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

Supporting Information for

Non-noble electrocatalysts discovered by instinctive scaling relations of Gibbs-free energies of key oxygen adsorbates in water oxidation

Jihyeon Park[a,b], Sinwoo Kang[a,b], Jaeyoung Lee[a,b,c,]*

[a] School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju 61005, South Korea.

[b] International Future Research Center of Chemical Energy Storage and Conversion Processes, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju 61005, South Korea.

[c] Ertl Center for Electrochemistry and Catalysis, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju 61005, South Korea.

AUTHOR INFORMATION

Corresponding Author

*E-mail: jaeyoung@gist.ac.kr

Tel.: +82-61-715-2579

Experimental methods

Preparation of database

The potentials (V_κ) at a specific current density (κ) were extracted from the cycled CV curves using Algorithm S1, which is visualized in Scheme S1. In the alkaline OER, the forward scan produces the oxidation peak of nickel (oxy)hydroxide; therefore, the backward scan of the CV cycles was used instead. The backward scan was conducted only in the potential range where the partial derivative of the time to voltage was negative (i.e., the first step in Algorithm S1). We then found the index ranges of the two current density points whose current density signs were reversed based on the specific current density (i.e., the third step). The potential (V_κ) located at the intersection of a linear function passing through two actual points ((V_i,j_i), (V_{i+1},j_{i+1})) and the specific current density becomes the desired value (i.e., the fourth and fifth steps). This process was repeated for each specific current density (κ: 1, 5, 10, and 20 mA cm^{-2}), and the intersectional potentials were obtained automatically for all cycles. Overpotentials (η_κ) were calculated by subtracting 1.23 from the potentials (V_κ).

Operational environment of deep symbolic regression (DSR)

All code was written in Python 3.6.13 with the Jupyter-Notebook. The version of the DSR algorithm was 1.1.dev0 requiring TensorFlow 1.14.0. Computer specifications were as follows: CPU: AMD Ryzen 9 5900X, a 12-core processor with a base clock of 3.70 GHz; RAM: Samsung DDR4-3200 16 GB (1600 MHz) × 2; and GPU: NVIDIA GeForce RTX3080 10 GB (8704 CUDA-core).

The hyperparameters for the DSR algorithm were as follows. The minimum and maximum lengths of expression were 4 and 30, respectively. A total of 4,000 equations were generated by the DSR algorithm at every step, and the DSR performed 10,000 steps in total (i.e., 40,000,000 empirical equations were evaluated at every specific current density). The mathematical symbol library included the following operators: $+,\ -,\ \times,\ \div,\ sin,\ cos,\ ln,\ exp, and\ reequations\ arec\ cureens\ \{\}0gth\ of\ ation.lon\ state.6666666666666666\ 6666666666666666666666666666666666666666666666666666666\ \sqrt{x}$.

Precision score evaluation was performed using the normalized root-mean-square error (NRMSE) (Eqs. S1 and S2):

$$precision\ score = 1/(1 + NRMSE). \tag{S1}$$

$$NRMSE = \frac{\sqrt{\frac{1}{n}\sum(\hat{y} - y)^2}}{\sigma} \tag{S2}$$

Tables

Table S1. The hyperparameter of the DSR algorithm for finding the empirical equation between Fe composition and the specific current density (@ 350 mV)

		specification
Dataset (X)		Fe composition ($0 < X < 1$)
Target value (y)		Specific current density (@ 350 mV)
Equations per step		100
Total steps		2000
Symbol library		$+,\ -,\ \times,\ \div,\ const$
Constant range	Min. Max.	*null* 10

Table S2. Physical properties as functions of the metal oxidation state

	N_d	χ [12]	***Radii*** **(Å)** [13]
Fe^{3+} (CN=6)	5	1.83	0.69
Fe^{4+} (CN=6)	4	1.83	0.725
Ni^{2+} (CN=6)	8	1.91	0.83
Ni^{3+} (CN=6)	7	1.91	0.7
$Ni^{3.5+}$ (CN=6)	6.5	1.91	0.66
Ni^{4+} (CN=6)	6	1.91	0.62

CN = Coordination number

Table S3. Calculative properties in terms of NiOOH ***(Potential limiting step)***

eV				**NiOOH**				**Avg.**
ΔG_1	1.77	***1.69***	0.854	1.35	1.21	-0.5	0.53	0.9863
ΔG_2	***1.97***	1.1	1.404	***2.17***	0.81	1.54	1.34	***1.4763***
ΔG_3	0.43	1.41	***1.659***	0.69	***1.6***	1.24	***1.88***	1.2727
ΔG_4	0.75	0.72	1.003	0.71	1.3	***2.63***	1.17	1.1833
$(\sum \Delta G_i)/4e$	1.23	1.23	1.23	1.23	1.23	1.23	1.23	1.230
References	1	6	9	10	14	15	16	

Table S4. Calculative properties in terms of FeOOH ***(Potential limiting step)***

eV				**FeOOH**				**Avg.**
ΔG_1	0.76	1.037	-0.08	0.377	-0.18	0.42	0.864	0.4569
ΔG_2	0.9	1.496	0.64	1.419	-0.09	1.46	***2.212***	1.1481
ΔG_3	***1.92***	***1.885***	***2.46***	1.546	***4.43***	***2.12***	1.002	***2.1947***
ΔG_4	1.3	0.502	1.9	***1.577***	0.76	0.92	0.842	1.1144
$(\sum \Delta G_i)/4e$	1.22	1.23	1.23	1.23	1.23	1.23	1.23	1.229
References	3	9	10	17	18	19	20	

Table S5. Effect of excluding a parameter

Excluded parameter	NRMSE	Best equation ($\eta^{empirical}_{10mA\ cm^{-2}}$)	R^2 based on the best equation
-	0.7201	$e^{\sin\left(\ln\left(\ln\left(\sqrt{\max(\Delta G_i)} + \frac{ESSI}{\max(\Delta G_i)}\right)\right)\right)}$	0.9894
$\max(\Delta G_i)$	0.7971	$\frac{ESSI + \sqrt{e^{\Delta G_2}}}{\Delta G_3 + e^{\sqrt{\gamma + \Delta G_2 \cdot ESSI + e^{\sin(\Delta G_4 \cdot e^{e^{\Delta G_1}}) \cdot \cos(N_d)}}}}$	0.7551
$ESSI$	0.8097	$e^{\cos\left(e^{\Delta G_1 \cdot e^{\Delta G_1} \cdot \sin(\Delta G_2) \cdot \sin(\sin(2 \cdot \max(\Delta G_i)) + \cos(\Delta G_2) \cdot \sin(\sin(\max(\Delta G_i + \sin(2 \cdot \max(\Delta G_i))))) + \sin(\cos(\cos(\chi))))}\right) \cdot \sin(\sin(3 \cdot \sin(\max(\Delta G_i) + \sin(\cos(\cos(\cos(e^{e^{\cos(\max(\Delta G_i) + \sin(\max(\Delta G_i)) \cdot \sin(\max(\Delta G_i) \cdot \sin(\sin(\sin(\sin(\sin(\max(\Delta G_i)))) \cdot \sin(\sin(\sin(\sin(\sin(\sin(\Delta G_2))))))))))}}))))))}$	0.9035

$\max\left(\Delta G_i\right), ESSI$	0.7907	$\dfrac{\chi}{N_d - e^{\sin\left(\Delta G_2 \cdot \left(\frac{N_d \cdot \chi \cdot \left(-\Delta G_2 + \ln\left(\Delta G_4\right)\right)}{\Delta G_3}\right) - \Delta G_2\right)}}$	0.9123

Algorithms

Algorithm S1. Finding the intersection point

Input potential V_i; current density j_i; time s; specific current density κ

Output list of intersection points $[V_\kappa]$

1: $V_i \leftarrow \left\{ \frac{\partial V_i}{\partial s} < 0 \right\}$ ▷ Select the backward scan

2: **repeat**

3: $i \leftarrow \{ (j_i - \kappa)(j_{i+1} - \kappa) < 0 \}$ ▷ Find the index range having intersection points

4: $x \leftarrow \left\{ (y - j_i) = \frac{j_i - j_{i+1}}{V_i - V_{i+1}} (x - V_i) \Big|_{y = \kappa} \right\}$ ▷ Find intersection points

5: $V_\kappa \leftarrow x$ ▷ Correspond finding values to intersection points

6: $[V_\kappa] \leftarrow append\ V_\kappa$ ▷ Append the list of intersection points

