Supporting Information

DFT insight into the stability of single metal atoms on Mo-based *o*-MXenes driven by the ligand effect

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The equation for the average electronegativity

The average electronegativity of PGM-MXene is evaluated using the following formula:

$$\chi_{avg} = (n_{Mo}\times\chi_{Mo} + n_{M''}\times\chi_{M''} + n_{C}\times\chi_{C} + n_{PGM}\times\chi_{PGM})/n \quad \text{(S1)}$$

$$n = n_{Mo} + n_{M''} + n_{C} + n_{PGM} \quad \text{(S2)}$$

where χ_{Mo}, $\chi_{M''}$, χ_{C} and χ_{PGM} stand for electronegativity of Mo, M'', C and PGM atom.

Figure Captions

Table Captions

Table S1. The comparison of lattice parameters a and bond lengths d for $MoTi_2C_3$ and Mo_2TiC_2.

Table S2. Binding energy E_b, formation energy E_f and energy difference ΔE_{diff} of PGM modified MXene.

Table S3. d band width W_d of PGM. Average Electronegativity χ_{avg} of PGM-MXene. d band center ε_d of PGM. Mulliken charge of PGM_I. The number of d valence electrons N_d of PGM. p band center ε_p of C atom that coordinate with PGM_I. Binding energy E_b of PGM_I. Adsorption energy E_{ads} of CO, CH_3 and NH_3 for PGM_I modified MXene.

Figure Captions

Figure S1. (a) Binding energy E_b of PGM on o-$Mo_2M"_2C_3$. (b) Binding energy E_b of PGM on o-$Mo_2M"C_2$. (c) Energy difference ΔE_{diff} between PGM_{IV} and PGM_V on $Mo_2M"_2C_3$ and $Mo_2M"C_2$. (d) The E_b difference between the strained system and the pristine system ΔE_{b1} and the E_b difference between the o-MXenes system and the strained system ΔE_{b2} of PGM_I.

Figure S2. (a) Formation energy E_f of PGM on o-$Mo_2M"_2C_3$. (b) Formation energy E_f of PGM on o-$Mo_2M"C_2$.

Figure S3. (a) Three possible adsorption sites for O, where $O_{M"}$ represents O adsorbed at a metal vacancy, O_C represents O adsorbed at a C vacancy, and O_{mix} denotes O adsorbed at metal vacancy and C vacancy respectively. (b) The atomic configurations of PGM-functionalized $Mo_2M"_2C_3O_2$, Model IV (dimer) and Model V(two single atoms). (c) The adsorption energies E_{ads}(O) on $Mo_2M"_2C_3$, wherein O adsorbed at different positions. (d) The adsorption energies E_{ads}(O) on $Mo_2M"C_2$, wherein O adsorbed at different positions. (e) Energy difference ΔE_{diff} between PGM_{IV} and PGM_V on $Mo_2M"_2C_3O_2$. (f) Energy difference ΔE_{diff} between PGM_{IV} and PGM_V on $Mo_2M"C_2O_2$.

Figure S4. (a) PDOS and COHP of Pt_I on o-$Mo_2M"_2C_3$. (b) PDOS and COHP of Pt_I on o-$Mo_2M"C_2$. (c) PDOS of PGM_I on Mo_4C_3 and $Mo_2Ti_2C_3$. (d) PDOS of PGM_I on Mo_3C_2 and Mo_2TiC_2.

Figure S5. (a) CDD of Pt_I on *o*-$Mo_2M"_2C_3$. (b) ELF of Pt_I on *o*-$Mo_2M"_2C_3$. (c) CDD of Pt_I on *o*-$Mo_2M"C_2$. (d) ELF of Pt_I on *o*-$Mo_2M"C_2$.

Figure S6. (a) CDD of PGM_I on Mo_4C_3 and $Mo_2Ti_2C_3$. (b) ELF of PGM_I on Mo_4C_3 and $Mo_2Ti_2C_3$.

Figure S7. (a) CDD of PGM_I on Mo_3C_2 and Mo_2TiC_2. (b) ELF of PGM_I on Mo_3C_2 and Mo_2TiC_2.

Figure S8. (a) The linear fitting between descriptor δ and the E_b of Ru_I, Rh_I, Pd_I, Os_I, Ir_I and Pt_I. Wherein δ is defined as the difference between the *p* band center (ε_p) of the C atoms adjacent to the PGM and the *d* band center (ε_d) of the PGM atom. (b) The linear fitting between the *d* band center ε_d and the E_b of Ru_I, Rh_I, Pd_I, Os_I, Ir_I and Pt_I.

Figure S9. The linear fittings between ML prediction and DFT evaluation when considering the *d* band center ε_d as the sole input.

Table S1. The comparison of lattice parameters *a* and bond lengths *d* for $MoTi_2C_3$ and Mo_2TiC_2.

		Ref[42]	This work	Relative difference
a (Å)	$Mo_2Ti_2C_3$	2.96	3.07	3.7%
	Mo_2TiC_2	2.94	3.04	3.4%
d(Mo-C) (Å)	$Mo_2Ti_2C_3$	2.13	2.10	1.4%
	Mo_2TiC_2	2.02	2.10	4.0%
d(Ti-C) (Å)	$Mo_2Ti_2C_3$	2.11	2.20	4.3%
	Mo_2TiC_2	2.26	2.15	4.9%

Table S2. Binding energy E_b, formation energy E_f and energy difference ΔE_{diff} of PGM modified MXene.

Systems	E_b (eV)			E_f (eV)			ΔE_{diff}
	PGM_I	PGM_{II}	PGM_{III}	PGM_I	PGM_{II}	PGM_{III}	(eV)
Mo_4C_3-Ru	–6.64	–5.68	–5.56	–0.13	0.95	0.83	0.07
$Mo_2Ti_2C_3$-Ru	–8.40	–5.71	–5.58	–1.89	0.94	0.80	–0.07
$Mo_2Zr_2C_3$-Ru	–7.91	–5.71	–5.60	–1.39	0.91	0.80	–0.05
$Mo_2Hf_2C_3$-Ru	–8.05	–5.73	–5.56	–1.54	0.96	0.78	–0.07
$Mo_2V_2C_3$-Ru	–8.00	–5.62	–5.45	–1.48	1.07	0.89	–0.09
$Mo_2Nb_2C_3$-Ru	–7.93	–5.46	–5.36	–1.42	1.16	1.05	0.004
$Mo_2Ta_2C_3$-Ru	–7.78	–5.49	–5.38	–1.27	1.13	1.03	0.004
Mo_3C_2-Ru	–7.21	–5.70	–5.49	–0.70	0.82	1.03	–0.07
Mo_2TiC_2-Ru	–8.98	–5.76	–5.55	–2.47	0.75	0.97	–0.02
Mo_2ZrC_2-Ru	–8.25	–5.73	–5.60	–1.73	0.78	0.91	–0.05
Mo_2HfC_2-Ru	–8.43	–5.67	–5.46	–1.92	0.84	1.05	–0.05
Mo_2VC_2-Ru	–8.19	–5.71	–5.50	–1.68	0.81	1.01	–0.06
Mo_2NbC_2-Ru	–8.03	–5.62	–5.43	–1.51	0.89	1.08	–0.08
Mo_2TaC_2-Ru	–7.98	–5.64	–5.42	–1.47	0.88	1.09	–0.09
Mo_4C_3-Rh	–5.99	–5.43	–5.26	–0.50	0.23	0.06	0.03
$Mo_2Ti_2C_3$-Rh	–7.55	–5.33	–5.12	–2.06	0.37	0.16	–0.20
$Mo_2Zr_2C_3$-Rh	–7.25	–5.35	–5.15	–1.77	0.34	0.14	–0.14
$Mo_2Hf_2C_3$-Rh	–7.34	–5.35	–5.12	–1.85	0.37	0.13	–0.18
$Mo_2V_2C_3$-Rh	–7.02	–5.30	–5.09	–1.53	0.40	0.18	–0.20
$Mo_2Nb_2C_3$-Rh	–6.98	–5.24	–5.08	–1.49	0.41	0.25	–0.01
$Mo_2Ta_2C_3$-Rh	–6.77	–5.26	–5.10	–1.28	0.39	0.23	–0.01
Mo_3C_2-Rh	–6.37	–5.39	–5.14	–0.88	0.10	0.35	–0.15
Mo_2TiC_2-Rh	–7.97	–5.36	–5.10	–2.49	0.13	0.39	–0.13
Mo_2ZrC_2-Rh	–7.46	–5.36	–5.15	–1.97	0.13	0.34	–0.14
Mo_2HfC_2-Rh	–7.57	–5.28	–5.03	–2.09	0.21	0.46	–0.16
Mo_2VC_2-Rh	–7.22	–5.34	–5.10	–1.73	0.15	0.39	–0.17
Mo_2NbC_2-Rh	–7.13	–5.29	–5.05	–1.65	0.19	0.43	–0.15
Mo_2TaC_2-Rh	–7.03	–5.30	–5.05	–1.55	0.18	0.44	–0.14
Mo_4C_3-Pd	–4.06	–4.06	–3.91	–0.53	–0.39	–0.53	–0.08
$Mo_2Ti_2C_3$-Pd	–5.20	–3.88	–3.67	–1.68	–0.15	–0.35	–0.36
$Mo_2Zr_2C_3$-Pd	–5.06	–3.90	–3.70	–1.53	–0.17	–0.38	–0.28
$Mo_2Hf_2C_3$-Pd	–5.09	–3.90	–3.68	–1.56	–0.15	–0.37	–0.32
$Mo_2V_2C_3$-Pd	–4.65	–3.92	–3.74	–1.12	–0.22	–0.39	–0.33
$Mo_2Nb_2C_3$-Pd	–4.46	–3.94	–3.79	–0.93	–0.27	–0.41	–0.05
$Mo_2Ta_2C_3$-Pd	–4.21	–3.94	–3.82	–0.68	–0.29	–0.42	–0.05
Mo_3C_2-Pd	–4.24	–4.01	–3.79	–0.71	–0.48	–0.26	–0.28
Mo_2TiC_2-Pd	–5.41	–3.87	–3.66	–1.88	–0.34	–0.13	–0.26
Mo_2ZrC_2-Pd	–5.15	–3.90	–3.70	–1.63	–0.38	–0.17	–0.27
Mo_2HfC_2-Pd	–5.17	–3.80	–3.59	–1.64	–0.28	–0.07	–0.27
Mo_2VC_2-Pd	–4.82	–3.90	–3.71	–1.30	–0.38	–0.18	–0.30

