Electronic Supplementary Information (ESI)

CuO-$Ni(OH)_2$ heterostructure nanosheets: a high-performance electrocatalyst for 5-hydroxymethylfurfural oxidation

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Experimental Section

Materials and Chemicals

Choline chloride (ChCl), oxalic acid ($H_2C_2O_4$), potassium chloride (KCl), copper acetylacetonate ($C_{10}H_{14}CuO_4$) were all obtained from Aladdin Chemistry Co., Ltd. Potassium hydroxide (KOH) and nickel chloride hexahydrate ($NiCl_2 \cdot 6H_2O$) were purchased from Sinopharm Chemical Regent Co., Ltd. 5-hydroxymethylfurfural (HMF), 2,5-furandicarboxylic acid (FDCA), 5-formyl furan2-carboxylic acid (FFCA) and 5-hydroxymethyl-2-furan-carboxylic acid (HMFCA) were purchased from Alfa-Aesar. 2,5-diformyl furan (DFF) was purchased from Tokyo Chemical Industry Co., Ltd. 5 wt% nafion solution was purchased from the Sigma Co., Ltd. Carbon cloth was obtained from Changsha Lyrun Material Co., Ltd. Nafion 115 membrane was purchased from Wuhan GaossUnion technology Co., Ltd.

Fabrication of choline chloride/oxalic acid (ChCl/OA) DES

The deep eutectic solvent (DES) was obtained following the procedures described in the literature.[1] To achieve the (ChCl/OA) DES, equimolar amounts of choline chloride and oxalic acid were magnetically stirred at 80 °C for 30 minutes.

Synthesis of CuO-Ni(OH)$_2$ Heterostructure Nanosheets

CuO-Ni(OH)$_2$ products with different initial Cu and Ni ratios were designated as CuO-Ni(OH)$_2$ (x:y), where x:y is the Cu/Ni atomic ratio of the initial feed. For the synthesis of the CuO-Ni(OH)$_2$ (1:3) product, a typical procedure involved dissolving 10.7 mg of $C_{10}H_{14}CuO_4$ and 29.3 mg of $NiCl_2 \cdot 6H_2O$ in 1 mL of ChCl/OA DES. The mixture was then ultrasonicated at 60 °C until a well-dispersed yellow solution was

obtained. The Cu/Ni-based precursor was generated by microwave heating the solution for 15 s at 100 W. The precursor was subsequently collected, washed multiple times with ethanol, and dried under vacuum at room temperature for 8 h. Next, 150 mg of the dried Cu/Ni-based precursor was refluxed with 15 mL of 2 M KOH at 100 °C for 5 h. After reaction, the product was obtained through centrifugation, and the achieved CuO-$Ni(OH)_2$ nanosheets were washed with water and ethanol before being dried overnight in a vacuum drying oven.

For comparison, CuO-$Ni(OH)_2$ (1:2) and CuO-$Ni(OH)_2$ (1:4) products were synthesized using the same method, where the 1 mL of ChCl/OA DES was used. However, there were differences in the amounts of $C_{10}H_{14}CuO_4$ and $NiCl_2{\cdot}6H_2O$ used for each synthesis. For CuO-$Ni(OH)_2$ (1:2), 14.2 mg of $C_{10}H_{14}CuO_4$ and 25.8 mg of $NiCl_2{\cdot}6H_2O$ were used. On the other hand, CuO-$Ni(OH)_2$ (1:4) was synthesized using 8.6 mg of $C_{10}H_{14}CuO_4$ and 31.4 mg of $NiCl_2{\cdot}6H_2O$. Additionally, CuO product was synthesized without the addition of $NiCl_2{\cdot}6H_2O$, while $Ni(OH)_2$ product was synthesized without the addition of $C_{10}H_{14}CuO_4$.

Characterizations

The X-ray diffraction (XRD) patterns were obtained using the Rigaku SmartLab 9KW X-ray diffractometer. Transmission electron microscopy (TEM) was performed on a JEM1400 microscope. Scanning electron microscopy (SEM) and energy-dispersive X-ray (EDX) characterization were conducted with the Zeiss Sigma 300 instrument. High-resolution transmission electron microscopy (HRTEM) images were acquired using the JEM-2100 microscope. High-angle annular dark field (HAADF)-scanning transmission

electron microscopy (STEM) and energy-dispersive X-ray (EDX) were tested on the FEI Titan G2 60-300. X-ray photoelectron spectroscopy (XPS) measurements were performed by a Thermo Fisher ESCALAB XI. Nitrogen adsorption-desorption tests were conducted on the micromeritics ASAP 2460. High performance liquid chromatography (HPLC) analysis was performed using an Agilent G7114A system.

Electrochemical Measurements

The electrochemical characterizations were conducted using a CHI760E workstation. The setup included a working electrode consisting of a catalyst loaded with carbon paper, a counter electrode made of platinum foil, and a reference electrode utilizing saturated Ag/AgCl. The electrolyte used was a 1 M KOH solution, either with or without addition of 10 mM HMF, and the volume of the electrolyte was 10 mL.

To prepare the catalyst ink, a mixture was made by adding 4 mg of catalyst to a solution containing Nafion (20 μL, 5 wt%), ethanol (120 μL), and water (100 μL). This mixture was then sonicated for 25 min to achieve a suspension of the catalyst. The resulting catalyst ink was coated on the carbon paper (1 × 1 cm^2), serving as working electrode. The catalyst on the electrode was 4 mg cm^{-2}.

Linear scanning voltammetry (LSV) was conducted at 10 mV s^{-1} within 1-2 V potential range. Electrochemical impedance spectroscopy (EIS) characterization was conducted using frequencies ranging from 1 Hz to 100 kHz. The capacitance (Cdl) was determined utilizing cyclic voltammetry (CV). All of the potentials were normalized to reversible hydrogen electrode (RHE) by the following equation:

$$E\ (RHE) = E\ (Ag/AgCl) + 0.197 + 0.059 \times pH \quad (1)$$

Products analysis

During the chronocurrent analysis at 1.48 V, a volume of 10 μL of electrolyte was extracted and diluted by ultrapure water to 500 μL for subsequent HPLC analysis. The UV-Vis detector utilized a wavelength of 265 nm. The HPLC mobile phase consisted of a mixture of 5 mM aqueous ammonium formate and methanol. Separation and quantification were carried out by isocratic elution with 5 mM aqueous ammonium formate (70% volume) and methanol (30% volume) at 0.6 mL min^{-1}.

HMF conversion, FDCA yield and Faradaic efficiency (FE) were achieved according to below equations:

$$\text{HMF conversion (\%)} = [n\text{ (HMF consumed)} / n\text{ (HMF initial)}] \times 100 \quad (2)$$

$$\text{FDCA yield (\%)} = [n\text{ (FDCA formed)} / n\text{ (HMF initial)}] \times 100 \quad (3)$$

$$\text{Faradaic efficiency (\%)} = [n\text{ (FDCA formed)} / (Q / (6 \times F))] \times 100 \quad (4)$$

where Q is the total passed charge, F is 96485 C mol^{-1} and n represents the number of moles of reactant, which is determined by calculating the concentration measured using HPLC.

Density functional theory (DFT) Calculation

Our spin-polarized density functional theory (DFT) calculations[2,3] were carried out in the the CP2K code.[4] All calculations employed a mixed Gaussian and planewave basis sets. Core electrons were represented with norm-conserving Goedecker-Teter-Hutter pseudopotentials,[5–7] and the valence electron wavefunction was expanded in a double-zeta basis set with polarization functions[8] along with an auxiliary plane wave basis set with an energy cutoff of 400 eV. The generalized gradient approximation

exchange-correlation functional of Perdew, Burke, and Enzerhof (PBE)[9] was used. Each configuration was optimized with the Broyden-Fletcher-Goldfarb-Shanno (BGFS) algorithm with SCF convergence criteria of 1.0×10^{-6} a.u. The van der Waals correction of Grimme's DFT-D3 model was also adopted.[10]

The adsorption energy between the HMF and the $Ni(OH)_2$ or $Ni(OH)_2$-CuO can be calculated using the following equation:

$$\Delta E_{ads} = E_{\mathrm{HMF@Ni(OH)_2/HMF@Ni(OH)_2-CuO}} - E_{\mathrm{Ni(OH)_2/Ni(OH)_2-CuO}} - E_{\mathrm{HMF}} \quad \text{(S1)}$$

In Eq. (S1), $E_{\mathrm{HMF@Ni(OH)_2/HMF@Ni(OH)_2-CuO}}$ and $E_{\mathrm{Ni(OH)_2/Ni(OH)_2-CuO}}$ represent the total energies of the the $Ni(OH)_2$ or $Ni(OH)_2$-CuO with and without the adsorption of adsorbate HMF, respectively. E_{HMF} is the total energy of the adsorbate HMF.

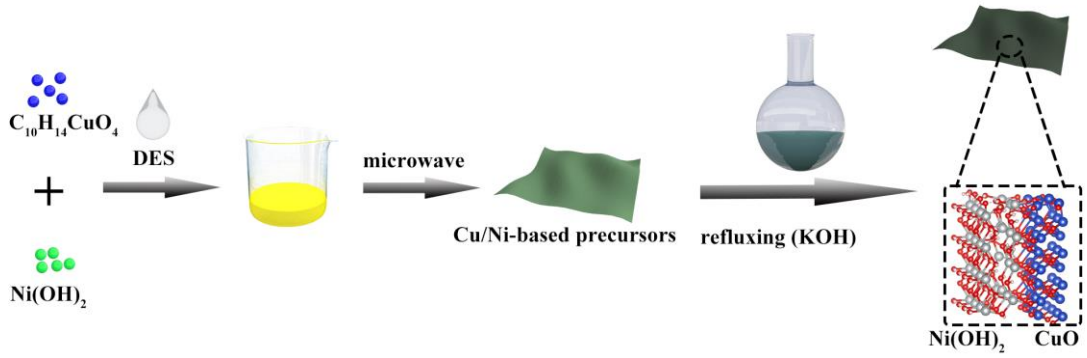

Fig. S1 Schematic diagram of CuO-$Ni(OH)_2$ nanosheet synthesis.

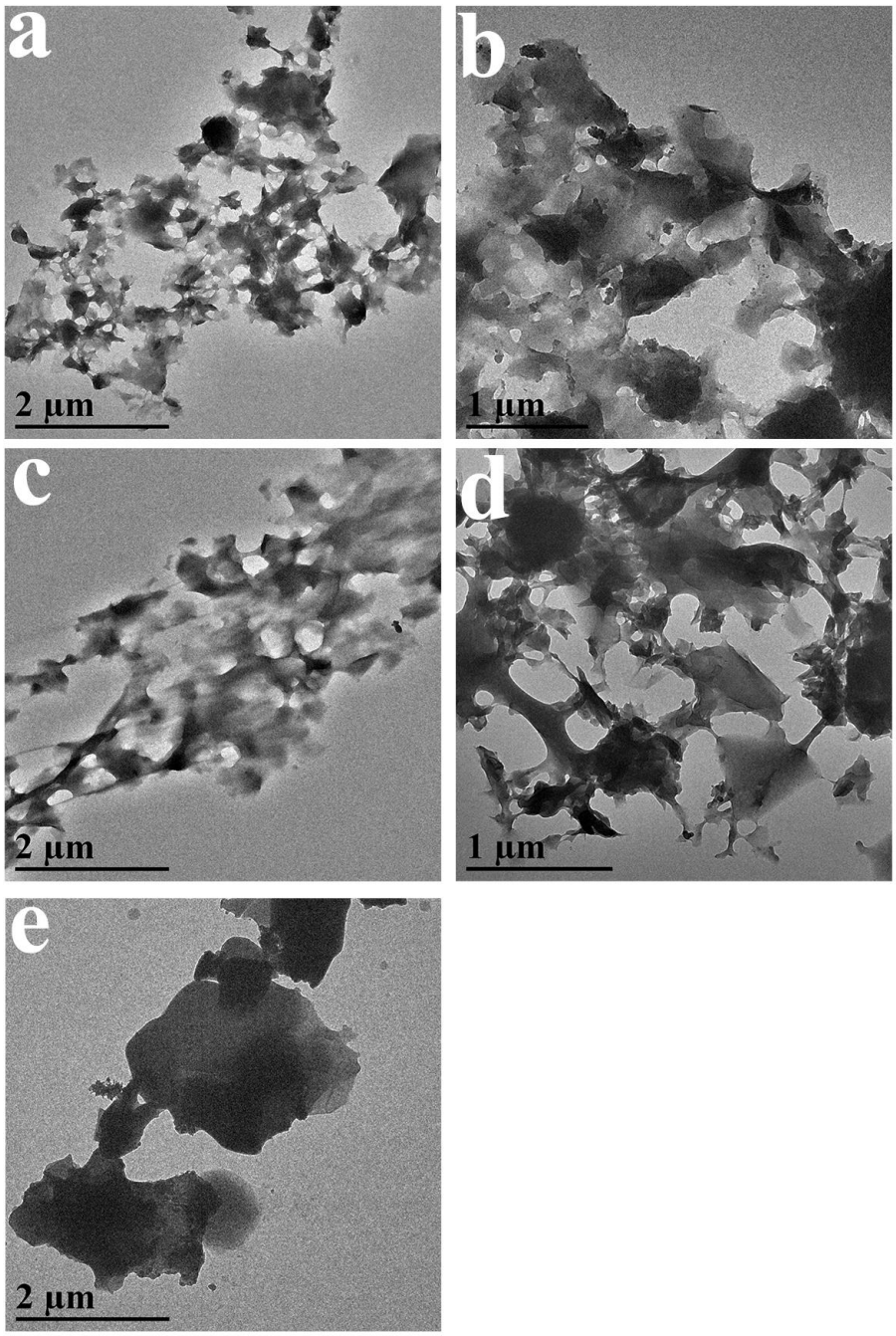

Fig. S2 TEM images of the precursors obtained after microwave heating 1 mL ChCl/OA DES with the presence of $C_{10}H_{14}CuO_4$ and $NiCl_2 \cdot 6H_2O$. (a) Ni precursor, (b) Cu/Ni precursor obtained with the initial mole ratio of Cu/Ni=1:2, (c) Cu/Ni precursor obtained with the initial mole ratio of Cu/Ni=1:3, (d) Cu/Ni precursor obtained with the initial mole ratio of Cu/Ni=1:4, (e) Cu precursor. The obtained precursors will be used for synthesizing $Ni(OH)_2$, CuO-$Ni(OH)_2$ (x:y) and CuO.

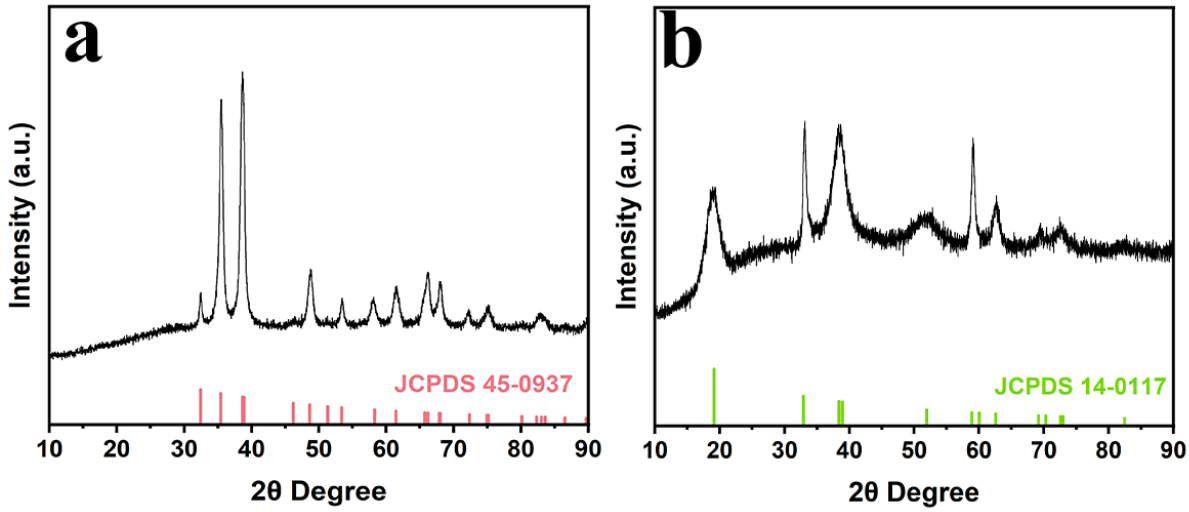

Fig. S3 XRD pattern of the synthesized (a) CuO, (b) $Ni(OH)_2$.

