

Electronic Supplementary Information (ESI)

CoO–NiO heterostructure nanosheets-enabled efficient electrooxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid

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Experimental Section

Materials and chemicals

Potassium chloride (KCl), oxalic acid ($\text{H}_2\text{C}_2\text{O}_4$), choline chloride (ChCl), nickel oxide (NiO) were all obtained from Aladdin Chemistry Co., Ltd. Potassium hydroxide (KOH), nickel chloride hexahydrate ($\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$), cobalt chloride hexahydrate ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$) were obtained from Sinopharm Chemical Reagent Co., Ltd. 5-hydroxymethylfurfural (HMF), 2,5-furandicarboxylic acid (FDCA), 5-formylfuran-2-carboxylic acid (FFCA) and 5-hydroxymethyl-2-furan-carboxylic acid (HMFCA) were bought from Alfa-Aesar. 5 wt% Nafion solution was purchased from the Sigma Co., Ltd. 2,5-diformyl furan (DFF) was bought from Tokyo Chemical Industry Co., Ltd. Carbon paper was obtained from Changsha Lyrun Material Co., Ltd. Nickel foam was purchased from Suzhou Siner Technology Co., Ltd. Nafion 115 membrane was bought from Wuhan GaossUnion technology Co., Ltd.

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

Deep eutectic solvent (DES) was fabricated based on the procedures specified in the literature¹, by mixing equimolar amounts of choline chloride (ChCl) and oxalic acid (OA), followed by magnetic stirring at 80 °C for 30 minutes.

Synthesis of CoO–NiO heterostructure nanosheets

The CoO–NiO products with various Co/Ni ratios are presented as CoO–NiO (x:y), where x:y denotes the initial molar feed ratio of Co and Ni salts. To synthesize the CoO–NiO (1:3) product, the Co/Ni-based precursor

was initially obtained by using a microwave-assisted DES method. In a standard

procedure, 10.0 mg of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and 30.0 mg $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ were dissolved in 1 mL CHCl_3/OA DES. The resulting mixture was then ultrasonicated at 60 °C until a well-dispersed blue solution was achieved. The precursor was obtained by heating the above mixture in a microwave for 15 seconds at 100 W. The precursors were then collected, washed several times with ethanol, and dried under vacuum overnight.

Next, the dried precursors were transferred to a quartz tube inside a tube furnace and heated for 1 hour at 350 °C, with 10 °C min^{-1} in a nitrogen atmosphere, to produce CoO-NiO nanosheets. Finally, the products were washed with water and ethanol, then dried in the vacuum oven.

For comparison, CoO-NiO (1:2) and CoO-NiO (1:4) products were prepared following the same procedure. To synthesize CoO-NiO (1:2), 13.3 mg $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and 26.7 mg $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ were utilized, whereas for CoO-NiO (1:4), 8.0 mg $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and 32.0 mg $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ were applied. Additionally, using a similar procedure, pyrolysis of the precursor with an initial Co/Ni molar feed ratio of 1:3 was conducted at 300 and 400 °C under N_2 for 1 h, and at 350 °C in air for 1 h.

Characterizations

X-ray diffraction (XRD) patterns were recorded using a Rigaku SmartLab 9KW X-ray diffractometer. X-ray photoelectron spectroscopy (XPS) measurements were performed using a Thermo Scientific K-Alpha system. Transmission electron microscopy (TEM) was conducted with a JEM-1400 microscope. High-resolution transmission electron microscopy (HRTEM), high-angle annular dark field (HAADF)-scanning transmission electron microscopy (STEM), Selected Area Electron

Diffraction (SAED) and energy-dispersive X-ray (EDX) analysis were performed on an FEI Talos F200x. High-performance liquid chromatography (HPLC) analysis was conducted with an Agilent G7114A system. Raman spectra were collected on a LabRAM Evolution micro-Raman spectrometer using a 532 nm laser. The Fourier transform infrared (FTIR) spectrum was obtained using the Thermo Fisher Scientific Nicolet iS20 instrument.