Mo_2NbC_2-Pd	–4.78	–3.91	–3.70	–1.25	–0.39	–0.17	–0.19
Mo_2TaC_2-Pd	–4.63	–3.92	–3.70	–1.11	–0.40	–0.17	–0.17
Mo_4C_3-Os	–7.39	–6.49	–6.37	0.55	1.57	1.44	-
$Mo_2Ti_2C_3$-Os	–9.41	–6.60	–6.47	–1.48	1.47	1.34	–0.07
$Mo_2Zr_2C_3$-Os	–8.78	–6.60	–6.52	–0.84	1.42	1.34	–0.09
$Mo_2Hf_2C_3$-Os	–8.95	–6.62	–6.46	–1.01	1.47	1.32	–0.10
$Mo_2V_2C_3$-Os	–8.97	–6.43	–6.24	–1.03	1.70	1.51	–0.11
$Mo_2Nb_2C_3$-Os	–8.71	–6.25	–6.17	–0.77	1.77	1.69	–0.05
$Mo_2Ta_2C_3$-Os	–8.53	–6.27	–6.19	–0.60	1.74	1.67	–0.06
Mo_3C_2-Os	–8.01	–6.54	–6.30	–0.07	1.40	1.63	–0.11
Mo_2TiC_2-Os	–10.11	–6.64	–6.40	–2.18	1.29	1.54	–0.06
Mo_2ZrC_2-Os	–9.23	–6.62	–6.49	–1.29	1.31	1.45	–0.07
Mo_2HfC_2-Os	–9.45	–6.56	–6.35	–1.51	1.37	1.59	–0.06
Mo_2VC_2-Os	–9.21	–6.55	–6.31	–1.28	1.39	1.63	–0.08
Mo_2NbC_2-Os	–8.90	–6.45	–6.26	–0.96	1.48	1.67	–0.12
Mo_2TaC_2-Os	–8.85	–6.47	–6.25	–0.91	1.47	1.69	–0.12
Mo_4C_3-Ir	–7.04	–6.59	–6.39	–0.01	0.63	0.43	0.11
$Mo_2Ti_2C_3$-Ir	–8.87	–6.58	–6.35	–1.85	0.67	0.44	–0.22
$Mo_2Zr_2C_3$-Ir	–8.44	–6.59	–6.40	–1.41	0.62	0.43	–0.15
$Mo_2Hf_2C_3$-Ir	–8.53	–6.60	–6.36	–1.51	0.66	0.42	–0.18
$Mo_2V_2C_3$-Ir	–8.29	–6.49	–6.22	–1.27	0.80	0.53	–0.24
$Mo_2Nb_2C_3$-Ir	–8.08	–6.39	–6.23	–1.06	0.79	0.63	–0.05
$Mo_2Ta_2C_3$-Ir	–7.84	–6.41	–6.26	–0.81	0.77	0.62	–0.06
Mo_3C_2-Ir	–7.43	–6.58	–6.27	–0.40	0.45	0.75	–0.21
Mo_2TiC_2-Ir	–9.46	–6.62	–6.30	–2.43	0.40	0.72	–0.18
Mo_2ZrC_2-Ir	–8.73	–6.60	–6.38	–1.71	0.42	0.65	–0.18
Mo_2HfC_2-Ir	–8.90	–6.54	–6.25	–1.88	0.49	0.77	–0.19
Mo_2VC_2-Ir	–8.55	–6.54	–6.24	–1.53	0.48	0.78	–0.21
Mo_2NbC_2-Ir	–8.30	–6.49	–6.22	–1.27	0.53	0.81	–0.19
Mo_2TaC_2-Ir	–8.18	–6.50	–6.21	–1.16	0.52	0.81	–0.19
Mo_4C_3-Pt	–5.52	–5.76	–5.57	–0.40	–0.46	–0.64	–0.12
$Mo_2Ti_2C_3$-Pt	–6.95	–5.65	–5.40	–1.83	–0.28	–0.53	–0.41
$Mo_2Zr_2C_3$-Pt	–6.67	–5.68	–5.46	–1.55	–0.34	–0.56	–0.32
$Mo_2Hf_2C_3$-Pt	–6.72	–5.68	–5.44	–1.60	–0.32	–0.56	–0.36
$Mo_2V_2C_3$-Pt	–6.34	–5.64	–5.39	–1.22	–0.27	–0.52	–0.43
$Mo_2Nb_2C_3$-Pt	–5.93	–5.65	–5.49	–0.81	–0.37	–0.53	–0.18
$Mo_2Ta_2C_3$-Pt	–5.63	–5.65	–5.51	–0.51	–0.40	–0.53	–0.21
Mo_3C_2-Pt	–5.70	–5.71	–5.42	–0.58	–0.59	–0.31	–0.40
Mo_2TiC_2-Pt	–7.33	–5.64	–5.34	–2.21	–0.52	–0.23	–0.33
Mo_2ZrC_2-Pt	–6.95	–5.79	–5.34	–1.83	–0.67	–0.42	–0.33
Mo_2HfC_2-Pt	–7.02	–5.69	–5.42	–1.91	–0.57	–0.30	–0.33
Mo_2VC_2-Pt	–6.57	–5.63	–5.35	–1.45	–0.51	–0.23	–0.39
Mo_2NbC_2-Pt	–6.37	–5.64	–5.37	–1.25	–0.53	–0.25	–0.29
Mo_2TaC_2-Pt	–6.20	–5.65	–5.37	–1.08	–0.53	–0.25	–0.29

Table S3. *d* band width W_d of PGM_I. Average Electronegativity χ_{avg} of PGM-MXene. *d* band center ε_d of PGM_I. Mulliken charge Q_{PGM} of PGM_I. The number of *d* valence electrons N_d of PGM_I. *p* band center ε_p of C atom that coordinate with PGM_I. Binding energy E_b of PGM_I. Adsorption energy E_{ads} of CO, CH_3 and NH_3 for PGM_I modified MXene.

