Supporting Information

Construction of Sc-NiFe-LDH electrocatalyst for highly efficient electrooxidation of 5-hydroxymethylfurfural at industrial current density

Yufeng Wu[1], Zhiyan Hou[1] and Changlong Wang[1]*,

1 Institute of Circular Economy, College of Materials Science and Engineering, Beijing University of Technology, Beijing 100124, P. R. China.

* Author to whom corresponce should be addressed:

E-mail: clwang1987@126.com.

Table of Contents

1. Supplementary Figures

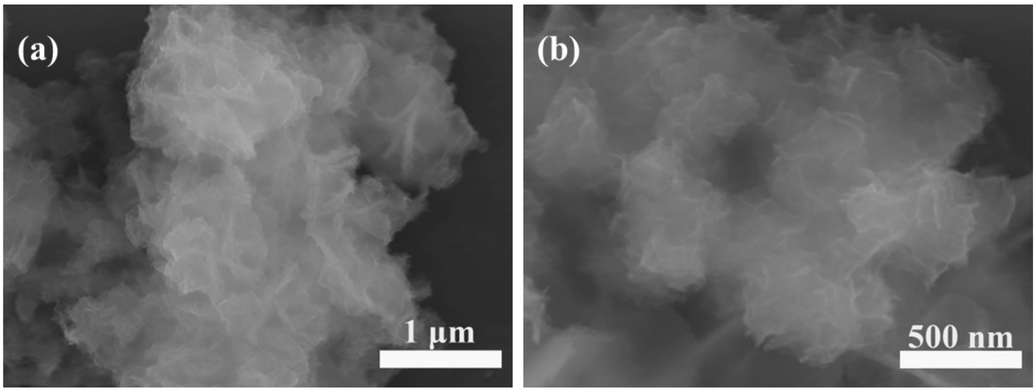

Figure S1 | SEM image of NiFe-LDH (a) 1μm, (b) 500 nm.

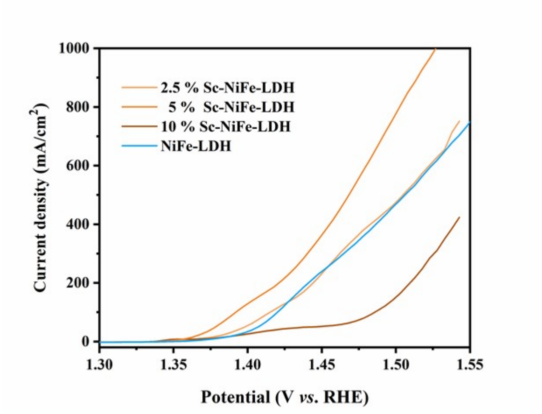

Figure S2 | LSV of Sc-NiFe-LDH with different Sc contents in 1 M KOH with 10 mM HMF.

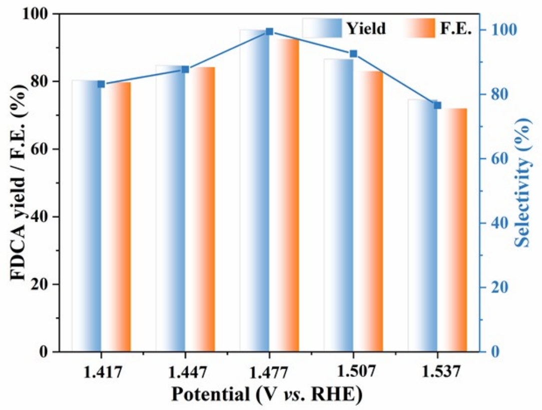

Figure S3 | The FDCA yield, FE and selectivity on Sc-NiFe-LDH at varied potentials in 10 mM HMF solution.

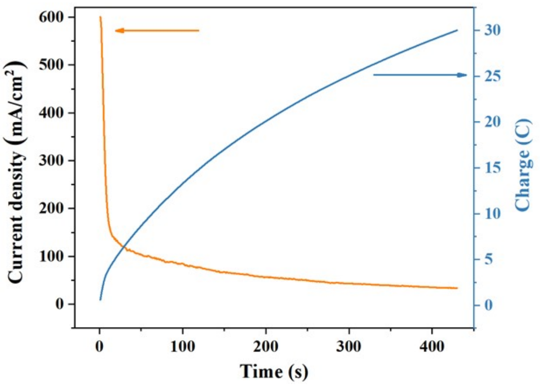

Figure S4 | Current densities, charges vs. time curves of Sc-NiFe-LDH.

