Supporting Information

Using machine learning to predict oxygen evolution activity for transition metal hydroxide electrocatalysts

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Synthesis

All hydroxide catalysts were synthesized using a modified aqueous sol-gel technique with metal chlorides as raw materials. The metal salts were weighed with the total metal ion amount of 0.27 mmol and dissolved in ethanol (4 ml) in a vial. Then a trace amount of deionized water (0.21 ml) was mixed with ethanol (2 ml) in another vial. After chilling, the solutions were mixed and propylene oxide (1 ml) was slowly added to the mixed solution. Thereafter, a wet gel was formed. The wet gel was aged for 24 h and soaked in acetone for another 5 days. Then the wet gel was dried in a vacuum at room temperature to obtain the final catalysts. For NiFeLa hydroxide, lanthanum nitrate was used as La source.

Material characterization

The phases were characterized using XRD on a Rigaku D/max-RB12 diffractometer with Cu Kα radiation in the 2-θ range of 5–90 °. XPS was performed on an X-ray photoelectron spectrometer (Thermo Escalab 250XI) using monochromatic Al Kα radiation (hv=1486.6 eV). SEM was conducted using an SU8100 electron microscope. TEM, HRTEM, and EDS mapping experiments were performed on a microscope (FEI Tecnai G2F30).

Electrochemical characterization

All the electrochemical tests were performed using a typical three-electrode system with a 1 M KOH solution as the electrolyte, and a platinum foil and an Hg/HgO electrode as the counter and reference electrodes, respectively. To prepare the working electrode, 5 mg of the as-prepared catalyst, 0.8 mg conductive carbon, and 20 μL of 5 wt.% Nafion solution were dispersed in a 980 μL mixture of water and ethanol (water:ethanol = 1:1) under ultrasonication for at least 2 h to form a homogeneous catalyst ink. Subsequently, 4 μL of the catalyst ink was cast onto a glassy carbon electrode (3 mm diameter). After drying at room temperature, the catalytic working electrode was used to perform the electrochemical study on an electrochemical workstation (CHI600E). The measured potentials vs. Hg/HgO were converted to potentials vs. RHE using the following equation: $E_{RHE}=E_{Hg/HgO}+0.059pH+0.098$.

The original dataset

The original data used in this work is collected and screened from published studies by experiment. The data set consists of 88 entries, shown in Table S1, covering the elemental composition in percent representing different hydroxide catalysts, the phase and morphology information of the sample, the measurement conditions including pH and electrode, and the target overpotential (OP) at 10 mA/cm^2. The source references of published studies can also be found in Table S1. To make phase, morphology and electrode to be machine-readable, we give label encoding to these categorical variables. The encoding detail is shown in Table S2. In order to simplify the display of Table S1, we describe the values of phase, morphology and electrode in Table S1 in the encoded way.

Table S1. The collected and screened hydroxides catalyst from published studies by experiment (compositions in mole fraction).

No.	Ni	Co	Fe	W	V	Ru	P	Au	Ce	Ir	Al	Mo	Zn	Mn	S	Se	Ti	Cr	Li	Pt	La	Morphology	Phase	pH	Eelectrode	Overpotential (mV)	Ref.
1	0.971	0	0	0.029	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	13.6	1	237	1
2	0.971	0	0	0.029	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	13.6	1	264	1
3	0.75	0	0.125	0	0.125	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	13.6	3	200	2
4	0	0.664	0.332	0	0	0.004	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	3	198	3
5	0	0.666	0.334	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	3	310	3
6	0	0.75	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13	1	348	4
7	0.75	0	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13	1	404	4
8	0.397	0	0.596	0	0	0.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	1	276	5
9	0.663	0	0.332	0	0	0.005	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	1	207	5
10	0.833	0	0.167	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	1	235	6
11	0.431	0.049	0.52	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	3	239	7
12	0.75	0	0.125	0	0.125	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	231	8
13	0	0.4	0.1	0.4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	13.6	2	250	9
14	0.187	0	0	0	0.748	0.065	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	190	10