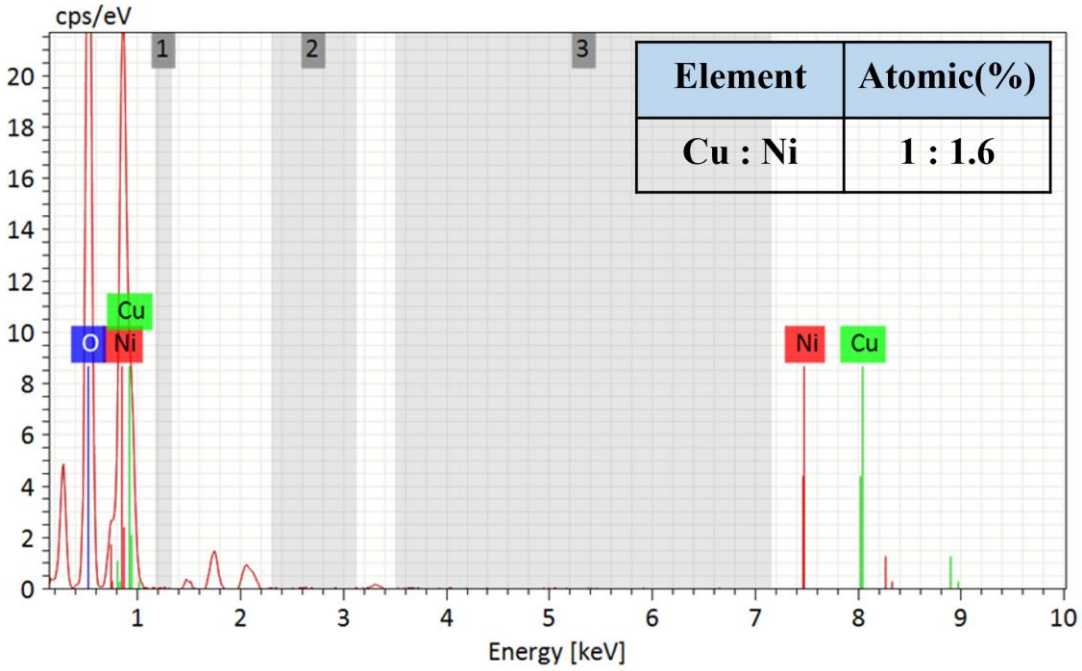

Fig. S4 EDX spectrum of CuO-$Ni(OH)_2$ (1:2) which was synthesized from the precursor obtained after microwave heating 1 mL ChCl/OA DES with 14.2 mg $C_{10}H_{14}CuO_4$ and 25.8 mg and $NiCl_2 \cdot 6H_2O$.

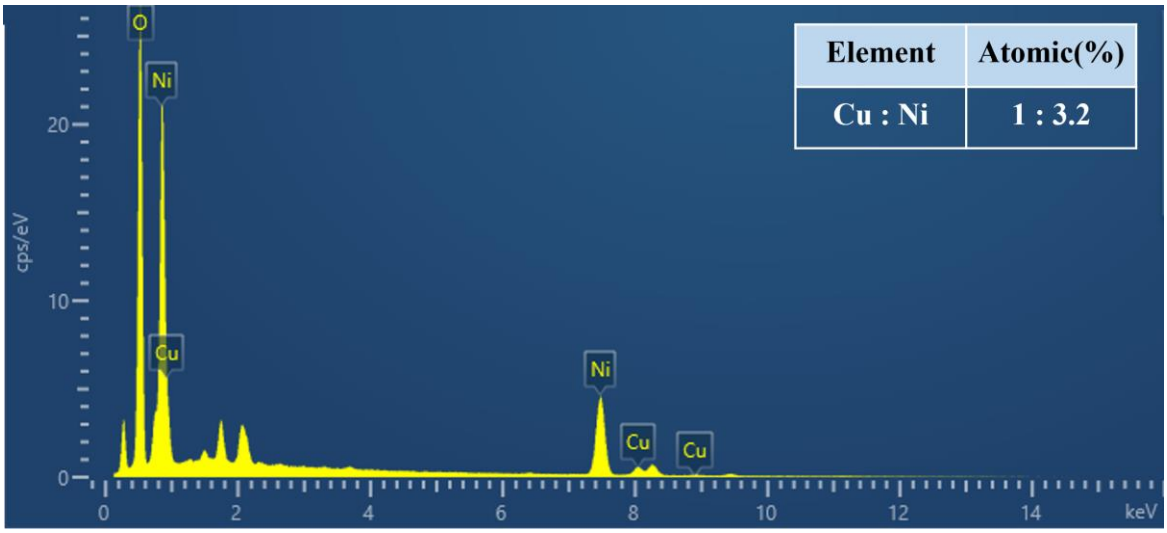

Fig. S5 EDX spectrum of CuO-$Ni(OH)_2$ (1:3) which was synthesized from the precursor obtained after microwave heating 1 mL ChCl/OA DES with 10.7 mg $C_{10}H_{14}CuO_4$ and 29.3 mg and $NiCl_2 \cdot 6H_2O$.

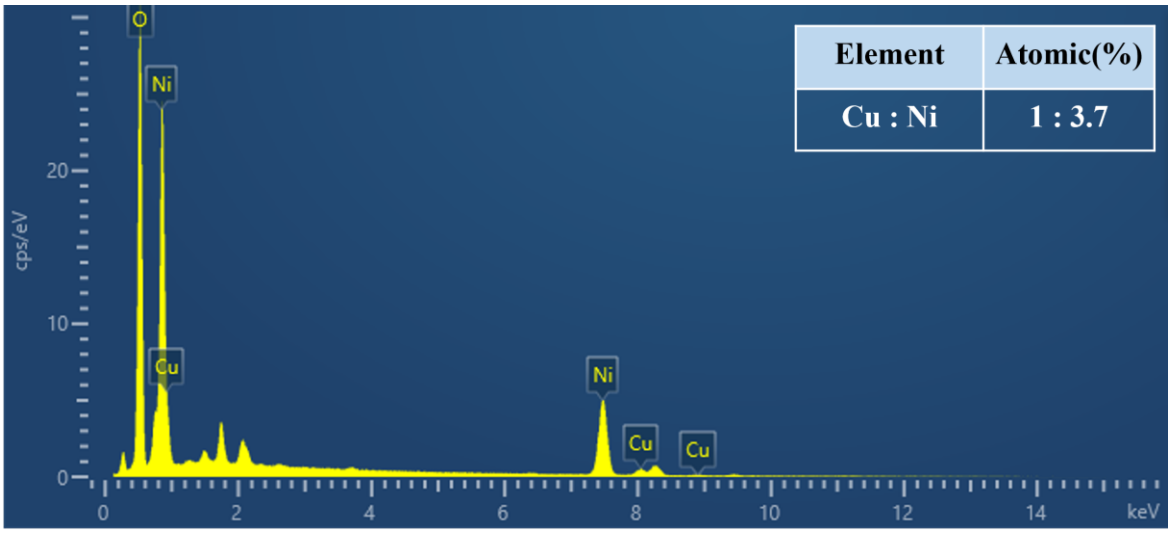

Fig. S6 EDX spectrum of CuO-$Ni(OH)_2$ (1:4) which was synthesized from the precursor obtained after microwave heating 1 mL ChCl/OA DES with 8.6 mg $C_{10}H_{14}CuO_4$ and 31.4 mg and $NiCl_2 \cdot 6H_2O$.

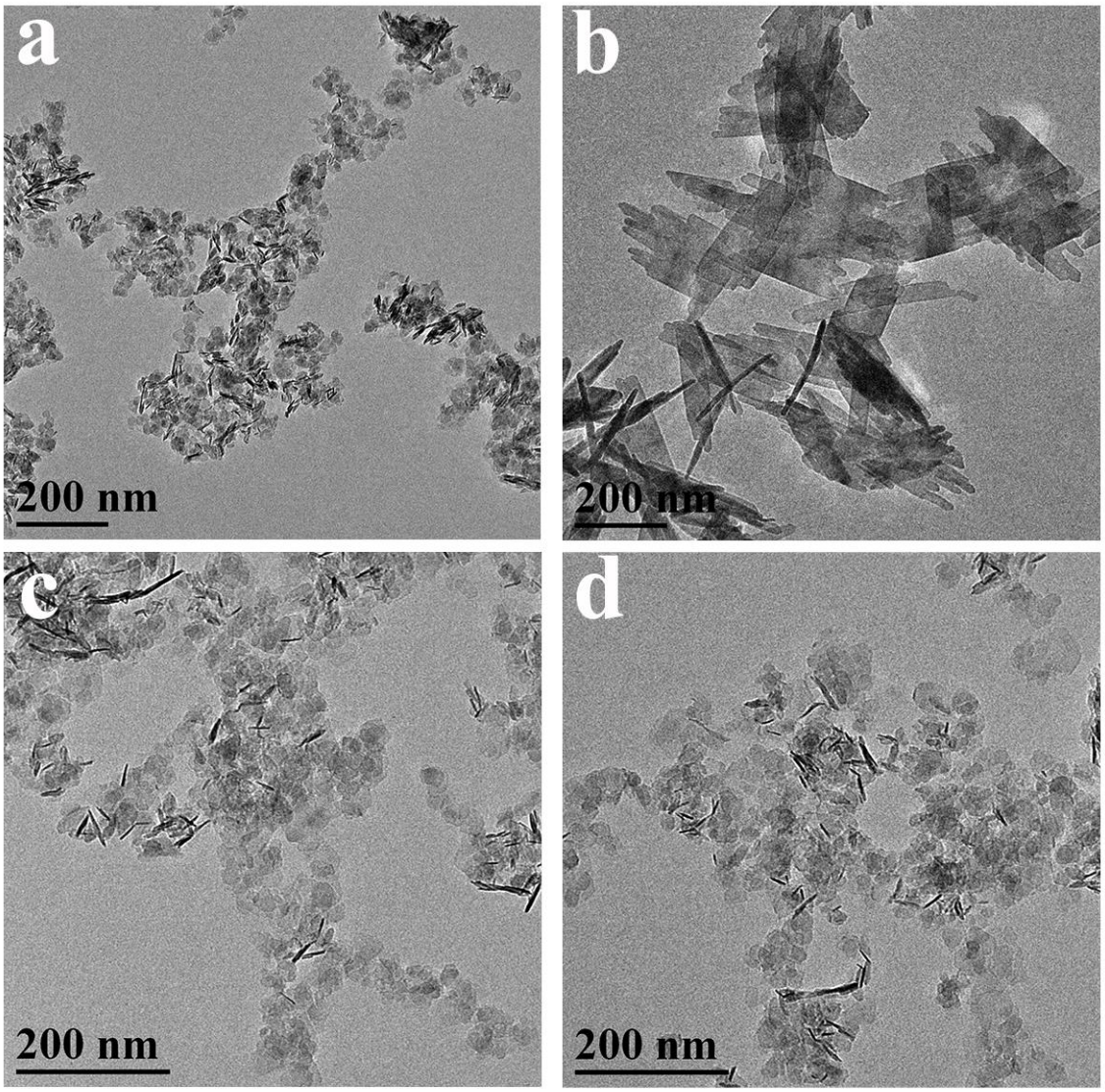

Fig. S7 TEM images of the synthesized (a) $Ni(OH)_2$, (b) CuO, (c) CuO-$Ni(OH)_2$ (1:2), (d) CuO-$Ni(OH)_2$ (1:4).

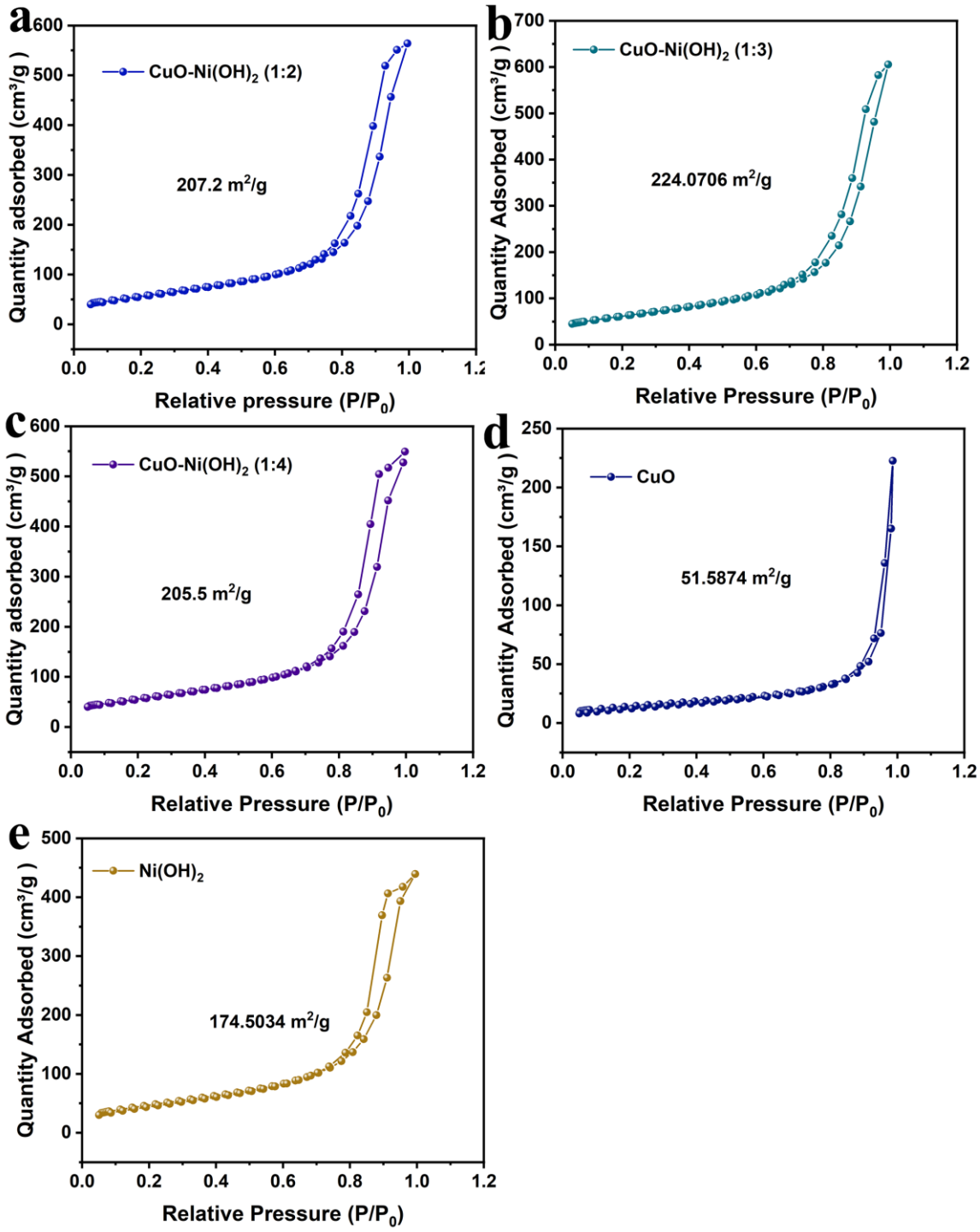

Fig. S8 N_2 adsorption-desorption isotherms of (a) CuO-$Ni(OH)_2$ (1:2), (b) CuO-$Ni(OH)_2$ (1:3), (c) CuO-$Ni(OH)_2$ (1:4), (d) CuO (e) $Ni(OH)_2$.