Electrochemical measurements

The electrochemical tests were performed with a CHI760E workstation. The three-electrode system was used for all electrochemical measurements, consisting of a catalyst-loaded carbon paper (working electrode), a platinum foil (counter electrode) and a saturated Ag/AgCl electrode (reference electrode). A 1.0 M KOH aqueous solution (10 mL) was used, with or without 10 mM HMF. The HMF-containing electrolyte was prepared by dissolving 12.611 mg of HMF in 10 mL of 1.0 M KOH aqueous solution. The amounts of KOH and HMF used in the other electrochemical tests in this article are the same (concentration, volume, mass).

To prepare the catalyst ink, 4 mg catalyst was mixed with ethanol (70 μL), Nafion solution (5 wt%, 20 μL) and deionized water (130 μL). The mixture was then sonicated for 20 minutes to achieve a suspension. Afterward, the suspension was applied onto a carbon paper ($1 \times 1 \text{ cm}^2$), with a loading of 4 mg cm^{-2} . For nickel foam electrodes, the catalyst ink was deposited in the same manner after the nickel foam was pre-cleaned.

Linear sweep voltammetry (LSV) was conducted at 10 mV s^{-1} . Electrochemical impedance spectroscopy (EIS) measurement was performed (0.01 Hz to 10 kHz). The

electrochemical double-layer capacitance (Cdl) was determined using cyclic voltammetry (CV), thereby estimating the electrochemical active surface area (ECSA) according to the following equation:

$$\text{ECSA} = \text{Cdl}/\text{Cs} \quad (1)$$

where Cs is taken as 0.04 mF cm⁻², a typical specific capacitance reported for electrodes in 1 M KOH.²

Potentials were referenced to reversible hydrogen electrode (RHE):

$$E (\text{RHE}) = E (\text{Ag/AgCl}) + 0.197 + 0.059 \times \text{pH} \quad (2)$$

Products analysis

The concentration of various compounds was monitored using high-performance liquid chromatography (HPLC). During chronoamperometry at 1.35 V for 7.6 h, 10 μL electrolyte was extracted, diluted with water to a final volume of 500 μL , and analyzed by HPLC (UV-Vis detector: 265 nm). Separation and quantification were performed through isocratic elution with a mixture of 5 mM aqueous ammonium formate (70% by volume) and methanol (30% by volume) at 0.6 mL min⁻¹, with the column oven temperature maintained at 30 °C.

HMF conversion, FDCA yield, and Faradaic efficiency (FE) were calculated:

$$\text{HMF conversion (\%)} = [\text{n (HMF consumed)} / \text{n (HMF initial)}] \times 100 \quad (3)$$

$$\text{FDCA yield (\%)} = [\text{n (FDCA formed)} / \text{n (HMF initial)}] \times 100 \quad (4)$$

$$\text{Faradaic efficiency (\%)} = [\text{n (FDCA formed)} / (\text{Q} / (6 \times \text{F}))] \times 100 \quad (5)$$

where Q is the transferred charge, F is 96485 C mol⁻¹, and n represents mole number of the reactant.

Density functional theory (DFT) Calculation

All density functional theory (DFT) calculations were performed using the Vienna Ab-initio Simulation Package (VASP)^{3,4}. The exchange-correlation effects were modeled using the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) approach^{5,6}. The core-valence interactions were treated with the projected augmented wave (PAW) method⁷. A DFT+U correction was introduced to capture strong correlation in the Ni and Co d states. The energy cutoff for plane wave expansions was set at 450 eV, and a 2×2×1 Monkhorst-Pack k-point grid was employed to sample the Brillouin zone, considering the large surface supercell and a thick vacuum layer, which allow reduced k-point sampling while maintaining a reasonable balance between computational accuracy and efficiency. Structural optimization was performed with energy and force convergence criteria of 1.0×10^{-5} eV and 0.05 eV \AA^{-1} , respectively. The DFT-D3 method was applied to model van der Waals (vdW) interactions⁸.