7: **return** $[V_\kappa]$

Equations

$$y = \frac{a(X - b)}{X^7 - cX^6 + dX^5 + eX^2 + f} \tag{S3}$$

$where, a = 0.1746584776011356,$

$b = 0.00013673749166442201,$

$c = 1.107216991218484,$

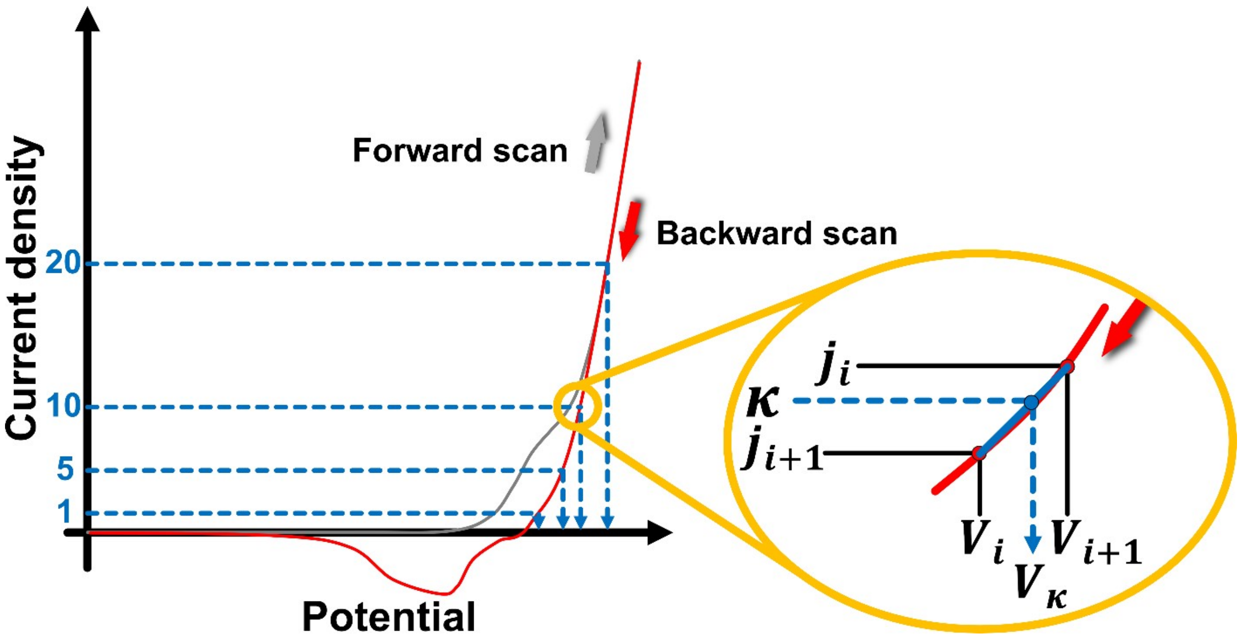
$d = 0.2909237571852588,$

$e = 0.013027824990815723,$

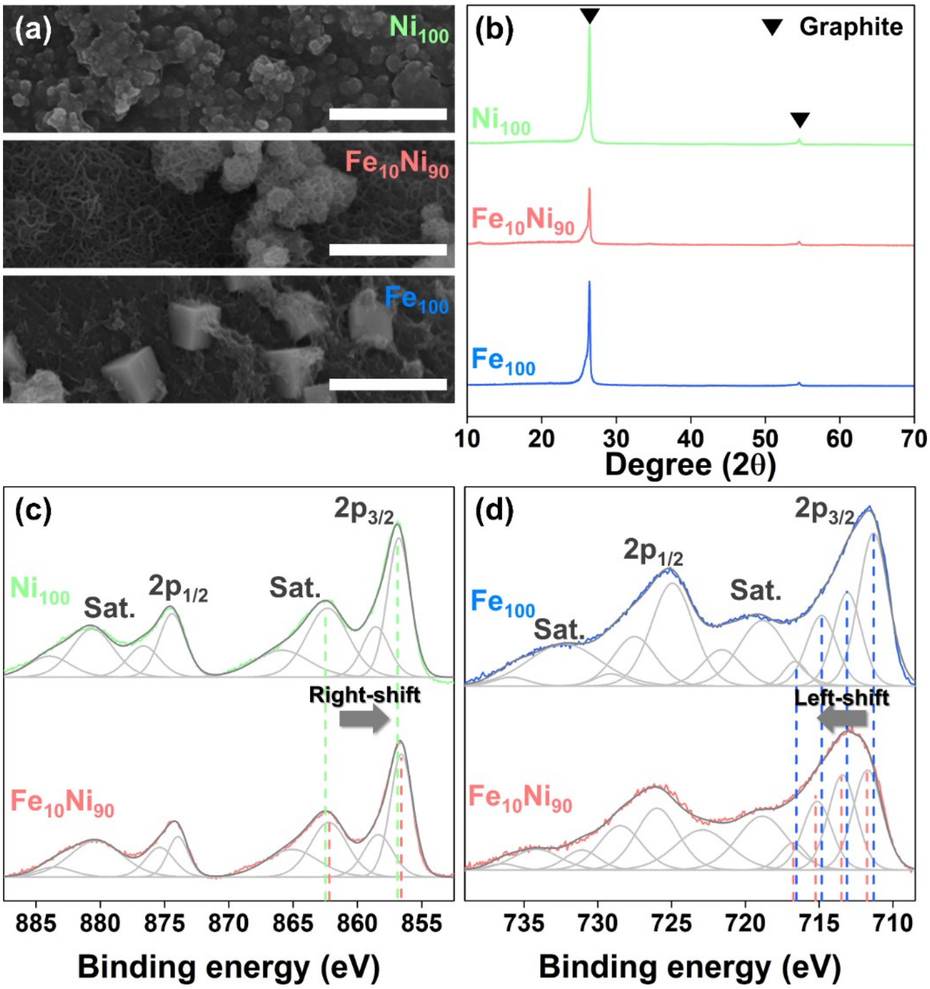
$f = 0.00010240969795094333$

$$(X, y)|_{y' = 0} = (0.0869, 75.33) \tag{S4}$$

Schemes



Scheme S1. Schematic of the algorithm extracting the specific potentials from the CV curve.



Figures

Figure S1. (a) SEM images of three different catalysts for OER; all scale bars for Fig. 1a correspond to 1 μm; (b) GI-XRD patterns that confirm the crystallinity of ultra-thin surface; and XPS profiles of (c) Ni 2p and (d) Fe 2p.

The morphological properties of the prepared catalysts, viz. $FeNiO_xH_y$ at three different ratios, were analyzed by FE-SEM (Figure S2a). A cube-like structure with a side of approximately 500 nm was observed on the electrodeposited surface of the pure Fe. In contrast, the surface-electrodeposited pure Ni appeared in the form of segregated nanoparticles. $FeNiO_xH_y$ of mixed ratio was uniformly electrodeposited on the carbon paper. Since the crystallinity of all samples (with the exception of the carbon paper) could not be detected by conventional XRD, we decided to use GI-XRD to analyze the crystallinity of the ultrathin film (Figure S2b). However, the crystallinity of the samples could not be confirmed using GI-XRD; thus, it was concluded that all catalysts were in amorphous phase. In Figure S2c, the XPS profiles of Ni $2p_{3/2}$ show two main peaks at ~856.8 and ~858.6 eV, corresponding to Ni^{2+} and Ni^{3+}, respectively.[21,22] Both peaks were right-shifted from Ni_{100} to $Fe_{10}Ni_{90}$, implying that Fe with a relatively low binding energy was successfully inserted into the Ni matrix. Similarly, compared to pure Fe, the four peak positions of $Fe_{10}Ni_{90}$ in Fe $2p_{3/2}$ were left-shifted because of the relatively higher binding energy of Ni (Figure S2d).[22–25] The changes in binding energy, as confirmed by XPS, indicated that the oxidation states of Fe and Ni were unpredictable with respect to the ratios.

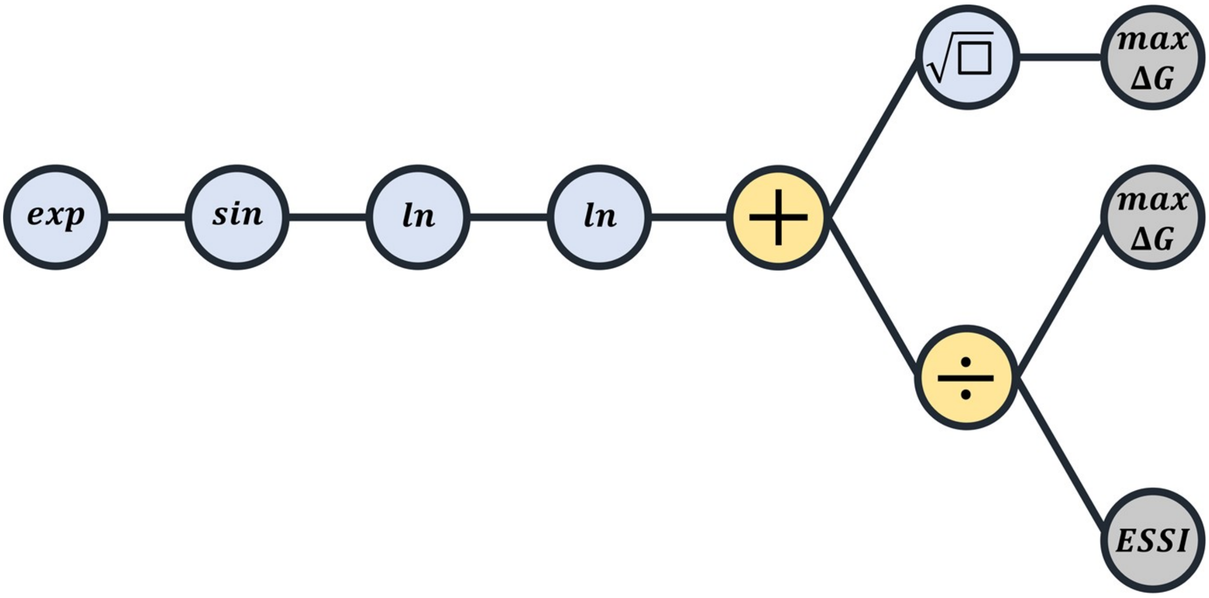


Figure S2. Tree-like structure of the completed equation.

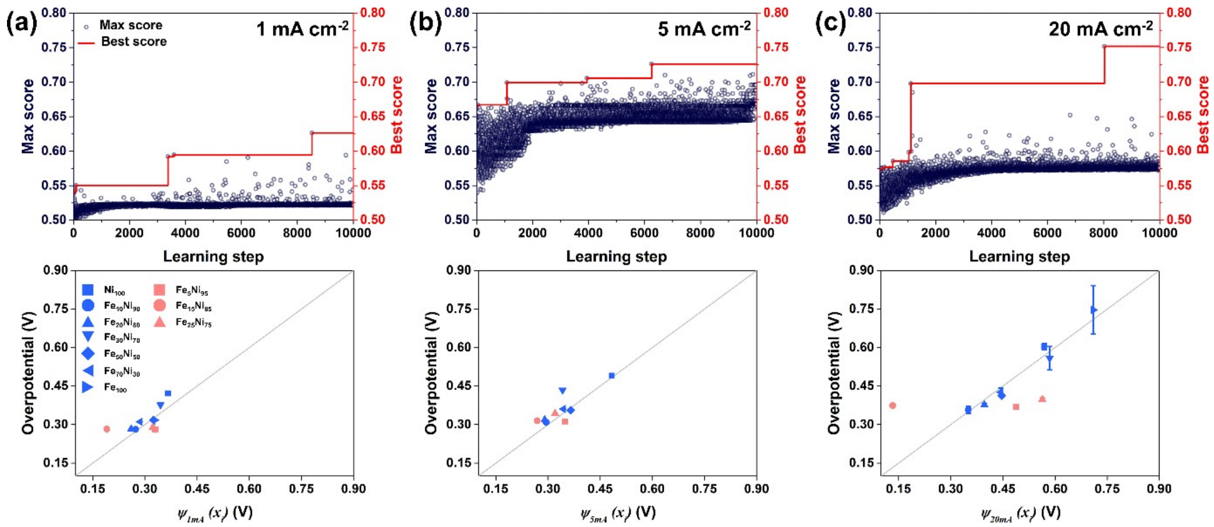


Figure S3. Score graph (upper) as a function of learning steps and reformatted graph (bottom) based on the best equation, with a gray solid line corresponding to the $y = x$ graph. The empirical equations express the overpotentials at (a) 1 mA cm^{-2}, (b) 5 mA cm^{-2}, and (c) 20 mA cm^{-2}, respectively.[a]

---

[a] The first-ranked equation

at 1mA cm^{-2}: $$\eta_{1mA\ cm^{-2}} = \frac{sin\left(\frac{\Delta G_4 \cdot \sqrt{ESSI}}{max(\Delta G_i)}\right)}{4\gamma}$$

, at 5mA cm^{-2}: $$\eta_{5\ mA\ cm^{-2}} = \frac{ESSI}{\Delta G_2 \cdot max(\Delta G_i) \cdot \left(\gamma + (\Delta G_2)^2 \cdot \left(\frac{-N_d \cdot \Delta G_2 + \gamma \cdot \Delta G_1}{\Delta G_3}\right) + sin(\gamma)\right) + \Delta G_4}$$

, and at 20 mA cm^{-2}: $$\eta_{20\ mA\ cm^{-2}} = -\gamma + max(\Delta G_i) - sin\left(\gamma - \frac{\Delta G_3}{N_d \cdot \gamma \cdot max(\Delta G_i) \cdot \sqrt{\gamma \cdot \Delta G_2 \cdot \left(\gamma^2 + \gamma + \Delta G_4\right) + \gamma}}\right)$$

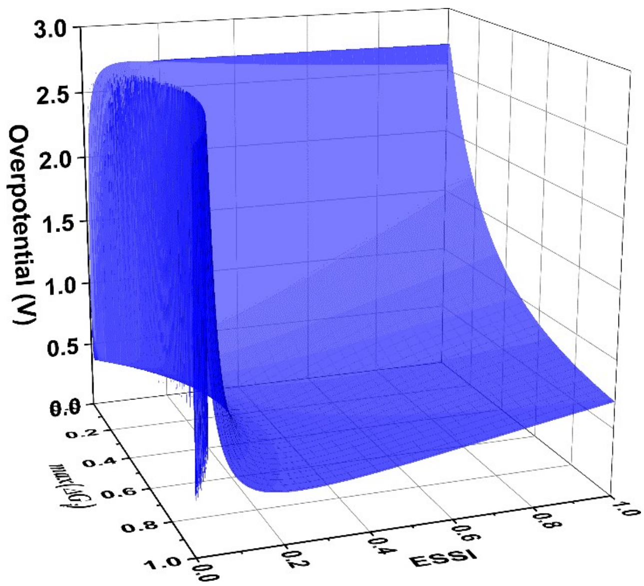


Figure S4. Three-dimensional graph of the first-ranked equation for the overpotential at 10 mA cm^{-2}.