Systems	W_d	χ_{avg}	ε_d	Q_{PGM}	N_d	ε_p	E_b	E_{ads}		
								CO	CH_3	NH_3
Mo_4C_3-Ru	9.96	2.33	–2.30	–0.061	7	–5.53	–6.64	–6.12	–6.14	–5.06
$Mo_2Ti_2C_3$-Ru	8.51	2.15	–1.61	–0.152	7	–4.24	–8.40	–5.20	–5.00	–4.03
$Mo_2Zr_2C_3$-Ru	7.82	2.09	–1.50	–0.181	7	–4.07	–7.91	–5.51	–5.36	–4.36
$Mo_2Hf_2C_3$-Ru	8.26	2.08	–1.51	–0.247	7	–4.16	–8.05	–5.28	–5.55	–4.13
$Mo_2V_2C_3$-Ru	8.84	2.18	–1.96	–0.131	7	–5.06	–8.00	–5.78	–5.70	–4.66
$Mo_2Nb_2C_3$-Ru	8.75	2.17	–2.03	–0.106	7	–5.06	–7.93	–4.84	–4.89	–3.80
$Mo_2Ta_2C_3$-Ru	9.53	2.14	–2.11	–0.125	7	–5.29	–7.78	–4.66	–4.71	–3.63
Mo_3C_2-Ru	9.5	2.32	–1.72	–0.113	7	–5.46	–7.21	–4.98	–4.94	–3.89
Mo_2TiC_2-Ru	8.59	2.19	–1.77	–0.186	7	–4.34	–8.98	–4.45	–4.84	–3.28
Mo_2ZrC_2-Ru	8.23	2.15	–1.53	–0.195	7	–4.23	–8.25	–4.98	–5.22	–3.82
Mo_2HfC_2-Ru	8.88	2.14	–1.57	–0.266	7	–4.32	–8.43	–4.75	–5.10	–3.58
Mo_2VC_2-Ru	8.99	2.21	–1.79	–0.138	7	–4.87	–8.19	–4.83	–5.21	–3.70
Mo_2NbC_2-Ru	9.09	2.20	–1.70	–0.145	7	–5.00	–8.03	–4.63	–4.54	–3.52
Mo_2TaC_2-Ru	9.55	2.18	–1.72	–0.167	7	–5.18	–7.98	–4.49	–4.38	–3.37
Mo_4C_3-Rh	8.84	2.33	–1.84	–0.254	8	–4.93	–5.99	–5.39	–6.24	–4.85
$Mo_2Ti_2C_3$-Rh	7.91	2.15	–1.95	–0.206	8	–4.27	–7.55	–4.73	–4.80	–3.74
$Mo_2Zr_2C_3$-Rh	7.36	2.09	–1.85	–0.234	8	–4.1	–7.25	–4.93	–5.02	–4.00
$Mo_2Hf_2C_3$-Rh	8.08	2.08	–1.88	–0.313	8	–4.2	–7.34	–4.76	–4.81	–3.81
$Mo_2V_2C_3$-Rh	8.64	2.18	–2.25	–0.196	8	–5.01	–7.02	–5.34	–5.51	–4.39
$Mo_2Nb_2C_3$-Rh	8.65	2.17	–2.42	–0.160	8	–5.12	–6.98	–4.36	–4.64	–3.49
$Mo_2Ta_2C_3$-Rh	9.51	2.14	–2.50	–0.184	8	–5.35	–6.77	–4.22	–4.48	–3.34
Mo_3C_2-Rh	9.06	2.32	–1.97	–0.178	8	–5.4	–6.37	–4.52	–4.73	–3.62
Mo_2TiC_2-Rh	8.46	2.19	–2.26	–0.250	8	–4.38	–7.97	–4.07	–4.69	–3.06
Mo_2ZrC_2-Rh	8.08	2.15	–1.99	–0.250	8	–4.27	–7.46	–4.50	–4.75	–3.53
Mo_2HfC_2-Rh	8.66	2.15	–2.05	–0.336	8	–4.38	–7.57	–4.31	–4.89	–3.32
Mo_2VC_2-Rh	8.95	2.21	–2.19	–0.202	8	–4.85	–7.22	–4.42	–4.56	–3.46
Mo_2NbC_2-Rh	8.91	2.21	–2.09	–0.197	8	–4.98	–7.13	–4.15	–4.32	–3.22
Mo_2TaC_2-Rh	9.54	2.19	–2.12	–0.221	8	–5.16	–7.03	–4.03	–4.19	–3.09
Mo_4C_3-Pd	9.19	2.33	–2.38	–0.180	10	–4.91	–4.06	–5.07	–5.32	–4.71
$Mo_2Ti_2C_3$-Pd	8.2	2.15	–2.83	–0.164	10	–4.26	–5.20	–4.02	–4.50	–3.50
$Mo_2Zr_2C_3$-Pd	7.78	2.09	–2.74	–0.162	10	–4.1	–5.06	–4.26	–4.67	–3.79
$Mo_2Hf_2C_3$-Pd	8.43	2.08	–2.78	–0.230	10	–4.21	–5.09	–4.09	–4.49	–3.60
$Mo_2V_2C_3$-Pd	8.94	2.18	–2.73	–0.188	10	–4.81	–4.65	–4.61	–5.19	–4.15
$Mo_2Nb_2C_3$-Pd	8.89	2.17	–2.83	–0.130	10	–5.07	–4.46	–3.89	–4.49	–3.43
$Mo_2Ta_2C_3$-Pd	9.75	2.14	–2.84	–0.153	10	–5.27	–4.21	–3.81	–4.41	–3.32
Mo_3C_2-Pd	9.38	2.32	–2.38	–0.159	10	–5.17	–4.24	–3.87	–4.36	–3.42
Mo_2TiC_2-Pd	8.86	2.19	–3.18	–0.222	10	–4.36	–5.41	–3.38	–3.94	–2.86