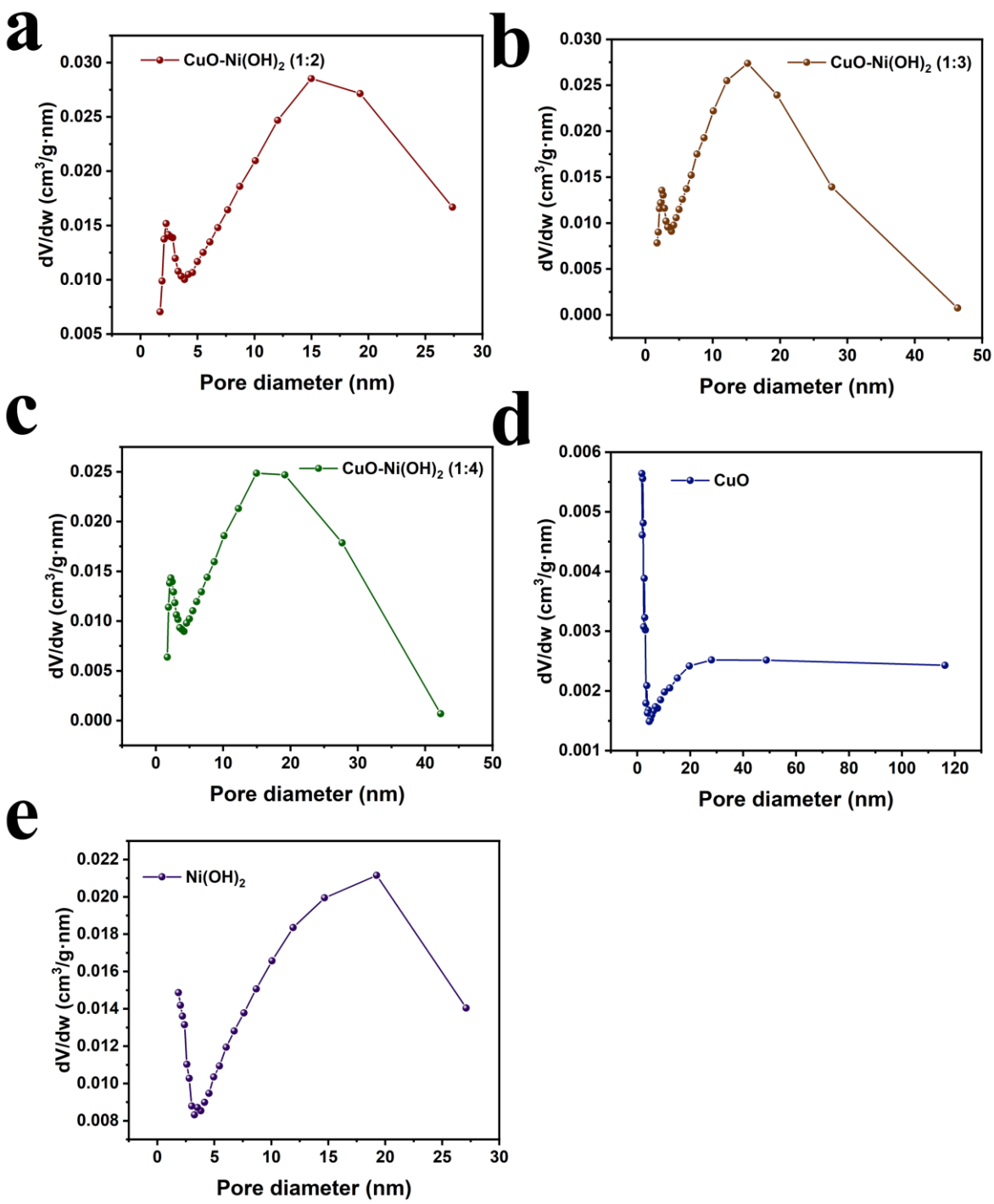

Fig. S9 Pore size distributions of the synthesized (a) CuO-$Ni(OH)_2$ (1:2), (b) CuO-$Ni(OH)_2$ (1:3), (c) CuO-$Ni(OH)_2$ (1:4), (d) CuO, (e) $Ni(OH)_2$.

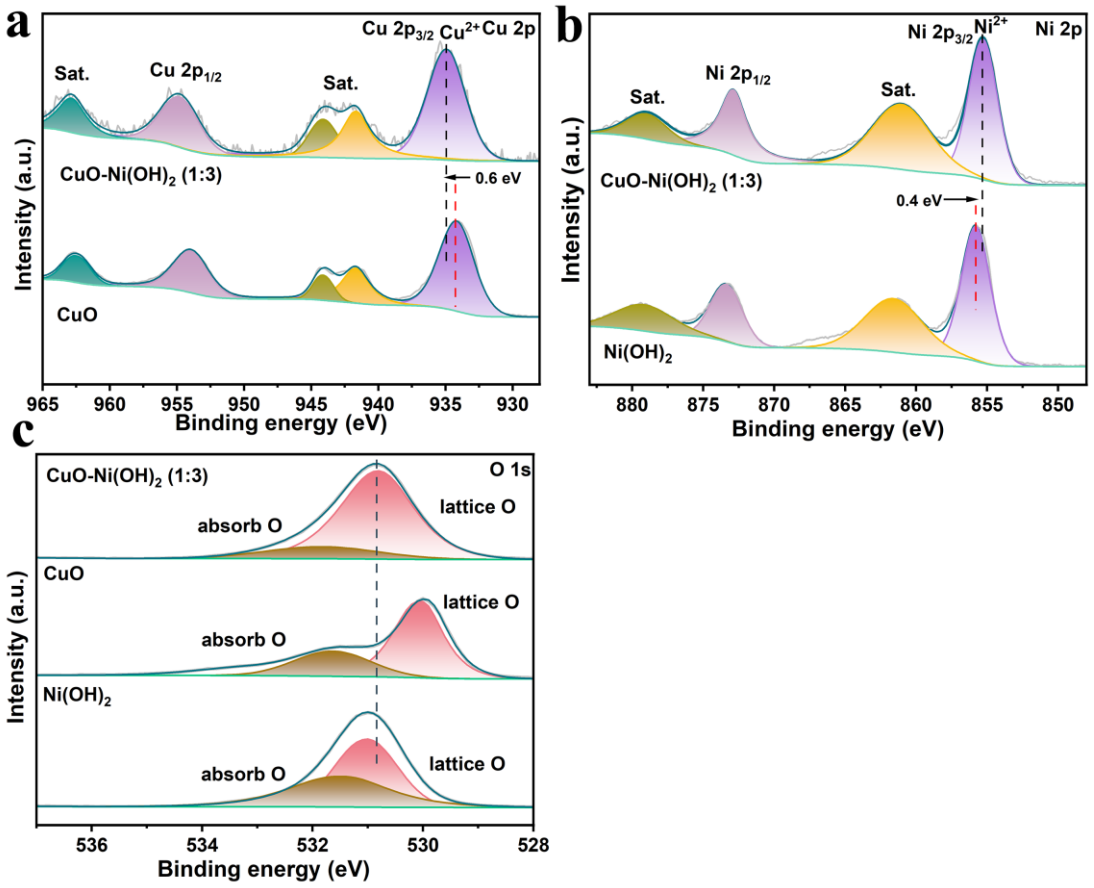

Fig. S10 High-resolution XPS spectra for CuO-Ni(OH)$_2$ (1:3): (a) Cu 2p, (b) Ni 2p and (c) O 1S.

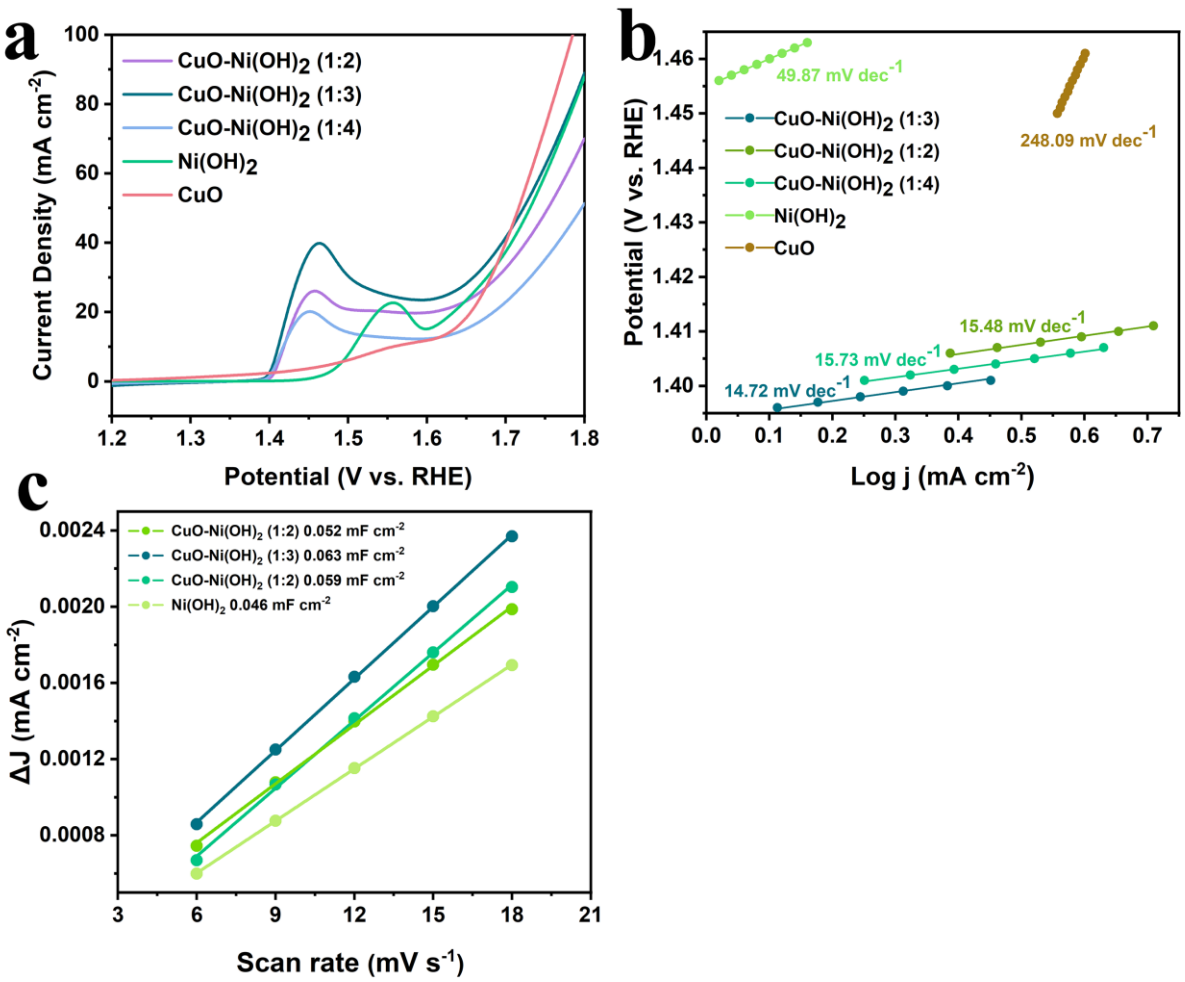

Fig. S11 (a) LSV curves (b) Tafel plots, and (c) electrochemical double layer capacitance (Cdl) of $Ni(OH)_2$, CuO-$Ni(OH)_2$ (1:2), CuO-$Ni(OH)_2$ (1:3) and CuO-$Ni(OH)_2$ (1:4) in 1.0 M KOH solution with 10 mM HMF.

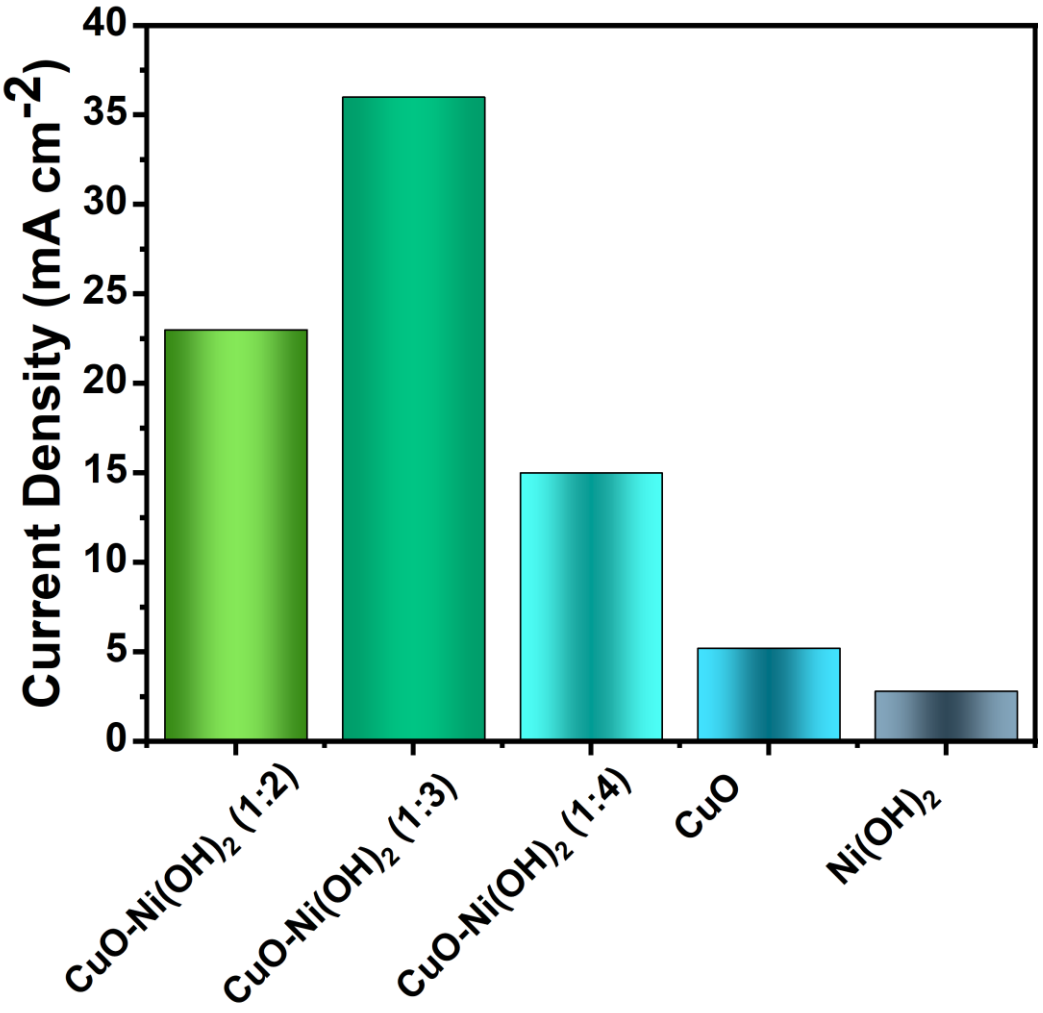

Fig. S12 Corresponding current densities at 1.48 V in 1 M KOH with 10 mM HMF.