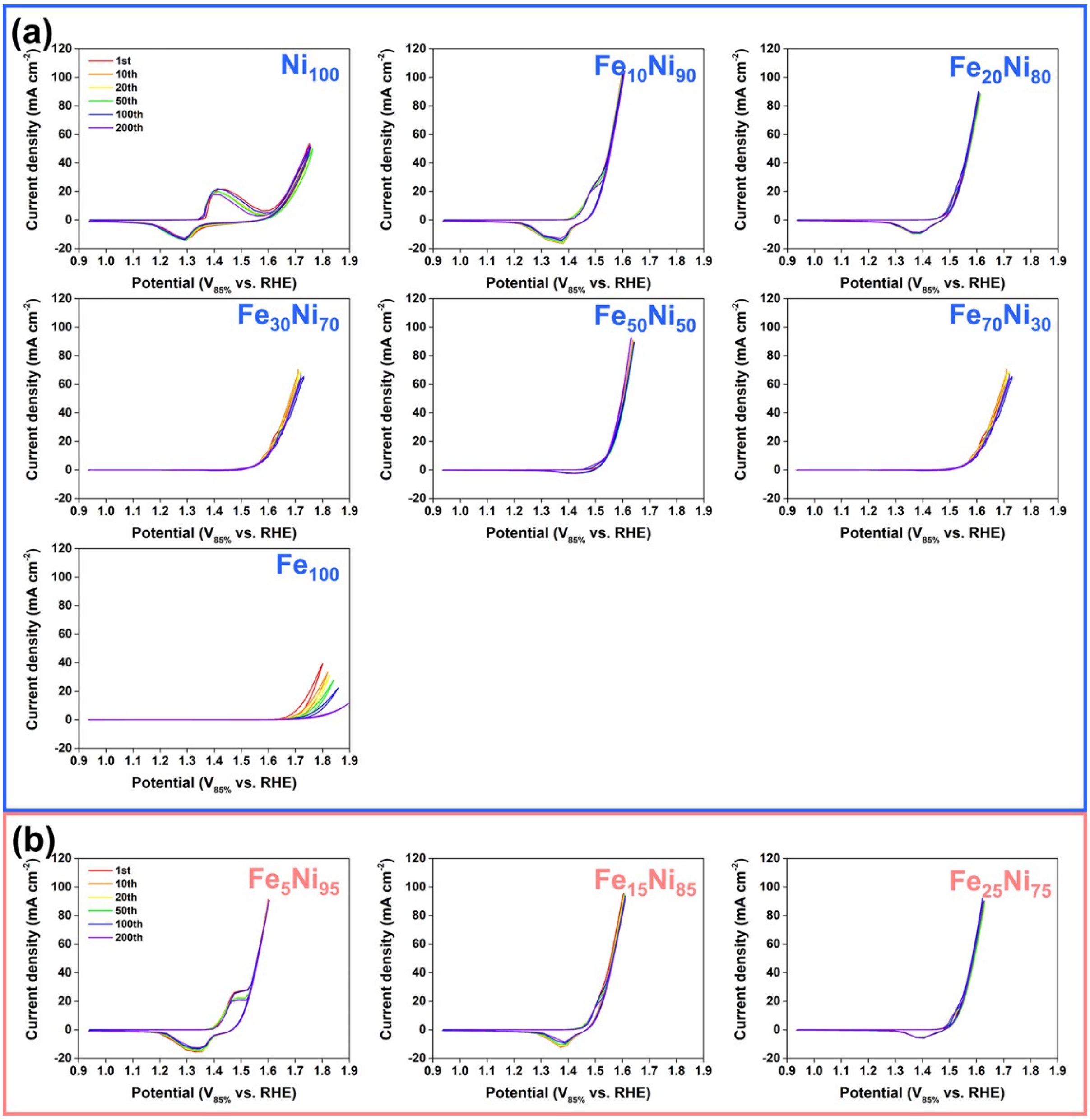


Figure S5. CV cycles of $FeNiO_xH_y$ at mixed ratio for (a) blue box (database) and (b) pink box (validation).

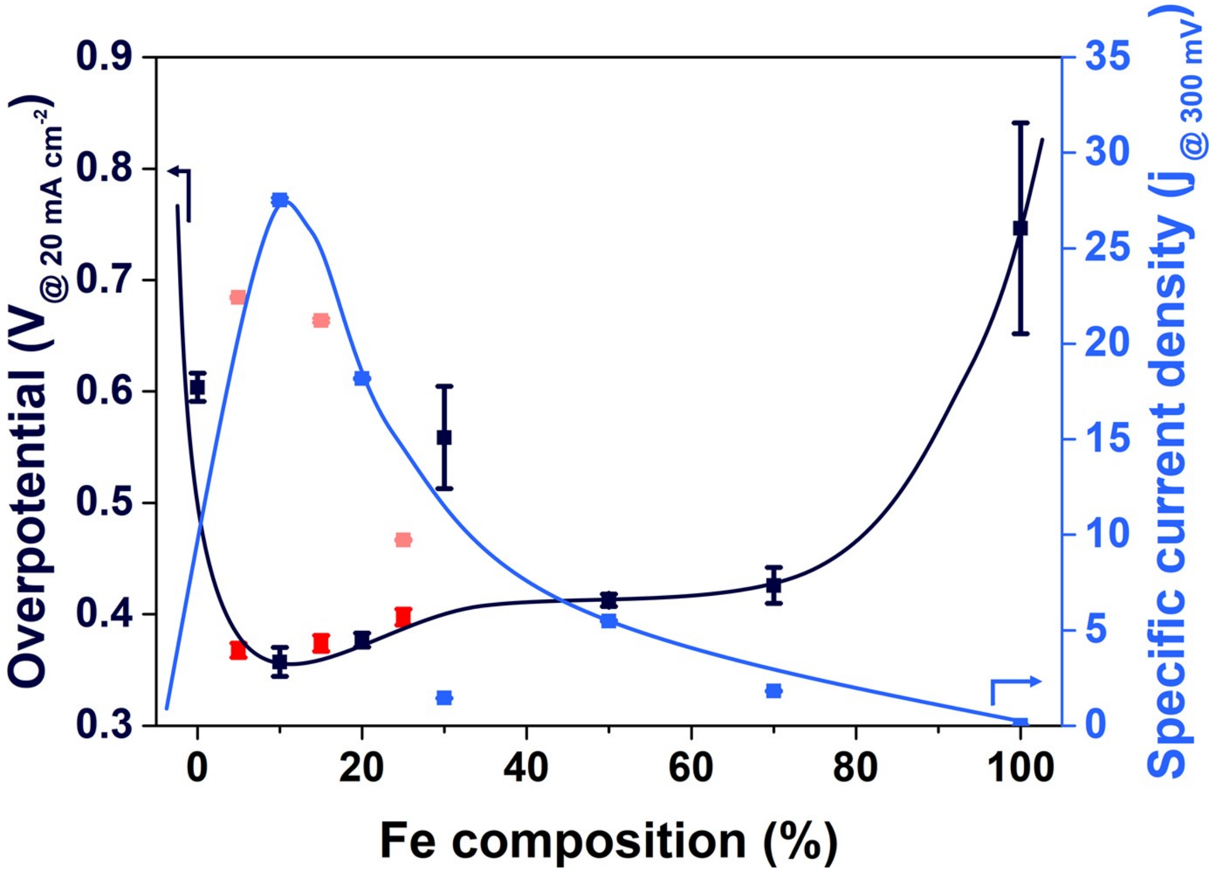


Figure S6. OER performance and overpotential of $FeNiO_xH_y$ catalysts at 300 mV and 20 mA cm^{-2}, respectively, as functions of Fe composition; blue and indigo-blue (Ni_{100}, $Fe_{10}Ni_{90}$, $Fe_{20}Ni_{80}$, $Fe_{30}Ni_{70}$, $Fe_{50}Ni_{50}$, $Fe_{70}Ni_{30}$, and Fe_{100} for database), pink and red (Fe_5Ni_{95}, $Fe_{15}Ni_{85}$, and $Fe_{25}Ni_{75}$ for validation).

Partial database for the empirical equation

NiO_xH_y	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.645843	1.717003	1.748985	1.815176
2	1.645061	1.715401	1.753105	1.82218
3	1.645822	1.715168	1.756521	1.820305
4	1.647236	1.717959	1.755978	1.817149
5	1.645052	1.718679	1.751491	1.817834
6	1.643673	1.716801	1.753288	1.823942
7	1.644022	1.715231	1.757384	1.823532
8	1.645688	1.717626	1.756455	1.818324
9	1.645653	1.719557	1.752525	1.821069
10	1.644153	1.717843	1.753986	1.826485
11	1.650385	1.718456	1.760278	1.825656
12	1.651531	1.721783	1.757627	1.82148
13	1.650988	1.722375	1.755281	1.825416
14	1.649514	1.71953	1.75826	1.83202
15	1.650473	1.718697	1.761321	1.829124
16	1.651756	1.721682	1.759824	1.823853
17	1.651309	1.722904	1.755982	1.826316
18	1.650111	1.720632	1.757675	1.83272
19	1.650368	1.719467	1.761525	1.830289
20	1.652006	1.721793	1.760236	1.825274
21	1.651731	1.723534	1.756357	1.828137
22	1.650303	1.720503	1.758951	1.834134
23	1.650856	1.719758	1.762016	1.83231
24	1.65217	1.72251	1.760285	1.826183
25	1.651686	1.723675	1.757038	1.830377
26	1.650463	1.720582	1.759695	1.835599
27	1.651503	1.720331	1.763041	1.830848
28	1.652422	1.72328	1.759423	1.827676
29	1.651487	1.723872	1.757318	1.833185
30	1.650512	1.72067	1.761706	1.836775
31	1.652024	1.721141	1.762816	1.830848

32	1.652482	1.724174	1.758182	1.829125
33	1.650941	1.723497	1.757822	1.835495
34	1.6507	1.720627	1.762564	1.836507
35	1.65271	1.722707	1.762505	1.830264
36	1.652456	1.724424	1.758435	1.832164
37	1.651027	1.721749	1.760668	1.838528
38	1.651683	1.720784	1.764099	1.835442
39	1.652833	1.723709	1.761154	1.831032
40	1.651896	1.724594	1.758743	1.83622
41	1.650926	1.721263	1.762509	1.839518
42	1.652556	1.722017	1.76389	1.832771
43	1.653093	1.724973	1.75921	1.831784
44	1.651169	1.723227	1.759912	1.839668
45	1.651426	1.721184	1.764247	1.838058
46	1.653059	1.723706	1.762517	1.832295
47	1.652383	1.72514	1.758688	1.836455
48	1.651219	1.721723	1.762436	1.841211
49	1.652283	1.721487	1.764762	1.836569
50	1.653038	1.724903	1.76063	1.832905
51	1.651947	1.724605	1.759564	1.839998
52	1.651178	1.721329	1.763427	1.841918
53	1.652836	1.722661	1.764773	1.834597
54	1.653246	1.725198	1.760489	1.833528
55	1.651559	1.724321	1.759932	1.841095
56	1.651544	1.721698	1.764116	1.841786
57	1.653152	1.723145	1.764554	1.834565
58	1.652958	1.725661	1.759972	1.836097
59	1.651777	1.723608	1.761005	1.842635
60	1.651726	1.721845	1.764922	1.841009
61	1.653341	1.724225	1.764014	1.835244
62	1.653037	1.725734	1.759859	1.837912
63	1.651493	1.722394	1.762917	1.84418
64	1.65239	1.721618	1.772885	1.84037
65	1.653526	1.725094	1.774905	1.835197
66	1.652062	1.725169	1.760141	1.841983