Mo_2ZrC_2-Pd	8.4	2.15	–2.76	–0.189	10	–4.27	–5.15	–3.80	–4.25	–3.30
Mo_2HfC_2-Pd	9.02	2.14	–2.89	–0.267	10	–4.39	–5.17	–3.63	–4.09	–3.11
Mo_2VC_2-Pd	9.13	2.21	–2.82	–0.189	10	–4.74	–4.82	–3.71	–4.30	–3.22
Mo_2NbC_2-Pd	9.12	2.20	–2.71	–0.161	10	–4.92	–4.78	–3.47	–4.06	–3.00
Mo_2TaC_2-Pd	9.76	2.18	–2.72	–0.182	10	–5.08	–4.63	–3.39	–3.97	–2.89
Mo_4C_3-Os	9.81	2.33	–2.62	–0.027	6	–5.7	–7.39	–6.37	–6.38	–5.06
$Mo_2Ti_2C_3$-Os	8.39	2.15	–1.75	–0.227	6	–4.42	–9.41	–5.46	–5.27	–4.06
$Mo_2Zr_2C_3$-Os	7.92	2.09	–1.65	–0.276	6	–4.26	–8.78	–5.83	–5.67	–4.44
$Mo_2Hf_2C_3$-Os	8.62	2.08	–1.66	–0.361	6	–4.35	–8.95	–5.58	–5.40	–4.19
$Mo_2V_2C_3$-Os	9.24	2.18	–2.19	–0.164	6	–5.26	–8.97	–6.01	–5.93	–4.69
$Mo_2Nb_2C_3$-Os	9.09	2.17	–2.24	–0.102	6	–5.24	–8.71	–5.14	–5.19	–3.87
$Mo_2Ta_2C_3$-Os	9.84	2.14	–2.31	–0.136	6	–5.47	–8.53	–4.95	–5.00	–3.69
Mo_3C_2-Os	9.8	2.32	–1.84	–0.160	6	–5.64	–8.01	–5.25	–5.20	–3.93
Mo_2TiC_2-Os	9.06	2.19	–1.98	–0.254	6	–4.51	–10.11	–4.64	–4.44	–3.28
Mo_2ZrC_2-Os	8.64	2.15	–1.75	–0.291	6	–4.42	–9.23	–5.25	–5.05	–3.87
Mo_2HfC_2-Os	9.22	2.14	–1.76	–0.378	6	–4.51	–9.45	–4.99	–4.78	–3.61
Mo_2VC_2-Os	9.37	2.21	–2.02	–0.182	6	–5.05	–9.21	–5.03	–4.91	–3.70
Mo_2NbC_2-Os	9.32	2.20	–1.86	–0.203	6	–5.2	–8.90	–4.89	–4.80	–3.56
Mo_2TaC_2-Os	9.91	2.18	–1.87	–0.245	6	–5.38	–8.85	–4.74	–4.65	–3.41
Mo_4C_3-Ir	9.38	2.33	–2.07	–0.302	7	–5.17	–7.04	–5.71	–6.25	–4.92
$Mo_2Ti_2C_3$-Ir	8.41	2.15	–2.17	–0.264	7	–4.45	–8.87	–5.02	–5.07	–3.74
$Mo_2Zr_2C_3$-Ir	7.96	2.09	–2.07	–0.300	7	–4.3	–8.44	–5.27	–5.34	–4.03
$Mo_2Hf_2C_3$-Ir	8.52	2.08	–2.06	–0.400	7	–4.4	–8.53	–5.10	–5.14	–3.84
$Mo_2V_2C_3$-Ir	9.24	2.18	–2.48	–0.248	7	–5.21	–8.29	–5.61	–5.78	–4.39
$Mo_2Nb_2C_3$-Ir	9.11	2.17	–2.74	–0.207	7	–5.33	–8.08	–4.63	–4.91	–3.47
$Mo_2Ta_2C_3$-Ir	9.84	2.14	–2.82	–0.241	7	–5.57	–7.84	–4.49	–4.75	–3.31
Mo_3C_2-Ir	9.56	2.32	–2.12	–0.242	7	–5.59	–7.43	–4.84	–5.03	–3.63
Mo_2TiC_2-Ir	8.93	2.19	–2.50	–0.315	7	–4.56	–9.46	–4.26	–4.58	–3.01
Mo_2ZrC_2-Ir	8.64	2.15	–2.21	–0.325	7	–4.47	–8.73	–4.80	–4.85	–3.54
Mo_2HfC_2-Ir	9.15	2.14	–2.28	–0.426	7	–4.58	–8.90	–4.58	–4.61	–3.31
Mo_2VC_2-Ir	9.39	2.21	–2.44	–0.259	7	–5.05	–8.55	–4.64	–4.79	–3.42
Mo_2NbC_2-Ir	9.22	2.20	–2.32	–0.261	7	–5.23	–8.30	–4.45	–4.61	–3.22
Mo_2TaC_2-Ir	9.97	2.18	–2.34	–0.297	7	–5.39	–8.18	–4.34	–4.48	–3.10
Mo_4C_3-Pt	9.22	2.33	–2.64	–0.271	9	–5.11	–5.52	–5.35	–5.59	–4.71
$Mo_2Ti_2C_3$-Pt	8.24	2.15	–3.35	–0.260	9	–4.44	–6.95	–4.23	–4.78	–3.38
$Mo_2Zr_2C_3$-Pt	7.94	2.09	–3.41	–0.269	9	–4.26	–6.67	–4.51	–4.99	–3.71
$Mo_2Hf_2C_3$-Pt	8.08	2.08	–3.38	–0.345	9	–4.4	–6.72	–4.35	–4.82	–3.52
$Mo_2V_2C_3$-Pt	8.82	2.18	–2.94	–0.276	9	–5.03	–6.34	–4.84	–5.47	–4.04
$Mo_2Nb_2C_3$-Pt	9.17	2.17	–3.12	–0.208	9	–5.32	–5.93	–4.13	–4.81	–3.32
$Mo_2Ta_2C_3$-Pt	9.84	2.14	–3.09	–0.241	9	–5.55	–5.63	–4.09	–4.73	–3.22
Mo_3C_2-Pt	9.45	2.32	–2.60	–0.257	9	–5.35	–5.70	–4.15	–4.67	–3.34
Mo_2TiC_2-Pt	8.82	2.19	–3.75	–0.314	9	–4.51	–7.33	–3.51	–4.13	–2.69
Mo_2ZrC_2-Pt	8.43	2.15	–3.26	–0.294	9	–4.47	–6.95	–3.94	–4.45	–3.10
Mo_2HfC_2-Pt	8.69	2.15	–3.36	–0.375	9	–4.58	–7.02	–3.74	–4.26	–2.89

Mo_2VC_2-Pt	9.12	2.21	–3.10	–0.277	9	–4.96	–6.57	–3.90	–4.53	–3.08
Mo_2NbC_2-Pt	8.76	2.21	–2.94	–0.249	9	–5.16	–6.37	–3.71	–4.35	–2.88
Mo_2TaC_2-Pt	9.65	2.19	–2.97	–0.278	9	–5.33	–6.20	–3.63	–4.25	–2.77