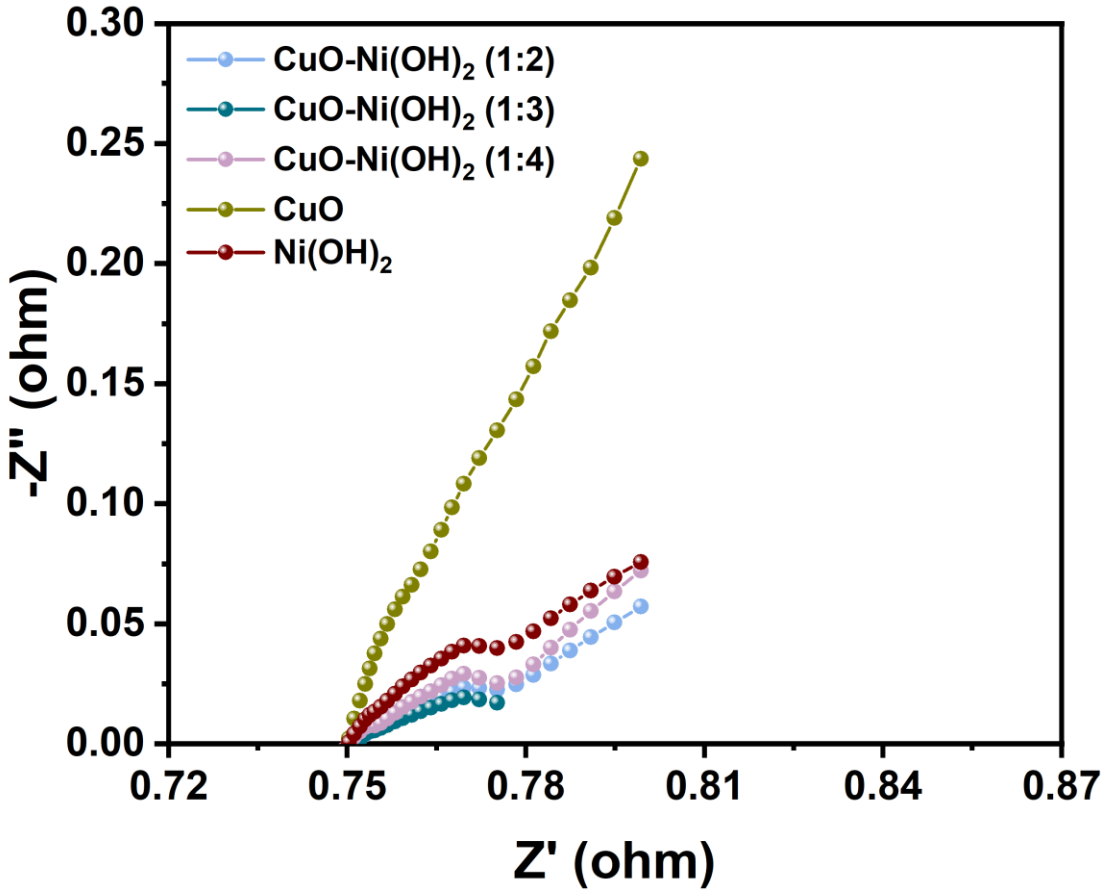

Fig. S13 Electrochemical impedance spectra of different catalysts at 1.48 V.

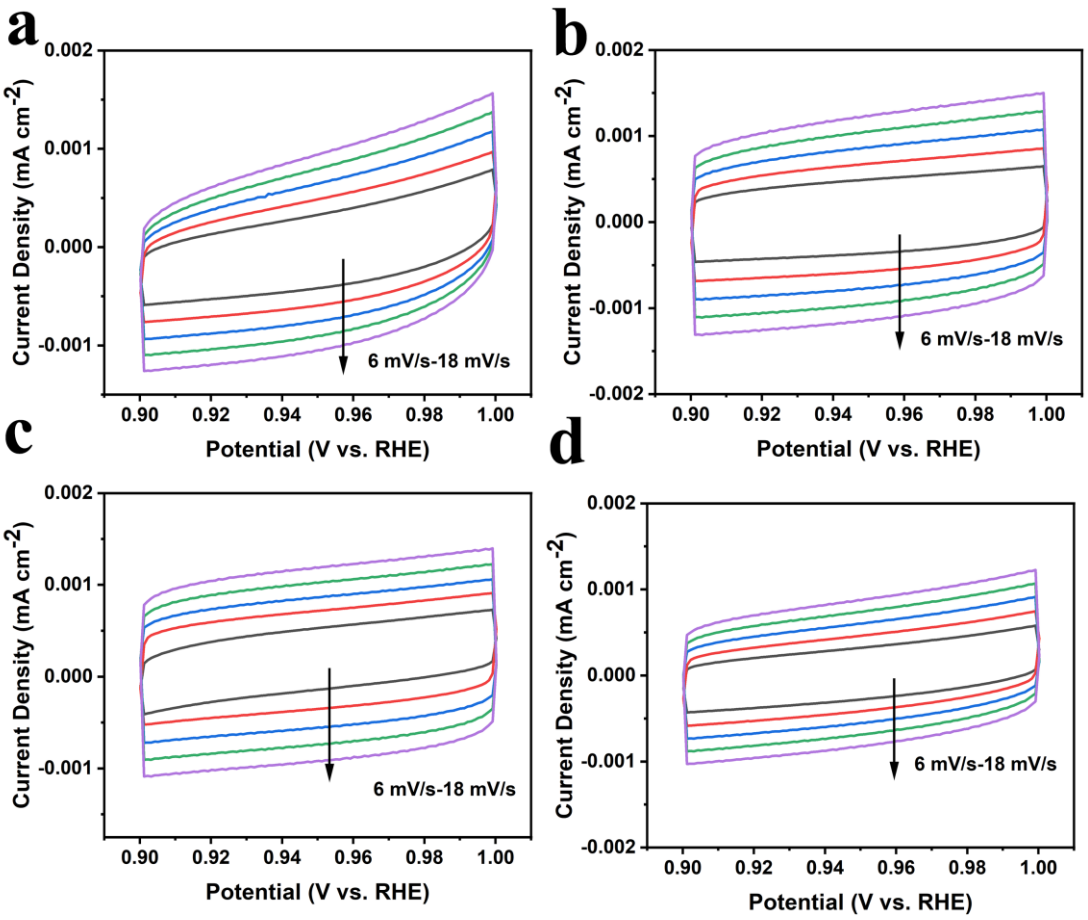

Fig. S14 Cyclic voltammograms of (a) CuO-$Ni(OH)_2$ (1:2), (b) CuO-$Ni(OH)_2$ (1:3), (c) CuO-$Ni(OH)_2$ (1:4), and (d) $Ni(OH)_2$ at different scan rates from 0.9 to 1 V vs. RHE.

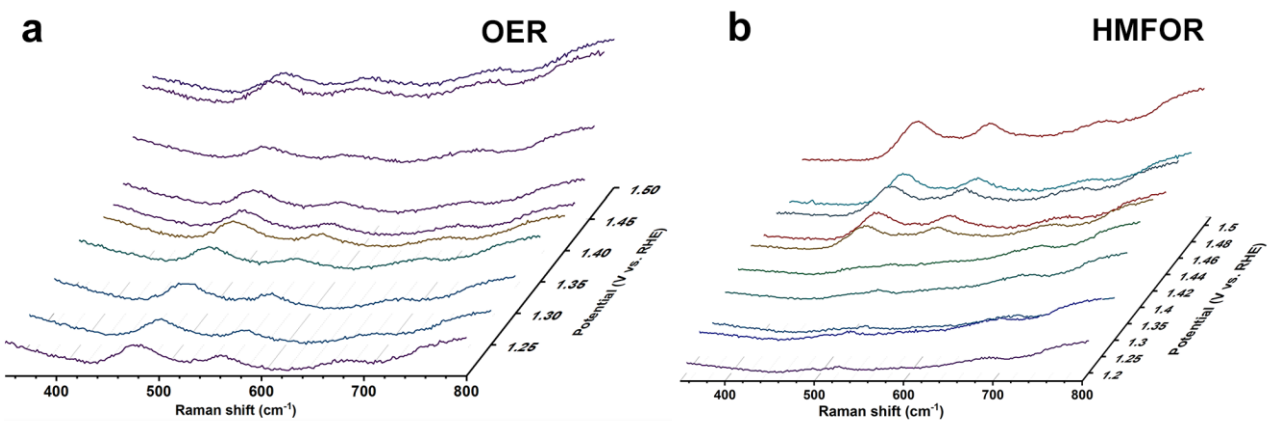

Fig. S15 In situ Raman spectra of CuO-$Ni(OH)_2$ for the OER (a), HMFOR(b).

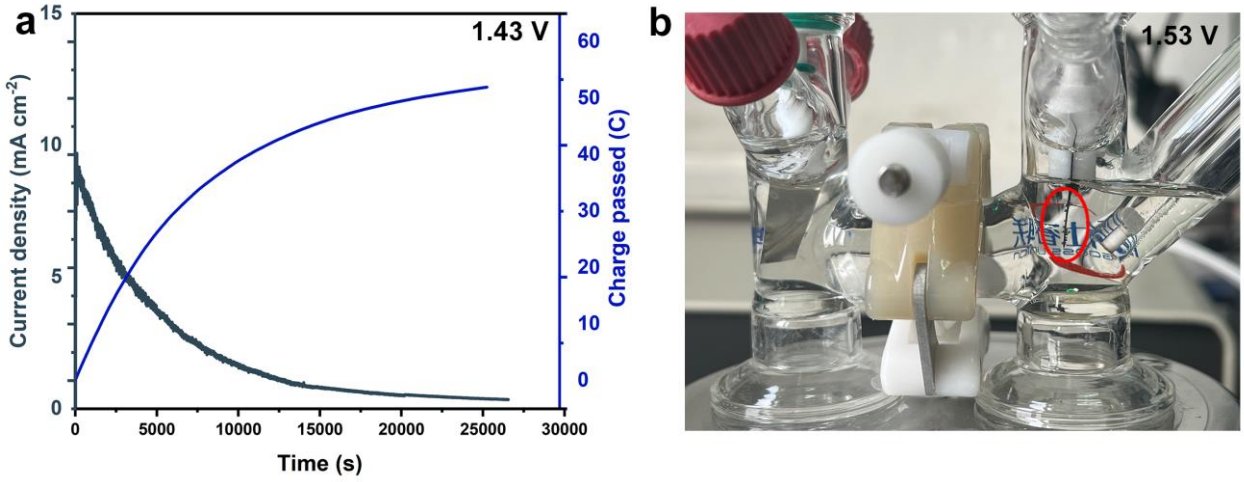

Fig. S16 (a) Corresponding current change and the accumulated charges over time of the chronoamperometry test of CuO-$Ni(OH)_2$ (1:3) at 1.43 V (b) the formed visible oxygen in the electrode at 1.53 V.

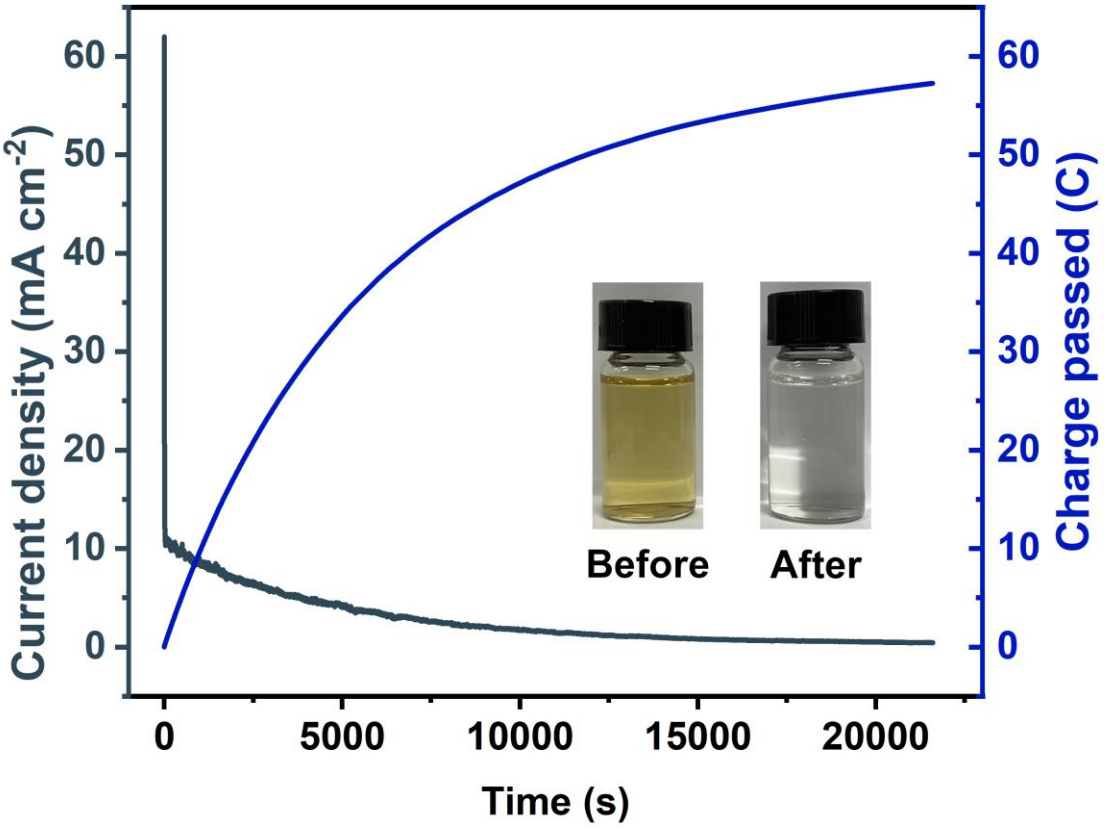

Fig. S17 Corresponding current change and the accumulated charges over time of the chronoamperometry test of CuO-$Ni(OH)_2$ (1:3) at 1.48 V in 1.0 M KOH solution with 10 mM HMF (insets: color change of the electrolyte before and after electrolysis).

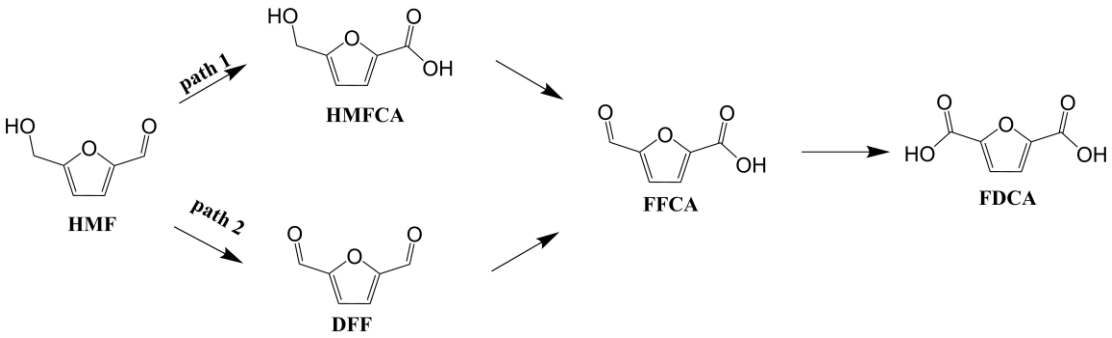

Fig. S18 Possible pathways for the oxidation of HMF to FDCA.