67	1.651734	1.72196	1.763608	1.844188
68	1.65295	1.722659	1.772635	1.837497
69	1.653599	1.725295	1.775702	1.835851
70	1.652174	1.724914	1.778921	1.842305
71	1.651547	1.72205	1.775594	1.844758
72	1.653215	1.722912	1.773175	1.837032
73	1.653345	1.725681	1.776578	1.836158
74	1.652021	1.724539	1.778707	1.842601
75	1.651835	1.721607	1.775796	1.845232
76	1.652999	1.723065	1.77291	1.837464
77	1.653873	1.725444	1.760908	1.836479
78	1.65209	1.724257	1.760489	1.844463
79	1.65195	1.7217	1.764823	1.845225
80	1.653565	1.722925	1.765072	1.837577
81	1.653596	1.725698	1.760866	1.837157
82	1.651948	1.724077	1.760787	1.844668
83	1.652153	1.7217	1.764883	1.844343
84	1.653458	1.723785	1.764945	1.837672
85	1.653581	1.725409	1.760566	1.838703
86	1.651884	1.722967	1.761763	1.84626
87	1.652406	1.721676	1.765673	1.843728
88	1.65383	1.72428	1.763637	1.837417
89	1.652961	1.725256	1.760065	1.8427
90	1.651764	1.721686	1.764012	1.84633
91	1.653201	1.721971	1.765372	1.840468
92	1.653782	1.724994	1.761298	1.837657
93	1.652259	1.724458	1.759675	1.844408
94	1.65188	1.72145	1.76408	1.845693
95	1.653236	1.722573	1.764918	1.83831
96	1.653426	1.725253	1.760036	1.838009
97	1.652412	1.724235	1.7602	1.844916
98	1.651851	1.721434	1.764494	1.845625
99	1.653357	1.722576	1.765107	1.838463
100	1.646368	1.713843	1.75145	1.821358

$Fe_{0.1}Ni_{0.9}O_xH_y$	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.510882	1.5354	1.558048	1.582248
2	1.511129	1.536879	1.55768	1.585669
3	1.510388	1.538409	1.556282	1.585172
4	1.510126	1.538797	1.556307	1.586143
5	1.50982	1.538631	1.556081	1.584645
6	1.509833	1.53787	1.5584	1.581404
7	1.510493	1.53664	1.559593	1.580199
8	1.510967	1.535931	1.559662	1.580543
9	1.510995	1.535717	1.559323	1.582386
10	1.510932	1.536259	1.55703	1.5842
11	1.510441	1.537496	1.556026	1.586089
12	1.509799	1.537964	1.555979	1.585413
13	1.509677	1.538415	1.555988	1.584627
14	1.50968	1.538048	1.556968	1.582526
15	1.509617	1.537064	1.558114	1.580889
16	1.510499	1.536226	1.559223	1.580369
17	1.510937	1.535512	1.558961	1.580101
18	1.510993	1.53542	1.558767	1.581874
19	1.511044	1.535832	1.557859	1.583081
20	1.510705	1.536908	1.55685	1.585254
21	1.510252	1.537805	1.555782	1.586178
22	1.509788	1.538096	1.555675	1.584613
23	1.509627	1.538183	1.556065	1.584178
24	1.509552	1.538038	1.556935	1.583092
25	1.509801	1.537355	1.558692	1.580212
26	1.510412	1.536192	1.559387	1.580601
27	1.510842	1.535692	1.55925	1.580953
28	1.510901	1.535576	1.559421	1.580069
29	1.511265	1.535745	1.559216	1.582488
30	1.511046	1.535989	1.558145	1.584278
31	1.510843	1.53697	1.557211	1.585472
32	1.510594	1.537627	1.55607	1.58614

33	1.510041	1.538226	1.555857	1.585383
34	1.509694	1.538213	1.555521	1.585469
35	1.509736	1.538244	1.556328	1.58387
36	1.50999	1.53848	1.557329	1.58273
37	1.50979	1.537568	1.558513	1.581153
38	1.510378	1.536997	1.55927	1.580844
39	1.510768	1.535941	1.559234	1.580784
40	1.510941	1.535885	1.560052	1.580772
41	1.511251	1.535726	1.559252	1.582492
42	1.511517	1.536231	1.559201	1.584074
43	1.511069	1.536283	1.558178	1.584778
44	1.510987	1.53749	1.557131	1.586642
45	1.510415	1.538216	1.556244	1.585881
46	1.510064	1.538383	1.556127	1.586927
47	1.51004	1.53862	1.556397	1.586295
48	1.509999	1.538818	1.556885	1.584369
49	1.50989	1.538084	1.557741	1.583325
50	1.510113	1.537828	1.559432	1.583186
51	1.510355	1.537375	1.559958	1.581058
52	1.510964	1.536241	1.560199	1.582453
53	1.511482	1.536355	1.560298	1.581636
54	1.511457	1.536245	1.560373	1.581716
55	1.511498	1.53622	1.559432	1.58437
56	1.511694	1.536929	1.55881	1.584836
57	1.511159	1.537127	1.558346	1.585259
58	1.510897	1.538073	1.556488	1.587404
59	1.510645	1.538607	1.556723	1.58645
60	1.510205	1.538954	1.556703	1.586294
61	1.510136	1.539105	1.556745	1.58709
62	1.510185	1.539123	1.557726	1.584779
63	1.510124	1.538291	1.558277	1.582978
64	1.510317	1.538147	1.559135	1.582766
65	1.510702	1.537628	1.560273	1.581476
66	1.51134	1.536757	1.560742	1.581715
67	1.511595	1.536552	1.560769	1.582886

68	1.511849	1.537028	1.561164	1.582415
69	1.51196	1.5369	1.5607	1.584016
70	1.5117	1.536837	1.559174	1.585305
71	1.511878	1.537049	1.559534	1.585421
72	1.511793	1.537579	1.559043	1.587039
73	1.511387	1.538324	1.558234	1.58732
74	1.511331	1.539201	1.558262	1.587333
75	1.510925	1.538977	1.557824	1.587905
76	1.510582	1.539336	1.55709	1.587497
77	1.510295	1.539543	1.557345	1.586199
78	1.51049	1.539665	1.557596	1.5876
79	1.510406	1.539605	1.55818	1.586629
80	1.510468	1.539391	1.559016	1.584847
81	1.510663	1.539075	1.559138	1.583952
82	1.510749	1.538967	1.559901	1.584137
83	1.510854	1.538722	1.56064	1.582939
84	1.511109	1.538382	1.561169	1.58353
85	1.511539	1.53791	1.561881	1.583041
86	1.51174	1.538018	1.561955	1.583632
87	1.51208	1.537391	1.561604	1.583704
88	1.512206	1.53753	1.561854	1.583889
89	1.512182	1.537633	1.561596	1.584105
90	1.512353	1.537751	1.561801	1.585078
91	1.512407	1.537749	1.561151	1.585567
92	1.51223	1.537783	1.560932	1.587939
93	1.512278	1.537882	1.559879	1.587351
94	1.512193	1.538488	1.559729	1.587966
95	1.511923	1.538956	1.558947	1.588822
96	1.51157	1.539713	1.558409	1.588879
97	1.511568	1.540192	1.558721	1.588802
98	1.511242	1.540303	1.558591	1.589252
99	1.511131	1.540464	1.558671	1.58818
100	1.510264	1.538137	1.559907	1.583268

$Fe_{0.2}Ni_{0.8}O_xH_y$	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.512921	1.547088	1.57227	1.604732
2	1.51313	1.549014	1.572701	1.605135
3	1.5131	1.54967	1.571678	1.60544
4	1.512271	1.550646	1.571237	1.60422
5	1.512146	1.551244	1.570893	1.606963
6	1.512278	1.5512	1.571271	1.609477
7	1.512093	1.550869	1.572387	1.611552
8	1.512149	1.550616	1.573533	1.611734
9	1.512522	1.549946	1.574472	1.61277
10	1.512911	1.548806	1.575606	1.612025
11	1.513442	1.548306	1.575807	1.611787
12	1.51352	1.54823	1.575448	1.61039
13	1.513562	1.548314	1.574911	1.608369
14	1.513483	1.5485	1.574243	1.606035
15	1.513395	1.548956	1.573284	1.605955
16	1.513071	1.550006	1.571592	1.605562
17	1.512496	1.551076	1.571364	1.604959
18	1.512269	1.551186	1.57119	1.606545
19	1.512141	1.551147	1.571567	1.607953
20	1.512169	1.551265	1.571555	1.609979
21	1.512176	1.550854	1.572109	1.611555
22	1.512457	1.550051	1.573835	1.613111
23	1.512618	1.549547	1.574976	1.612808
24	1.513108	1.548881	1.575414	1.613172
25	1.515229	1.54761	1.575824	1.612101
26	1.513698	1.548409	1.575619	1.610647
27	1.515483	1.547433	1.575319	1.609119
28	1.513621	1.54841	1.574357	1.606028
29	1.513909	1.548814	1.574068	1.606747
30	1.513409	1.549336	1.573004	1.60648
31	1.513207	1.55029	1.571868	1.606095
32	1.51262	1.551023	1.571444	1.605894

33	1.512475	1.55096	1.571468	1.606809
34	1.512198	1.551381	1.571172	1.607996
35	1.512163	1.551388	1.571107	1.609734
36	1.51223	1.550915	1.571999	1.61092
37	1.512167	1.550641	1.573308	1.611863
38	1.512401	1.550065	1.574318	1.612733
39	1.512859	1.549107	1.574851	1.61275
40	1.513505	1.548215	1.576075	1.611489
41	1.513505	1.548407	1.575731	1.612153
42	1.513799	1.547993	1.575436	1.610088
43	1.51373	1.548491	1.574563	1.606895
44	1.513649	1.54857	1.573514	1.606512
45	1.513354	1.549563	1.57218	1.605742
46	1.512835	1.550722	1.571513	1.604803
47	1.512425	1.550993	1.571026	1.606402
48	1.512308	1.550948	1.570826	1.608015
49	1.51223	1.550897	1.57142	1.609871
50	1.51258	1.550741	1.57237	1.611426
51	1.512459	1.550057	1.573784	1.612475
52	1.51305	1.549073	1.574955	1.612494
53	1.513479	1.548274	1.575782	1.612298
54	1.513648	1.547907	1.575261	1.611092
55	1.513652	1.548331	1.574548	1.607065
56	1.51343	1.548958	1.572722	1.605875
57	1.513104	1.549855	1.571178	1.606195
58	1.512484	1.550841	1.570905	1.606161
59	1.51222	1.551085	1.570753	1.607903
60	1.512207	1.550617	1.571271	1.611701
61	1.512256	1.550131	1.573131	1.611497
62	1.512872	1.549076	1.57485	1.61197
63	1.513415	1.54803	1.575475	1.611625
64	1.513694	1.54796	1.574886	1.609384
65	1.513724	1.548071	1.573855	1.606465
66	1.513482	1.548512	1.572543	1.605125
67	1.512702	1.550312	1.570546	1.604325

68	1.512227	1.550872	1.569876	1.606281
69	1.512186	1.550627	1.570977	1.608983
70	1.512261	1.550043	1.572842	1.610747
71	1.513108	1.548701	1.574493	1.611708
72	1.513323	1.547673	1.575083	1.609758
73	1.513537	1.547824	1.574245	1.608156
74	1.513584	1.547998	1.572521	1.605415
75	1.512939	1.549947	1.570708	1.604266
76	1.512139	1.550514	1.569934	1.605486
77	1.512264	1.550382	1.570437	1.609664
78	1.512356	1.549434	1.573075	1.609474
79	1.513008	1.548047	1.574516	1.611686
80	1.513698	1.547537	1.5748	1.609331
81	1.513579	1.547672	1.573377	1.605532
82	1.513152	1.549159	1.571036	1.604352
83	1.512391	1.550175	1.569878	1.604769
84	1.51213	1.550154	1.569872	1.60799
85	1.512258	1.549645	1.572116	1.610032
86	1.513139	1.547701	1.574171	1.611214
87	1.513541	1.547226	1.574516	1.608818
88	1.513622	1.547637	1.572906	1.604572
89	1.513088	1.549067	1.570144	1.604107
90	1.512536	1.550333	1.569981	1.6038
91	1.512134	1.550176	1.570354	1.608832
92	1.512736	1.548551	1.573319	1.610859
93	1.513429	1.547525	1.574346	1.609194
94	1.513499	1.547288	1.573234	1.604604
95	1.513287	1.548522	1.570783	1.603313
96	1.512233	1.550173	1.569625	1.603831
97	1.512071	1.549869	1.569969	1.608484
98	1.512762	1.54814	1.573114	1.610702
99	1.513444	1.547119	1.573811	1.608697
100	1.514215	1.543896	1.570485	1.602227