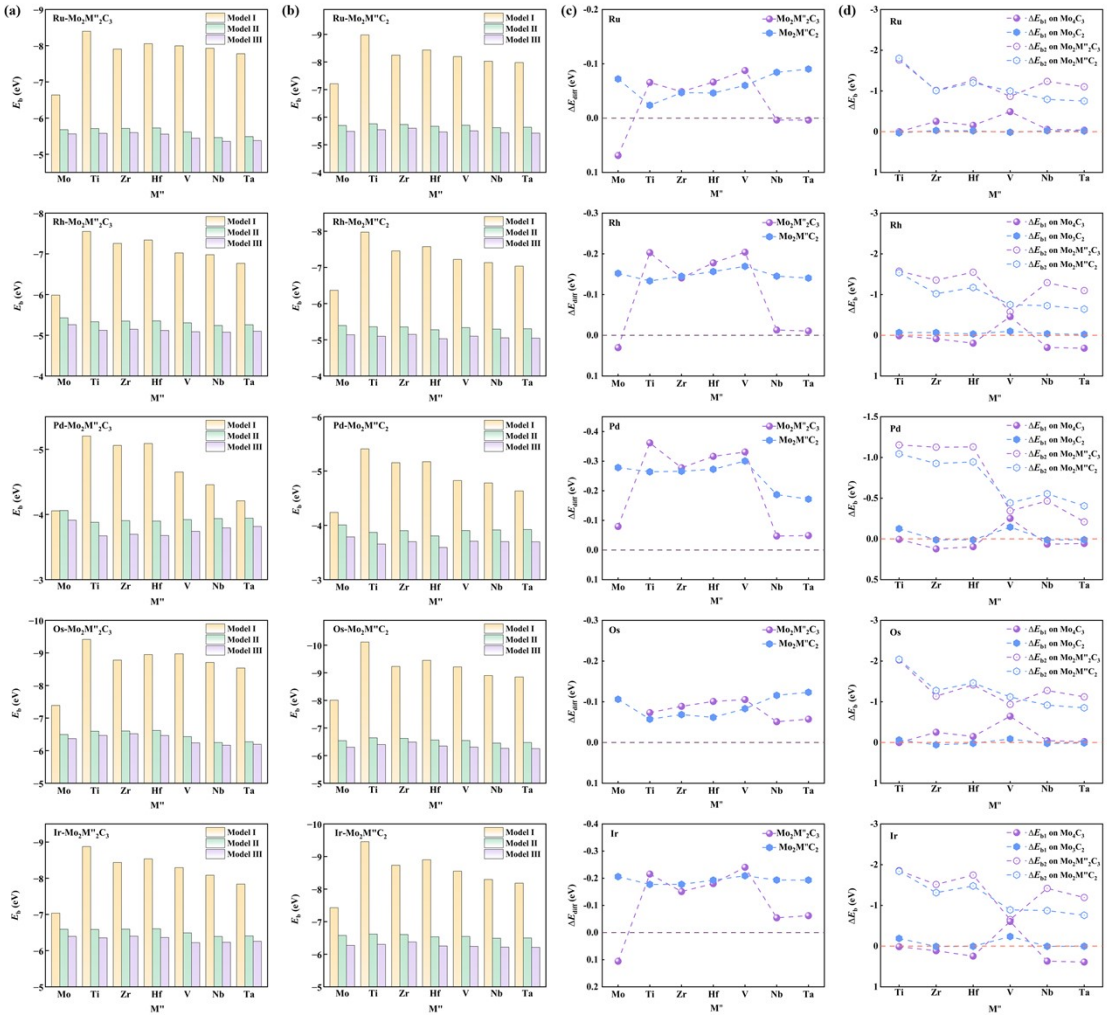

Figure S1. (a) Binding energy E_b of PGM on *o*-$Mo_2M"_2C_3$. (b) Binding energy E_b of PGM on *o*-$Mo_2M"C_2$. (c) Energy difference ΔE_{diff} between PGM_{IV} and PGM_V on $Mo_2M"_2C_3$ and $Mo_2M"C_2$. (d) The E_b difference between the strained system and the pristine system ΔE_{b1} and the E_b difference between the *o*-MXenes system and the strained system ΔE_{b2} of PGM_I.

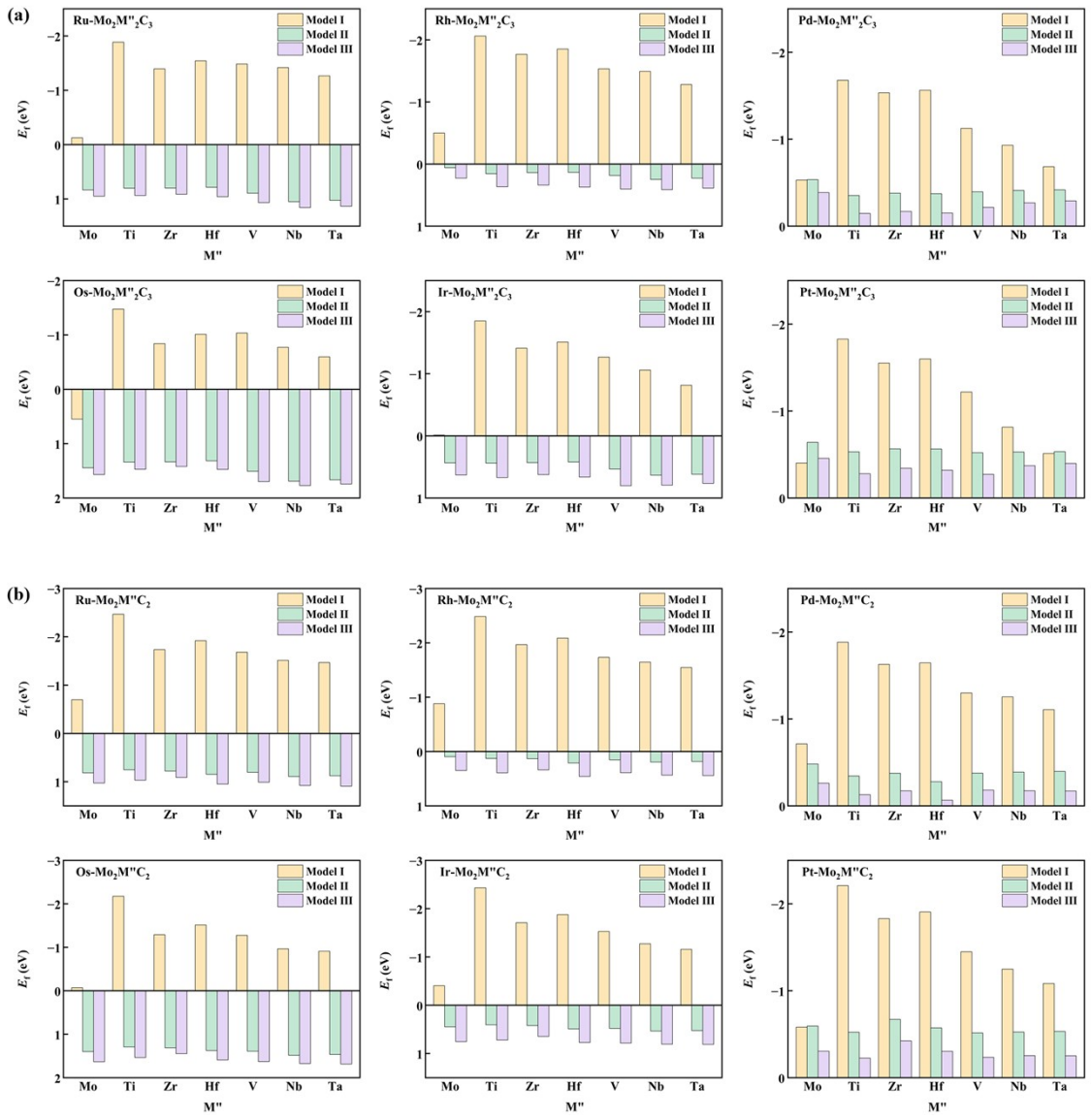

Figure S2. (a) Formation energy E_f of PGM on *o*-$Mo_2M''_2C_3$. (b) Formation energy E_f of PGM on *o*-$Mo_2M''C_2$.

