond in water. A number of initial water molecule conformations are used while the most stable one 1/8 ($H_2O/Å^2$) is used for the barrier simulation.

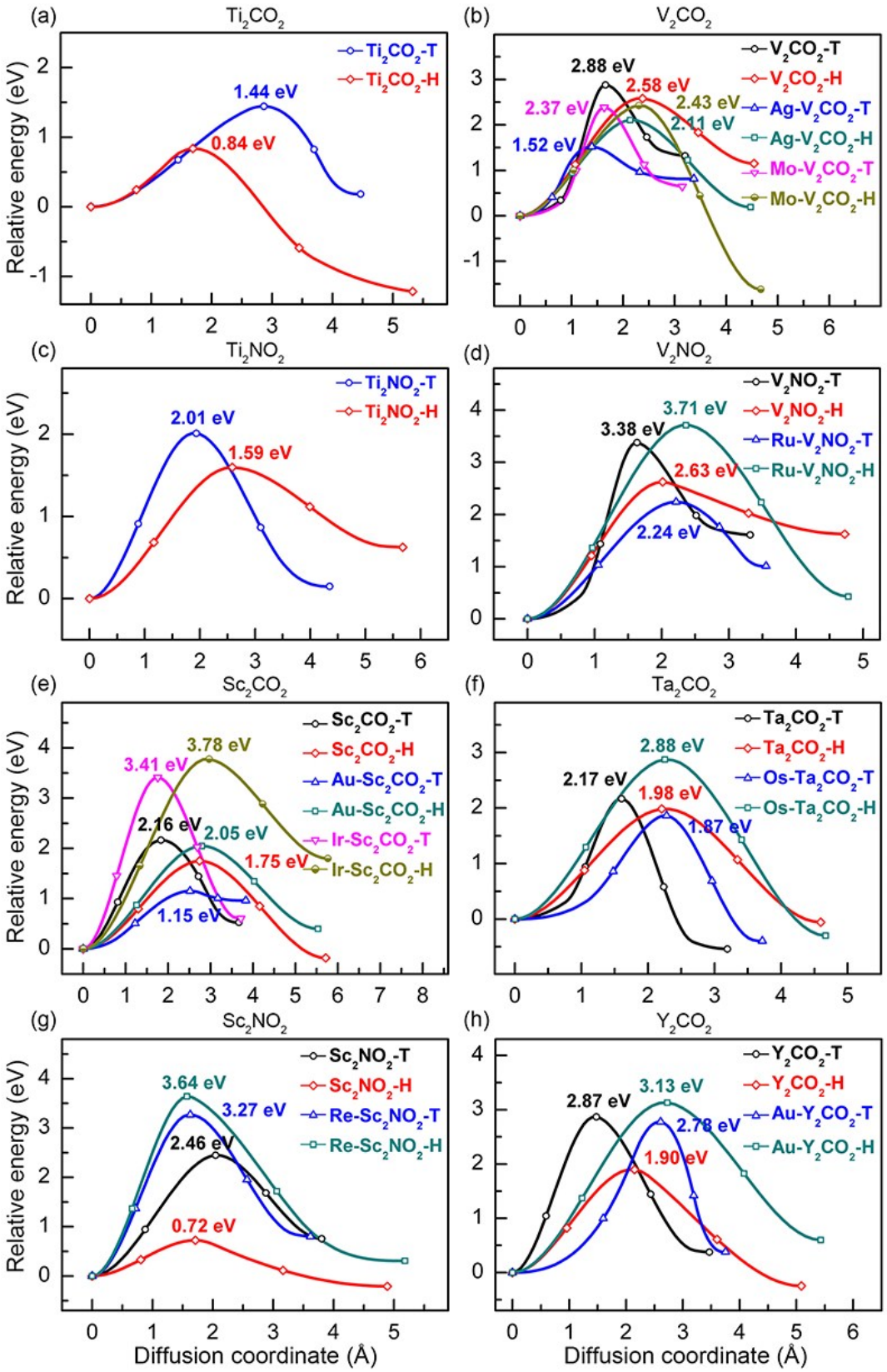

Figure S3. The transition energy barriers of materials with catalytic activity in modified MXenes (a) Ti_2CO_2, (b)V_2CO_2, Ag- and Mo-modified V_2CO_2, (c)Ti_2NO_2, (d)V_2NO_2 and Ru-modified V_2NO_2, (e) Sc_2CO_2, Au- and Ir-modified Sc_2CO_2, (f) Ta_2CO_2 and Os-modified Ta_2CO_2, (g) Sc_2NO_2 and Re-modified Sc_2NO_2, (h) Y_2CO_2 and Au-modified Y_2CO_2.The "-T" represents the Tafel reaction while the "-H" typifies the Heyrovsky reaction in the figure.

7. The Bader charge and its effect on energy barrier and ΔG_H

Table S4. Bader charge of O ion in different MXenes were calculated by Bader charge scheme. e_S represents the charge of O ion on stable site, e_T represents the charge of O ion on transition site. The value with "-" means the ion gain electron comparing with isolated atom state while the value with "+" means the ion loss electron. Δe represents the charge difference between e_S and e_T ($\Delta e' = e_S - e_T$) in the table. O-H is the distance between the H atom and the O atom.

System	Reaction	Barrier (eV)	O^- ion charge (e)			O-H (Å)	H^+ ion charge (e)		
		E_A	e_S	e_T	$\Delta e'$		e_S	e_T	$\Delta e'$
Ti_2CO_2	Tafel	**1.44**	-1.30	-1.16	**0.14**	2.06	+0.65	+0.30	**0.35**
	Heyrovsky	**0.84**	-1.26	-1.16	**0.10**	3.64	+0.64	+0.34	**0.30**
Nb_2CO_2	Tafel	**1.82**	-1.29	-1.11	**0.18**	2.21	+0.63	+0.24	**0.39**
	Heyrovsky	**1.37**	-1.27	-1.14	**0.13**	3.01	+0.63	+0.29	**0.34**
Zr_2CO_2	Tafel	**1.62**	-1.38	-1.23	**0.15**	2.62	+0.67	+0.29	**0.38**
	Heyrovsky	**1.00**	-1.37	-1.25	**0.12**	3.19	+0.65	+0.33	**0.32**
Ir-Zr_2CO_2	Tafel	**0.55**	-1.35	-1.26	**0.09**	3.70	+0.64	+0.34	**0.30**
