SUPPLEMENTARY INFORMATION
Predicting Aqueous Stability of Solid with Computed Pourbaix Diagram using SCAN Functional

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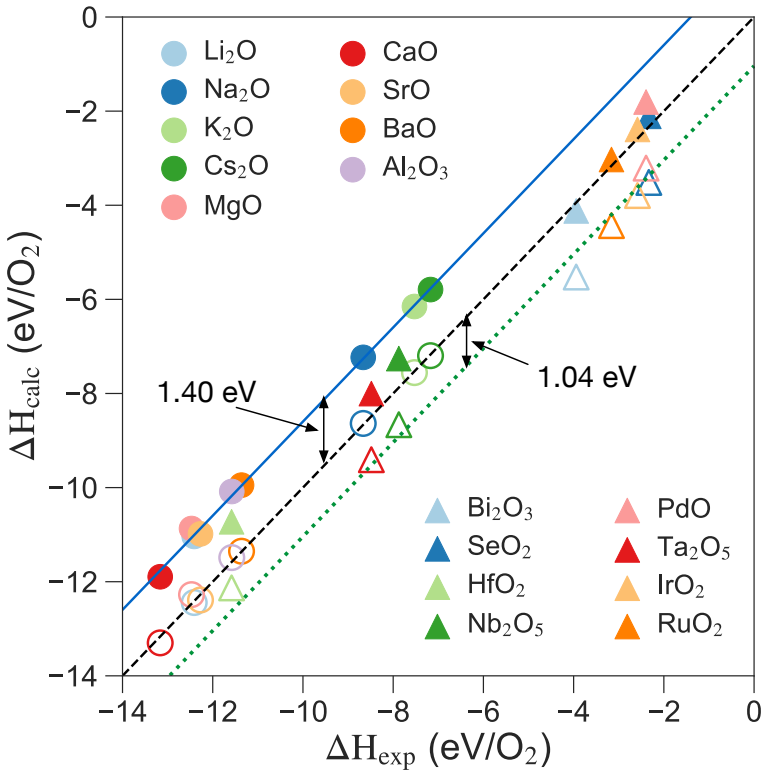
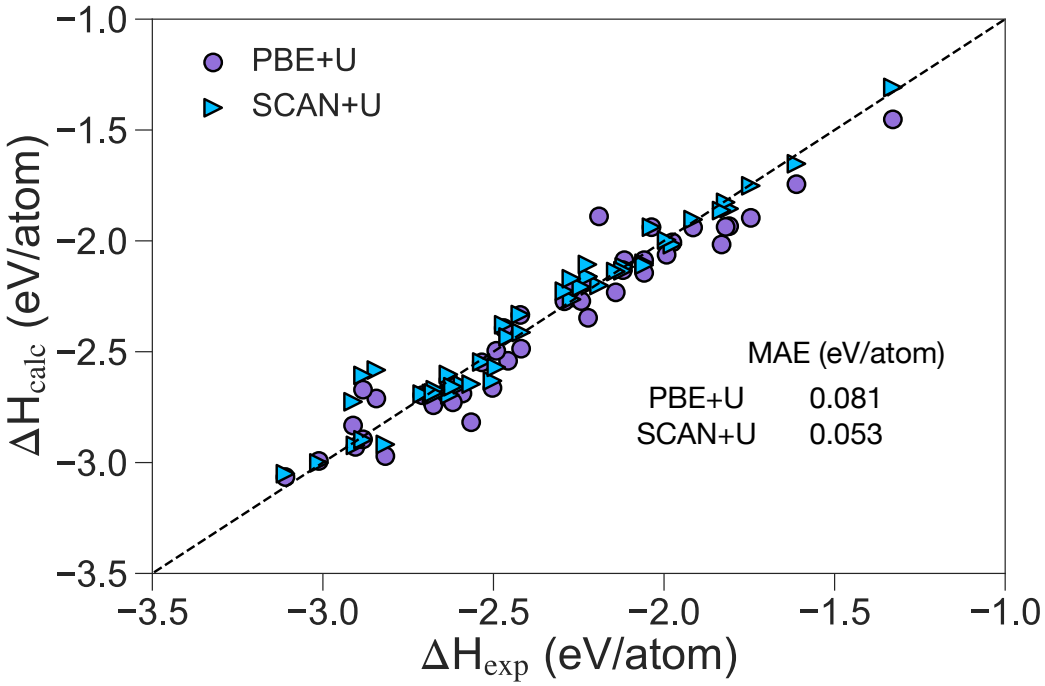