15	0.193	0	0	0	0.77	0.037	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	180	10
16	0.2	0	0	0	0.8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	200	10
17	0.73	0	0.266	0	0	0	0	0.004	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	5	237	11
18	0.6	0	0.4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	1	227	12
19	0.921	0	0	0	0	0	0	0	0	0.079	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	3	215	13
20	0.992	0	0	0	0	0	0	0	0	0.008	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	3	338	13
21	0.954	0	0	0	0	0	0	0	0	0.046	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	3	257	13
22	0	0	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	0	0	0	0	1	0	13.6	4	287	14
23	0.9	0	0.05	0	0	0	0	0	0	0	0	0.05	0	0	0	0	0	0	0	0	0	1	0	13.6	2	240	15
24	0	0.8	0	0	0	0	0	0	0	0	0	0	0.2	0	0	0	0	0	0	0	0	1	0	13.6	1	235	16
25	0	0.505	0.495	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	13	1	308	17
26	0.75	0	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	4	13.6	2	215	18
27	0.6	0.4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13	2	420	19
28	0.075	0	0.16	0	0	0	0	0	0	0	0.765	0	0	0	0	0	0	0	0	0	0	1	3	13	1	275	20
29	0.22	0	0.447	0	0	0	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	13.6	2	260	21
30	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	170	22

31	0.5	0	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	7	199	23
32	0.5	0	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	13.6	2	208	24
33	0.667	0	0.222	0	0	0	0	0	0	0	0	0	0	0.111	0	0	0	0	0	0	0	1	0	13.6	3	262	25
34	0.667	0	0	0	0	0	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	13.6	2	290	26
35	0	0.159	0.628	0	0	0	0	0	0	0	0	0	0	0	0.213	0	0	0	0	0	0	1	0	13.6	1	270	27
36	0.727	0.182	0.091	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	1	224	28
37	0.909	0	0.091	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	1	242	28
38	0.818	0.091	0.091	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	1	232	28
39	0.6	0	0.4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	13	6	280	29
40	0.9	0	0.1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	13.6	6	336	30
41	0.88	0	0.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	13.6	6	280	31
42	0.8	0	0.2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	1	13.6	1	215	32
43	0.78	0	0.22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	3	280	33
44	0.764	0	0.227	0	0	0	0	0	0	0	0	0	0	0	0	0	0.003	0	0	0	0.006	1	1	13.6	3	260	33
45	0.75	0	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.6	1	300	34
46	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.6	1	335	34

47	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.6	1	350	34
48	0	0.25	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	0	1	0	13	3	350	35
49	0.165	0.165	0.165	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	0	1	0	13	3	300	35
50	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	13.6	0	360	36
51	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	1	13.6	0	400	36
52	0.183	0.726	0.091	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	3	280	37
53	0.2	0.8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	3	330	37
54	0.611	0	0.204	0	0	0	0	0	0	0	0.185	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	300	38
55	0.569	0	0.19	0	0	0	0	0	0	0	0.241	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	323	38
56	0.445	0	0.149	0	0	0	0	0	0	0	0.406	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	327	38
57	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	0	0	0	0	0	0	1	1	13.6	1	420	39
58	0.75	0	0	0	0	0	0	0	0	0	0	0	0	0.25	0	0	0	0	0	0	0	1	1	13.6	1	350	39
59	0.767	0	0.106	0	0.127	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	13.6	2	192	40
60	0.83	0	0.17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	13.6	1	245	41
61	0.95	0	0	0	0	0	0	0	0.05	0	0	0	0	0	0	0	0	0	0	0	0	5	0	13.6	6	271	42
62	0.678	0	0.315	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.007	0	1	1	13.6	1	230	43

63	0.75	0	0	0	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.6	1	218	44
64	0.75	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.6	1	347	44
65	0.75	0	0	0	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.6	2	300	44
66	0.615	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.385	0	0	0	0	1	0	13.6	1	320	45
67	0	0.2	0	0	0	0	0.6	0	0	0	0	0	0	0.2	0	0	0	0	0	0	0	6	0	13.6	4	288	46
68	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	6	0	13.6	4	408	46
69	0	0.25	0	0	0	0	0.75	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	13.6	4	322	46
70	0	0.4	0.3	0	0.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	13.6	1	307	47
71	0	0.6	0.4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	13.6	3	283	48
72	0	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	13.6	1	314	49
73	0	0.67	0	0	0	0	0	0	0	0	0	0	0.33	0	0	0	0	0	0	0	0	2	0	13.6	1	324	50
74	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	1	338	50
75	0	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.33	0	0	2	0	13.6	1	340	51
76	0	0.375	0.368	0.257	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	4	13.6	1	223	52
77	0	0.375	0.368	0.257	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	4	13.6	6	191	52
78	0	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	13.	2	232	53