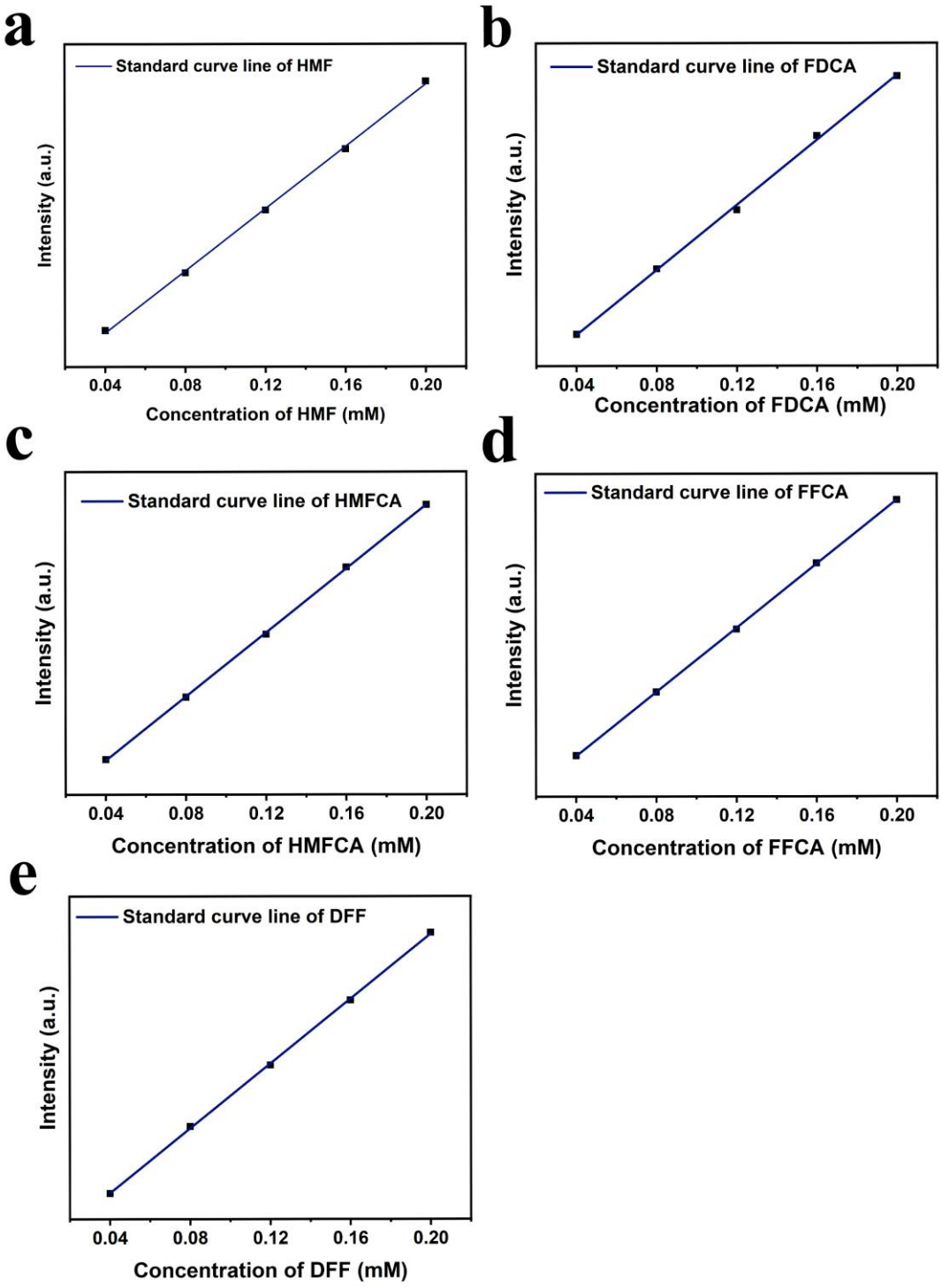

Fig. S19 Standard curves of the HPLC for (a) HMF, (b) FDCA, (c) HMFCA, (d) FFCA and (e) DFF.

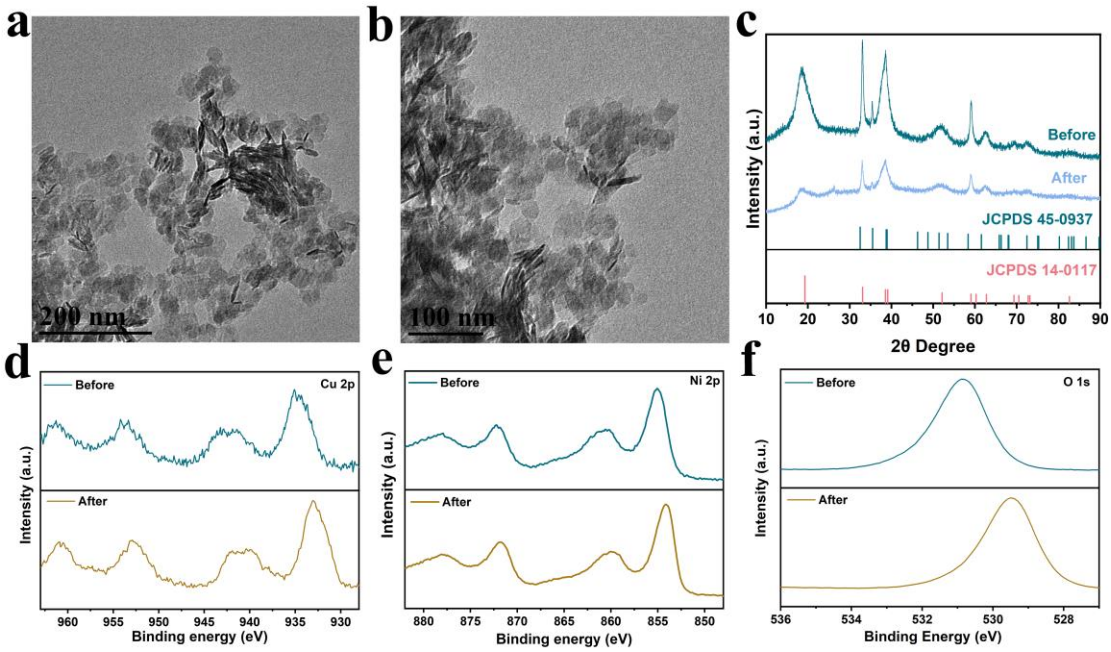

Fig. S20 (a, b) TEM images of CuO-Ni(OH)$_2$ (1:3) after five electrolysis cycles. (c) XRD patterns, XPS spectra of (d) Cu 2p, (e) Ni 2p, (f) O 1s of CuO-Ni(OH)$_2$ (1:3) before and after five electrolysis cycles.

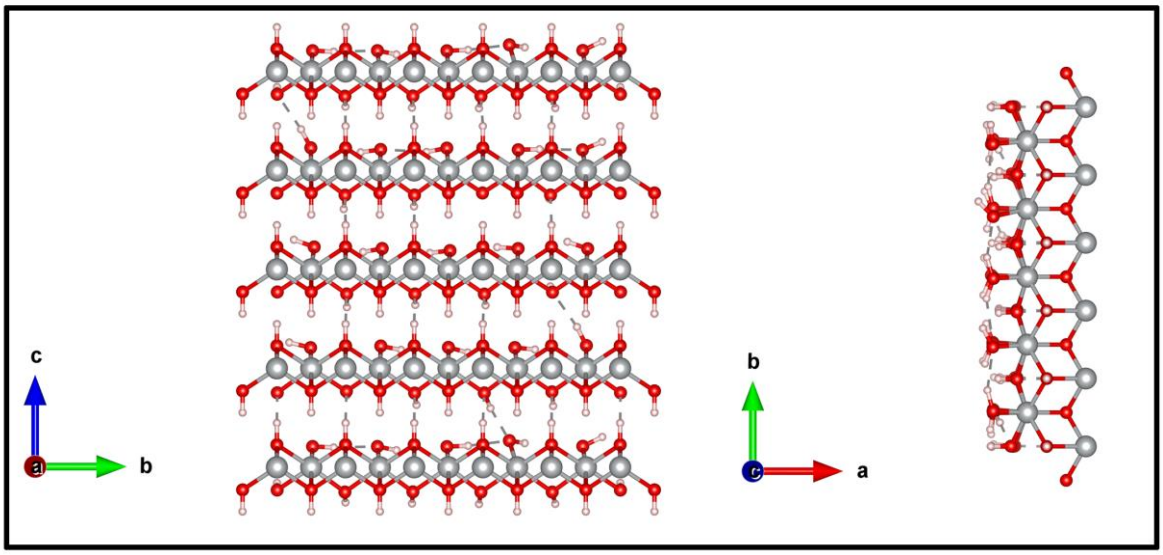

Fig. S21 Side and top views of an optimized structure for the $Ni(OH)_2$

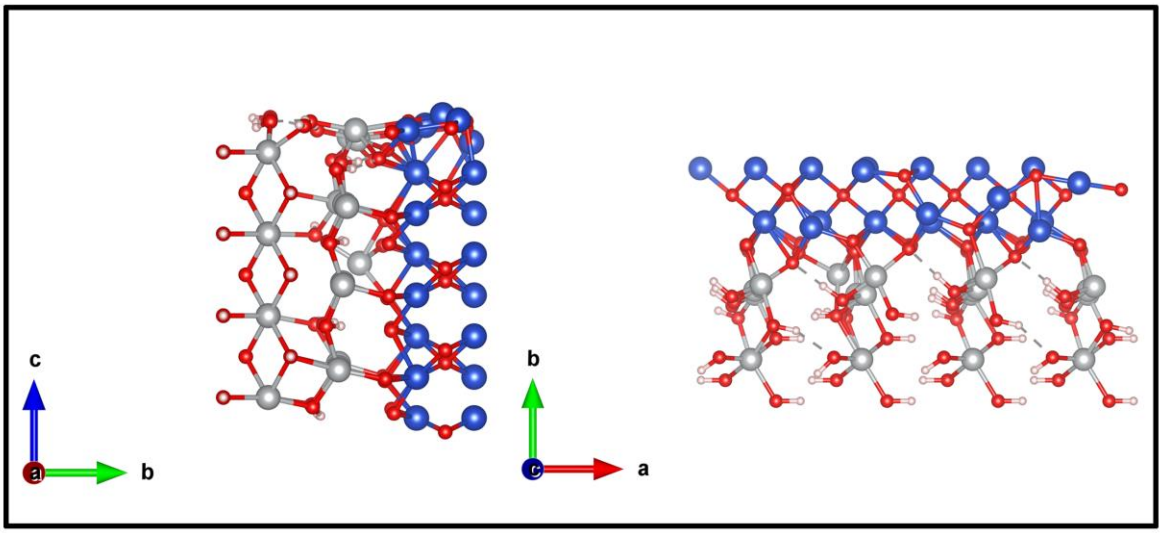

Fig. S22 Side and top views of an optimized structure for the CuO-$Ni(OH)_2$ (1:3).

Table S1 Recently reported electrocatalytic HMF catalysts.

Catalysts	C_{HMF} (mM)	Potential (V *vs.* RHE)	Conv. (%)	FDCA Yield (%)	FE. (%)
CuO-PdO[11]	50	~	99.5	96.2	93.7
CF-$Cu(OH)_2$[12]	100	1.81	100	98.7	~
$Ni_{0.9}Cu_{0.1}(OH)_2$[13]	5	1.45	~	~	91.2
NiVWv-LMH[14]	10	1.434	100	97.2	~
14%Ce-$Ni(OH)_2$[15]	10	1.56	99.8	97.8	86.6
Ni(NS)/CP[16]	5	1.36	99.7	99.4	95.3
NF/Co_4N@CeO_2[17]	10	1.425	91.1	93.6	84.5
Mn-5Ni_2P[18]	10	1.43	100	98	97.8
NiS_x/Ni_2P[19]	10	1.46	100	98.5	95.1
NiS_x/β$Ni(OH)_2$/Ni[20]	10	1.32	99.4	97.7	98.3
CF−CuO/CeO_2[21]	10	1.61	100	99.7	97.9
$NiMo_3S_4$-R[22]	10	1.45	99.3	98.7	98.5
Rh-SA/NiFe NMLDH[23]	50	1.3	98	99.8	98.5
V_O-Sc_2O_3[24]	10	1.46	~	<95	<90
δ-MnO_2[25]	10	1.457	~	98	98
P-Co_3O_4-NBA@NF[26]	10	1.636	100	96.9	97
CoO-$CoSe_2$[27]	10	1.43	~	99	97.9
Co_9S_8–Ni_3S_2@NSOC[28]	10	1.4	99.5	98.8	98.6
$NiCo_2O_4$-CFP[29]	10	1.43	~	94.3	89.6
$CuCo_2O_4$[30]	50	1.45	~	93.7	94
CuO-$Ni(OH)_2$ (This work)	**10**	**1.48**	**100**	**99.8**	**98.4**

Table S2 Adsorption energy of HMF on different surfaces

Adsorbed sites	$\mathbf{E_{ad/sub}}$	$\mathbf{E_{ad}}$	$\mathbf{E_{sub}}$
$Ni(OH)_2$	-8186.665005	-8100.911164	-85.721
$CuO\text{-}Ni(OH)_2$	-8023.060820	-7937.279332	-85.721

*Where Ead/sub, Ead, and Esub are the total energies of the optimized adsorbate/substrate system, the adsorbate in the gas phase, and the clean substrate, respectively.

Table S3 Bader charge analysis of CuO-$Ni(OH)_2$

#	X	Y	Z	CHARGE	MIN DIST	ATOMIC VOL
1	4.033173	2.872355	4.489622	0.57051	0.349311	31.34739
2	4.033173	2.872355	10.64763	0.587202	0.344224	26.07612
3	4.033173	7.939588	7.568624	0.516397	0.319646	21.66782
4	-4.03317	4.561433	7.568624	0.58795	0.349527	21.26747
5	4.033173	2.872355	16.80511	0.593075	0.389886	26.26739
6	4.033173	7.939588	13.72611	0.621584	0.386649	23.96316
7	-4.03317	4.561433	13.72611	0.599491	0.387057	21.15626
8	4.033173	7.939588	19.88411	0.657412	0.389506	24.59482
9	-4.03317	4.561433	19.88411	0.604297	0.375454	21.24078
10	13.05766	2.872355	4.489622	0.571861	0.37192	32.29933
11	13.05766	2.872355	10.64763	0.572256	0.367379	26.28074
12	13.05766	7.939588	7.568624	0.580611	0.374581	25.39997
13	4.991583	4.561433	7.568624	0.597392	0.392819	21.51213
14	13.05766	2.872355	16.80511	0.554521	0.37391	25.24428
15	13.05766	7.939588	13.72611	0.557843	0.377897	25.66687
16	4.991583	4.561433	13.72611	0.581362	0.409246	20.69363
17	13.05766	7.939588	19.88411	0.585717	0.375415	28.26469
18	4.991583	4.561433	19.88411	0.598068	0.39829	21.20074
19	22.08215	2.872355	4.489622	0.57478	0.379995	31.4497
20	22.08215	2.872355	10.64763	0.579984	0.418666	26.20067

21	22.08215	7.939588	7.568624	0.60238	0.39152	27.7042
22	14.01607	4.561433	7.568624	0.586874	0.375034	21.20074
23	22.08215	2.872355	16.80511	0.572916	0.390329	25.88484
24	22.08215	7.939588	13.72611	0.582074	0.407999	27.69531
25	14.01607	4.561433	13.72611	0.564622	0.378346	20.3778
26	22.08215	7.939588	19.88411	0.629633	0.430597	29.29226
27	14.01607	4.561433	19.88411	0.569112	0.375866	20.33777
28	4.033173	2.872355	22.96311	0.61937	0.355133	29.39902
29	13.05766	2.872355	22.96311	0.585214	0.367061	27.99335
30	22.08215	2.872355	22.96311	0.605405	0.423334	27.86879
31	-2.62724	10.20523	3.100002	0.492226	0.142551	32.73971
32	-2.99869	11.71094	9.866458	0.541305	0.213422	26.62326
33	-2.8376	12.0263	16.22133	0.498343	0.213823	21.81017
34	6.212608	10.1037	3.13675	0.477969	0.152438	31.06714
35	5.471601	10.0714	10.25022	0.529463	0.193465	25.23538
36	5.231457	9.749578	17.39361	0.54313	0.249728	20.1109
37	15.06924	9.948021	3.293194	0.506058	0.220882	33.46479
38	14.73515	11.21283	10.1216	0.528253	0.225877	28.83408
39	14.87674	11.80201	16.29483	0.485854	0.198661	22.68649
40	3.673905	8.58876	25.01001	0.504157	0.265214	20.93384
41	-3.99933	5.365668	24.81996	0.55153	0.269743	22.72652
42	-3.0041	12.57025	21.70106	0.514969	0.263434	17.14832