$Fe_{0.3}Ni_{0.7}O_xH_y$	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.561513	1.646772	1.718274	1.704118
2	1.561795	1.647021	1.718066	1.797451
3	1.561754	1.64682	1.718066	1.797451
4	1.561934	1.647153	1.716877	1.797059
5	1.560155	1.650595	1.716583	1.803469
6	1.560238	1.650448	1.716373	1.803061
7	1.560214	1.650824	1.716667	1.802653
8	1.56021	1.650672	1.717857	1.8
9	1.560497	1.651061	1.716456	1.7992
10	1.560669	1.651061	1.716162	1.802245
11	1.560446	1.650451	1.718346	1.7988
12	1.560871	1.650758	1.716837	1.7988
13	1.560642	1.651217	1.718041	1.7988
14	1.560605	1.651212	1.717048	1.802245
15	1.560832	1.651379	1.718135	1.801837
16	1.560984	1.651231	1.716327	1.801429
17	1.561255	1.653557	1.718848	1.801429
18	1.562908	1.647794	1.718848	1.80102
19	1.563006	1.648007	1.718229	1.80102
20	1.562832	1.648364	1.71701	1.80102
21	1.563006	1.64829	1.71701	1.80102
22	1.56331	1.648507	1.718635	1.800612
23	1.563286	1.648148	1.71671	1.80102
24	1.563091	1.648074	1.718947	1.800612
25	1.563104	1.648148	1.717617	1.80102
26	1.563193	1.648216	1.718635	1.800612
27	1.563441	1.648141	1.717708	1.800612
28	1.613184	1.648642	1.717188	1.799796
29	1.61307	1.648496	1.717801	1.799796
30	1.613387	1.648277	1.71811	1.799796
31	1.613413	1.648134	1.719048	1.803333
32	1.613413	1.648792	1.717493	1.799796

33	1.613529	1.648717	1.717493	1.799796
34	1.613488	1.648935	1.717585	1.714694
35	1.613328	1.649008	1.716971	1.71625
36	1.613714	1.649084	1.717277	1.714694
37	1.613455	1.648855	1.658995	1.71449
38	1.613481	1.648931	1.659467	1.71449
39	1.613507	1.649234	1.659626	1.71449
40	1.613409	1.648931	1.659467	1.71449
41	1.613435	1.649008	1.659626	1.71449
42	1.613735	1.649157	1.658839	1.716042
43	1.613501	1.64969	1.659358	1.715833
44	1.613293	1.649154	1.659517	1.715833
45	1.613375	1.649535	1.658886	1.715833
46	1.613605	1.649	1.6592	1.714286
47	1.613531	1.649457	1.660054	1.715625
48	1.613485	1.649305	1.6592	1.717447
49	1.611697	1.652996	1.659892	1.715625
50	1.613521	1.649305	1.65973	1.714082
51	1.613715	1.649457	1.658421	1.715833
52	1.613599	1.649455	1.659249	1.715625
53	1.613636	1.649688	1.659091	1.715417
54	1.614446	1.653443	1.659783	1.715417
55	1.613822	1.649455	1.659249	1.718696
56	1.613748	1.649455	1.660274	1.720444
57	1.613636	1.649688	1.659091	1.720667
58	1.613525	1.649455	1.660109	1.718696
59	1.613908	1.649609	1.659946	1.720444
60	1.61386	1.649922	1.658777	1.720444
61	1.613882	1.6493	1.659946	1.720444
62	1.613845	1.649765	1.659621	1.720222
63	1.613819	1.649921	1.658981	1.720222
64	1.614057	1.650079	1.659836	1.715
65	1.613943	1.650079	1.659836	1.72
66	1.613879	1.65	1.659511	1.716596
67	1.613803	1.65	1.659511	1.716596

68	1.613917	1.650238	1.660894	1.716596
69	1.614119	1.649921	1.659511	1.716596
70	1.613967	1.650159	1.659189	1.715
71	1.61394	1.65056	1.660055	1.716596
72	1.613891	1.650398	1.659189	1.716596
73	1.614041	1.650159	1.659563	1.719778
74	1.613887	1.6504	1.659563	1.716383
75	1.614129	1.65032	1.659945	1.71617
76	1.613976	1.650482	1.659079	1.71617
77	1.614104	1.650402	1.660111	1.71617
78	1.614195	1.650402	1.65978	1.717826
79	1.614234	1.650726	1.659615	1.71617
80	1.614104	1.675526	1.65978	1.717826
81	1.614207	1.675163	1.66	1.715957
82	1.614117	1.674967	1.659945	1.71617
83	1.614286	1.675329	1.659452	1.717826
84	1.614286	1.675479	1.659128	1.715957
85	1.614156	1.675049	1.659615	1.71617
86	1.614246	1.675395	1.66	1.719111
87	1.61401	1.675347	1.659504	1.721136
88	1.614299	1.675281	1.659178	1.717609
89	1.61414	1.675629	1.659504	1.8296
90	1.614062	1.675629	1.659669	1.8296
91	1.614206	1.675149	1.660224	1.832857
92	1.614486	1.675298	1.660056	1.8296
93	1.614193	1.675017	1.660224	1.832857
94	1.614538	1.675298	1.660224	1.832449
95	1.614393	1.675667	1.659722	1.719111
96	1.614259	1.675395	1.659392	1.8292
97	1.614272	1.675953	1.659392	1.832449
98	1.614313	1.675819	1.660795	1.8288
99	1.614272	1.676216	1.660282	1.8288
100	1.614615	1.675133	1.659669	1.8288

$Fe_{0.5}Ni_{0.5}O_xH_y$	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.544592	1.582123	1.604774	1.638813
2	1.545288	1.582788	1.606574	1.639355
3	1.546719	1.581975	1.60755	1.64247
4	1.546562	1.583067	1.607101	1.643405
5	1.545129	1.583665	1.606962	1.64201
6	1.545003	1.581384	1.605766	1.63912
7	1.54484	1.581824	1.605657	1.639223
8	1.544864	1.583557	1.606342	1.639149
9	1.54522	1.582962	1.607057	1.640765
10	1.545555	1.582846	1.606832	1.64055
11	1.544979	1.583128	1.60603	1.640769
12	1.5454	1.583188	1.606788	1.639684
13	1.54534	1.582389	1.606351	1.6399
14	1.545381	1.584243	1.606931	1.640728
15	1.546989	1.583215	1.607548	1.640758
16	1.547118	1.583038	1.608279	1.642117
17	1.545552	1.584232	1.607414	1.641397
18	1.547075	1.583582	1.607698	1.640703
19	1.547263	1.583266	1.608339	1.641823
20	1.547354	1.584005	1.608244	1.643168
21	1.547168	1.583791	1.608515	1.641679
22	1.547413	1.583448	1.60865	1.642105
23	1.545291	1.583669	1.607281	1.642229
24	1.545734	1.583809	1.606792	1.639624
25	1.545742	1.583527	1.607679	1.640586
26	1.545413	1.584108	1.607374	1.641575
27	1.545964	1.584335	1.607495	1.641324
28	1.54625	1.584923	1.609526	1.643834
29	1.545834	1.585452	1.608973	1.64354
30	1.546103	1.585007	1.608922	1.642445
31	1.546264	1.585191	1.609856	1.64391
32	1.545903	1.585897	1.609036	1.643504

33	1.546383	1.585396	1.609599	1.642797
34	1.546362	1.58572	1.610283	1.644239
35	1.546052	1.58579	1.609161	1.643226
36	1.547813	1.583909	1.609171	1.642792
37	1.546088	1.585009	1.608954	1.643281
38	1.547698	1.584753	1.608848	1.64211
39	1.546721	1.586115	1.61095	1.645325
40	1.546406	1.58681	1.611019	1.645053
41	1.54673	1.586561	1.610365	1.644466
42	1.54661	1.58554	1.610354	1.644528
43	1.54638	1.586336	1.609418	1.643871
44	1.546781	1.585992	1.610339	1.644091
45	1.546556	1.586251	1.610698	1.644707
46	1.546514	1.586395	1.609865	1.643085
47	1.546763	1.585519	1.610841	1.644615
48	1.546534	1.586557	1.610163	1.644588
49	1.546725	1.585633	1.610056	1.642559
50	1.546625	1.586011	1.610798	1.645762
51	1.546623	1.586559	1.609938	1.643614
52	1.546793	1.586348	1.611218	1.644753
53	1.546705	1.586552	1.610259	1.644487
54	1.546752	1.586063	1.610285	1.643525
55	1.546803	1.586501	1.610939	1.64465
56	1.54691	1.586847	1.610617	1.64394
57	1.547038	1.586567	1.610959	1.645054
58	1.546821	1.586839	1.610271	1.644243
59	1.547107	1.586339	1.611026	1.643417
60	1.546889	1.586998	1.611416	1.645472
61	1.547134	1.586938	1.610762	1.645447
62	1.547231	1.586919	1.611591	1.645983
63	1.546834	1.587105	1.610432	1.644846
64	1.547099	1.586072	1.611141	1.644944
65	1.54686	1.587009	1.610633	1.645988
66	1.547318	1.58704	1.611598	1.644634
67	1.547117	1.58756	1.611476	1.64614

68	1.547232	1.587547	1.611405	1.645715
69	1.547373	1.587434	1.611932	1.646367
70	1.547083	1.587327	1.610893	1.645324
71	1.547443	1.58694	1.611891	1.645707
72	1.547088	1.587706	1.611365	1.646001
73	1.547625	1.587407	1.611561	1.64536
74	1.54733	1.586905	1.611564	1.646105
75	1.547096	1.58711	1.61063	1.644061
76	1.547384	1.586229	1.610889	1.645113
77	1.547151	1.587283	1.610785	1.644768
78	1.547458	1.58678	1.611039	1.644575
79	1.547095	1.587021	1.610802	1.645153
80	1.547387	1.58725	1.611313	1.644277
81	1.54766	1.58776	1.61217	1.646893
82	1.547398	1.587977	1.611721	1.644798
83	1.547888	1.587719	1.612835	1.647039
84	1.547772	1.588647	1.612119	1.646311
85	1.547713	1.587708	1.612904	1.646767
86	1.547837	1.588387	1.611759	1.646719
87	1.548166	1.587933	1.612497	1.646445
88	1.547853	1.588784	1.613097	1.647661
89	1.547737	1.588818	1.612608	1.646646
90	1.548082	1.58847	1.613051	1.647997
91	1.547965	1.588816	1.612569	1.646188
92	1.547986	1.588256	1.613409	1.646753
93	1.547935	1.588402	1.611855	1.646329
94	1.548039	1.587714	1.612343	1.645601
95	1.547516	1.588053	1.611642	1.64604
96	1.547785	1.588255	1.611817	1.644988
97	1.547721	1.58787	1.612056	1.646141
98	1.547612	1.588316	1.611529	1.645174
99	1.547814	1.587698	1.612035	1.646813
100	1.549148	1.585754	1.610094	1.644365

$Fe_{0.7}Ni_{0.3}O_xH_y$	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.540909	1.576629	1.64489	1.641155
2	1.544271	1.594032	1.599269	1.639987
3	1.545619	1.586337	1.629124	1.651598
4	1.54414	1.583544	1.636243	1.647516
5	1.5447	1.595139	1.602953	1.651362
6	1.544623	1.584831	1.619468	1.596142
7	1.544357	1.579724	1.614285	1.648566
8	1.541742	1.584982	1.627098	1.641655
9	1.542222	1.595456	1.606757	1.652474
10	1.546576	1.582933	1.707273	2.12255
11	1.543267	1.595503	1.62843	1.654731
12	1.544126	1.609178	1.590075	1.640472
13	1.5422	1.583608	1.681338	1.662772
14	1.543843	1.584322	1.619454	1.654868
15	1.542845	1.599968	1.595694	1.658088
16	1.539586	1.579967	1.657662	1.610381
17	1.54093	1.579479	1.641436	1.677062
18	1.54273	1.582568	1.616629	1.650387
19	1.542472	1.605482	1.603486	1.614732
20	1.542966	1.586438	1.617328	1.665829
21	1.541217	1.578267	1.617917	1.620295
22	1.54328	1.584709	1.598475	1.652141
23	1.544108	1.622135	1.596199	1.67101
24	1.542154	1.580321	1.60116	1.653167
25	1.541747	1.57943	1.618905	1.622376
26	1.543928	1.575548	1.627567	1.656801
27	1.537675	1.595379	1.605006	1.59916
28	1.539453	1.5896	1.630111	1.660848
29	1.541657	1.582806	1.628295	1.743021
30	1.540038	1.592006	1.613979	1.655154
31	1.545352	1.623207	1.599697	1.626354
32	1.540271	1.58647	1.595348	1.662098