																								6			
79	0.5	0	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	3	13.6	1	280	54
80	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	13.6	1	300	55
81	0.75	0	0.25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	13.6	3	230	56
82	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	13.6	1	293	57
83	0.364	0.227	0.409	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	13.6	6	400	58
84	0.167	0	0.167	0	0	0	0	0	0	0	0	0	0	0	0	0.666	0	0	0	0	0	5	0	13.6	3	280	59
85	0	0.667	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.333	0	0	0	1	1	13	1	340	60
86	0	0.667	0	0	0	0	0	0	0	0	0	0	0	0.333	0	0	0	0	0	0	0	2	1	13.6	1	324	61
87	0	0.741	0.259	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	13	1	350	62
88	0	0.54	0.46	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	13	1	390	63

Table S2. The label encoding method for the phase and morphology information of the sample and the measurement electrode.

Morphology		Phase		Electrode	
common plate	1	layered double hydroxide	1	glass carbon	1
exfoliated/ultrathin anosheet	2	α phase	2	Ni foam	2
porous sheet	3	γ phase	3	carbon cloth/paper	3
film	4	amorphous phase	4	Iron foam	4
nanoparticle	5	unknown	0	Ti mesh	5
nanowire	6	-	-	Au/AuO/Pt supporter	6
flower	7	-	-	copper foam	7
unknown	0	-	-	unknown	0

Data set after feature construction

Table S3. The data set in dense representation (compositions in mole fraction).

No.	1st_componentatom_number	1st_component_element_fraction	2nd_component_atom_number	2nd_component_element_fraction	3rd_component_atom_number	3rd_component_element_fraction	Morphology	Phase	pH	Eelectrode	Overpotential (mV)	Ref.
1	28	0.971	74	0.029	0	0	2	2	13.6	1	237	1
2	28	0.971	74	0.029	0	0	1	2	13.6	1	264	1
3	28	0.75	26	0.125	23	0.125	1	2	13.6	3	200	2
4	27	0.664	26	0.332	44	0.004	1	1	13.6	3	198	3
5	27	0.666	26	0.334	0	0	1	1	13.6	3	310	3
6	27	0.75	26	0.25	0	0	1	1	13	1	348	4
7	28	0.75	26	0.25	0	0	1	1	1	1	404	4

									3			
8	28	0.397	26	0.596	44	0.007	2	0	13.6	1	276	5
9	28	0.663	26	0.332	44	0.005	2	0	13.6	1	207	5
10	28	0.833	26	0.167	0	0	1	1	13.6	1	235	6
11	28	0.431	26	0.52	27	0.049	1	1	13.6	3	239	7
12	28	0.75	26	0.125	23	0.125	1	1	13.6	2	231	8
13	27	0.4	74	0.4	26	0.1	7	0	13.6	2	250	9
14	23	0.748	28	0.187	44	0.065	1	1	13.6	2	190	10
15	23	0.77	28	0.193	44	0.037	1	1	13.6	2	180	10
16	23	0.8	28	0.2	0	0	1	1	13.6	2	200	10
17	28	0.73	26	0.266	79	0.004	1	1	13.6	5	237	11
18	28	0.6	26	0.4	0	0	1	1	13.	1	227	12

									6			
19	28	0.921	77	0.079	0	0	2	0	13.6	3	215	13
20	28	0.992	77	0.008	0	0	2	0	13.6	3	338	13
21	28	0.954	77	0.046	0	0	2	0	13.6	3	257	13
22	26	0.5	34	0.5	0	0	1	0	13.6	4	287	14
23	28	0.9	26	0.05	42	0.05	1	0	13.6	2	240	15
24	27	0.8	30	0.2	0	0	1	0	13.6	1	235	16
25	27	0.505	26	0.495	0	0	1	0	13	1	308	17
26	28	0.75	26	0.25	0	0	1	4	13.6	2	215	18
27	28	0.6	27	0.4	0	0	1	1	13	2	420	19
28	13	0.765	26	0.16	28	0.075	1	3	13	1	275	20
29	26	0.447	15	0.333	28	0.22	1	0	13.6	2	260	21
30	28	1	0	0	0	0	1	1	13.6	2	170	22
3	28	0.5	26	0.5	0	0	1	1	1	7	199	23