43	13.32217	9.718811	25.00371	0.483874	0.257991	22.126
44	5.45671	5.10323	25.51871	0.512652	0.203408	26.07167
45	5.898824	12.20228	22.31319	0.532348	0.253244	15.93837
46	21.77675	9.019798	25.36594	0.509532	0.279812	22.73097
47	14.19557	5.374282	25.17905	0.50554	0.21618	24.2434
48	15.16021	13.0179	22.23287	0.508966	0.224387	16.47662
49	0	6.25051	4.489622	17.12351	1.57645	130.514
50	0	6.25051	10.64763	17.00655	1.764651	85.47468
51	0	6.25051	16.80511	16.96372	1.760569	87.07607
52	9.024486	6.25051	4.489622	17.1245	1.595471	131.079
53	9.024486	6.25051	10.64763	16.9093	1.758944	77.89027
54	9.024486	6.25051	16.80511	16.94094	1.759598	77.28975
55	18.04924	6.25051	4.489622	17.11161	1.554023	127.9162
56	18.04924	6.25051	10.64763	16.95639	1.759708	82.66778
57	18.04924	6.25051	16.80511	16.97324	1.758635	85.51471
58	0	6.25051	22.96311	16.86118	1.536375	81.40445
59	9.024486	6.25051	22.96311	16.94694	1.574149	89.54045
60	18.04924	6.25051	22.96311	16.95358	1.499744	89.03334
61	0.336256	11.5448	6.565389	17.09104	1.587505	111.6976
62	0.340046	11.86416	12.95439	17.11013	1.601162	99.97623
63	0.843076	12.17582	18.86618	17.0931	1.627539	83.66865
64	8.633	11.53957	7.05572	17.08592	1.592416	113.3257

65	7.110915	13.13296	14.59862	17.08893	1.534465	96.71116
66	9.310655	11.53403	19.19219	17.12662	1.62809	98.93532
67	17.9423	11.54695	6.728133	17.0729	1.590466	113.9262
68	18.1061	11.85523	13.11555	17.06671	1.616252	104.5091
69	18.44912	12.01337	19.03207	17.05773	1.609391	93.91761
70	0.847949	12.34288	24.11649	17.02099	1.525537	99.58478
71	10.1494	12.98282	23.94797	16.99143	1.491511	92.41852
72	19.11974	12.82192	24.60735	17.05509	1.57617	111.017
73	2.058957	2.872355	4.489622	6.77525	1.32668	130.0158
74	3.024406	19.58284	7.089843	7.074428	1.523021	60.00353
75	7.536785	19.58284	1.889925	6.912324	1.553162	116.1059
76	2.058957	2.872355	10.64763	6.73698	1.325414	117.8763
77	2.058957	7.939588	7.568624	6.993673	1.496395	92.72545
78	-2.05896	4.561433	7.568624	6.846574	1.327547	104.9317
79	3.024406	19.58284	13.24732	7.104101	1.534949	60.60851
80	7.536785	19.58284	8.047405	7.105623	1.549813	60.50175
81	2.058957	2.872355	16.80511	6.729682	1.327239	119.7758
82	2.058957	7.939588	13.72611	6.940209	1.328368	89.45148
83	-2.05896	4.561433	13.72611	6.895755	1.328487	106.9735
84	3.024406	19.58284	19.40533	7.151795	1.536899	62.0898
85	7.536785	19.58284	14.20541	7.10807	1.507132	61.60048
86	2.058957	7.939588	19.88411	6.928085	1.327664	86.69797

87	-2.05896	4.561433	19.88411	6.883478	1.327783	104.6781
88	7.536785	19.58284	20.36289	7.075032	1.510439	59.0338
89	11.08344	2.872355	4.489622	6.793932	1.439477	130.4517
90	12.04889	19.58284	7.089843	7.073275	1.540438	60.3594
91	16.56127	19.58284	1.889925	6.938284	1.542628	117.8185
92	11.08344	2.872355	10.64763	6.786664	1.43831	119.5266
93	11.08344	7.939588	7.568624	6.939983	1.440167	98.28587
94	6.9658	4.561433	7.568624	6.870674	1.384028	103.8285
95	12.04889	19.58284	13.24732	7.120055	1.559056	61.25351
96	16.56127	19.58284	8.047405	7.088677	1.516928	60.73751
97	11.08344	2.872355	16.80511	6.779808	1.439992	121.4795
98	11.08344	7.939588	13.72611	6.925597	1.441033	110.9191
99	6.9658	4.561433	13.72611	6.862741	1.384929	104.1532
100	12.04889	19.58284	19.40533	7.136793	1.533511	61.32024
101	16.56127	19.58284	14.20541	7.098215	1.53969	60.99996
102	11.08344	7.939588	19.88411	6.94204	1.440384	88.77978
103	6.9658	4.561433	19.88411	6.870917	1.384254	103.3792
104	16.56127	19.58284	20.36289	7.079367	1.523125	67.93491
105	20.1082	2.872355	4.489622	6.811821	1.382956	131.3192
106	21.07365	19.58284	7.089843	7.082286	1.526692	60.37274
107	25.58576	19.58284	1.889925	6.935323	1.549991	115.4342
108	20.1082	2.872355	10.64763	6.769558	1.381742	119.758

109	20.1082	7.939588	7.568624	6.956092	1.383674	98.5928
110	15.99029	4.561433	7.568624	6.880084	1.440244	104.7226
111	21.07365	19.58284	13.24732	7.123375	1.522361	61.20013
112	25.58576	19.58284	8.047405	7.076669	1.553432	60.47506
113	20.1082	2.872355	16.80511	6.705484	1.383493	119.6512
114	20.1082	7.939588	13.72611	6.96795	1.384575	98.48159
115	15.99029	4.561433	13.72611	6.924925	1.44111	106.5375
116	21.07365	19.58284	19.40533	7.098643	1.519847	62.37449
117	25.58576	19.58284	14.20541	7.09746	1.52091	60.4884
118	20.1082	7.939588	19.88411	6.933857	1.3839	94.70051
119	15.99029	4.561433	19.88411	6.892118	1.440461	105.6701
120	25.58576	19.58284	20.36289	7.095814	1.543493	63.8113

Table S4 Unit-cell and position parameters of $Ni(OH)_2$ optimization model.

	$Ni(OH)_2$		
a (Å)	19.46900		
b (Å)	15.48110		
c (Å)	17.80660		
α (deg)	90.0		
β (deg)	90.0		
γ (deg)	90.0		
Atom Coordinates	**x**	**y**	**z**
H2	0.95409	0.10000	-0.11173
H3	0.90818	0.00000	0.11173
H4	0.95409	0.30000	-0.11173
H5	0.90818	0.20000	0.11173
H6	0.95409	0.50000	-0.11173
H7	0.90818	0.40000	0.11173
H8	0.95409	0.70000	-0.11173
H9	0.90818	0.60000	0.11173
H10	0.95409	0.90000	-0.11173
H11	0.90818	0.80000	0.11173
H12	0.95409	0.10000	0.13827
H13	0.90818	0.00000	0.36173

H14	0.95409	0.30000	0.13827
H15	0.90818	0.20000	0.36173
H16	0.95409	0.50000	0.13827
H17	0.90818	0.40000	0.36173
H18	0.95409	0.70000	0.13827
H19	0.90818	0.60000	0.36173
H20	0.95409	0.90000	0.13827
H21	0.90818	0.80000	0.36173
H22	0.95409	0.10000	0.38827
H23	0.90818	0.00000	0.61173
H24	0.95409	0.30000	0.38827
H25	0.90818	0.20000	0.61173
H26	0.95409	0.50000	0.38827
H27	0.90818	0.40000	0.61173
H28	0.95409	0.70000	0.38827
H29	0.90818	0.60000	0.61173
H30	0.95409	0.90000	0.38827
H31	0.90818	0.80000	0.61173
H32	0.95409	0.10000	0.63827
H33	0.90818	0.00000	0.86173
H34	0.95409	0.30000	0.63827
H35	0.90818	0.20000	0.86173

H36	0.95409	0.50000	0.63827
H37	0.90818	0.40000	0.86173
H38	0.95409	0.70000	0.63827
H39	0.90818	0.60000	0.86173
H40	0.95409	0.90000	0.63827
H41	0.90818	0.80000	0.86173
H42	0.76888	0.16548	0.04996
H43	0.77640	0.00030	-0.03954
H44	0.75838	0.34799	0.04300
H45	0.79416	0.19961	-0.08886
H46	0.76788	0.55690	0.05427
H47	0.79556	0.39354	-0.09149
H48	0.74780	0.72181	0.06087
H49	0.79624	0.58878	-0.09293
H50	0.77661	0.94788	0.07648
H51	0.79668	0.81107	-0.09243
H52	0.77749	0.03611	0.31527
H53	0.78330	0.00613	0.18574
H54	0.76607	0.36154	0.29651
H55	0.78439	0.20372	0.18177
H56	0.76125	0.55576	0.28991
H57	0.79608	0.40655	0.15768

H58	0.76286	0.75159	0.29748
H59	0.80273	0.62209	0.14934
H60	0.79527	0.87417	0.35463
H61	0.79902	0.80477	0.15494
H62	0.77537	0.04965	0.57486
H63	0.77921	0.00067	0.44626
H64	0.75880	0.25133	0.54378
H65	0.79781	0.20380	0.40440
H66	0.75953	0.44576	0.54143
H67	0.79495	0.40316	0.41038
H68	0.76792	0.64172	0.55600
H69	0.79542	0.60786	0.40910
H70	0.77325	0.84640	0.56963
H71	0.77706	0.79645	0.45678
H72	0.79815	0.07034	0.85383
H73	0.77931	-0.00127	0.69868
H74	0.76297	0.24404	0.79577
H75	0.79950	0.19466	0.65227
H76	0.76657	0.43609	0.79665
H77	0.79525	0.39935	0.65908
H78	0.77050	0.76508	0.80347
H79	0.77911	0.59883	0.69963

H80	0.76782	0.94719	0.82218
H81	0.78493	0.79332	0.67851
Ni82	0.86227	0.10000	0.00000
Ni83	1.00000	0.00000	0.00000
Ni84	0.86227	0.30000	0.00000
Ni85	1.00000	0.20000	0.00000
Ni86	0.86227	0.50000	0.00000
Ni87	1.00000	0.40000	0.00000
Ni88	0.86227	0.70000	0.00000
Ni89	1.00000	0.60000	0.00000
Ni90	0.86227	0.90000	0.00000
Ni91	1.00000	0.80000	0.00000
Ni92	0.86227	0.10000	0.25000
Ni93	1.00000	0.00000	0.25000
Ni94	0.86227	0.30000	0.25000
Ni95	1.00000	0.20000	0.25000
Ni96	0.86227	0.50000	0.25000
Ni97	1.00000	0.40000	0.25000
Ni98	0.86227	0.70000	0.25000
Ni99	1.00000	0.60000	0.25000
Ni100	0.86227	0.90000	0.25000
Ni101	1.00000	0.80000	0.25000

Ni102	0.86227	0.10000	0.50000
Ni103	1.00000	0.00000	0.50000
Ni104	0.86227	0.30000	0.50000
Ni105	1.00000	0.20000	0.50000
Ni106	0.86227	0.50000	0.50000
Ni107	1.00000	0.40000	0.50000
Ni108	0.86227	0.70000	0.50000
Ni109	1.00000	0.60000	0.50000
Ni110	0.86227	0.90000	0.50000
Ni111	1.00000	0.80000	0.50000
Ni112	0.86227	0.10000	0.75000
Ni113	1.00000	0.00000	0.75000
Ni114	0.86227	0.30000	0.75000
Ni115	1.00000	0.20000	0.75000
Ni116	0.86227	0.50000	0.75000
Ni117	1.00000	0.40000	0.75000
Ni118	0.86227	0.70000	0.75000
Ni119	1.00000	0.60000	0.75000
Ni120	0.86227	0.90000	0.75000
Ni121	1.00000	0.80000	0.75000
O122	0.95409	0.10000	-0.05704
O123	0.90818	0.00000	0.05704

O124	0.95409	0.30000	-0.05704
O125	0.90818	0.20000	0.05704
O126	0.95409	0.50000	-0.05704
O127	0.90818	0.40000	0.05704
O128	0.95409	0.70000	-0.05704
O129	0.90818	0.60000	0.05704
O130	0.95409	0.90000	-0.05704
O131	0.90818	0.80000	0.05704
O132	0.95409	0.10000	0.19296
O133	0.90818	0.00000	0.30704
O134	0.95409	0.30000	0.19296
O135	0.90818	0.20000	0.30704
O136	0.95409	0.50000	0.19296
O137	0.90818	0.40000	0.30704
O138	0.95409	0.70000	0.19296
O139	0.90818	0.60000	0.30704
O140	0.95409	0.90000	0.19296
O141	0.90818	0.80000	0.30704
O142	0.95409	0.10000	0.44296
O143	0.90818	0.00000	0.55704
O144	0.95409	0.30000	0.44296
O145	0.90818	0.20000	0.55704

O146	0.95409	0.50000	0.44296
O147	0.90818	0.40000	0.55704
O148	0.95409	0.70000	0.44296
O149	0.90818	0.60000	0.55704
O150	0.95409	0.90000	0.44296
O151	0.90818	0.80000	0.55704
O152	0.95409	0.10000	0.69296
O153	0.90818	0.00000	0.80704
O154	0.95409	0.30000	0.69296
O155	0.90818	0.20000	0.80704
O156	0.95409	0.50000	0.69296
O157	0.90818	0.40000	0.80704
O158	0.95409	0.70000	0.69296
O159	0.90818	0.60000	0.80704
O160	0.95409	0.90000	0.69296
O161	0.90818	0.80000	0.80704
O162	0.78189	0.10397	0.05256
O163	0.82399	0.00074	-0.05763
O164	0.78154	0.29286	0.05258
O165	0.83813	0.19811	-0.06257
O166	0.78228	0.49527	0.05226
O167	0.83792	0.39612	-0.06208

O168	0.78247	0.67725	0.06733
O169	0.83794	0.59446	-0.06254
O170	0.78158	0.89112	0.05311
O171	0.83821	0.80206	-0.06263
O172	0.78247	0.09807	0.30223
O173	0.83321	0.00103	0.18819
O174	0.78314	0.30272	0.30639
O175	0.83359	0.20253	0.19216
O176	0.78170	0.49975	0.30291
O177	0.83807	0.40122	0.18758
O178	0.78217	0.69321	0.30253
O179	0.83785	0.60422	0.18786
O180	0.78070	0.90163	0.30760
O181	0.83739	0.80134	0.19051
O182	0.78270	0.10865	0.55659
O183	0.82928	0.00115	0.44285
O184	0.78151	0.30676	0.55279
O185	0.83780	0.20334	0.43790
O186	0.77810	0.50432	0.54746
O187	0.83845	0.40201	0.43784
O188	0.78188	0.70269	0.55251
O189	0.83829	0.60439	0.43754

O190	0.78171	0.90536	0.55218
O191	0.82537	0.80289	0.44241
O192	0.78310	0.09891	0.80711
O193	0.82913	0.00014	0.69241
O194	0.78159	0.30230	0.80291
O195	0.83789	0.19848	0.68773
O196	0.78327	0.49501	0.80640
O197	0.83808	0.40078	0.68771
O198	0.78242	0.70306	0.80221
O199	0.82906	0.59896	0.69286
O200	0.77816	0.89021	0.80196
O201	0.83413	0.79709	0.68794