The adsorption energy (E_{ads}) between the HMF and the NiO or CoO–NiO is calculated:

$$E_{\text{ads}} = E_{*\text{HMF}} - E_{\text{HMF}} - E_{\text{sub}} \quad (6)$$

where E_{HMF} and $E_{*\text{HMF}}$ denote the energies before and after the adsorption of HMF on the substrates, respectively. E_{sub} represents the energy of NiO and CoO–NiO surfaces.

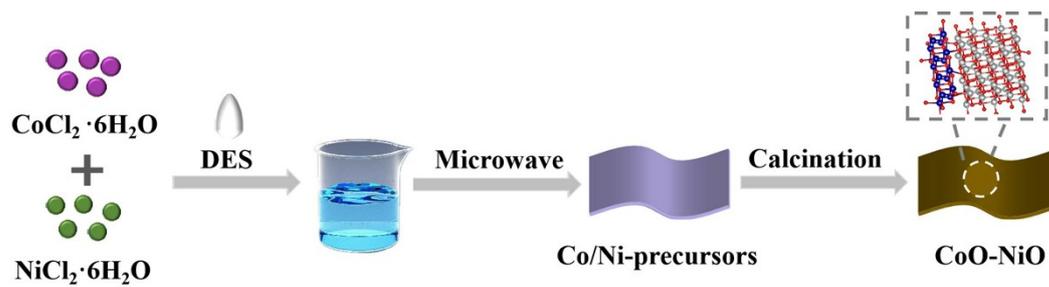


Fig. S1 Schematic diagram of CoO–NiO heterostructure nanosheet synthesis.