33	1.539747	1.58145	1.626635	1.603138
34	1.545485	1.58937	1.59572	1.653138
35	1.543451	1.585248	1.592421	1.666106
36	1.538334	1.5855	1.637678	1.671375
37	1.541295	1.577166	1.610025	1.630677
38	1.542764	1.589778	1.596156	1.589956
39	1.53795	1.588054	1.621174	1.662129
40	1.538559	1.588884	1.744543	1.62508
41	1.539508	1.586498	1.633377	1.659161
42	1.540007	1.59027	1.599665	1.597781
43	1.539097	1.587875	1.594178	1.657733
44	1.539665	1.583486	1.630263	1.657379
45	1.542124	1.597536	1.597567	1.666938
46	1.539965	1.585045	1.586286	1.614646
47	1.537308	1.584043	1.616195	1.606416
48	1.539227	1.574718	1.614363	1.657555
49	1.538087	1.580933	1.596982	1.676066
50	1.537937	1.586955	1.62812	1.671039
51	1.537571	1.576396	1.61622	1.633128
52	1.538259	1.596679	1.604175	1.663236
53	1.539906	1.586555	1.636248	1.613348
54	1.539701	1.578961	1.629376	1.657317
55	1.538092	1.599644	1.607318	1.621726
56	1.538794	1.585218	1.629489	1.669567
57	1.539644	1.582092	1.608704	1.783201
58	1.540567	1.59008	1.595685	1.667052
59	1.542201	1.592583	1.620273	1.667269
60	1.538341	1.586502	1.64327	1.655825
61	1.541597	1.581103	1.609157	1.608597
62	1.541855	1.612491	1.59585	1.661422
63	1.538782	1.587041	1.724574	1.585059
64	1.538922	1.581537	1.62612	1.668113
65	1.539044	1.598584	1.592603	1.686659
66	1.539196	1.580866	1.622401	1.662197
67	1.537707	1.586979	1.629406	1.636891

68	1.538804	1.56978	1.609572	1.668463
69	1.542091	1.582624	1.606597	1.588912
70	1.539092	1.603437	1.607108	1.657273
71	1.538089	1.586668	1.809726	1.634631
72	1.54113	1.582465	1.623502	1.659814
73	1.538026	1.608006	1.599387	1.743942
74	1.539162	1.588098	1.680685	1.670677
75	1.536418	1.58245	1.63404	1.624949
76	1.536548	1.589619	1.604319	1.669153
77	1.539627	1.588788	1.605151	1.642708
78	1.539672	1.590774	1.649726	1.6198
79	1.539908	1.583062	1.617673	1.65703
80	1.540095	1.597629	1.611539	1.709573
81	1.538328	1.588724	1.644023	1.659208
82	1.537672	1.582983	1.616528	1.646064
83	1.542095	1.590058	1.605335	1.658048
84	1.538586	1.621793	1.624288	1.595002
85	1.539298	1.590302	1.737252	1.669088
86	1.542212	1.584373	1.633437	1.683581
87	1.537925	1.630929	1.61119	1.641024
88	1.539067	1.592145	1.693232	1.662036
89	1.542526	1.583253	1.642133	1.597037
90	1.538045	1.596495	1.610516	1.655573
91	1.541489	1.593271	1.610892	1.701424
92	1.54062	1.586609	1.630409	1.665474
93	1.539475	1.587162	1.612712	1.636915
94	1.544352	1.604944	1.59786	1.662569
95	1.539683	1.586914	1.651167	1.618026
96	1.539513	1.586801	1.627673	1.659521
97	1.542603	1.596817	1.594624	1.7239
98	1.540798	1.589437	1.644134	1.677414
99	1.539307	1.587718	1.621878	1.64273
100	1.536141	1.596342	1.621777	1.670025

FeO_xH_y	Current density (mA cm^{-2})			
Measurements	1	5	10	20
1	1.719327	1.775505	1.815462	1.882823
2	1.723995	1.782122	1.826549	1.881729
3	1.728602	1.787689	1.835652	1.889335
4	1.730539	1.788304	1.838137	1.899023
5	1.734972	1.793494	1.837285	1.909229
6	1.738761	1.80336	1.843091	1.916414
7	1.745295	1.805919	1.847215	1.912723
8	1.746962	1.810779	1.843966	1.912659
9	1.746226	1.809728	1.84636	1.921432
10	1.748219	1.809377	1.852374	1.919674
11	1.750503	1.813799	1.849547	1.916011
12	1.749343	1.814347	1.849249	1.924778
13	1.750287	1.812543	1.861112	1.925522
14	1.753002	1.816411	1.862439	1.919454
15	1.752023	1.817651	1.868247	1.927095
16	1.751978	1.815523	1.865489	1.929874
17	1.754833	1.818525	1.864428	1.923644
18	1.755022	1.820697	1.870166	1.928718
19	1.754076	1.818113	1.868934	1.933182
20	1.756787	1.820389	1.866484	1.926423
21	1.757304	1.823477	1.872224	1.92985
22	1.7558	1.820458	1.871811	1.936524
23	1.758365	1.82211	1.868443	1.93008
24	1.759083	1.825785	1.873709	1.951854
25	1.757745	1.822965	1.874928	1.944116
26	1.760128	1.823638	1.871119	1.94833
27	1.760903	1.8281	1.875849	1.954048
28	1.759266	1.825417	1.877327	1.947242
29	1.760454	1.827149	1.873508	1.950835
30	1.761777	1.831433	1.877271	1.956928
31	1.759854	1.828917	1.87953	1.949432
32	1.761989	1.829252	1.875336	1.951624

33	1.763584	1.83351	1.879381	1.958986
34	1.762943	1.829398	1.881482	1.951301
35	1.764663	1.829268	1.877185	1.952737
36	1.766346	1.8337	1.880855	1.960513
37	1.764717	1.832012	1.883686	1.954325
38	1.766366	1.843691	1.878701	1.95487
39	1.766964	1.840426	1.882213	1.963187
40	1.765287	1.841691	1.885648	1.956637
41	1.76706	1.845379	1.880651	1.95748
42	1.768633	1.84204	1.883977	1.964401
43	1.766944	1.843244	1.886836	1.957501
44	1.768421	1.846213	1.88218	1.958852
45	1.770369	1.843304	1.886461	1.966099
46	1.768406	1.844507	1.888553	1.959794
47	1.770436	1.847852	1.883996	1.962358
48	1.771835	1.8443	1.888415	1.968063
49	1.770096	1.846237	1.890418	1.961478
50	1.772087	1.84907	1.885719	1.965219
51	1.773449	1.845836	1.890458	1.970071
52	1.771516	1.848649	1.897744	1.962875
53	1.774039	1.850391	1.903861	1.968101
54	1.774826	1.846863	1.900842	1.971691
55	1.77277	1.850332	1.899525	1.964943
56	1.776158	1.851352	1.905816	1.971777
57	1.775838	1.848203	1.901551	1.972502
58	1.774587	1.852235	1.902223	1.966619
59	1.778338	1.851853	1.906967	1.974881
60	1.776807	1.849565	1.902446	1.973812
61	1.784393	1.854398	1.906004	1.968958
62	1.782218	1.851842	1.90846	1.978313
63	1.784036	1.851569	1.903946	1.9732
64	1.78513	1.856142	1.9092	1.97299
65	1.783076	1.853116	1.910056	1.990004
66	1.785532	1.853783	1.905241	1.995335
67	1.786002	1.857602	1.911439	1.999697

68	1.784088	1.85409	1.910732	1.99152
69	1.786889	1.856393	1.907226	1.999241
70	1.786331	1.858842	1.913897	2.000485
71	1.785115	1.855469	1.910219	1.99376
72	1.78801	1.858628	1.909666	2.002303
73	1.786201	1.859627	1.915955	1.999422
74	1.786366	1.85685	1.911007	1.996124
75	1.788916	1.86085	1.913263	2.00616
76	1.786921	1.860457	1.917348	1.999991
77	1.78789	1.858341	1.911882	1.999306
78	1.789663	1.863316	1.916207	2.008342
79	1.787722	1.860575	1.918679	2.000491
80	1.789565	1.860616	1.913915	2.004518
81	1.790649	1.865048	1.919126	2.010353
82	1.78859	1.861306	1.919626	2.002126
83	1.7913	1.86336	1.91569	2.008384
84	1.791157	1.866414	1.922161	2.012427
85	1.789611	1.862736	1.920336	2.005458
86	1.792578	1.866363	1.918632	2.013439
87	1.791031	1.867805	1.924934	2.011996
88	1.791443	1.864592	1.920375	2.007663
89	1.793883	1.868942	1.922329	2.017763
90	1.791551	1.86844	1.927139	2.011375
91	1.792916	1.866164	1.922176	2.011421
92	1.795001	1.871189	1.925865	2.020588
93	1.792468	1.869826	1.928883	2.013987
94	1.794204	1.868359	1.924023	2.015494
95	1.795905	1.873667	1.929577	2.023809
96	1.793589	1.870921	1.931354	2.0158
97	1.795877	1.87152	1.926352	2.019868
98	1.796738	1.875854	1.932261	2.025598
99	1.794532	1.872202	1.932956	2.0181
100	1.793976	1.873132	1.931663	2.020366

Top 50 equations from the DSR algorithm

Definitions of x_i

x1: number of *d*-electrons (N_d)
x2: Pauling electronegativity (χ)
x3: atomic radii (γ)
x4: ΔG_1
x5: ΔG_2
x6: ΔG_3
x7: ΔG_4
x8: $\max(\Delta G_i)$
x9: *ESSI*

◆ *1 mA cm^{-2}*

rank	score	expression
1	0.626387386	sin(x7*sqrt(x9)/x8)/(4*x3)
2	0.594619589	log(x7**2*(sqrt(x8)/x6 + exp(sqrt(x3))/(5*x3)))
3	0.594123018	x4*exp(-x3/sqrt(x2 + log(x8)))
4	0.59234255	x1*x7*sqrt(x8)*exp(-3*x3)/x6
5	0.590715766	x2*x8/(-x3 + exp(x6) - log(x3 + exp(4*x3**2)))
6	0.584795341	x4*sqrt(x8)*exp(-x3)/x3
7	0.580427469	x4*sqrt(x8*exp(x2)/(x3*x7*(x3 + exp(x3 + exp(x3)))))
8	0.57518221	sqrt(x8)/(-2*x3 + x6*exp(x3))
9	0.566854688	cos(sqrt(x6 - log(x2*sqrt(x8))))
10	0.563985324	x4*sqrt(x8*exp(sin(x4))/(x3*x7**2*(x2 + x3 + exp(x3))))
11	0.560703461	sin(x4*sqrt(x8/(x6*x7)))
12	0.559206693	x2*log(sqrt(x5 + x8))/x6
13	0.558947051	x4*x5*sqrt(x8/log((x3 + (exp(x8) + exp(x2 + 2*x3 + x7))/x2)/x7))
14	0.558221956	exp(-x6 + x7*x8)
15	0.558221956	exp(-x6 + x7*x8)
16	0.557844488	sqrt(x7)*exp(-x6 + x8)
17	0.554737789	exp(x3 - x6 + x8 - sin(x3))
18	0.553639807	log(log(x5*x7*(x2 + sqrt(x8*exp(x4*x5*x8)/x7))))
19	0.553203063	x4*sqrt(x8*(-x3 + x7))
20	0.552592728	log(log(sqrt(exp(x5*x7*(sqrt(x5)*x8/x7 + x5)))))