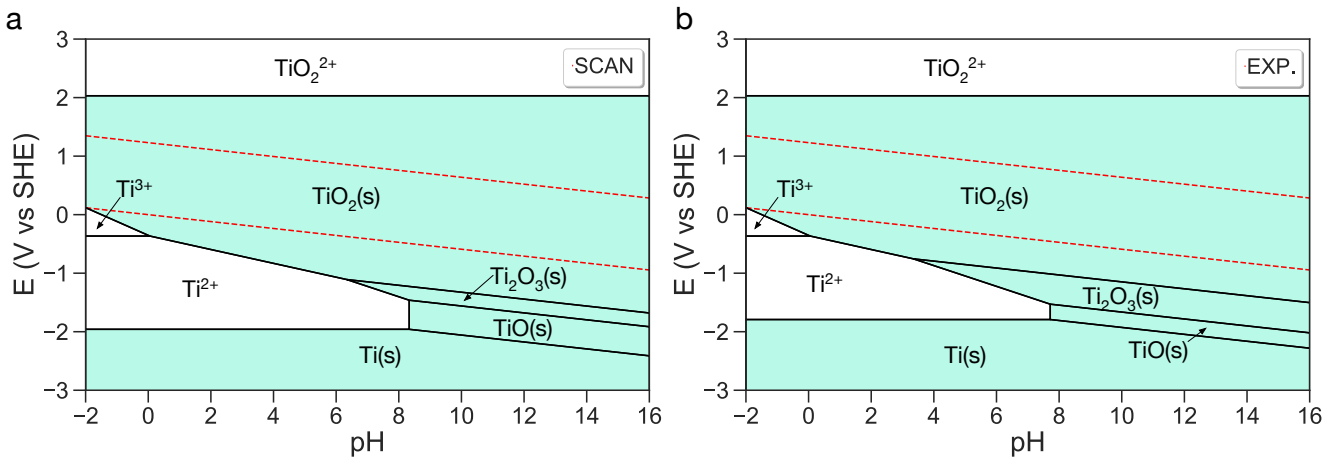
Supplementary Figure 1. Calculated formation enthalpies of representative oxides as a function of the experimental enthalpies. The solid and open symbols refer to data of raw PBE and PBE with O_2 correction, respectively. The solid blue line gives the fitted O_2 correction (1.40 eV/fu) adopted in the Materials Project (MP) for oxide compounds. The dotted line is the best fit (1.04 eV/fu) for the eight representative oxides deviating from the experimental values after applying the MP O_2 correction. All PBE data were retrieved from the Materials Project[1–3] and the experimental formation enthalpies were obtained from 4–6



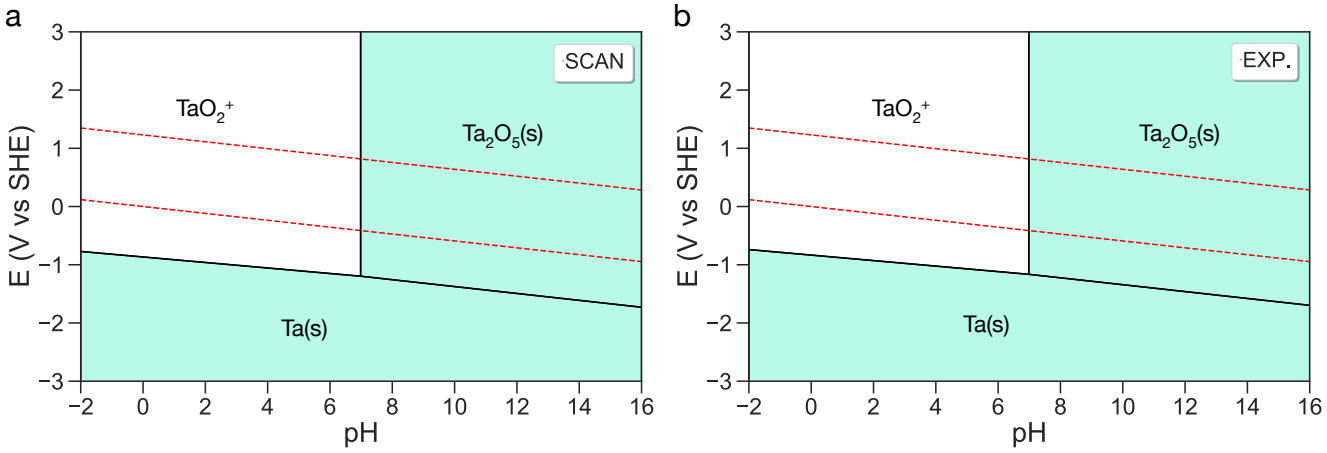
Supplementary Figure 2. Calculated formation enthalpies of 47 ternary transition metal oxides as a function of experiment formation enthalpies. The PBE+U data were retrieved from the Materials Project.[1–3] and the experimental enthalpies were obtained from Ref 4,5,7. The raw data for this plot are provided in Table 4.