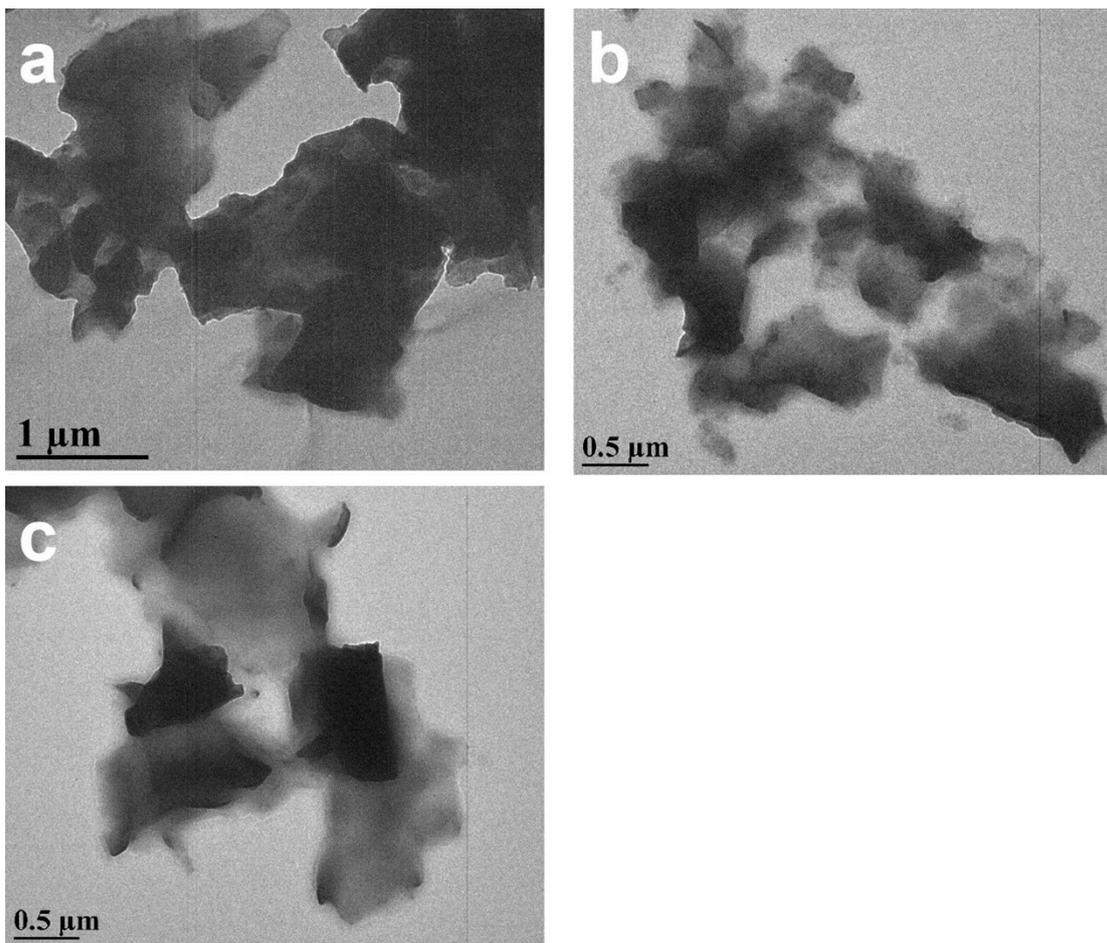


Fig. S2 TEM images of the precursors obtained after microwave heating 1 mL ChCl/OA DES with the presence of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$. (a) Co/Ni precursor obtained with the initial Co/Ni molar feed ratio of 1:2 (13.3 mg $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and 26.7mg $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$), (b) Co/Ni precursor obtained with the initial Co/Ni molar feed ratio of 1:3 (10.0 mg $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and 30.0 mg $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$), (c) Co/Ni precursor obtained with the initial Co/Ni molar feed ratio of 1:4 (8.0 mg $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and 32.0 mg $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$) These obtained precursors will be used for synthesizing CoO–NiO (x:y).

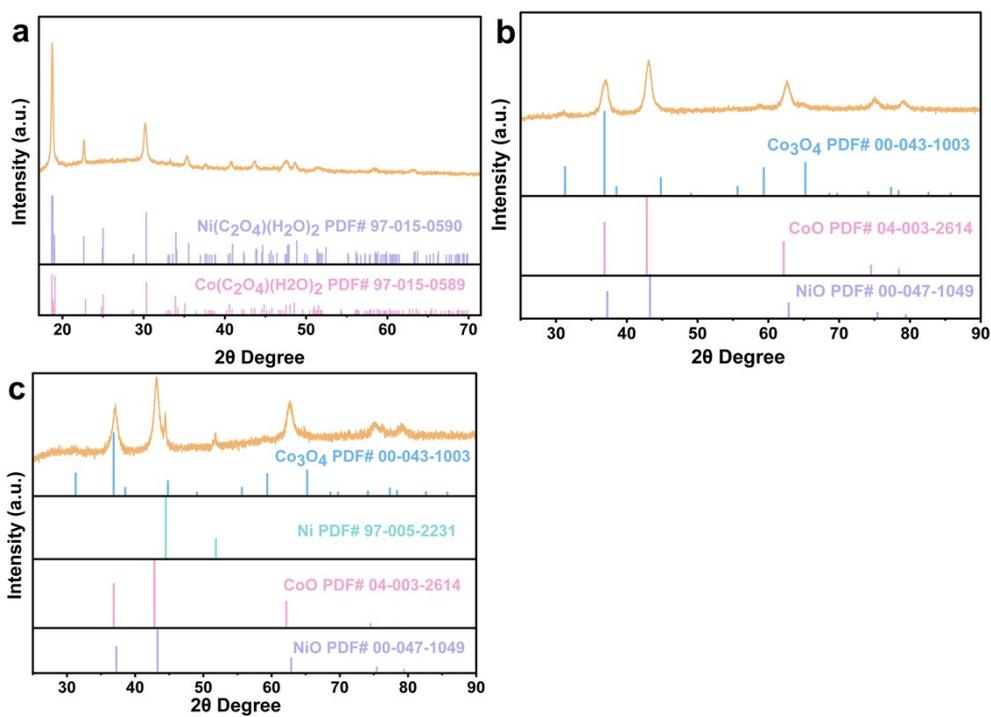


Fig. S3 XRD patterns of the precursors (the initial Co/Ni molar feed ratio of 1:3) pyrolyzed for 1 h: (a) 300 °C under N_2 , (b) 400 °C under N_2 , and (c) 350 °C in air.