	Heyrovsky	**1.03**	-1.39	-1.26	**0.13**	3.06	+0.66	+0.31	**0.35**
Ta_2CO_2	Tafel	**2.17**	-1.32	-1.16	**0.16**	2.43	+0.66	+0.30	**0.36**
	Heyrovsky	**1.98**	-1.35	-1.20	**0.15**	3.13	+0.63	+0.29	**0.34**
Os-Ta_2CO_2	Tafel	**1.87**	-1.24	-1.15	**0.09**	3.78	+0.63	+0.30	**0.33**
	Heyrovsky	**2.88**	-1.33	-1.16	**0.17**	2.35	+0.66	+0.26	**0.40**
V_2CO_2	Tafel	**2.88**	-1.23	-0.98	**0.25**	1.91	+0.65	+0.20	**0.45**
	Heyrovsky	**2.58**	-1.24	-1.01	**0.23**	2.29	+0.64	+0.20	**0.44**
Mo-V_2CO_2	Tafel	**2.37**	-1.23	-1.04	**0.19**	3.02	+0.63	+0.24	**0.39**
	Heyrovsky	**2.46**	-1.28	-1.07	**0.21**	2.64	+0.65	+0.23	**0.42**
Ag-V_2CO_2	Tafel	**1.52**	-1.26	-1.10	**0.16**	3.73	+0.65	+0.31	**0.34**
	Heyrovsky	**2.11**	-1.32	-1.14	**0.18**	3.40	+0.62	+0.24	**0.38**
Sc_2CO_2	Tafel	**2.16**	-1.35	-1.23	**0.12**	2.91	+0.59	+0.19	**0.40**
	Heyrovsky	**1.75**	-1.38	-1.29	**0.09**	3.53	+0.64	+0.29	**0.35**
Ir-Sc_2CO_2	Tafel	**3.41**	-1.33	-1.16	**0.17**	2.44	+0.61	+0.18	**0.43**
	Heyrovsky	**3.78**	-1.34	-1.13	**0.21**	2.18	+0.61	+0.14	**0.47**
Au-Sc_2CO_2	Tafel	**1.15**	-1.34	-1.28	**0.06**	3.70	+0.56	+0.24	**0.32**
	Heyrovsky	**2.05**	-1.33	-1.23	**0.10**	3.12	+0.61	+0.22	**0.39**
Y_2CO_2	Tafel	**2.87**	-1.38	-1.27	**0.11**	2.79	+0.60	+0.15	**0.45**
	Heyrovsky	**1.90**	-1.37	-1.31	**0.06**	3.76	+0.59	+0.22	**0.37**
Au-Y_2CO_2	Tafel	**2.78**	-1.37	-1.28	**0.09**	3.28	+0.60	+0.16	**0.44**
	Heyrovsky	**3.13**	-1.35	-1.19	**0.16**	2.37	+0.58	+0.11	**0.47**
Ti_2NO_2	Tafel	**2.10**	-1.34	-1.16	**0.18**	2.21	+0.69	+0.26	**0.43**
	Heyrovsky	**1.59**	-1.27	-1.15	**0.12**	3.41	+0.62	+0.30	**0.32**
Nb_2NO_2	Tafel	**2.92**	-1.26	-1.07	**0.19**	2.14	+0.63	+0.22	**0.41**
	Heyrovsky	**2.22**	-1.24	-1.07	**0.17**	2.32	+0.61	+0.24	**0.37**
W-Nb_2NO_2	Tafel	**2.06**	-1.26	-1.11	**0.15**	2.52	+0.62	+0.27	**0.35**