Supplementary Table 1. Calibrated Hubbard U parameters (eV) and the corresponding energy adjustment (ΔE_M, M=metal, eV) when mixing the SCAN and SCAN+U energies in the formation enthalpy calculation for transition metal oxides. Detailed fitting procedures were described in Ref 7.

Element	Hubbard U	ΔE_M
V	0.66	0
Cr	0.22	0.552
Mn	2.93	-0.941
Fe	2.86	-1.116
Co	2.86	-1.118
Ni	2.43	-0.641
Mo	2.05	-1.624



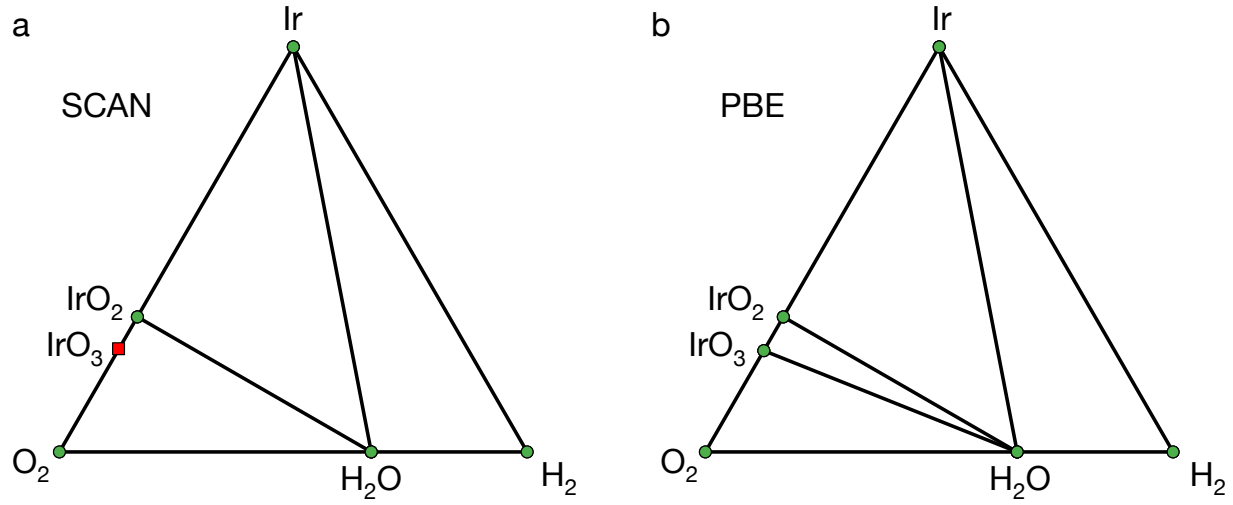
Supplementary Figure 3. Ti Pourbaix diagrams generated with aqueous ion concentrations of 10^{-6} M at 25°C. (a) SCAN-calculated and (b) experimental Pourbaix diagram generated without TiH_2. Regions with solid are shaded in Lake blue. The water stability window is shown in red dashed line.