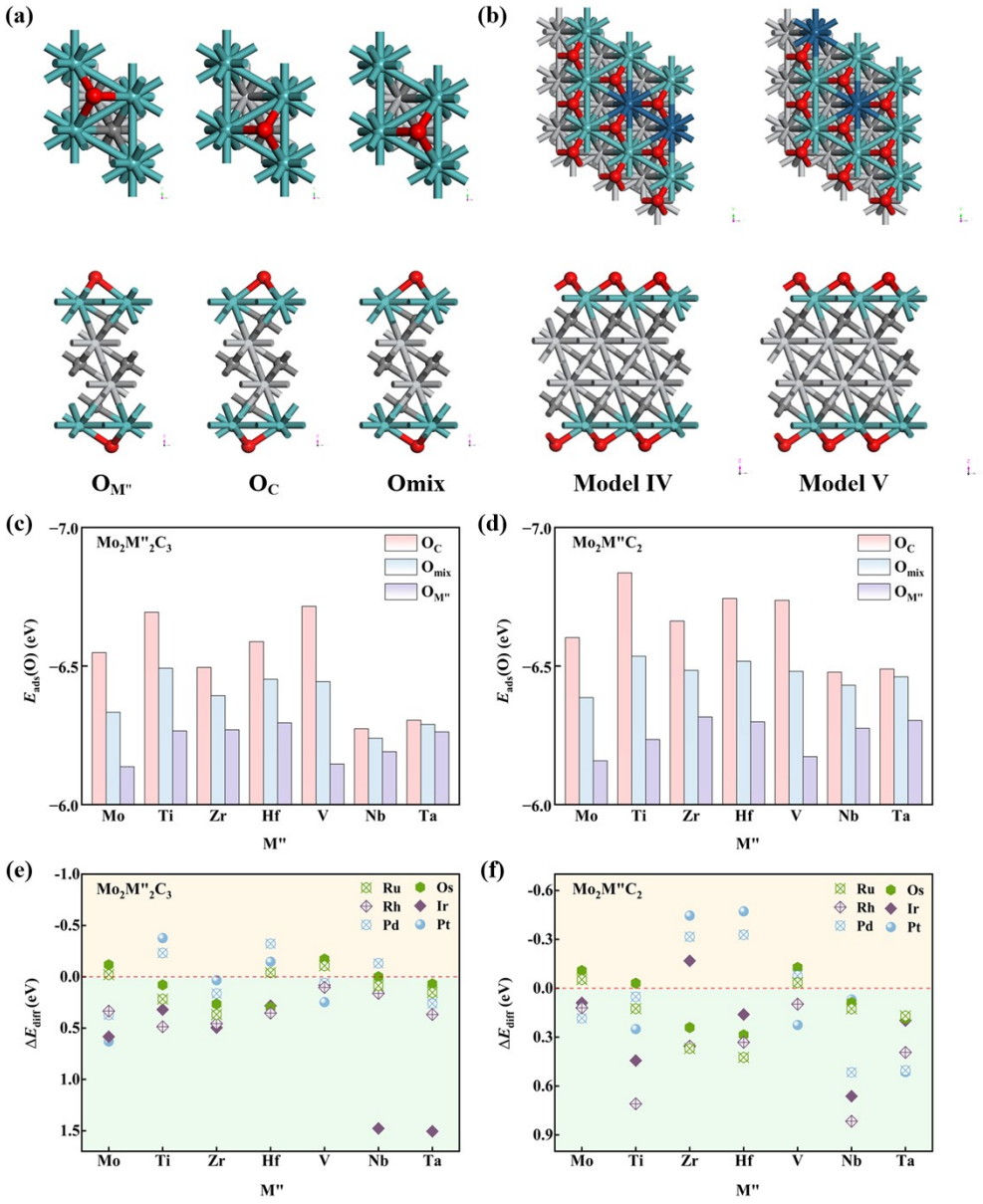

Figure S3. (a) Three possible adsorption sites for O, where $O_{M''}$ represents O adsorbed at a metal vacancy, O_C represents O adsorbed at a C vacancy, and O_{mix} denotes O adsorbed at metal vacancy and C vacancy respectively. (b) The atomic configurations of PGM-functionalized $Mo_2M''_2C_3O_2$, Model IV (dimer) and Model V(two single atoms). (c) The adsorption energies E_{ads}(O) on $Mo_2M''_2C_3$, wherein O adsorbed at different positions. (d) The adsorption energies E_{ads}(O) on $Mo_2M''C_2$, wherein O adsorbed at different positions. (e) Energy difference ΔE_{diff} between PGM_{IV} and PGM_V on $Mo_2M''_2C_3O_2$. (f) Energy difference ΔE_{diff} between PGM_{IV} and PGM_V on $Mo_2M''C_2O_2$.

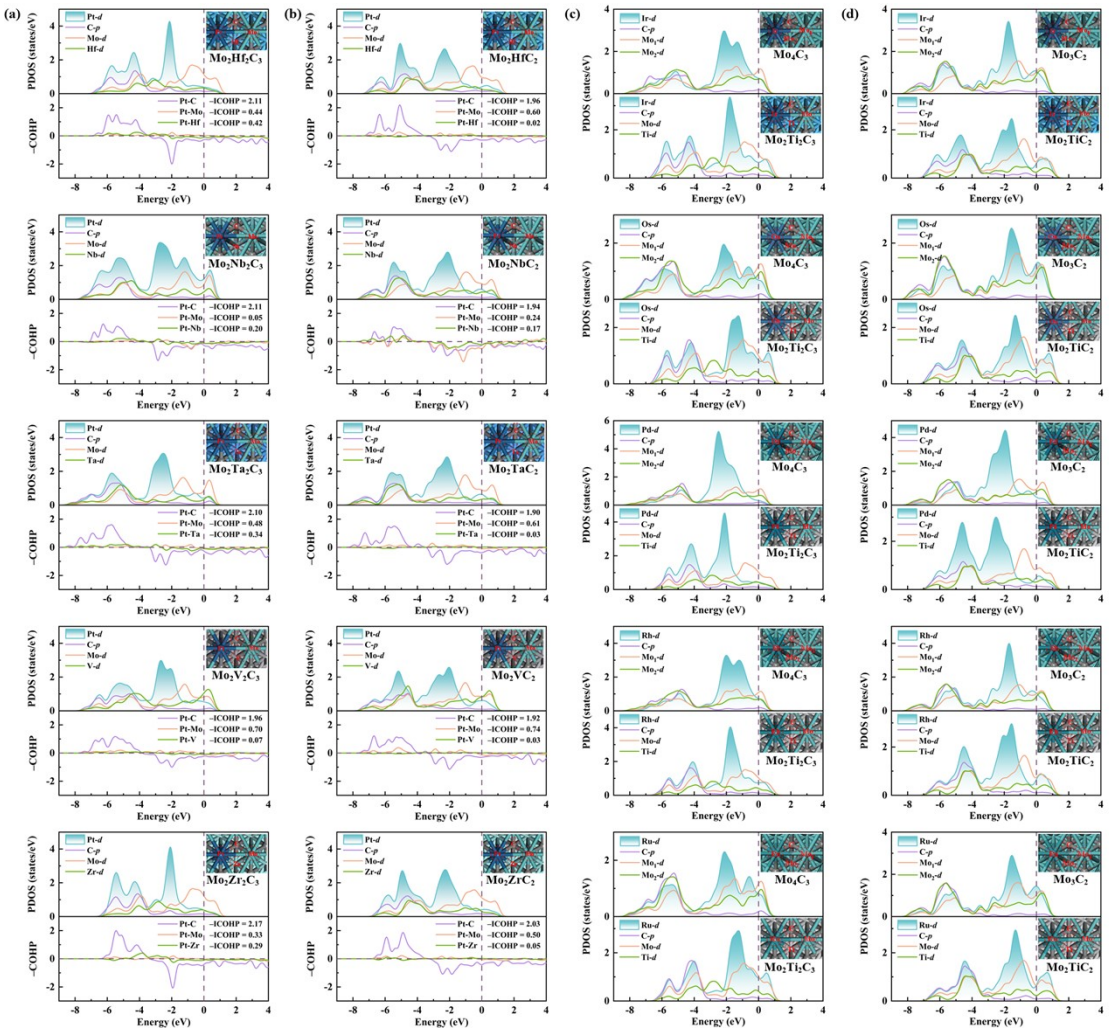

Figure S4. (a) PDOS and COHP of Pt_I on *o*-$Mo_2M''_2C_3$. (b) PDOS and COHP of Pt_I on *o*-$Mo_2M''C_2$. (c) PDOS of PGM_I on Mo_4C_3 and $Mo_2Ti_2C_3$. (d) PDOS of PGM_I on Mo_3C_2 and Mo_2TiC_2.