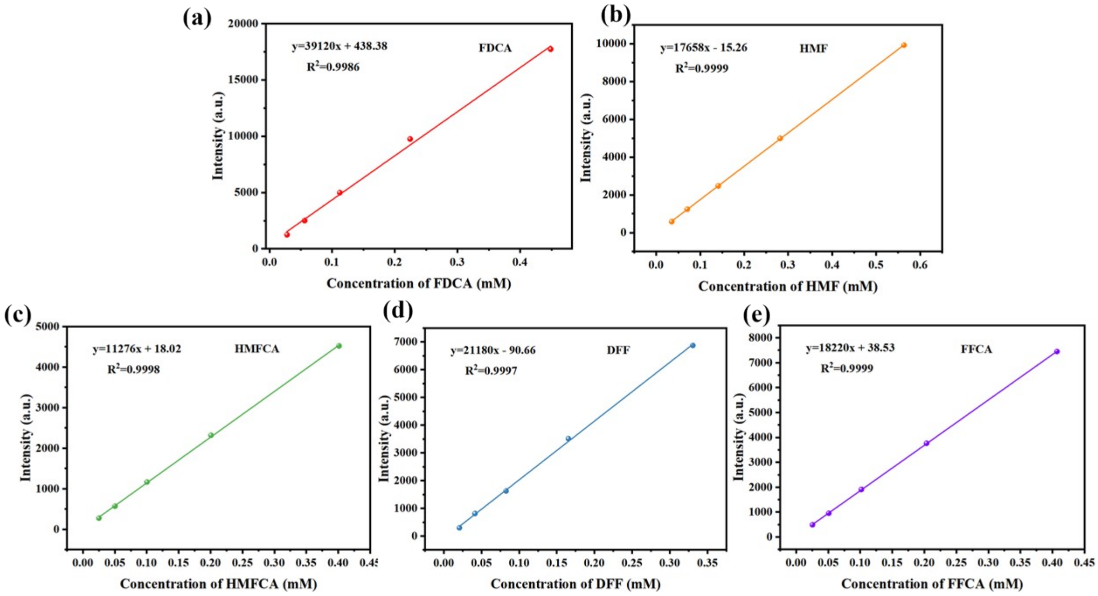

Figure S5 | (a-e) The HPLC standard curves of HMF and corresponding products.

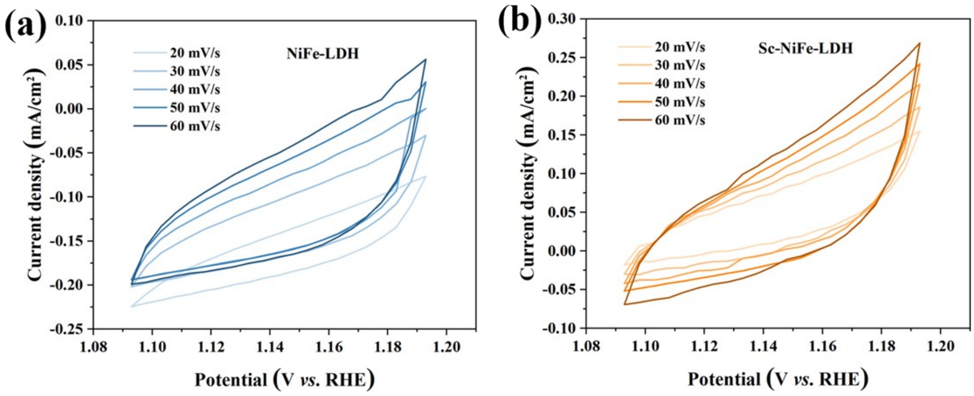

Figure S6 | CV curves of different electrodes in 1 M KOH with 10 mM HMF at different scan rates. (a) NiFe-LDH, (b) Sc-NiFe-LDH.