21	0.551895858	log(log(log(x7*x8*(x3 + x5)*exp(exp(x5))*sin(x5)/x3)))
22	0.55136384	x8*(x3 + x5)*exp(x4)*exp(-x6)
23	0.551203443	x4*sqrt(sin(x8/(x6*x7)))
24	0.550416944	exp(-x6/sqrt(x7) + x8)
25	0.550294923	log(sin(x5 + exp(x8*(-2*x3 + x8 - exp(x3))))/x3)
26	0.549986321	sin(log(sqrt(x4*exp(sqrt(x2*x5*x8/x7)))))
27	0.54941232	exp((-x6 + sin(x8))*sin(x7))
28	0.548366252	x5*(x4 + x8)/log((-x3 + exp(x3 + 2*exp(x3)))/x3)
29	0.548222776	exp(x5*x8 - x6)
30	0.545415629	sqrt(sqrt(x8)/(x6**2*(-x5 + x7*exp(x7)*sin(x7))))
31	0.544197821	x8*exp(-sin((x4 + x5)/sqrt(x7*exp(-x4))))
32	0.544117733	sqrt(x4*sqrt(x8)*(x5 + x7)/(x3*(x3 + exp(4*x3))))
33	0.543721375	(x4 + x8)*exp(-sqrt(x6))
34	0.543261733	x5*(-x3 + cos(x3 - x8))
35	0.543089844	exp(x7*sin(3*x7/x3))
36	0.542590164	x4*exp(x8)/log(x7*(-x3 + sqrt(x3 + exp(exp(3*x3))))/x2)
37	0.541330811	log(sqrt(exp(x7*log(x2 + exp(x5))*sin(exp(x8)/x6)/(2*x3 + x7))))
38	0.541315043	sin(x8/(exp(x8) + log(exp(x6)/(4*x3 + x5 + 2*x7))))
39	0.541077507	x4*exp(x8)/(x3 + x6 + x7)
40	0.540946398	x4*x5*x7*x8*sin(x7*exp(-x8))/(2*x3**2)
41	0.540723129	x4*exp(x8)/(-x3 + exp(sqrt(x3)) + exp(x3))
42	0.540334714	x7 - sin(sqrt(x2*(x2 + x8*log(x5 + x5/x9 - x7 - x9))))
43	0.53842398	sin(log(x4 + sqrt(x8)))
44	0.53842398	sin(log(x4 + sqrt(x8)))
45	0.53842398	sin(log(x4 + sqrt(x8)))
46	0.538416256	log(x2 - log(sqrt(exp(sqrt(cos(x3*(2*x3 + exp(exp(x3)))))))))
47	0.538370757	(x4 + x8)/(2*x3**2*x6 + x3 + x4 + sqrt(x8))
48	0.538111251	x3*cos(x7)/sin(exp(exp(x3)))
49	0.538075781	sqrt(log(log(sqrt(x5)*(x5 + exp(x8*(x7 - log(x2)))))))
50	0.538018053	sqrt(sin(x4*x8)) - cos(x5)

◆ ***5 mA cm^{-2}***

rank	score	expression
1	0.726103885	x9/(x5*x8*(x3 + x5**2*(-x2*x5 + x3*x4)/x6 + sin(x3)) + x7)
2	0.711196932	exp(cos(x2/(2*x3**7*x5*(x3 + 2*x5)) + x3))

3	0.710022782	exp(sin(x1 - x3*(x3*(4*x3 + x5)*exp(x5) - x3)))
4	0.709312752	exp(cos(x2*x7/(4*x3**6*x5**2) + x3))
5	0.705596347	exp(-sin(x1*x4**2*x8/(x3*(x3 + x9)) + x3 - x7))
6	0.70384991	exp(cos(x2/(x3**5*x5*x7*(2*x3 + x5)) + x3))
7	0.700509974	exp(cos(x1*x5*x6 + x3*x5*(2*x3 + x5)))
8	0.700509974	exp(cos(x1*x5*x6 + x3*x5*(2*x3 + x5)))
9	0.700509974	exp(cos(x1*x5*x6 + x3*x5*(2*x3 + x5)))
10	0.69954978	exp(cos(x2/(4*x3**6*x5**2) + x7))
11	0.69954978	exp(cos(x2/(4*x3**6*x5**2) + x7))
12	0.699154378	x9 - log(log(x2*log(x9 + exp(-x8 + x9)/x4) + x2))
13	0.698446224	x8*exp(x3*sin(x5*(x3 + x5)**2) - x3 + sin(x6))
14	0.698260809	exp(cos(x3**2*(x3 + exp(x3**2*(x3*x5 + x3 + x4 + x5))) + x3 - x7))
15	0.697945366	exp(sin(exp(x3*(x3*(2*x3 + 2*x5) - x3))))
16	0.697874996	exp(cos(sqrt(x3*(x3**2*exp(5*x3**2*x5) - 2*x3))))
17	0.697262399	exp(cos(x2*(-x3*(x3*(x3*x5*(2*x3 + 2*x5) + x3) + x3) + x7)))
18	0.695874403	exp(cos(x6/log(5*x3**4*x5)))
19	0.695874403	exp(cos(x6/log(5*x3**4*x5)))
20	0.695874403	exp(cos(x6/log(5*x3**4*x5)))
21	0.695874403	exp(cos(x6/log(5*x3**4*x5)))
22	0.695874403	exp(cos(x6/log(5*x3**4*x5)))
23	0.695874403	exp(cos(x6/log(5*x3**4*x5)))
24	0.694832465	exp(cos(x2*x3**2*(x3*(4*x3 + x5) + x3) - x8))
25	0.694708598	exp(cos(exp(x3**3*x7*(4*x3*x5 + x3) - x3)))
26	0.694120206	exp(cos(x5*(x2 + x9)/(x3**2*(x3*x5*x7 + x3))))
27	0.693631434	exp(cos(x2*x3**(3/2)*x6*(x2*x4*x5 + x2*x5) + x5))
28	0.69264789	exp(cos(sqrt(x1)*(x3**3*(2*x3 + 3*x5) - x3)))
29	0.692083671	exp(cos(x3**3*(x3*(4*x3 + x5)*exp(x5) + x3) - x7))
30	0.691631932	exp(cos(exp(x3*(x3**3*x5*(3*x3 + 2*x5) - x3))))
31	0.691353983	log(x3*sin(x5*(4*x3*x5 + x3)) + exp(x8))
32	0.690518655	exp(cos((-x3 + exp(x3**2*(x3*(x3*x5*(3*x3 + x5) + x3) - x3)))/x3))
33	0.690300574	exp(cos(x2*exp(x3)/(x3**4*x5*(3*x3 + x5))))
34	0.689867328	exp(cos(x5*sqrt(x6)*(4*x3**2*x5 + x3 + exp(x3))))
35	0.68905286	exp(cos(x6*(-x3**2*(5*x3 + x4 + x5) - x3 + x6)))
36	0.688958088	exp(cos(x3**3*(x3 + x7*exp(x3**2*(x4 + 2*x5))) - x3 + x7))

37	0.688605381	exp(cos(x6*(-x3*(x3**2*(x3 + x5*(3*x3 + x5)) + 2*x3) - x3 + x6)))
38	0.688603669	exp(cos(exp(x2)/(x3**3*x5*(4*x3 + x5))))
39	0.688603669	exp(cos(exp(x2)/(x3**3*x5*(4*x3 + x5))))
40	0.688603669	exp(cos(exp(x2)/(x3**3*x5*(4*x3 + x5))))
41	0.688043202	exp(cos(x2 + x7/(x3**6*x5**2*(3*x3 + x5))))
42	0.688043202	exp(cos(x2 + x7/(x3**6*x5**2*(3*x3 + x5))))
43	0.688043202	exp(cos(x2 + x7/(x3**6*x5**2*(3*x3 + x5))))
44	0.688043202	exp(cos(x2 + x7/(x3**6*x5**2*(3*x3 + x5))))
45	0.688043202	exp(cos(x2 + x7/(x3**6*x5**2*(3*x3 + x5))))
46	0.686984535	exp(cos(x2*x3**2*(x3**2*(3*x3 + 2*x5) + 2*x3) - x8))
47	0.686847126	exp(sin(x3**2*(8*x3*x5 + x5)))
48	0.686497603	exp(sin(log(log(log(2*x3**3*(2*x3 + x5))/x3**2))))
49	0.685992094	exp(cos(x2*(x3**2*(x3*x5*(4*x3 + x5) + x3) - x3)))
50	0.685257292	log(x4*(x7*sin((x5*x7**2*x8 + x7)/x7) + x8) + x9)

◆ ***10 mA cm^{-2}***

rank	score	expression
1	0.72010348	exp(sin(log(log(sqrt(x8) + x9/x8))))
2	0.71734414	x4*x7**2*x8 + x9 + log(x4)
3	0.716224351	x4 + x9 - cos(x4*x5**3*x7*x8)
4	0.714385626	exp(sin(x6/log((x6 + x9)/x6)))
5	0.712262645	exp(sin(log(log(log(x1*x7*x9 + x2)))))
6	0.709186794	exp(cos(x9 + exp(x9/x8) + log(x6)))
7	0.707559694	exp(sin(x1/(-x7 + x8*x9 + log(x5))))
8	0.707340129	log(x4**2 + x9 + sqrt(sin(x8)))
9	0.705611295	sin(sqrt(x7*sqrt(x8*(x1*x8**2*x9**3 + x8))) + log(x4))
10	0.704769814	sqrt(x8*(x5 + cos(x9 - exp(x5))))
11	0.70373112	(x7*sin(x7*x8**2*x9**2) + x7)*sin(log(x4 + sqrt(x8)))
12	0.702439762	exp(-sin(x8 - log(x9/(x4*x7))))
13	0.701975412	exp(sin(log(x9*log(x5 + x9/x8))))
14	0.701571966	cos(sqrt(x2) - x7 + x8 + x9 - sqrt(exp(x6*x7/x5)))
15	0.70130261	(x4 + x8 - cos(x7) - cos(x7 + x9))/x6
16	0.700089296	exp(sin(x4*log(x9/(x7 + x8))))
17	0.699996664	exp(cos(-x1*x7 + x3/x9 + x4))

18	0.699830724	exp(sin(log(log(sqrt(x2) + x9 + log(x3)))))
19	0.698943694	exp(sin(x7*log(x9) - x8 + log((x8*x9 + x8)/x8)))
20	0.698394733	log(x8 + log(x5)) + sin(x9/(x5*x7**2*x8**2))
21	0.69805703	exp(cos(2*x6 - x8 + x9))
22	0.69805703	exp(cos(2*x6 - x8 + x9))
23	0.696663774	sqrt(x8)/cos(x8**2*x9) + log(x4)
24	0.695694613	x4 + x5*log(x2 - cos(x9))/x8
25	0.695416159	exp(sin(log(x8*(-x5 + x8) + sqrt(x9))))
26	0.695256754	exp(sin(log(log(x3 + (x7*x9*(x9**2 + x9)*exp(x9))**(1/4)))))
27	0.695233868	exp(sin(x7*(x3 + x8)*log(x9/x7)))
28	0.695013437	exp(sin(-x7**2*x8 + x8*x9 + log(x9)))
29	0.695006388	exp(sin(x7*(-x7 + log(exp(x9) + log(x9/(x7*x8))))))
30	0.694301322	exp(sin(x7*log(x3*x5*x9)))
31	0.693951765	exp(sin(x1*x5*sqrt(x7*x9)))
32	0.692677022	exp(-x6*cos(x9) + sqrt(x8))
33	0.692531829	sin(x5 + x6 - (x7*x8**4*x9**2)**(1/4))
34	0.692436227	log(x5*x7**2*sin(x5*x7*log(x5)) + x9 + sin(x8))
35	0.69212699	sin(x4*sqrt(x8)*log(sqrt(x4))/x9 + sqrt(x8))
36	0.691802405	sqrt(exp(-x7 + sin(x7**2*log(x9)) + sin(x8)/x2))
37	0.691582201	exp(sin((x7*x8*exp((x5 - x9)*exp(-x8)) + x7)*exp(x4)))
38	0.691490977	exp(sin(log(x9*(x3 + x9*(-x9**2 + x9)))))
39	0.691389776	x4 + sin(x7 + (x5*sqrt(x7**2*x8*x9) - 2*x7)/x7)
40	0.690984489	exp(sin(log(x2 - x7)/x9))
41	0.690984489	exp(sin(log(x2 - x7)/x9))
42	0.69089839	sin(sqrt(log(x5 + x9*(x9 + log(x8)))))
43	0.690829094	exp(sin(exp(x7*exp(x9)/(x3 + x9))))
44	0.690742822	exp(sin(log(x3*sqrt(x7)*x9)))
45	0.690742822	exp(sin(log(x3*sqrt(x7)*x9)))
46	0.690742822	exp(sin(log(x3*sqrt(x7)*x9)))
47	0.690742822	exp(sin(log(x3*sqrt(x7)*x9)))
48	0.690742822	exp(sin(log(x3*sqrt(x7)*x9)))
49	0.690323148	exp(sin(log(sqrt(x3**(3/2)*x9**2))))
50	0.689778152	exp(sin(log(sqrt(x3)*x9/x7)))