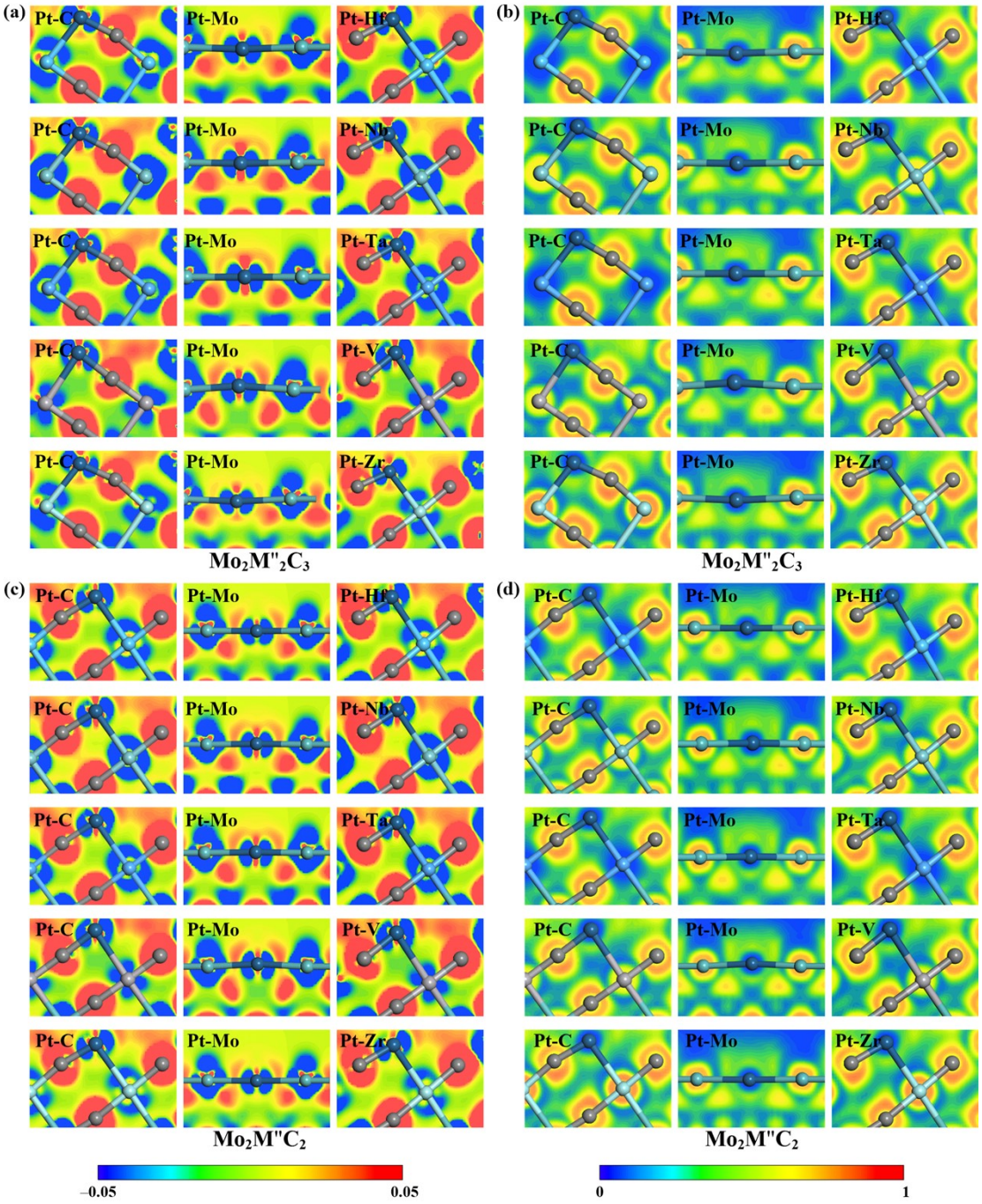

Figure S5. (a) CDD of Pt_I on *o*-$Mo_2M"_2C_3$. (b) ELF of Pt_I on *o*-$Mo_2M"_2C_3$. (c) CDD of Pt_I on *o*-$Mo_2M"C_2$. (d) ELF of Pt_I on *o*-$Mo_2M"C_2$.

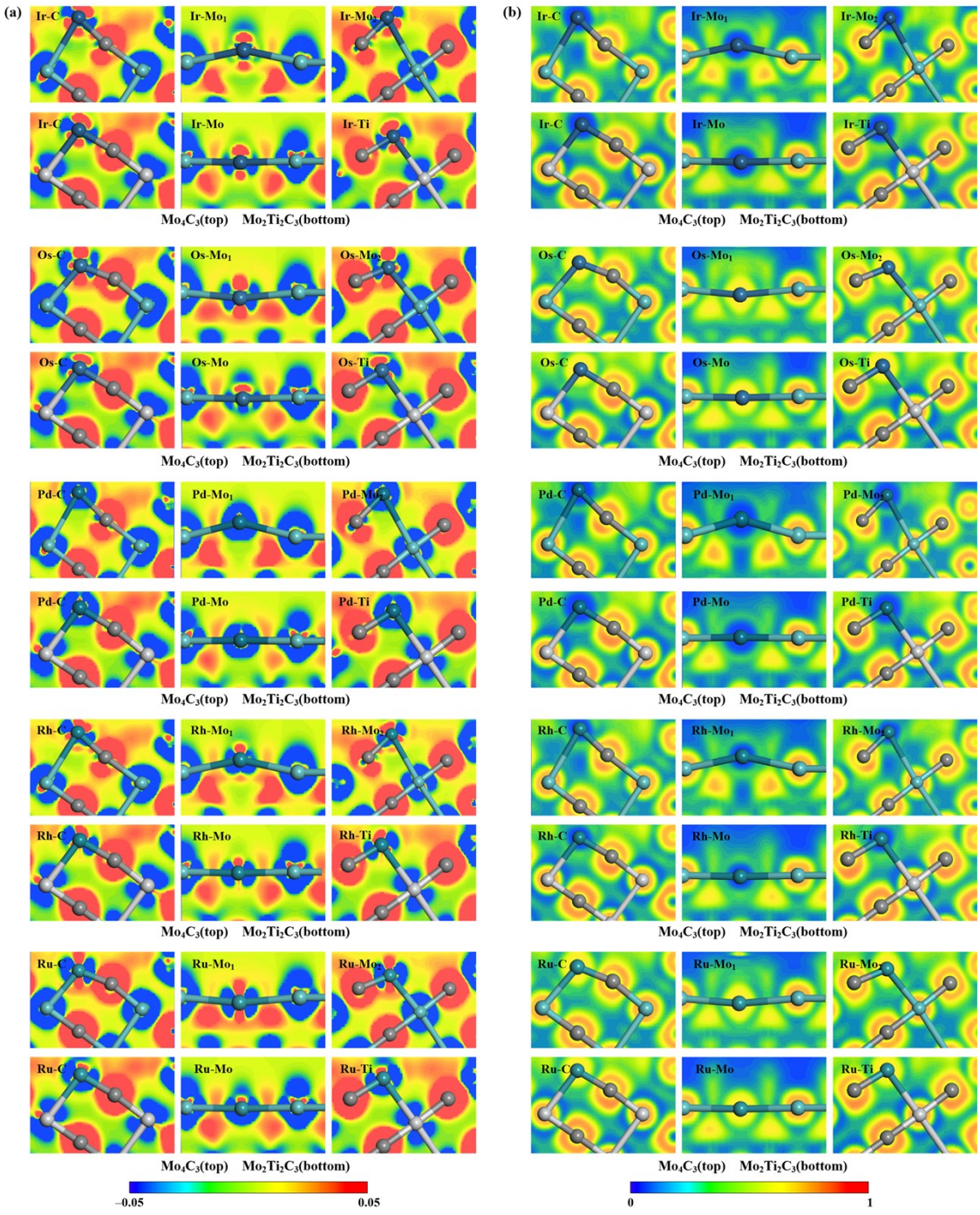

Figure S6. (a) CDD of PGM_I on Mo_4C_3 and $Mo_2Ti_2C_3$. (b) ELF of PGM_I on Mo_4C_3 and $Mo_2Ti_2C_3$.