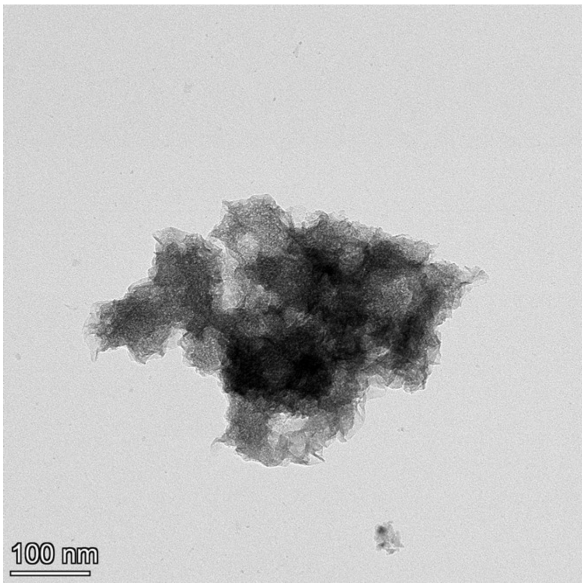

Figure S7 | TEM image of the Sc-NiFe-LDH after six successive electrolysis cycles.

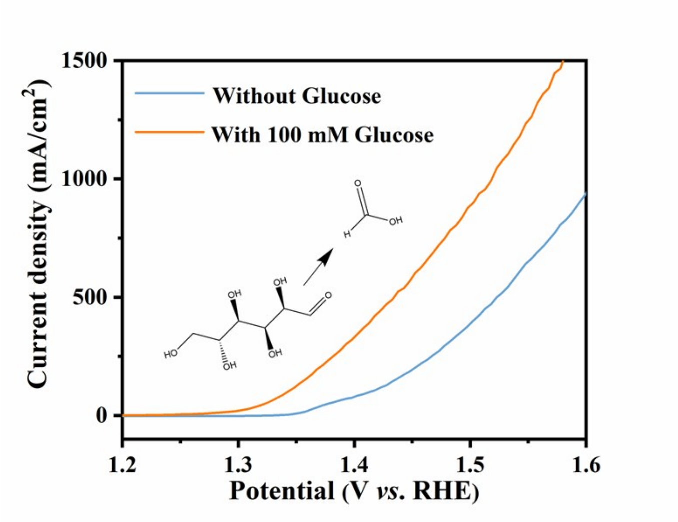

Figure S8 | LSV curves for Sc-NiFe-LDH in 1 M KOH with and without 0.1 M Glucose.

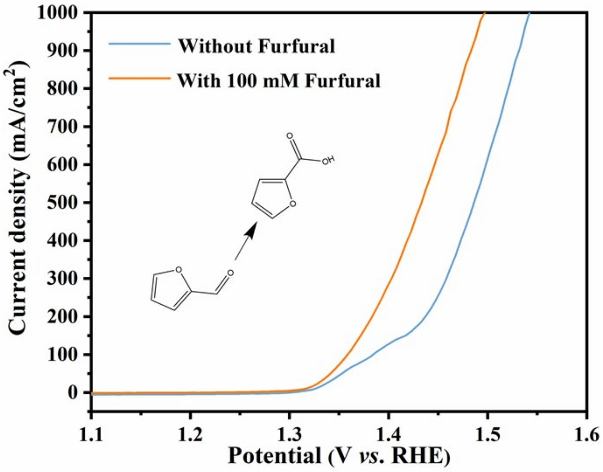

Figure S9 | LSV curves for Sc-NiFe-LDH in 1 M KOH with and without 0.1 M Furfural.

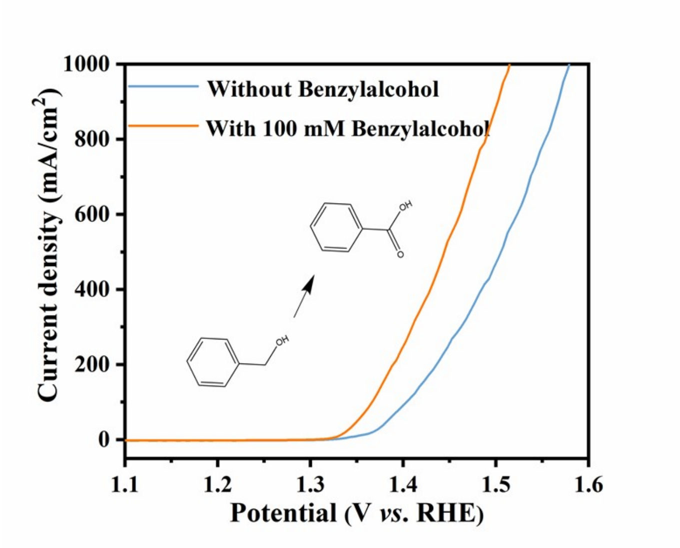

Figure S10 | LSV curves for Sc-NiFe-LDH in 1 M KOH with and without 0.1 M Benzylalcohol.