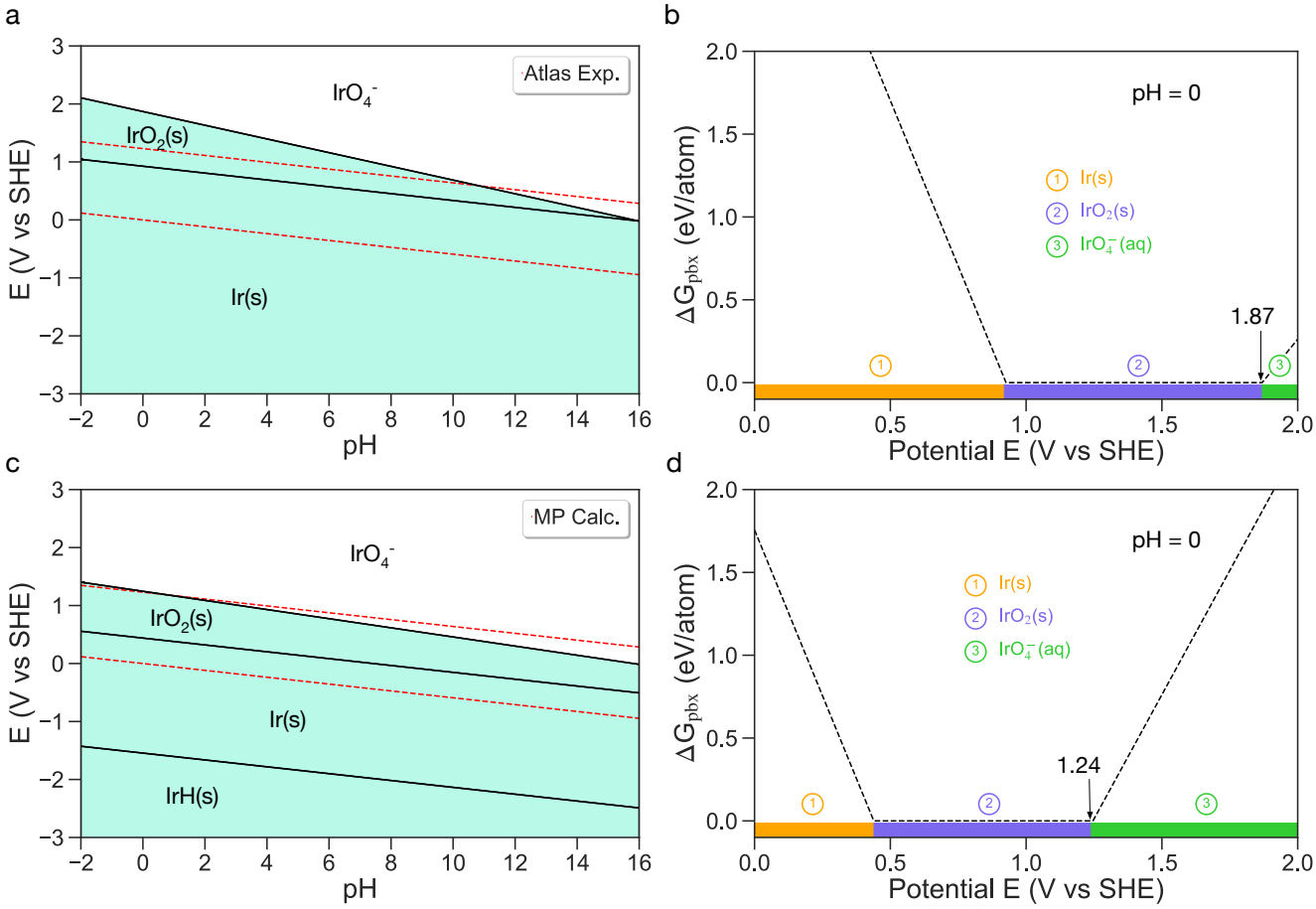
Supplementary Figure 4. Ta Pourbaix diagrams generated with aqueous ion concentration of 10^{-6} M at 25°C. (a) SCAN-calculated and (b) experimental Ta Pourbaix diagram without TaO_2^{2+}. Regions with solid are shaded in Lake blue. The water stability window is shown in red dashed line.

Supplementary Table 2. The experimental formation Gibbs free energy (eV/fu) of Co solids and aqueous ions. Values used in this work are highlighted in bold font. Wagman's data are used by the Materials Project.

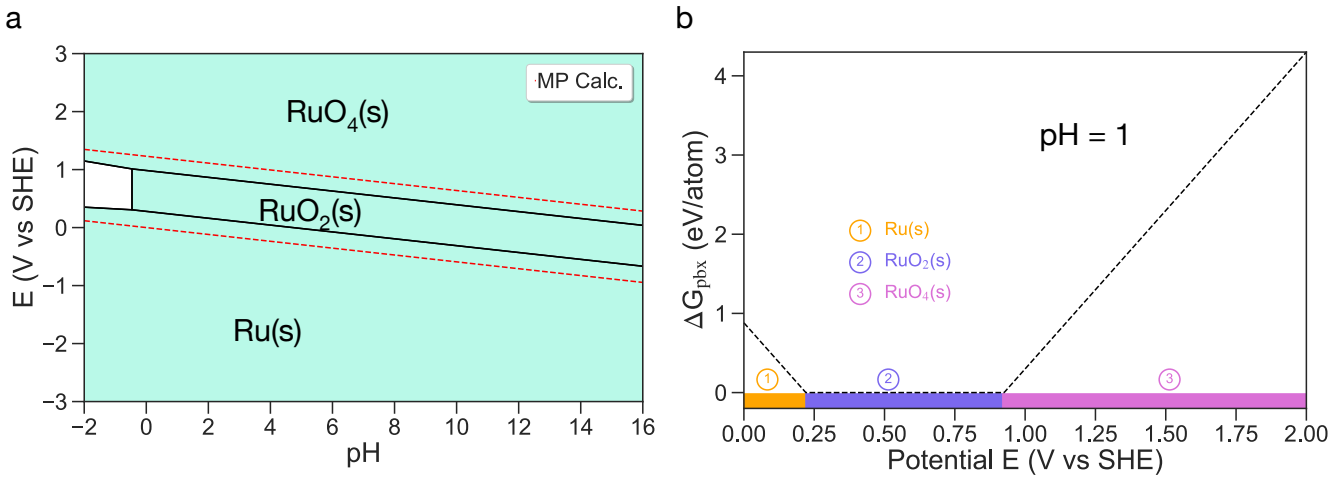
Species	Pourbaix[8]	Wagman[6]	Barin[9]	Hem[10]
Co^{2+}	**-0.555**	-0.564		-
Co^{3+}	**1.253**	1.386	-	-
$HCoO_2^-$	**-3.598**	-4.224	-	-
$Co(OH)_2$(aq)	-	-3.825	-	-
CoO	-2.125	-2.220	**-2.220**	-
Co_3O_4	-7.278	-8.022	**-8.238**	-
Co_2O_3(hydr)	**-4.992**	-	-	-
CoO_2	**-2.248**	-	-	-
$Co(OH)_2$	-4.727	-4.748	**-4.797**	-
CoOOH	-	-	-	**-4.003**