	Heyrovsky	**3.18**	-1.31	-1.10	**0.21**	2.01	+0.65	+0.20	**0.45**
Ag-Nb_2NO_2	Tafel	**0.47**	-1.31	-1.23	**0.08**	3.82	+0.66	+0.38	**0.28**
	Heyrovsky	**0.91**	-1.36	-1.25	**0.11**	3.58	+0.62	+0.31	**0.31**
Re-Nb_2NO_2	Tafel	**2.03**	-1.25	-1.13	**0.12**	3.04	+0.61	+0.28	**0.33**
	Heyrovsky	**2.88**	-1.30	-1.11	**0.19**	2.21	+0.66	+0.26	**0.40**
V_2NO_2	Tafel	**3.38**	-1.24	-1.00	**0.24**	2.36	+0.66	+0.21	**0.45**
	Heyrovsky	**2.63**	-1.22	-1.02	**0.20**	2.88	+0.63	+0.21	**0.42**
Ru-V_2NO_2	Tafel	**2.24**	-1.18	-1.00	**0.18**	3.07	+0.63	+0.24	**0.39**
	Heyrovsky	**3.71**	-1.25	-0.99	**0.26**	1.94	+0.65	+0.15	**0.50**
Sc_2NO_2	Tafel	**2.46**	-1.36	-1.25	**0.11**	2.81	+0.63	+0.26	**0.37**
	Heyrovsky	**0.72**	-1.36	-1.30	**0.06**	3.63	+0.59	+0.28	**0.31**
Re-Sc_2NO_2	Tafel	**3.27**	-1.36	-1.17	**0.19**	2.69	+0.63	+0.21	**0.42**
	Heyrovsky	**3.64**	-1.34	-1.13	**0.21**	2.04	+0.62	+0.17	**0.46**

Table S5. e_O is the charge on O^- ion, the Δe is the charge difference of O^- ion before and after the addition of single transition metal atom ($\Delta e = e_O - e_{TM-O}$), meanwhile, the difference of ΔG_H defined as $\Delta G_{H-TM-O} - \Delta G_{H-o}$.