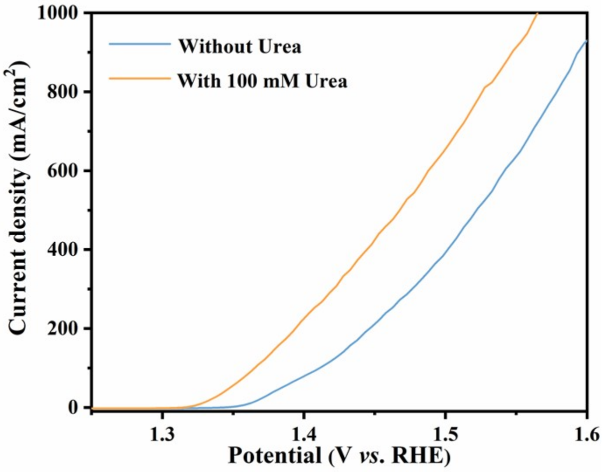

Figure S11 | LSV curves for Sc-NiFe-LDH in 1 M KOH with and without 0.1 M Urea.

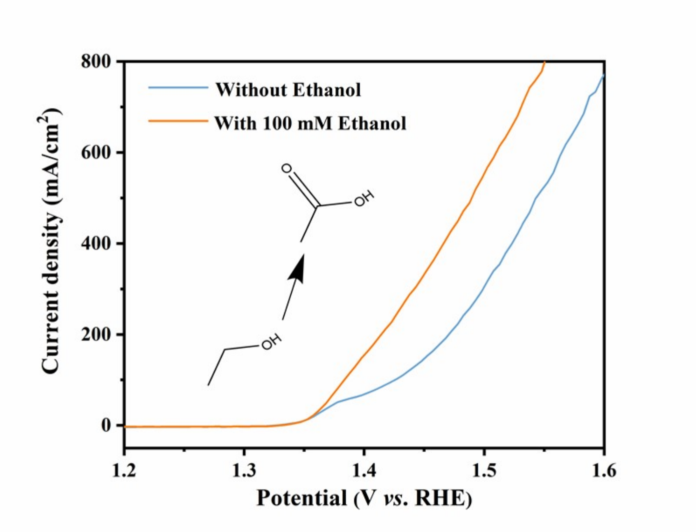

Figure S12 | LSV curves for Sc-NiFe-LDH in 1 M KOH with and without 0.1 M Ethanol.

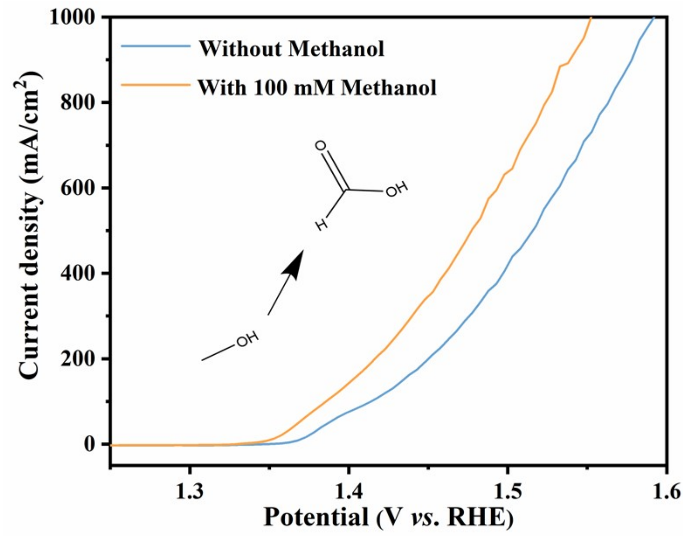

Figure S13 | LSV curves for Sc-NiFe-LDH in 1 M KOH with and without 0.1 M Methanol.