Supplementary Figure 5. DFT calculated phase diagram in the Ir-O-H composition spaces using the (a) SCAN and (b) PBE functionals. The green solid circle and the red solid square labels stable and metastable phases, respectively. The PBE data were retrieved from the Materials Project.[1–3]



Supplementary Figure 6. (a) Experimental and (c) the Materials Project (MP) PBE calculated Ir Pourbaix diagrams generated using aqueous ion concentration of 10^{-6} M at 25°C. Regions with solid are shaded in Lake blue. The water stability window is shown in red dashed line. (b-d) Computed Pourbaix decomposition free energy (ΔG_{pbx}) of IrO_2 in experimental and the MP PBE diagrams from the potential 0−2.0 V at pH = 0, respectively. The projection of ΔG_{pbx} onto the potential axis highlights the stable species at the corresponding regions. The labels with arrow show the onset dissolution potential of IrO_2 under OER conditions. The experimental and the MP PBE data were retrieved from Ref 8 and the Materials Project[1–3], respectively.



Supplementary Figure 7. (a) The Materials Project (MP) PBE calculated Ru Pourbaix diagrams generated using aqueous ion concentration of 10^{-6} M at 25°C. Regions with solid are shaded in Lake blue. The water stability window is shown in red dashed line.. (b) Computed Pourbaix decomposition free energy (ΔG_{pbx}) of RuO_2 in (a) from the potential 0−2.0 V at pH = 1. The projection of ΔG_{pbx} onto the potential axis highlights the stable species at the corresponding regions. All data were retrieved from the Materials Project.[1–3]

Supplementary Table 3. Calculated and experimental formation enthalpies (eV/atom) of 114 binary oxides. ΔH_{SCAN} and ΔH_{SCAN+U} are data calculated using the SCAN functional and the SCAN+U functional for transition metal oxides, respectively. ΔH_{MP} refers to the PBE(+U) data retrieved from the Materials Project.[1–3] The experimental data were obtained from Ref 4, 5.