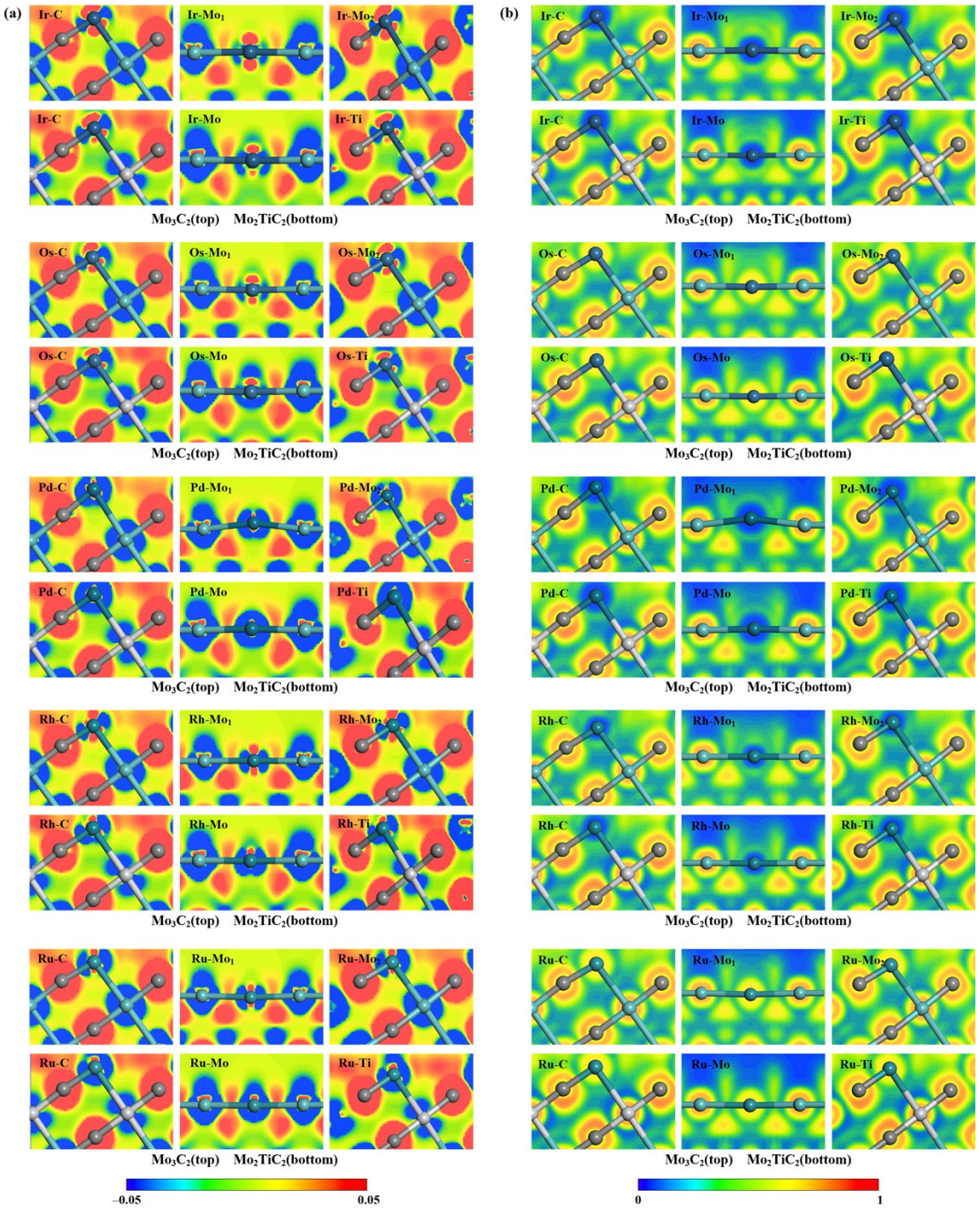

Figure S7. (a) CDD of PGM_I on Mo_3C_2 and Mo_2TiC_2. (b) ELF of PGM_I on Mo_3C_2 and Mo_2TiC_2.

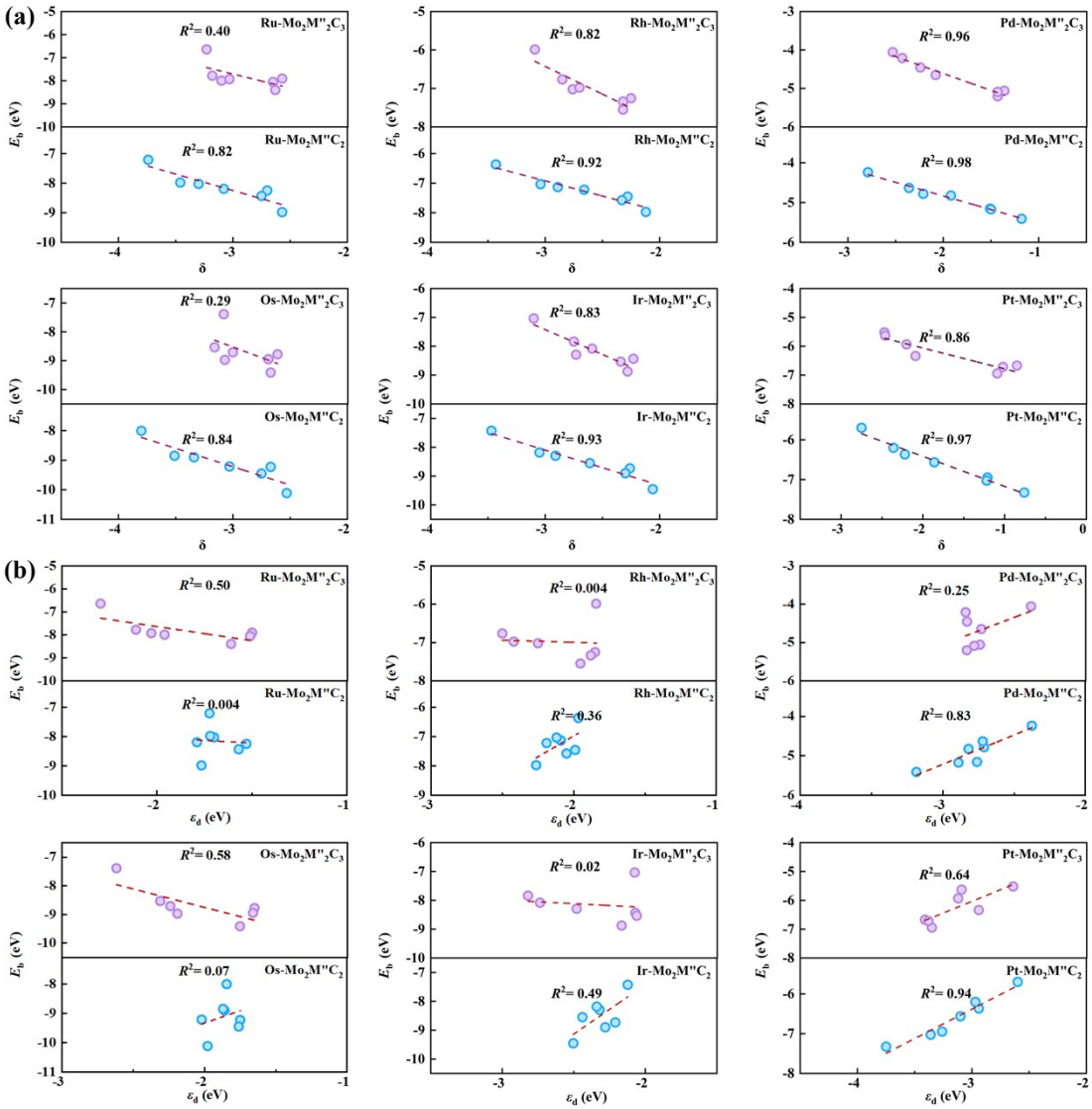

Figure S8. (a) The linear fitting between descriptor δ and the E_b of Ru_I, Rh_I, Pd_I, Os_I, Ir_I and Pt_I. Wherein δ is defined as the difference between the *p* band center (ε_p) of the C atoms adjacent to the PGM and the *d* band center (ε_d) of the PGM atom. (b) The linear fitting between the *d* band center ε_d and the E_b of Ru_I, Rh_I, Pd_I, Os_I, Ir_I and Pt_I.

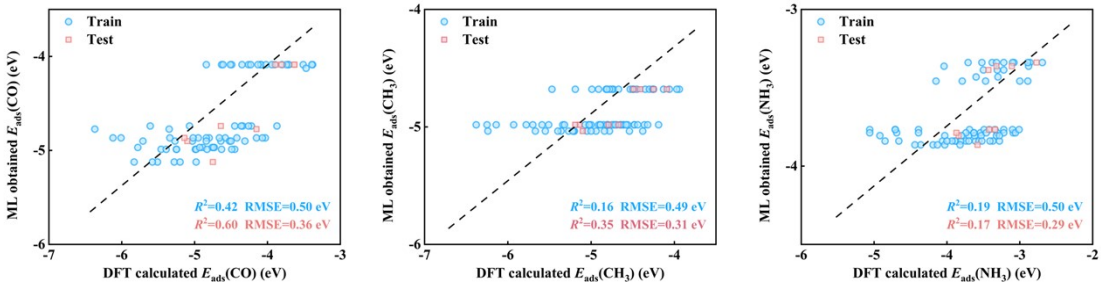

Figure S9. The linear fittings between ML prediction and DFT evaluation when considering the *d* band center ε_d as the sole input.