System	Site	e_O (e)	Δe (e)	ΔG_H/eV	ΔG_H difference between TM-modified and pristine system
		Without H absorbed			
Zr_2CO_2		-1.25		0.81	
Ir-Zr_2CO_2	S_0	-1.16	-0.09	0.15	-0.66
	S_1	-1.18	-0.07	0.18	-0.63
	S_2	-1.18	-0.07	0.11	-0.70
Re-Zr_2CO_2	S_0	-1.18	-0.07	0.18	-0.63
Ta_2CO_2		-1.16		0.63	
Os-Ta_2CO_2	S_0	-1.08	-0.08	0.05	-0.58
	S_1	-1.11	-0.05	-0.38	-1.01
	S_2	-1.10	-0.06	-0.03	-0.66
V_2CO_2		-0.97		-0.43	
W-V_2CO_2	S_1	-1.04	0.07	-0.10	0.33
Mo-V_2CO_2	S_0	-1.03	0.06	-0.31	0.12
	S_1	-1.02	0.05	-0.09	0.34
	S_2	-1.01	0.04	-0.01	0.42
Os-V_2CO_2	S_2	-1.01	0.04	-0.09	0.34
Ru-V_2NO_2	S_2	-1.00	0.03	-0.16	0.27
Ag-V_2CO_2	S_0	-1.07	0.10	-0.17	0.26
	S_1	-1.05	0.08	-0.20	0.23
	S_2	-1.06	0.09	-0.17	0.26
Sc_2CO_2		-1.29		0.36	
Os-Sc_2CO_2	S_0	-1.15	-0.14	0.12	-0.24

Ru-Sc_2NO_2	S_0	-1.20	-0.09	-0.14	-0.50
Pt-Sc_2CO_2	S_2	-1.26	-0.03	-0.10	-0.46
Ir-Sc_2CO_2	S_0	-1.12	-0.17	-0.27	-0.63
	S_1	-1.20	-0.09	0.07	-0.29
	S_2	-1.16	-0.13	-0.02	-0.38
Au-Sc_2CO_2	S_0	-1.25	-0.04	-0.34	-0.70
	S_1	-1.24	-0.05	-0.07	-0.43
	S_2	-1.28	-0.01	-0.07	-0.43
Y_2CO_2		-1.31		0.87	
Pt-Y_2CO_2	S_0	-1.25	-0.06	0.17	-0.70
Pd-Y_2CO_2	S_2	-1.28	-0.03	0.18	-0.69
Ru-Y_2CO_2	S_0	-1.25	-0.06	-0.19	-1.06
Ir-Y_2CO_2	S_0	-1.18	-0.13	0.03	-0.84
Ag-Y_2CO_2	S_1	-1.28	-0.03	0.04	-0.83
Au-Y_2CO_2	S_0	-1.27	-0.04	-0.35	-1.22
	S_1	-1.28	-0.03	-0.14	-1.01
	S_2	-1.29	-0.02	-0.09	-0.96
Ta_2NO_2		-1.18		0.45	
Mo-Ta_2NO_2	S_0	-1.16	-0.02	-0.12	-0.57
Rh-Ta_2NO_2	S_0	-1.15	-0.03	-0.16	-0.61
Re-Ta_2NO_2	S_0	-1.10	-0.08	-0.04	-0.49
V_2NO_2		-1.00		-0.26	
W-V_2NO_2	S_2	-1.06	0.06	-0.08	0.18
Mo-V_2NO_2	S_1	-1.09	0.09	0.05	0.31
Ir-V_2NO_2	S_0	-1.01	0.01	-0.19	0.07
Rh-V_2NO_2	S_0	-1.00	0.00	-0.02	0.24
Ru-V_2NO_2	S_0	-1.07	0.07	0.21	0.47
	S_1	-1.03	0.03	-0.12	0.14
	S_2	-1.05	0.05	-0.03	0.23
Sc_2NO_2		-1.11		-0.95	
Mo-Sc_2NO_2	S_2	-1.19	0.08	0.18	1.13
Re-Sc_2NO_2	S_0	-1.18	0.07	0.74	1.69
	S_1	-1.15	0.04	-0.07	0.88
	S_2	-1.16	0.05	-0.08	0.87

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