1									3.6			
32	28	0.5	26	0.5	0	0	1	0	13.6	2	208	24
33	28	0.667	26	0.222	25	0.111	1	0	13.6	3	262	25
34	28	0.667	15	0.333	0	0	1	0	13.6	2	290	26
35	26	0.628	16	0.213	27	0.159	1	0	13.6	1	270	27
36	28	0.727	27	0.182	26	0.091	1	1	13.6	1	224	28
37	28	0.909	26	0.091	0	0	1	1	13.6	1	242	28
38	28	0.818	27	0.091	26	0.091	1	1	13.6	1	232	28
39	28	0.818	26	0.091	0	0	4	0	13	6	280	29
40	28	0.818	26	0.091	0	0	4	0	13.6	6	336	30
41	28	0.818	26	0.091	0	0	4	0	13.6	6	280	31
42	28	0.818	26	0.091	0	0	5	1	13.	1	215	32

									6			
43	28	0.818	26	0.091	0	0	1	1	13.6	3	280	33
44	28	0.76389	26	0.22743	57	0.006	1	1	13.6	3	260	33
45	28	0.75	26	0.25	0	0	2	1	13.6	1	300	34
46	27	0.67	28	0.33	0	0	2	1	13.6	1	335	34
47	28	1	0	0	0	0	2	1	13.6	1	350	34
48	3	0.5	27	0.25	26	0.25	1	0	13	3	350	35
49	3	0.5	28	0.165	27	0.165	1	0	13	3	300	35
50	27	0.67	28	0.33	0	0	1	0	13.6	0	360	36
51	27	0.67	28	0.33	0	0	5	1	13.6	0	400	36
52	27	0.726	28	0.183	26	0.091	1	1	13.6	3	280	37
53	27	0.8	28	0.2	0	0	1	1	13.6	3	330	37
54	28	0.611	26	0.204	13	0.185	1	1	13.	2	300	38

									6			
55	28	0.569	13	0.241	26	0.19	1	1	13.6	2	323	[38]
56	28	0.445	13	0.406	26	0.149	1	1	13.6	2	327	[38]
57	28	0.5	25	0.5	0	0	1	1	13.6	1	420	[39]
58	28	0.75	25	0.25	0	0	1	1	13.6	1	350	[39]
59	28	0.7672	23	0.127	26	0.1058	1	1	13.6	2	192	[40]
60	28	0.83	26	0.17	0	0	1	0	13.6	1	245	[41]
61	28	0.95	58	0.05	0	0	5	0	13.6	6	271	[42]
62	28	0.678	26	0.315	78	0.007	1	1	13.6	1	230	[43]
63	28	0.75	23	0.25	0	0	2	1	13.6	1	218	[44]
64	28	0.75	27	0.25	0	0	2	1	13.6	1	347	[44]
65	28	0.75	23	0.25	0	0	2	1	13.	2	300	[44]

									6			
66	28	0.615	22	0.385	0	0	1	0	13.6	1	320	45
67	15	0.6	27	0.2	25	0.2	6	0	13.6	4	288	46
68	25	1	0	0	0	0	6	0	13.6	4	408	46
69	15	0.75	27	0.25	0	0	0	0	13.6	4	322	46
70	27	0.4	26	0.3	23	0.3	5	0	13.6	1	307	47
71	27	0.6	26	0.4	0	0	4	0	13.6	3	283	48
72	26	0.67	27	0.33	0	0	5	0	13.6	1	314	49
73	27	0.67	30	0.33	0	0	2	0	13.6	1	324	50
74	27	0.67	28	0.33	0	0	2	0	13.6	1	338	50
75	27	0.67	3	0.33	0	0	2	0	13.6	1	340	51
76	27	0.375	26	0.368	74	0.257	5	4	13.	1	223	52

									6			
77	27	0.375	26	0.368	74	0.257	5	4	13.6	6	191	[52]
78	27	0.5	26	0.5	0	0	2	1	13.6	2	232	[53]
79	28	0.5	26	0.5	0	0	2	3	13.6	1	280	[54]
80	27	1	0	0	0	0	2	0	13.6	1	300	[55]
81	28	0.75	26	0.25	0	0	5	0	13.6	3	230	[56]
82	27	1	0	0	0	0	6	0	13.6	1	293	[57]
83	26	0.409	28	0.364	27	0.227	6	0	13.6	6	400	[58]
84	34	0.666	28	0.167	26	0.167	5	0	13.6	3	280	[59]
85	27	0.667	24	0.333	0	0	1	1	13	1	340	[60]
86	27	0.667	25	0.333	0	0	2	1	13.6	1	324	[61]
87	27	0.741	26	0.259	0	0	0	1	13	1	350	[62]
88	27	0.54	26	0.46	0	0	6	0	13	1	390	[63]

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