Formula	ΔH_{exp}	ΔH_{MP}	ΔH_{SCAN}	ΔH_{SCAN+U}	Formula	ΔH_{exp}	ΔH_{MP}	ΔH_{SCAN}	ΔH_{SCAN+U}
Ag_2O	-0.107	-0.334	-0.165		Nb_2O_5	-2.812	-3.094	-2.789	
Ag_2O_3	0.07	-0.377	-0.14		NbO	-2.175	-1.476	-2.154	
AgO	-0.063	-0.46	-0.217		NbO_2	-2.747	-2.917	-2.708	
Al_2O_3	-3.473	-3.446	-3.436		Nd_2O_3	-3.748	-3.803	-3.721	
As_2O_3	-1.38	-1.649	-1.336		NiO	-1.242	-0.937	-1.27	-1.238
As_2O_5	-1.362	-1.584	-1.261		OsO_2	-1.018	-1.367	-1.003	
Au_2O_3	-0.007	-0.471	-0.255		OsO_4	-0.816	-1.553	-0.975	
B_2O_3	-2.64	-2.816	-2.622		P_2O_5	-2.228	-2.461	-2.212	
BaO	-2.84	-2.838	-2.761		Pb_3O_4	-1.064	-1.471	-1.113	
BaO_2	-2.191	-2.173	-2.122		PbO	-1.137	-1.491	-1.191	
BeO	-3.158	-3.125	-3.087		PbO_2	-0.948	-1.318	-0.921	
Bi_2O_3	-1.183	-1.658	-1.226		PdO	-0.599	-0.803	-0.687	
CaO	-3.291	-3.325	-3.275		Pr_2O_3	-3.751	-3.755	-3.674	
CdO	-1.339	-1.386	-1.263		Pt_3O_4	-0.4	-0.849	-0.699	
Ce_2O_3	-3.731	-3.781	-3.72		PtO	-0.37	-0.599	-0.425	
CeO_2	-3.767	-3.95	-3.844		PtO_2	-0.57	-0.945	-0.762	
Co_3O_4	-1.347	-1.421	-1.536	-1.224	Rb_2O	-1.171	-1.12	-1.097	
CoO	-1.232	-1.333	-1.162	-1.338	Re_2O_7	-1.438	-2.053	-1.562	
Cr_2O_3	-2.352	-2.349	-2.609	-2.339	ReO_2	-1.495	-1.917	-1.546	
CrO_2	-2.07	-2.032	-2.345	-2.096	ReO_3	-1.583	-2.16	-1.67	
CrO_3	-1.521	-1.542	-1.713	-1.507	Rh_2O_3	-0.737	-1.095	-1.025	
Cs_2O	-1.195	-1.199	-1.145		RuO_2	-1.054	-1.478	-1.261	
CsO_2	-0.989	-0.975	-0.978		SO_3	-1.136	-1.766	-1.214	
Cu_2O	-0.598	-0.651	-0.519		Sb_2O_3	-1.484	-1.771	-1.441	
CuO	-0.839	-0.955	-0.842		Sb_2O_5	-1.492	-1.771	-1.459	
Dy_2O_3	-3.861	-4.031	-3.972		SbO_2	-1.567	-1.859	-1.55	
Er_2O_3	-3.934	-4.078	-4.014		Sc_2O_3	-3.956	-3.989	-3.925	
Eu_2O_3	-3.447	-3.186	-3.058		SeO_2	-0.778	-1.172	-0.804	
EuO	-3.057	-3.14	-3.097		SiO_2	-3.147	-3.289	-3.087	
Fe_2O_3	-1.711	-1.89	-1.629	-1.699	Sm_2O_3	-3.778	-3.883	-3.8	
Fe_3O_4	-1.66	-1.844	-1.623	-1.629	SnO	-1.455	-1.648	-1.37	
FeO	-1.41	-1.682	-1.306	-1.42	SnO_2	-1.995	-2.129	-1.882	
Ga_2O_3	-2.258	-2.288	-2.098		SrO	-3.068	-3.097	-3.036	
Gd_2O_3	-3.786	-3.913	-3.772		SrO_2	-2.189	-2.211	-2.169	
GeO_2	-2.004	-2.099	-1.784		Ta_2O_5	-3.03	-3.36	-3.102	

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Supplementary Table 3 – *Continued from previous page*

Formula	ΔH_{exp}	ΔH_{MP}	ΔH_{SCAN}	ΔH_{SCAN+U}	Formula	ΔH_{exp}	ΔH_{MP}	ΔH_{SCAN}	ΔH_{SCAN+U}
HfO_2	-3.861	-4.044	-3.927		Tb_2O_3	-3.866	-4.007	-3.94	
HgO	-0.471	-0.65	-0.355		TbO_2	-3.356	-3.214	-3.03	
Ho_2O_3	-3.899	-4.056	-3.99		TeO_2	-1.093	-1.514	-1.155	
In_2O_3	-1.919	-2.018	-1.871		ThO_2	-4.238	-4.392	-4.25	
IrO_2	-0.862	-1.265	-0.936		Ti_2O_3	-3.153	-3.323	-3.226	
K_2O	-1.255	-1.259	-1.211		Ti_3O_5	-3.186	-3.403	-3.287	
K_2O_2	-1.285	-1.299	-1.248		TiO	-2.812	-2.924	-2.854	
KO_2	-0.983	-0.981	-0.99		TiO_2	-3.261	-3.523	-3.395	
La_2O_3	-3.721	-3.898	-3.803		Tl_2O	-0.578	-0.826	-0.685	
Li_2O	-2.068	-2.074	-2.076		Tl_2O_3	-0.809	-1.122	-0.779	
Li_2O_2	-1.642	-1.654	-1.644		Tm_2O_3	-3.915	-4.112	-4.046	
Lu_2O_3	-3.893	-4.143	-4.081		U_3O_8	-3.368	-3.725	-3.396	
MgO	-3.118	-3.069	-3.051		UO_2	-3.748	-3.781	-3.469	
Mn_2O_3	-1.986	-2.032	-2.183	-2.01	UO_3	-3.171	-3.635	-3.255	
Mn_3O_4	-2.054	-2.067	-2.148	-2.047	V_2O_3	-2.526	-2.538	-2.701	-2.549
MnO	-1.995	-2.004	-1.889	-1.996	V_2O_5	-2.295	-2.306	-2.485	-2.283
MnO_2	-1.8	-1.814	-2.155	-1.778	VO_2	-2.466	-2.49	-2.673	-2.483
MoO_2	-2.031	-2.142	-2.077	-2.03	WO_2	-2.037	-2.033	-2.109	
MoO_3	-1.931	-2.029	-2.133	-1.932	WO_3	-2.183	-2.189	-2.329	
Na_2O	-1.444	-1.439	-1.412		Y_2O_3	-3.949	-3.99	-3.972	
Na_2O_2	-1.33	-1.303	-1.279		ZnO	-1.816	-1.801	-1.656	
NaO_2	-0.901	-0.903	-0.913		ZrO_2	-3.803	-3.838	-3.845	