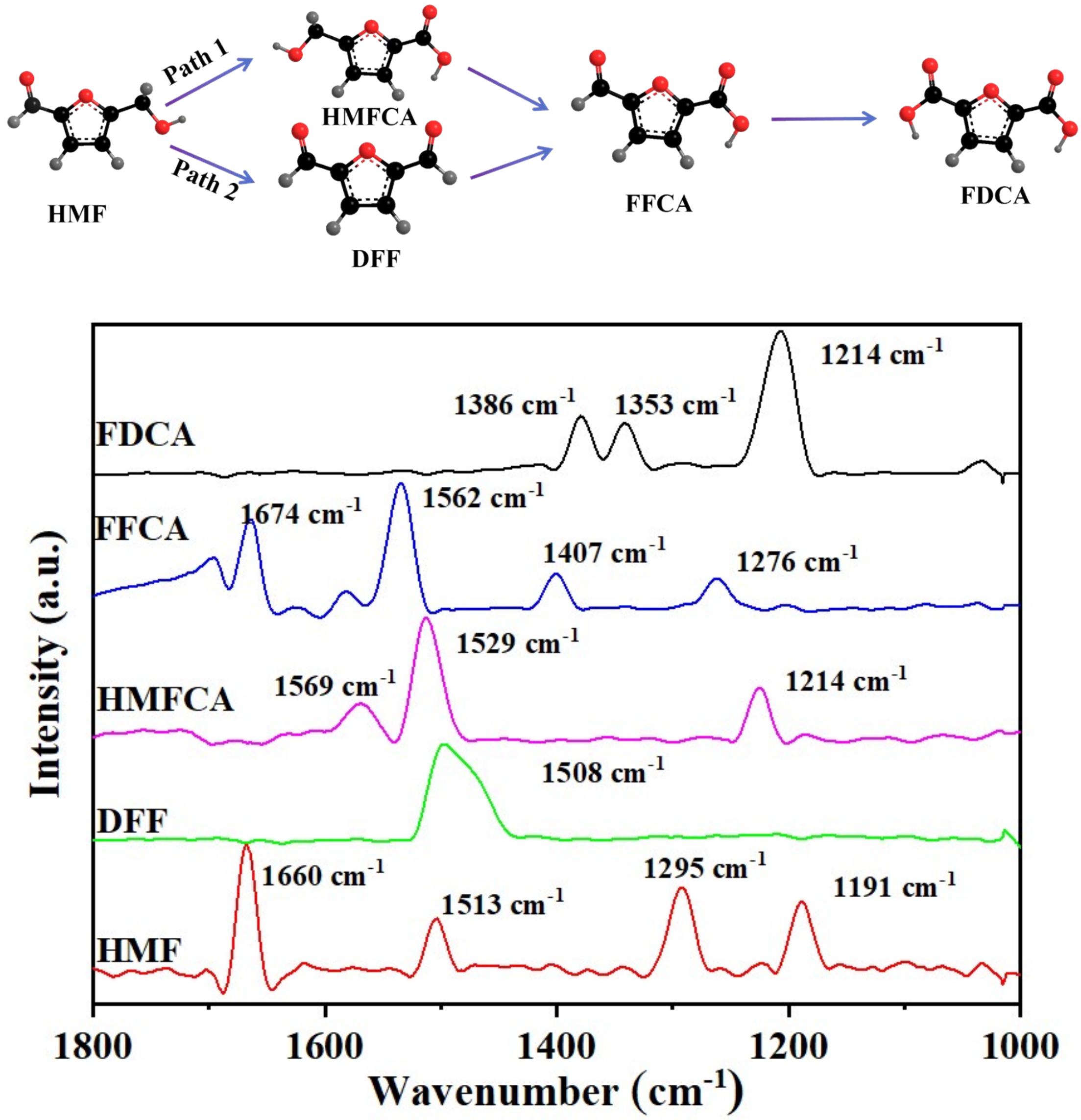

Figure S14 | Two possible pathways for the oxidation of HMF to FDCA, and the FTIR of each pure product.

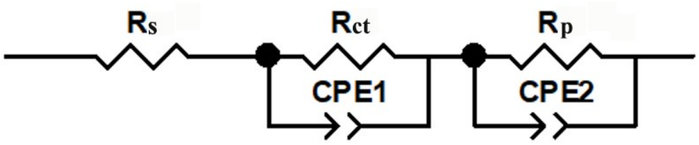

Figure S15 | The equivalent circuit used for modeling the measured electrochemical response.