◆ ***20 mA cm^{-2}***

rank	score	expression
1	0.751827993	-x3 + x8 - sin(x3 - x6/(x2*x3*x8*sqrt(x3*x5*(x3**2 + x3 + x7) + x3)))
2	0.697920925	x3**2*exp(sin(x5 + exp(exp(sqrt(x1*x2*x5)))))
3	0.685037173	exp(cos(exp(sqrt(x7)*(x2 + 2*x3))))
4	0.652181114	exp(cos(exp(-x3 + log(x5*x6/(x3**4*(2*x3 + x7)))/x3)))
5	0.647320156	exp(cos(exp(x6)*log(log(x3*(x3**2*(4*x3 + 3*x5) - x3)))/x3))
6	0.646359666	exp(cos(x3**2/(x3*log(x3*x5*(6*x3**2 + x3)) - x3)))
7	0.635930883	exp(cos(exp(log(x1)*log((x3**2*(x3*(2*x3 + x4) + 3*x3) - x3)/x3)/x3)))
8	0.631275806	exp(cos(x5/(x3*log(x3**2*(x3*(3*x3 + 3*x4) + x3)))))
9	0.627682476	exp(sin(x7)*cos(x2/(x3*(x2*x3**2*(x3*x5 + x3) - x3))))
10	0.624317782	exp(sin(exp(x7 - (x3*x9 - x8)*(x3*(x3*(x3**2 + x3) + 3*x3) + x3)/x3)))
11	0.622635186	exp(-sin(x3*x9/(3*x3**4*x7 - x3) - x9/x2))
12	0.622030016	exp(sin(exp(x3**2*(x3*(x3*exp(x3*x5**2*x7) + x9) + x3))))
13	0.621733408	exp(cos(2*x3 - x5*x6/(x3**4*(x3*(x3**2 + 2*x3) + x3))))
14	0.61824896	exp(cos(1/(x3*log(x3**2*(x3*(x3 + x4*x5) + 3*x3)))))
15	0.617720184	exp(sin(log(-x3**5*x8*(x3 + x7)/(x3 + x9) + x9)))
16	0.616441035	exp(sin(x8 - sqrt(exp(x3)) + exp(x2**2*x3)))
17	0.61441548	x8*(-x3*exp(sin(x3**3*x6)) - x3 + x5*exp(cos(x3)))/x3
18	0.614003434	exp(sin(x1*(x2*x3**2*x5 + x6)))
19	0.612971851	exp(x3*(x3**2*sin(x3 + exp(x7/(x2*x5 - x3**2 - 2*x3))) - x3))
20	0.612470228	sqrt(exp(log(x1)*cos(x3 + 1/(x3**5*(x3*(x4 + x5) + x3)))))
21	0.609504993	exp(sin(x3*(-x3 + x5*(-x3 + x7*exp(2*x3*(x3**2 + x3))))))
22	0.608961897	exp(cos(exp(log(x2)/(x3*(x3*(x3*(x3 + x4) + 3*x3) - 2*x3)))))
23	0.608536392	exp(sin(x2/log(x3**2*x5*x7*(x3**2*x7 + 2*x3))))
24	0.60830422	exp(cos(1/(x5*log(x7*(x3**3*(x3**2*x7 + x3) + x3)))))
25	0.607953404	x3*sin(x3*exp((x3*x4*x5*x7 + x3 + x4)*log(x1)))
26	0.606795533	sqrt(exp(-x2*exp(x3)*log(x3*(x3*(x3*x5 + 2*x3) + x3)) + sin(x3/x8)))
27	0.605203056	cos(x7)/sin(x7/(x3*log(x3*(x3*(x3 + x5**2) + 2*x3))))
28	0.602861872	exp(-sin(2*x3 - x3*x9*exp(x9)/(x2*log(x3**2*x7*(x3*x7 + 2*x3)))))
29	0.602830864	exp(cos(sqrt(exp(exp(log(x7)/(x3**2*(x3**2*x7*(x3*x4 + 2*x3) -

		x3)))))))
30	0.601776646	exp(cos(x3/log(x3*(x3**3*(x3*x4*x5**2 + x3) + x7))))
31	0.601754198	exp(cos(x1*x5*log(x3**2*(x3*(x3**2 + x3) + x3) + x3)))
32	0.601721368	x5*sqrt(x8)*cos(x3 + log(x3**3*(x3*x7 + 4*x3)))
33	0.60161463	log(x7 + exp(cos((x3**2*x7*(x3*(x3*x5*x7 + x3) + x3) - x3)*exp(x2))))
34	0.601061156	exp(cos(x3*x6/log(x3**3*(x3*x5 + 5*x3))))
35	0.600992451	exp(sin(log(-x3*x8/(x2 + x3**4*x5*x7) + x9)))
36	0.600830232	exp(cos(x3 + log(x6/log(x3**2*(2*x3*x5 + 3*x3) - x3))))
37	0.600367642	exp(cos(x1*x3**4*(x3*(x3 + x5) + 2*x3) - x7))
38	0.600248909	x8*(-x3**2*(x3**3 + 3*x3) + x4 + x5)/x3
39	0.599679916	exp(cos(x7 - exp(x1*x3**4)))
40	0.599411826	sin(sqrt(x8*(x2*x7 - x3*(x3*(x3*(2*x3 + x7) + x3) + x3))/x3))
41	0.599167343	exp(sin(x3*exp(x3*(x3*(2*x3*x4*x5 + 2*x3) + x3)) - x3 + x9))
42	0.598702034	x3*x9*cos(x1)/log(x3*(x3**2*(2*x3**4 + x3) + 2*x3))
43	0.598643842	sqrt(x8*cos(log(x2*x5/(6*x3**3) - x3)))
44	0.598456984	sqrt(exp(-x3 + cos(x3**2*exp(x3*x5*x7*(x3*(2*x3**2 + x3) + x3)) - x3)))
45	0.598249875	x3*x8/sin(x3*x4*x5*(x3**3 + 4*x3))
46	0.598193536	2*x3 + sin(x3**2*x7*(x1 + x6))
47	0.597715653	x3/(x2 + log(sin((x3**4*(2*x3 + 3*x5) - x3)/x3))/x3)
48	0.597664628	exp(cos(x3)*cos(x7*log(x6/(x3*log(x3*(3*x3 + x5) + x3) - x3))))
49	0.597629801	sqrt(x8*cos(x3 - (-x3*(x3**2*(4*x3**2 + x3) + x3) + x5)/x3))
50	0.597354556	exp(cos(x2*(log(x4) + log(x7*(x3*(x3**2*(x3**2 + x3) + x3) - x3)))))

REFERENCES

1 T. Wang, X. Li, Y. Pang, X. Gao, Z. Kou, J. Tang and J. Wang, *Chem. Eng. J.*, 2021, **425**, 131491.
2 A. J. Tkalych, H. L. Zhuang and E. A. Carter, *ACS Catal*, 2017, 11.
3 P. Gono and A. Pasquarello, *J. Chem. Phys.*, 2021, **154**, 024706.
4 H. Xiao, H. Shin and W. A. Goddard, *Proc. Natl. Acad. Sci.*, 2018, **115**, 5872–5877.
5 J. M. P. Martirez and E. A. Carter, *J. Am. Chem. Soc.*, 2019, **141**, 693–705.
6 Y.-F. Li and A. Selloni, *ACS Catal.*, 2014, **4**, 1148–1153.
7 S. Kang, K. Ham, H.-K. Lim and J. Lee, *Electrochimica Acta*, 2021, **386**, 138401.
8 J. Wang, Y. Gao, H. Kong, J. Kim, S. Choi, F. Ciucci, Y. Hao, S. Yang, Z. Shao and J. Lim, *Chem. Soc. Rev.*, 2020, **49**, 9154–9196.
9 K. Wang, H. Du, S. He, L. Liu, K. Yang, J. Sun, Y. Liu, Z. Du, L. Xie, W. Ai and W. Huang, *Adv. Mater.*, 2021, **33**, 2005587.
10 P. Yan, Q. Liu, H. Zhang, L. Qiu, H. Bin Wu and X.-Y. Yu, *J. Mater. Chem. A*, 2021, **9**, 15586–15594.
11 O. Piqué, F. Illas and F. Calle-Vallejo, *Phys. Chem. Chem. Phys.*, 2020, **22**, 6797–6803.
12 *Wikipedia*, 2022.
13 Radii for All Species, http://abulafia.mt.ic.ac.uk/shannon/radius.php, (accessed February 11, 2022).
14 H. Shin, H. Xiao and W. A. Goddard, *J. Am. Chem. Soc.*, 2018, **140**, 6745–6748.
15 Z. Xue, X. Zhang, J. Qin and R. Liu, *J. Mater. Chem. A*, 2019, **7**, 23091–23097.
16 Y. Zhou and N. López, *ACS Catal.*, 2020, **10**, 6254–6261.
17 J. Dong, Y. Lu, X. Tian, F.-Q. Zhang, S. Chen, W. Yan, H.-L. He, Y. Wang, Y.-B. Zhang, Y. Qin, M. Sui, X.-M. Zhang and X. Fan, *Small*, 2020, **16**, 2003824.
18 S. Niu, W.-J. Jiang, Z. Wei, T. Tang, J. Ma, J.-S. Hu and L.-J. Wan, *J. Am. Chem. Soc.*, 2019, **141**, 7005–7013.
19 C. Gang, J. Chen, Q. Chen and Y. Chen, *J. Colloid Interface Sci.*, 2021, **600**, 594–601.
20 Z. Zhao, P. Schlexer Lamoureux, A. Kulkarni and M. Bajdich, *ChemCatChem*, 2019, **11**, 3423–3431.
21 J. Park, S. Bae, J.-S. Park, S. Bong and J. Lee, *ACS Appl. Nano Mater.*, 2021, acsanm.1c01388.
22 W. Guo, D. Li, D. Zhong, S. Chen, G. Hao, G. Liu, J. Li and Q. Zhao, *Nanoscale*, 2020, **12**, 983–990.
23 L. Li, P. Ma, S. Hussain, L. Jia, D. Lin, X. Yin, Y. Lin, Z. Cheng and L. Wang, *Sustain. Energy Fuels*, 2019, **3**, 1749–1756.
24 X. Ji, Y. Lin, J. Zeng, Z. Ren, Z. Lin, Y. Mu, Y. Qiu and J. Yu, *Nat. Commun.*, 2021, **12**, 1380.
25 L. Cai, J. Zhao, H. Li, J. Park, I. S. Cho, H. S. Han and X. Zheng, *ACS Energy Lett.*, 2016, **1**, 624–632.