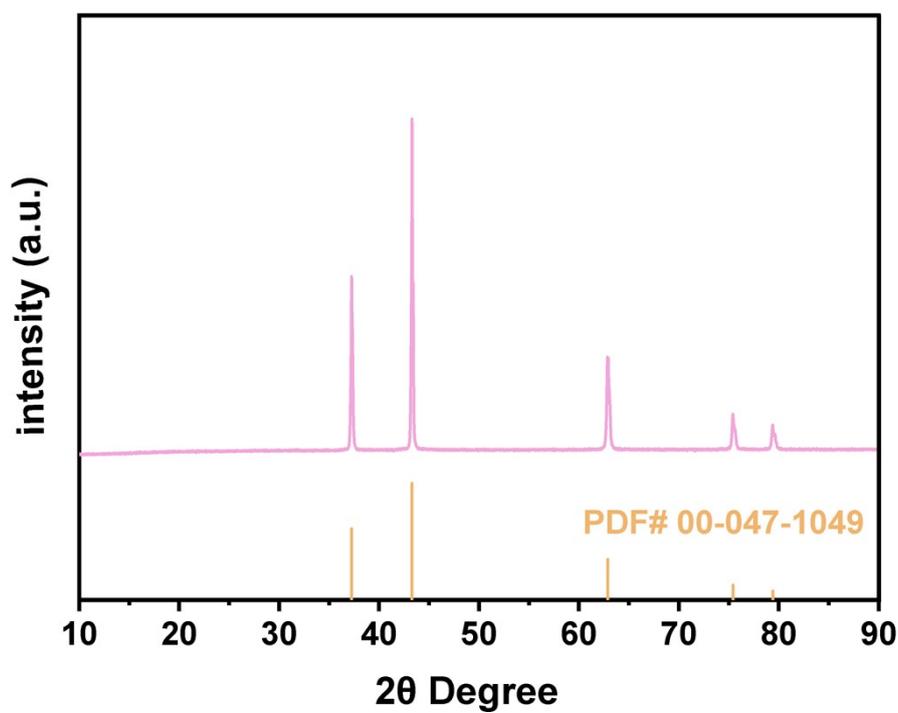


Fig. S4 XRD pattern of NiO .