Table S5 Unit-cell and position parameters of CuO-$Ni(OH)_2$ (1:3) optimization model

	CuO-$Ni(OH)_2$ (1:3)
a (Å)	14.32680
b (Å)	16.28090
c (Å)	27.78070
α (deg)	90.0
β (deg)	90.0
γ (deg)	90.0

Atom Coordinates	**x**	**y**	**z**
H2	0.14897	0.09336	0.08552
H3	0.14897	0.09336	0.20282
H4	0.14897	0.25806	0.14417
H5	-0.14897	0.14826	0.14417
H6	0.14897	0.09336	0.32011
H7	0.14897	0.25806	0.26146
H8	-0.14897	0.14826	0.26146
H9	0.14897	0.25806	0.37876
H10	-0.14897	0.14826	0.37876
H11	0.48230	0.09336	0.08552
H12	0.48230	0.09336	0.20282
H13	0.48230	0.25806	0.14417

H14	0.18437	0.14826	0.14417
H15	0.48230	0.09336	0.32011
H16	0.48230	0.25806	0.26146
H17	0.18437	0.14826	0.26146
H18	0.48230	0.25806	0.37876
H19	0.18437	0.14826	0.37876
H20	0.81563	0.09336	0.08552
H21	0.81563	0.09336	0.20282
H22	0.81563	0.25806	0.14417
H23	0.51770	0.14826	0.14417
H24	0.81563	0.09336	0.32011
H25	0.81563	0.25806	0.26146
H26	0.51770	0.14826	0.26146
H27	0.81563	0.25806	0.37876
H28	0.51770	0.14826	0.37876
H29	0.14897	0.09336	0.43741
H30	0.48230	0.09336	0.43741
H31	0.81563	0.09336	0.43741
H32	-0.09704	0.33170	0.05905
H33	-0.11076	0.38064	0.18794
H34	-0.10481	0.39089	0.30899
H35	0.22947	0.32840	0.05975

H36	0.20210	0.32735	0.19525
H37	0.19323	0.31689	0.33132
H38	0.55660	0.32334	0.06273
H39	0.54426	0.36445	0.19280
H40	0.54949	0.38360	0.31039
H41	0.13570	0.27916	0.47640
H42	-0.14772	0.17440	0.47278
H43	-0.11096	0.40857	0.41337
H44	0.49207	0.31589	0.47628
H45	0.20155	0.16587	0.48609
H46	0.21788	0.39661	0.42503
H47	0.80435	0.29317	0.48318
H48	0.52433	0.17468	0.47962
H49	0.55996	0.42312	0.42350
Ni50	0.00000	0.20316	0.08552
Ni51	0.00000	0.20316	0.20282
Ni52	0.00000	0.20316	0.32011
Ni53	0.33333	0.20316	0.08552
Ni54	0.33333	0.20316	0.20282
Ni55	0.33333	0.20316	0.32011
Ni56	0.66667	0.20316	0.08552
Ni57	0.66667	0.20316	0.20282

Ni58	0.66667	0.20316	0.32011
Ni59	0.00000	0.20316	0.43741
Ni60	0.33333	0.20316	0.43741
Ni61	0.66667	0.20316	0.43741
Ni62	0.01242	0.37524	0.12506
Ni63	0.01256	0.38562	0.24676
Ni64	0.03114	0.39575	0.35937
Ni65	0.31887	0.37507	0.13440
Ni66	0.26265	0.42686	0.27808
Ni67	0.34390	0.37489	0.36558
Ni68	0.66272	0.37531	0.12816
Ni69	0.66877	0.38533	0.24983
Ni70	0.68144	0.39047	0.36253
Ni71	0.03132	0.40118	0.45938
Ni72	0.37488	0.42198	0.45617
Ni73	0.70621	0.41675	0.46873
O74	0.07605	0.09336	0.08552
O75	0.11171	0.63650	0.13505
O76	0.27838	0.63650	0.03600
O77	0.07605	0.09336	0.20282
O78	0.07605	0.25806	0.14417
O79	-0.07605	0.14826	0.14417

O80	0.11171	0.63650	0.25234
O81	0.27838	0.63650	0.15329
O82	0.07605	0.09336	0.32011
O83	0.07605	0.25806	0.26146
O84	-0.07605	0.14826	0.26146
O85	0.11171	0.63650	0.36964
O86	0.27838	0.63650	0.27059
O87	0.07605	0.25806	0.37876
O88	-0.07605	0.14826	0.37876
O89	0.27838	0.63650	0.38788
O90	0.40938	0.09336	0.08552
O91	0.44504	0.63650	0.13505
O92	0.61171	0.63650	0.03600
O93	0.40938	0.09336	0.20282
O94	0.40938	0.25806	0.14417
O95	0.25729	0.14826	0.14417
O96	0.44504	0.63650	0.25234
O97	0.61171	0.63650	0.15329
O98	0.40938	0.09336	0.32011
O99	0.40938	0.25806	0.26146
O100	0.25729	0.14826	0.26146
O101	0.44504	0.63650	0.36964

O102	0.61171	0.63650	0.27059
O103	0.40938	0.25806	0.37876
O104	0.25729	0.14826	0.37876
O105	0.61171	0.63650	0.38788
O106	0.74272	0.09336	0.08552
O107	0.77838	0.63650	0.13505
O108	0.94504	0.63650	0.03600
O109	0.74272	0.09336	0.20282
O110	0.74272	0.25806	0.14417
O111	0.59062	0.14826	0.14417
O112	0.77838	0.63650	0.25234
O113	0.94504	0.63650	0.15329
O114	0.74272	0.09336	0.32011
O115	0.74272	0.25806	0.26146
O116	0.59062	0.14826	0.26146
O117	0.77838	0.63650	0.36964
O118	0.94504	0.63650	0.27059
O119	0.74272	0.25806	0.37876
O120	0.59062	0.14826	0.37876
O121	0.94504	0.63650	0.38788
O122	0.07605	0.09336	0.43741
O123	0.40938	0.09336	0.43741

O124	0.74272	0.09336	0.43741
O125	-0.03767	0.31213	0.07175
O126	0.15001	0.51047	0.06289
O127	0.31287	0.48417	0.11569
O128	-0.05554	0.34445	0.18747
O129	0.14971	0.50489	0.18417
O130	0.30705	0.49494	0.22832
O131	-0.05003	0.35388	0.30611
O132	0.14418	0.48421	0.30353
O133	0.31216	0.48813	0.34011
O134	0.28760	0.31222	0.07545
O135	0.47547	0.50531	0.06885
O136	0.64950	0.48881	0.10944
O137	0.26884	0.31761	0.19044
O138	0.48232	0.50501	0.18480
O139	0.65028	0.49522	0.22830
O140	0.25687	0.31816	0.31855
O141	0.48126	0.50001	0.30614
O142	0.65076	0.50119	0.34655
O143	0.61831	0.30870	0.07478
O144	0.81751	0.51116	0.06282
O145	0.99279	0.48928	0.11203

O146	0.60632	0.33840	0.19070
O147	0.81901	0.50465	0.18151
O148	0.98750	0.49854	0.23085
O149	0.60626	0.34861	0.30899
O150	0.81287	0.49914	0.30618
O151	0.98668	0.50509	0.34401
O152	0.06794	0.29177	0.47483
O153	-0.09382	0.20859	0.48118
O154	-0.05685	0.36954	0.41228
O155	0.12539	0.45802	0.42475
O156	0.11224	0.65111	0.47157
O157	0.30610	0.51520	0.46254
O158	0.42530	0.32281	0.46888
O159	0.24989	0.20818	0.48729
O160	0.27505	0.35982	0.42533
O161	0.47451	0.49451	0.44079
O162	0.46191	0.68800	0.47206
O163	0.65629	0.54615	0.48114
O164	0.73730	0.30638	0.48096
O165	0.57994	0.20839	0.48455
O166	0.61165	0.38127	0.42191
O167	0.79337	0.47419	0.42797

O168	0.85635	0.68794	0.48125
O169	0.98759	0.50551	0.46578
Cu170	0.04164	0.56595	0.05622
Cu171	0.01521	0.70702	0.11487
Cu172	0.18188	0.70702	0.05618
Cu173	0.20831	0.56595	0.11482
Cu174	0.04164	0.56595	0.17351
Cu175	0.01521	0.70702	0.23216
Cu176	0.18188	0.70702	0.17347
Cu177	0.20831	0.56595	0.23212
Cu178	0.04164	0.56595	0.29081
Cu179	0.01521	0.70702	0.34946
Cu180	0.18188	0.70702	0.29077
Cu181	0.20831	0.56595	0.34941
Cu182	0.04164	0.56595	0.40810
Cu183	0.18188	0.70702	0.40806
Cu184	0.37497	0.56595	0.05622
Cu185	0.34855	0.70702	0.11487
Cu186	0.51521	0.70702	0.05618
Cu187	0.54164	0.56595	0.11482
Cu188	0.37497	0.56595	0.17351
Cu189	0.34855	0.70702	0.23216

Cu190	0.51521	0.70702	0.17347
Cu191	0.54164	0.56595	0.23212
Cu192	0.37497	0.56595	0.29081
Cu193	0.34855	0.70702	0.34946
Cu194	0.51521	0.70702	0.29077
Cu195	0.54164	0.56595	0.34941
Cu196	0.37497	0.56595	0.40810
Cu197	0.51521	0.70702	0.40806
Cu198	0.70831	0.56595	0.05622
Cu199	0.68188	0.70702	0.11487
Cu200	0.84855	0.70702	0.05618
Cu201	0.87497	0.56595	0.11482
Cu202	0.70831	0.56595	0.17351
Cu203	0.68188	0.70702	0.23216
Cu204	0.84855	0.70702	0.17347
Cu205	0.87497	0.56595	0.23212
Cu206	0.70831	0.56595	0.29081
Cu207	0.68188	0.70702	0.34946
Cu208	0.84855	0.70702	0.29077
Cu209	0.87497	0.56595	0.34941
Cu210	0.70831	0.56595	0.40810
Cu211	0.84855	0.70702	0.40806

Cu212	-0.01467	0.66867	0.48316
Cu213	0.18204	0.55169	0.46542
Cu214	0.33877	0.70063	0.45167
Cu215	0.53143	0.58745	0.47573
Cu216	0.74443	0.62975	0.49065
Cu217	0.86715	0.54307	0.46918

Table S6 Unit-cell and position parameters of the optimized model for the adsorption of HMF on $Ni(OH)_2$

	HMF@$Ni(OH)_2$
a (Å)	19.46900
b (Å)	15.48110
c (Å)	17.80660
α (deg)	90.0
β (deg)	90.0
γ (deg)	90.0

Atom Coordinates	**x**	**y**	**z**
H2	0.95409	0.10000	-0.11173
H3	0.90818	0.00000	0.11173
H4	0.95409	0.30000	-0.11173
H5	0.90818	0.20000	0.11173
H6	0.95409	0.50000	-0.11173
H7	0.90818	0.40000	0.11173
H8	0.95409	0.70000	-0.11173
H9	0.90818	0.60000	0.11173
H10	0.95409	0.90000	-0.11173
H11	0.90818	0.80000	0.11173
H12	0.95409	0.10000	0.13827

H13	0.90818	0.00000	0.36173
H14	0.95409	0.30000	0.13827
H15	0.90818	0.20000	0.36173
H16	0.95409	0.50000	0.13827
H17	0.90818	0.40000	0.36173
H18	0.95409	0.70000	0.13827
H19	0.90818	0.60000	0.36173
H20	0.95409	0.90000	0.13827
H21	0.90818	0.80000	0.36173
H22	0.95409	0.10000	0.38827
H23	0.90818	0.00000	0.61173
H24	0.95409	0.30000	0.38827
H25	0.90818	0.20000	0.61173
H26	0.95409	0.50000	0.38827
H27	0.90818	0.40000	0.61173
H28	0.95409	0.70000	0.38827
H29	0.90818	0.60000	0.61173
H30	0.95409	0.90000	0.38827
H31	0.90818	0.80000	0.61173
H32	0.95409	0.10000	0.63827
H33	0.90818	0.00000	0.86173
H34	0.95409	0.30000	0.63827

H35	0.90818	0.20000	0.86173
H36	0.95409	0.50000	0.63827
H37	0.90818	0.40000	0.86173
H38	0.95409	0.70000	0.63827
H39	0.90818	0.60000	0.86173
H40	0.95409	0.90000	0.63827
H41	0.90818	0.80000	0.86173
H42	0.76004	0.15302	0.04248
H43	0.80357	-0.03156	-0.10349
H44	0.76862	0.35905	0.05508
H45	0.80522	0.16097	-0.10598
H46	0.74513	0.51806	0.05422
H47	0.80196	0.36899	-0.10140
H48	0.76446	0.75740	0.04591
H49	0.79644	0.60141	-0.09305
H50	0.76045	0.95210	0.04119
H51	0.79467	0.79142	-0.08972
H52	0.76301	0.15720	0.29468
H53	0.79405	0.00497	0.16116
H54	0.76317	0.35095	0.30018
H55	0.79631	0.20888	0.15759
H56	0.76176	0.55257	0.29369

H57	0.80172	0.42382	0.15053
H58	0.75955	0.74856	0.30015
H59	0.79744	0.60669	0.15510
H60	0.76427	0.95469	0.30107
H61	0.79417	0.80683	0.16113
H62	0.76586	0.15458	0.55208
H63	0.79204	0.00949	0.41602
H64	0.80111	0.27084	0.60385
H65	0.79797	0.20764	0.40609
H66	0.78365	0.45473	0.59345
H67	0.78399	0.40294	0.42734
H68	0.76575	0.64343	0.55187
H69	0.79816	0.61562	0.40409
H70	0.76444	0.83257	0.54643
H71	0.79979	0.80197	0.40337
H72	0.75245	0.06959	0.81813
H73	0.79624	-0.00542	0.65679
H74	0.76769	0.24700	0.81534
H75	0.77683	0.19631	0.70300
H76	0.76371	0.45104	0.80694
H77	0.77883	0.39649	0.69661
H78	0.75610	0.65772	0.78944

H79	0.80234	0.58435	0.64985
H80	0.76186	0.85077	0.80320
H81	0.79703	0.79088	0.65597
H82	0.42633	0.57972	0.61372
H83	0.53060	0.65982	0.53641
H84	0.64984	0.59425	0.47170
H85	0.61012	0.51956	0.41028
H86	0.39755	0.41329	0.64386
H87	0.71320	0.48581	0.51871
Ni88	0.86227	0.10000	0.00000
Ni89	1.00000	0.00000	0.00000
Ni90	0.86227	0.30000	0.00000
Ni91	1.00000	0.20000	0.00000
Ni92	0.86227	0.50000	0.00000
Ni93	1.00000	0.40000	0.00000
Ni94	0.86227	0.70000	0.00000
Ni95	1.00000	0.60000	0.00000
Ni96	0.86227	0.90000	0.00000
Ni97	1.00000	0.80000	0.00000
Ni98	0.86227	0.10000	0.25000
Ni99	1.00000	0.00000	0.25000
Ni100	0.86227	0.30000	0.25000