Supplementary Table 4. Calculated and experimental formation enthalpies (eV/atom) of 47 ternary oxides. ΔH_{SCAN+U} are data calculated using the SCAN+U functional. ΔH_{MP} are the PBE(+U) data retrieved from the Materials Project.[1–3] The experimental data were from Ref 4, 5, 7

Compound	ΔH_{exp}	ΔH_{MP}	ΔH_{SCAN+U}	Compound	ΔH_{exp}	ΔH_{MP}	ΔH_{SCAN+U}
Al_2CoO_4	-2.882	-2.895	-2.897	$Mg_2V_2O_7$	-2.671	-2.698	-2.694
Al_2CuO_4	-2.882	-2.671	-2.607	$MgCr_2O_4$	-2.632	-2.629	-2.603
Al_2FeO_4	-2.912	-2.833	-2.726	$MgMoO_4$	-2.419	-2.486	-2.413
Al_2NiO_4	-2.843	-2.711	-2.583	MgV_2O_6	-2.534	-2.548	-2.546
$BaMoO_4$	-2.619	-2.728	-2.658	$Mn(FeO_2)_2$	-1.819	-1.937	-1.826
BaV_2O_6	-2.628	-2.712	-2.695	$MnAl_2O_4$	-3.11	-3.065	-3.05
$Ca_2Fe_2O_5$	-2.457	-2.541	-2.434	$MnMoO_4$	-2.058	-2.144	-2.109
$Ca_2V_2O_7$	-2.905	-2.929	-2.922	Na_2CrO_4	-1.976	-2.007	-2.017
$Ca_3V_2O_8$	-3.012	-2.993	-3.002	$Na_2Mo_2O_7$	-2.225	-2.183	-2.106
$Ca(FeO_2)_2$	-2.191	-1.89	-2.201	Na_2MoO_4	-2.272	-2.215	-2.171
$CaCr_2O_4$	-2.709	-2.696	-2.691	$Na_4V_2O_7$	-2.421	-2.334	-2.332
$CaMoO_4$	-2.671	-2.715	-2.671	$NaCrO_2$	-2.271	-2.256	-2.264
CaV_2O_6	-2.682	-2.718	-2.688	$NaFeO_2$	-1.809	-1.934	-1.855
Cr_2CoO_4	-2.121	-2.132	-2.135	$NaVO_3$	-2.47	-2.393	-2.378
Cr_2CuO_4	-1.915	-1.94	-1.904	$SrMoO_4$	-2.676	-2.741	-2.686
Cr_2FeO_4	-2.142	-2.232	-2.138	$Ti(FeO_2)_2$	-2.223	-2.347	-2.161
Cr_2NiO_4	-2.037	-1.938	-1.938	$TiCoO_3$	-2.503	-2.663	-2.631
Cs_2CrO_4	-2.116	-2.087	-2.117	$TiFeO_3$	-2.565	-2.818	-2.646
Cs_2MoO_4	-2.243	-2.272	-2.209	$TiMn_2O_4$	-2.591	-2.689	-2.649
Fe_2CoO_4	-1.612	-1.744	-1.652	$TiMnO_3$	-2.817	-2.971	-2.918
$FeCuO_2$	-1.329	-1.452	-1.308	$TiNiO_3$	-2.492	-2.496	-2.57
$FeMoO_4$	-1.831	-2.016	-1.863	$Zn(FeO_2)_2$	-1.746	-1.896	-1.752
K_2CrO_4	-2.058	-2.087	-2.101	$ZnCr_2O_4$	-2.292	-2.272	-2.227
$LiFeO_2$	-1.992	-2.063	-1.996				

Supplementary Table 5. Calculated and experimental formation Gibbs free energy (eV/formula) of solid and aqueous ions for element Pourbaix diagram studied in this work. The referenced solid of each element Pourbaix diagram are highlighted in bold. The experimental data were obtained from Ref 5, 6, 8, 11