2. Supplementary Tables

Table S1 | Comparison of the catalytic performances of Sc-NiFe-LDH and known catalysts for the electrooxidation of 100 mM HMF

Catalysts	HMF concentration (mM)	Yield (%)	E_{10} (vs. RHE)/HMFOR	Current density at 1.50 V vs. RHE (mA/cm^2)	E_{50} (vs. RHE)/HMFOR	Conc. (%)	FE	Stability (h)	Selectivity (%)	Reference
Sc-NiFe-LDH	10	96.72	1.357	802.82	1.37	100	96.54	110	99.47	This work
d-NiFe LDH/CP	10	96.8	1.48	15	1.64	97.35	84.47	/	99.4	Ind Eng Chem Res, **2020**, 59: 17348-17356.
InOOH-OV	10	92.41	1.421	40	1.616	98.68	90	25	88.4	Nat. Commun. **2023**, 14, 2040
Co-P@NF	10	89.8	1.392	/	1.53	100	/	2	89.5	Chem. Eng. J. **2023**, 469, 143832
VN/NiF	10	97	1.36	140	1.373	99	86	/	/	Adv. Funct. Mater. **2019**, 29, 1904780

Table S2 | Comparison of FDCA yield with several electrochemical HMF catalysts reported recently.

Catalysts	Condition	E (V vs. RHE)/Current density (mA/cm^2)	FE	Time (h)	Reference
Sc-NiFe-LDH	1 M KOH 10 mM HMF	1.50 V/802.8 mA/cm^2	96.5	110	This work
Ni_3S_2/NF	1 M KOH+10 mM HMF	1.423 V/100 mA/cm^2	98	/	J. Am. Chem. Soc. 2016, 138, 13639-13646
NixB/NF	1 M KOH+10 mM HMF	1.45 V/100 mA/cm^2	100	/	Angew. Chem., Int. Ed. 2018, 57, 11460-11464
CoNW/NF	1 M KOH+10 mM HMF	1.764 V/100 mA/cm^2	96.6	/	Green Chem. 2019, 21, 6699-6706
CoO/$CoSe_2$	1 M KOH+10 mM HMF	1.48 V/100 mA/cm^2	97.9	/	Green Chem. 2020, 22, 843-849
E-CoAl-LDH-NSA	1 M KOH+10 mM HMF	1.59V/100 mA/cm^2	99.4	/	Appl. Catal., B. 2021, 299, 120669
Co_3O_4/CF	1 M KOH+10 mM HMF	1.40 V /100 mA/cm^2	92.9	/	Appl. Catal., B. 2022, 307, 121209

Catalysts	Condition	E (V vs. RHE)/Current density (mA/cm^2)	FE	Time (h)	Reference
$Ni(OH)_2$-NiOOH/NiFeP	1 M KOH+10 mM HMF	1.437 V /100 mA/cm^2	94	/	Appl. Catal., B. 2022, 311, 121357
Co-NixP@C	1 M KOH+10 mM HMF	1.54 V /100 mA/cm^2	98.9	/	J. Colloid Interface Sci. 2022, 629, 451-460
NiRu NPs	1 M KOH+10 mM HMF	1.5 V /110 mA/cm^2	99.7	/	ACS Sustainable Chem. Eng. 2023, 11, 13441-13450
Co_3S_4/Ni_3S_2	1 M KOH+10 mM HMF	1.489 V /100 mA/cm^2	100	/	Green Chem. 2023, 25, 8698-8705
CuH_NWs@Ce: NiH_NSs/Cu	1 M KOH+10 mM HMF	1.43 V /100 mA/cm^2	98.0	30	Inorg. Chem. 2023, 62, 12534-12547
$NiMo_3S_4$-R	1 M KOH+10 mM HMF	1.395 V /100 mA/cm^2	98.5	12	Appl. Catal., B. 2023, 323, 122126
Co_9S_8@Ni_3S_2/NF	1 M KOH+10 mM HMF	1.46 V /100 mA/cm^2	89.04	/	Mater. Today Nano. 2023, 23, 100373
CoO–Co@C/CF	1 M KOH+10 mM HMF	1.471 V /100 mA/cm^2	99.4	20	Molecules. 2023, 28, 3040

Catalysts	Condition	E (V vs. RHE)/Current density (mA/cm^2)	FE	Time (h)	Reference
P-Co_3O_4-NBA@NF	1 M KOH+10 mM HMF	1.524 V /100 mA/cm^2	97.01	/	Appl. Catal., A. 2024, 669, 119497

Table S3 | The resistance of each component for Sc-NiFe-LDH in 1 M KOH.