Ni101	1.00000	0.20000	0.25000
Ni102	0.86227	0.50000	0.25000
Ni103	1.00000	0.40000	0.25000
Ni104	0.86227	0.70000	0.25000
Ni105	1.00000	0.60000	0.25000
Ni106	0.86227	0.90000	0.25000
Ni107	1.00000	0.80000	0.25000
Ni108	0.86227	0.10000	0.50000
Ni109	1.00000	0.00000	0.50000
Ni110	0.86227	0.30000	0.50000
Ni111	1.00000	0.20000	0.50000
Ni112	0.86227	0.50000	0.50000
Ni113	1.00000	0.40000	0.50000
Ni114	0.86227	0.70000	0.50000
Ni115	1.00000	0.60000	0.50000
Ni116	0.86227	0.90000	0.50000
Ni117	1.00000	0.80000	0.50000
Ni118	0.86227	0.10000	0.75000
Ni119	1.00000	0.00000	0.75000
Ni120	0.86227	0.30000	0.75000
Ni121	1.00000	0.20000	0.75000
Ni122	0.86227	0.50000	0.75000

Ni123	1.00000	0.40000	0.75000
Ni124	0.86227	0.70000	0.75000
Ni125	1.00000	0.60000	0.75000
Ni126	0.86227	0.90000	0.75000
Ni127	1.00000	0.80000	0.75000
O128	0.95409	0.10000	-0.05704
O129	0.90818	0.00000	0.05704
O130	0.95409	0.30000	-0.05704
O131	0.90818	0.20000	0.05704
O132	0.95409	0.50000	-0.05704
O133	0.90818	0.40000	0.05704
O134	0.95409	0.70000	-0.05704
O135	0.90818	0.60000	0.05704
O136	0.95409	0.90000	-0.05704
O137	0.90818	0.80000	0.05704
O138	0.95409	0.10000	0.19296
O139	0.90818	0.00000	0.30704
O140	0.95409	0.30000	0.19296
O141	0.90818	0.20000	0.30704
O142	0.95409	0.50000	0.19296
O143	0.90818	0.40000	0.30704
O144	0.95409	0.70000	0.19296

O145	0.90818	0.60000	0.30704
O146	0.95409	0.90000	0.19296
O147	0.90818	0.80000	0.30704
O148	0.95409	0.10000	0.44296
O149	0.90818	0.00000	0.55704
O150	0.95409	0.30000	0.44296
O151	0.90818	0.20000	0.55704
O152	0.95409	0.50000	0.44296
O153	0.90818	0.40000	0.55704
O154	0.95409	0.70000	0.44296
O155	0.90818	0.60000	0.55704
O156	0.95409	0.90000	0.44296
O157	0.90818	0.80000	0.55704
O158	0.95409	0.10000	0.69296
O159	0.90818	0.00000	0.80704
O160	0.95409	0.30000	0.69296
O161	0.90818	0.20000	0.80704
O162	0.95409	0.50000	0.69296
O163	0.90818	0.40000	0.80704
O164	0.95409	0.70000	0.69296
O165	0.90818	0.60000	0.80704
O166	0.95409	0.90000	0.69296

O167	0.90818	0.80000	0.80704
O168	0.78279	0.09884	0.05684
O169	0.83354	-0.01028	-0.06213
O170	0.78334	0.29743	0.05643
O171	0.83328	0.18770	-0.06222
O172	0.78240	0.47935	0.06765
O173	0.83381	0.39042	-0.06230
O174	0.78217	0.69840	0.05234
O175	0.83792	0.59932	-0.06232
O176	0.78188	0.89622	0.05258
O177	0.83813	0.79662	-0.06264
O178	0.78201	0.09886	0.30236
O179	0.83773	0.00047	0.18788
O180	0.78207	0.29207	0.30231
O181	0.83815	0.20292	0.18772
O182	0.78216	0.49534	0.30238
O183	0.83785	0.40605	0.18785
O184	0.78230	0.69278	0.30772
O185	0.83801	0.60368	0.18753
O186	0.78300	0.89613	0.30616
O187	0.83778	0.80184	0.18783
O188	0.78244	0.09446	0.55207

O189	0.83803	0.00440	0.43727
O190	0.78609	0.30122	0.55780
O191	0.84019	0.20242	0.43573
O192	0.78227	0.51035	0.56745
O193	0.83333	0.40071	0.43792
O194	0.78216	0.70342	0.55242
O195	0.83350	0.60415	0.44230
O196	0.78225	0.89076	0.55761
O197	0.84146	0.80089	0.43386
O198	0.78224	0.12003	0.81764
O199	0.83773	-0.00076	0.68779
O200	0.78264	0.30724	0.80726
O201	0.82479	0.20391	0.68822
O202	0.78211	0.50971	0.80271
O203	0.82881	0.40099	0.69251
O204	0.78257	0.70766	0.80690
O205	0.83808	0.59873	0.68790
O206	0.78455	0.90667	0.81064
O207	0.83797	0.79711	0.68755
O208	0.54175	0.44781	0.54153
O209	0.67629	0.46310	0.48416
O210	0.45839	0.31288	0.60931

C211	0.48245	0.46194	0.58217
C212	0.46953	0.54996	0.58540
C213	0.52323	0.59114	0.54527
C214	0.56588	0.52650	0.51922
C215	0.62798	0.52847	0.46871
C216	0.44425	0.39033	0.61357

Table S7 Unit-cell and position parameters of the optimized model for the adsorption of HMF on CuO-$Ni(OH)_2$ (1:3)

	HMF@CuO-$Ni(OH)_2$
a (Å)	14.32680
b (Å)	16.28090
c (Å)	27.78070
α (deg)	90.0
β (deg)	90.0
γ (deg)	90.0

Atom Coordinates	**x**	**y**	**z**
H2	0.14897	0.09336	0.08552
H3	0.14897	0.09336	0.20282
H4	0.14897	0.25806	0.14417
H5	-0.14897	0.14826	0.14417
H6	0.14897	0.09336	0.32011
H7	0.14897	0.25806	0.26146
H8	-0.14897	0.14826	0.26146
H9	0.14897	0.25806	0.37876
H10	-0.14897	0.14826	0.37876
H11	0.48230	0.09336	0.08552
H12	0.48230	0.09336	0.20282

H13	0.48230	0.25806	0.14417
H14	0.18437	0.14826	0.14417
H15	0.48230	0.09336	0.32011
H16	0.48230	0.25806	0.26146
H17	0.18437	0.14826	0.26146
H18	0.48230	0.25806	0.37876
H19	0.18437	0.14826	0.37876
H20	0.81563	0.09336	0.08552
H21	0.81563	0.09336	0.20282
H22	0.81563	0.25806	0.14417
H23	0.51770	0.14826	0.14417
H24	0.81563	0.09336	0.32011
H25	0.81563	0.25806	0.26146
H26	0.51770	0.14826	0.26146
H27	0.81563	0.25806	0.37876
H28	0.51770	0.14826	0.37876
H29	0.14897	0.09336	0.43741
H30	0.48230	0.09336	0.43741
H31	0.81563	0.09336	0.43741
H32	-0.09072	0.33478	0.05686
H33	-0.11354	0.37847	0.18883
H34	-0.11382	0.39556	0.30221

H35	0.22832	0.32835	0.05903
H36	0.21337	0.35952	0.19338
H37	0.22457	0.38369	0.30920
H38	0.56559	0.33476	0.06202
H39	0.54989	0.35939	0.19617
H40	0.54466	0.37204	0.30455
H41	0.15992	0.31297	0.47850
H42	-0.11433	0.15596	0.49487
H43	-0.10506	0.38992	0.42754
H44	0.46408	0.25965	0.48299
H45	0.18431	0.17569	0.47145
H46	0.22524	0.42262	0.42017
H47	0.81181	0.26264	0.47614
H48	0.55581	0.14197	0.49096
H49	0.54068	0.34365	0.43501
H50	0.30026	0.36034	0.72986
H51	0.42481	0.45464	0.67892
H52	0.43040	0.50360	0.58728
H53	0.31697	0.54534	0.57915
H54	0.14001	0.28166	0.70505
H55	0.33778	0.49952	0.51133
Ni56	0.00000	0.20316	0.08552

Ni57	0.00000	0.20316	0.20282
Ni58	0.00000	0.20316	0.32011
Ni59	0.33333	0.20316	0.08552
Ni60	0.33333	0.20316	0.20282
Ni61	0.33333	0.20316	0.32011
Ni62	0.66667	0.20316	0.08552
Ni63	0.66667	0.20316	0.20282
Ni64	0.66667	0.20316	0.32011
Ni65	0.00000	0.20316	0.43741
Ni66	0.33333	0.20316	0.43741
Ni67	0.66667	0.20316	0.43741
Ni68	0.00625	0.38022	0.12804
Ni69	0.01261	0.38549	0.24380
Ni70	0.01240	0.38538	0.35637
Ni71	0.33122	0.37501	0.12811
Ni72	0.34374	0.38531	0.24679
Ni73	0.35623	0.39581	0.36246
Ni74	0.66879	0.37508	0.13418
Ni75	0.68110	0.38534	0.25010
Ni76	0.62489	0.41127	0.37182
Ni77	0.04982	0.42183	0.45009
Ni78	0.36888	0.39496	0.46259

Ni79	0.70630	0.38009	0.45015
O80	0.07605	0.09336	0.08552
O81	0.11171	0.63650	0.13505
O82	0.27838	0.63650	0.03600
O83	0.07605	0.09336	0.20282
O84	0.07605	0.25806	0.14417
O85	-0.07605	0.14826	0.14417
O86	0.11171	0.63650	0.25234
O87	0.27838	0.63650	0.15329
O88	0.07605	0.09336	0.32011
O89	0.07605	0.25806	0.26146
O90	-0.07605	0.14826	0.26146
O91	0.11171	0.63650	0.36964
O92	0.27838	0.63650	0.27059
O93	0.07605	0.25806	0.37876
O94	-0.07605	0.14826	0.37876
O95	0.27838	0.63650	0.38788
O96	0.40938	0.09336	0.08552
O97	0.44504	0.63650	0.13505
O98	0.61171	0.63650	0.03600
O99	0.40938	0.09336	0.20282
O100	0.40938	0.25806	0.14417

O101	0.25729	0.14826	0.14417
O102	0.44504	0.63650	0.25234
O103	0.61171	0.63650	0.15329
O104	0.40938	0.09336	0.32011
O105	0.40938	0.25806	0.26146
O106	0.25729	0.14826	0.26146
O107	0.44504	0.63650	0.36964
O108	0.61171	0.63650	0.27059
O109	0.40938	0.25806	0.37876
O110	0.25729	0.14826	0.37876
O111	0.61171	0.63650	0.38788
O112	0.74272	0.09336	0.08552
O113	0.77838	0.63650	0.13505
O114	0.94504	0.63650	0.03600
O115	0.74272	0.09336	0.20282
O116	0.74272	0.25806	0.14417
O117	0.59062	0.14826	0.14417
O118	0.77838	0.63650	0.25234
O119	0.94504	0.63650	0.15329
O120	0.74272	0.09336	0.32011
O121	0.74272	0.25806	0.26146
O122	0.59062	0.14826	0.26146

O123	0.77838	0.63650	0.36964
O124	0.94504	0.63650	0.27059
O125	0.74272	0.25806	0.37876
O126	0.59062	0.14826	0.37876
O127	0.94504	0.63650	0.38788
O128	0.07605	0.09336	0.43741
O129	0.40938	0.09336	0.43741
O130	0.74272	0.09336	0.43741
O131	-0.03777	0.31273	0.07467
O132	0.14984	0.51104	0.06298
O133	0.31816	0.48522	0.11228
O134	-0.05661	0.34435	0.18749
O135	0.14918	0.50092	0.18446
O136	0.31850	0.49563	0.22814
O137	-0.06244	0.35418	0.29998
O138	0.14429	0.49521	0.30652
O139	0.31881	0.50493	0.34421
O140	0.28846	0.31188	0.07225
O141	0.48177	0.51083	0.06280
O142	0.65016	0.48492	0.11265
O143	0.27525	0.33371	0.19060
O144	0.48169	0.50427	0.18463

O145	0.65060	0.49479	0.22800
O146	0.28158	0.34941	0.30641
O147	0.47539	0.49503	0.30641
O148	0.64895	0.50400	0.34054
O149	0.61982	0.31223	0.07843
O150	0.81664	0.51150	0.06277
O151	0.98694	0.48974	0.10955
O152	0.61175	0.33336	0.19435
O153	0.81894	0.50473	0.18174
O154	0.98726	0.49945	0.22809
O155	0.60671	0.34947	0.31242
O156	0.81426	0.50014	0.30339
O157	0.98186	0.49979	0.34362
O158	0.09478	0.32324	0.46889
O159	-0.08859	0.20871	0.48521
O160	-0.04490	0.35951	0.41859
O161	0.14919	0.49979	0.44059
O162	0.10611	0.68291	0.46871
O163	0.33120	0.58445	0.48066
O164	0.39961	0.28143	0.47802
O165	0.23859	0.20848	0.48084
O166	0.26985	0.37563	0.41588

O167	0.44375	0.46376	0.42488
O168	0.58051	0.62956	0.49072
O169	0.64198	0.47168	0.43017
O170	0.74377	0.28080	0.47503
O171	0.58039	0.19749	0.48715
O172	0.59889	0.32749	0.41882
O173	0.81176	0.43672	0.45016
O174	0.84350	0.66113	0.48122
O175	0.97620	0.51103	0.45918
O176	0.24030	0.39593	0.61692
O177	0.34912	0.44970	0.53276
O178	0.09702	0.27620	0.63480
Cu179	0.04164	0.56595	0.05622
Cu180	0.01521	0.70702	0.11487
Cu181	0.18188	0.70702	0.05618
Cu182	0.20831	0.56595	0.11482
Cu183	0.04164	0.56595	0.17351
Cu184	0.01521	0.70702	0.23216
Cu185	0.18188	0.70702	0.17347
Cu186	0.20831	0.56595	0.23212
Cu187	0.04164	0.56595	0.29081
Cu188	0.01521	0.70702	0.34946

Cu189	0.18188	0.70702	0.29077
Cu190	0.20831	0.56595	0.34941
Cu191	0.04164	0.56595	0.40810
Cu192	0.18188	0.70702	0.40806
Cu193	0.37497	0.56595	0.05622
Cu194	0.34855	0.70702	0.11487
Cu195	0.51521	0.70702	0.05618
Cu196	0.54164	0.56595	0.11482
Cu197	0.37497	0.56595	0.17351
Cu198	0.34855	0.70702	0.23216
Cu199	0.51521	0.70702	0.17347
Cu200	0.54164	0.56595	0.23212
Cu201	0.37497	0.56595	0.29081
Cu202	0.34855	0.70702	0.34946
Cu203	0.51521	0.70702	0.29077
Cu204	0.54164	0.56595	0.34941
Cu205	0.37497	0.56595	0.40810
Cu206	0.51521	0.70702	0.40806
Cu207	0.70831	0.56595	0.05622
Cu208	0.68188	0.70702	0.11487
Cu209	0.84855	0.70702	0.05618
Cu210	0.87497	0.56595	0.11482

Cu211	0.70831	0.56595	0.17351
Cu212	0.68188	0.70702	0.23216
Cu213	0.84855	0.70702	0.17347
Cu214	0.87497	0.56595	0.23212
Cu215	0.70831	0.56595	0.29081
Cu216	0.68188	0.70702	0.34946
Cu217	0.84855	0.70702	0.29077
Cu218	0.87497	0.56595	0.34941
Cu219	0.70831	0.56595	0.40810
Cu220	0.84855	0.70702	0.40806
Cu221	-0.02324	0.67833	0.47849
Cu222	0.19569	0.59540	0.47574
Cu223	0.44739	0.63685	0.48928
Cu224	0.53719	0.52676	0.46011
Cu225	0.71033	0.65042	0.48747
Cu226	0.84333	0.54186	0.46854
C227	0.22410	0.35975	0.66117
C228	0.29526	0.38009	0.69267
C229	0.35953	0.42862	0.66633
C230	0.32364	0.43634	0.62049
C231	0.35708	0.48725	0.57951
C232	0.14766	0.30225	0.66707

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