Species	ΔG_{exp}	ΔG_{calc}	Species	ΔG_{exp}	ΔG_{calc}
Ti	0	0	$Fe(OH)_2$[+]	-4.540	-4.573
TiO	-5.130	-5.391	$Fe(OH)_3$(aq)	-6.834	-6.867
Ti_2O_3	-14.865	-15.180	$Fe_2(OH)_2$[4+]	-4.843	-4.909
TiO_2	-9.219	-9.553	FeO_2[-]	-3.817	-3.850
Ti_3O_5	-24.019	-24.710	FeO_4[2-]	-3.339	-3.373
TiH_2	-1.089	-1.250	Co	0	0
Ti[2+]	-3.229	-3.563	CoO	-2.220	-2.382
Ti[3+]	-3.595	-3.929	**Co_3O_4**	-8.238	-8.858
TiO[2+]	-5.934	-6.268	Co_2O_3	-4.992	-5.612
$HTiO_3$[-]	-9.823	-10.157	CoO_2	-2.248	-2.008
TiO_2[2+]	-4.801	-5.136	$Co(OH)_2$	-4.797	-5.020
Ta	0	0	CoOOH	-4.277	-4.000
Ta_2O_5	-19.808	-20.131	Co[2+]	-0.555	-0.762
TaO_2+	-8.733	-8.895	Co[3+]	1.253	1.046
Se	0	0	$HCoO_2$[-]	-3.598	-3.805
SeO_2	-1.777	-1.779	Ni	0	0
Se[2-]	1.847	1.844	NiO	-2.194	-2.256
H_2Se(aq)	0.228	0.225	**$Ni(OH)_2$**	-4.696	-4.848
HSe[-]	0.453	0.451	Ni_3O_4	-7.378	-6.269
H_2SeO_3(aq)	-4.418	-4.421	Ni_2O_3	-4.868	-4.095
$HSeO_3$[-]	-4.267	-4.269	NiO_2	-2.230	-1.513
SeO_3[2-]	-3.836	-3.838	Ni[2+]	-0.480	-0.631
$HSeO_4$[-]	-4.688	-4.690	NiOH[+]	-2.355	-2.507
SeO_4[2-]	-4.575	-4.578	$Ni(OH)_3$[-]	-6.079	-6.231
H_2SeO_4(aq)	-4.571	-4.573	$Ni(OH)_4$[2-]	-7.709	-7.860
Mn	0	0	$HNiO_2$[-]	-3.619	-3.771
MnO	-3.761	-3.731	NiO_2[2-]	-2.784	-2.935
MnO_2	-4.821	-4.701	NiO(aq)	-1.706	-1.857
Mn_2O_3	-9.132	-9.097	**Ir**	0	0
Mn_3O_4	-13.299	-13.127	Ir_2O_3	-1.821	-
$Mn(OH)_2$	-6.374	-6.378	IrO_2	-1.214	-2.173
Mn[2+]	-2.362	-2.345	IrO_3	-	-1.538

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Supplementary Table 5 – *Continued from previous page*

Species	ΔG_{exp}	ΔG_{calc}	Species	ΔG_{exp}	ΔG_{calc}
$Mn[3+]$	-0.850	-0.832	$IrO_4[2-]$	-2.038	-2.038
$MnO_4[2-]$	-5.189	-5.172	Ru	0	0
$MnO_4[-]$	-4.634	-4.617	**RuO_2**	-2.623	-3.149
$MnOH[+]$	-4.199	-4.181	RuO_4	-1.653	-2.394
$Mn(OH)_3[-]$	-7.715	-7.697	$Ru[2+]$	1.558	1.032
$HMnO_2[-]$	-5.243	-5.225	$Ru[3+]$	1.797	1.272
Fe	0	0	$Ru(OH)[2+]$	-0.529	-1.054
FeO	-2.553	-2.523	$H_2RuO_5(aq)$	-4.054	-4.580
Fe_3O_4	-10.524	-10.649	$HRuO_5[-]$	-3.372	-3.898
Fe_2O_3	-7.693	-7.759	$RuO_4[-]$	-2.592	-3.118
$Fe[2+]$	-0.817	-0.851	$RuO_4[2-]$	-3.178	-3.703
$Fe[3+]$	-0.048	-0.081	$Ru(OH)_2[2+]$	-2.299	-2.824
$FeO_2[2-]$	-3.061	-3.094	$Ru(OH)_2[+]$	-2.911	-3.437
$FeOH[+]$	-2.874	-2.907	$Ru_4(OH)_{12}[4+]$	-19.453	-21.555
$FeOH[2+]$	-2.380	-2.413	$RuO_4(aq)$	-1.596	-2.122
$FeHO_2[-]$	-3.916	-3.949	-	-	-

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