Potential	R_s	R_p	R_{ct}	CPE1	CPE2
1.15 V vs. RHE	0.3342	44.9	10330	0.003889	0.00378
1.20 V vs. RHE	0.3385	28.43	2511	0.005315	0.003971
1.25 V vs.RHE	0.3485	19.83	1117	0.01025	0.005325
1.30 V vs. RHE	0.3517	19.71	514.4	0.007785	0.02177
1.35 V vs. RHE	0.3296	4.236	80.01	0.01796	0.08332
1.40 V vs. RHE	0.3012	0.6041	20.34	0.405	0.7023
1.45 V vs. RHE	0.2902	0.01239	1.078	1	0.97
1.50 V vs. RHE	0.2840	0.01024	0.1022	1.8417	1
1.55 V vs. RHE	0.2891	0.009233	0.08389	1	0.6787
1.60 V vs. RHE	0.2521	$1*10^{-12}$	0.05324	0.3131	0.9005

Table S4 | The resistance of each component for Sc-NiFe-LDH in 1 M KOH with 10 M HMF.

Potential	R_s	R_p	R_{ct}	**CPE1**	**CPE2**
1.15V vs. RHE	0.4096	15.8	$2.629*10^{9}$	0.003907	0.004842
1.20V vs. RHE	0.412	10.48	2331	0.006598	0.004051
1.25 V vs. RHE	0.41	5.121	975.8	0.005165	0.01016
1.30 V vs. RHE	0.4108	3.687	383.1	0.007383	0.01613
1.35 V vs. RHE	0.4003	1.402	95.88	0.01225	0.02463
1.40 V vs. RHE	0.394	1.089	16.65	0.03679	0.1019
1.45 V vs. RHE	0.3559	0.7132	6.873	0.2368	0.872
1.50 V vs. RHE	0.3476	0.4402	0.02964	1	0.3404
1.55 V vs. RHE	0.2455	0.2834	0.4876	$1*10^{-12}$	1
1.60 V vs. RHE	0.6271	0.06972	0.4227	0.1547	1

Table S5 | The resistance of each component for NiFe-LDH in 1 M KOH.

Potential	R_s	R_p	R_{ct}	CPE1	CPE2
1.15 V vs. RHE	0.3941	179.7	$5.572*10^{10}$	0.001312	0.002968
1.20 V vs. RHE	0.3904	14.24	6239	0.002307	0.002861
1.25 V vs.RHE	0.3889	10.48	2869	0.00357	0.00149
1.30 V vs. RHE	0.392	4.203	350.9	0.004616	0.008771
1.35 V vs. RHE	0.3216	2.586	66.71	0.01914	0.06565
1.40 V vs. RHE	0.2789	0.6035	13.42	0.4021	1
1.45 V vs. RHE	0.2768	1.35	0.06531	1	0.6748
1.50 V vs. RHE	0.2748	0.2853	0.06952	0.8851	0.3722
1.55 V vs. RHE	0.2771	0.1253	0.05063	0.7845	0.2642
1.60 V vs. RHE	0.2851	0.04092	0.08101	0.2267	0.7646

Table S6 | The resistance of each component for NiFe-LDH in 1 M KOH with 10 M HMF.

Potential	R_s	R_p	R_{ct}	CPE1	CPE2
1.15 V vs. RHE	0.4069	79.27	$2.479*10^{10}$	0.002392	0.005983
1.20 V vs. RHE	0.4178	10.55	1753	0.002043	0.007201
1.25 V vs. RHE	0.4162	5.668	711.9	0.00254	0.01042
1.30 V vs. RHE	0.4094	3.123	251.1	0.003964	0.01715
1.35 V vs. RHE	0.3967	1.862	68.75	0.008578	0.03028
1.40 V vs. RHE	0.3708	1.203	1.914	0.3168	0.0823
1.45 V vs. RHE	0.3118	0.06084	1.801	0.4673	1
1.50 V vs. RHE	0.3181	0.08432	0.4478	0.2844	1
1.55 V vs. RHE	0.06071	0.08432	0.4478	0.1745	1

s