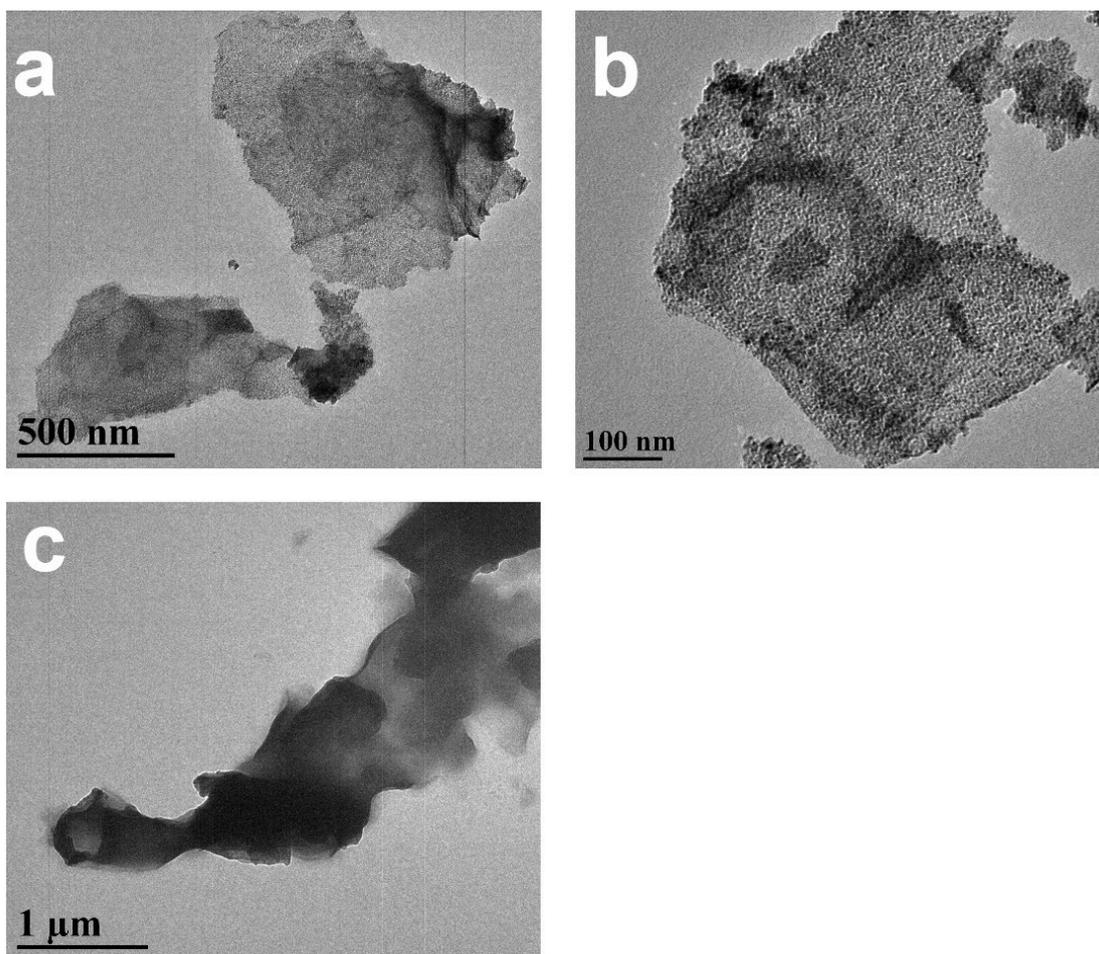


Fig. S5 TEM images of (a) CoO–NiO (1:2), (b) CoO–NiO (1:4), (c) NiO.

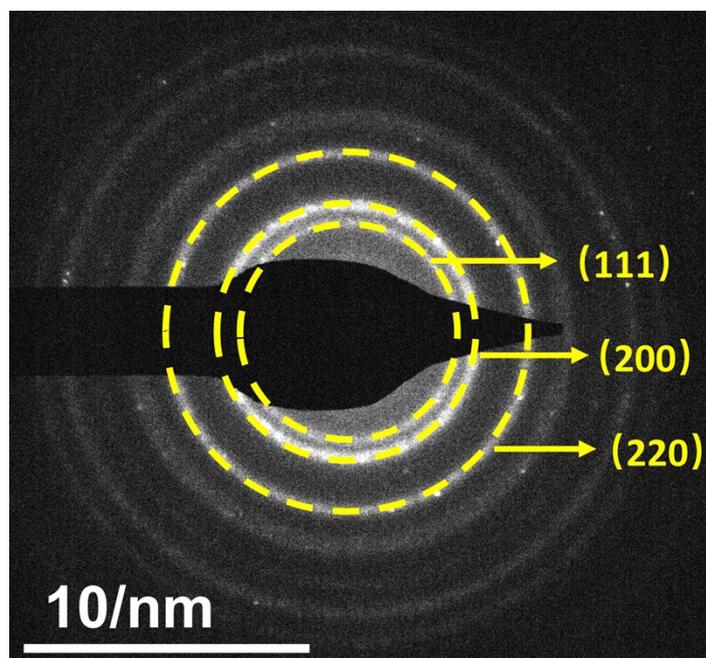


Fig. S6 SAED pattern of CoO–NiO (1:3), showing rock-salt diffraction rings (111), (200), and (220).

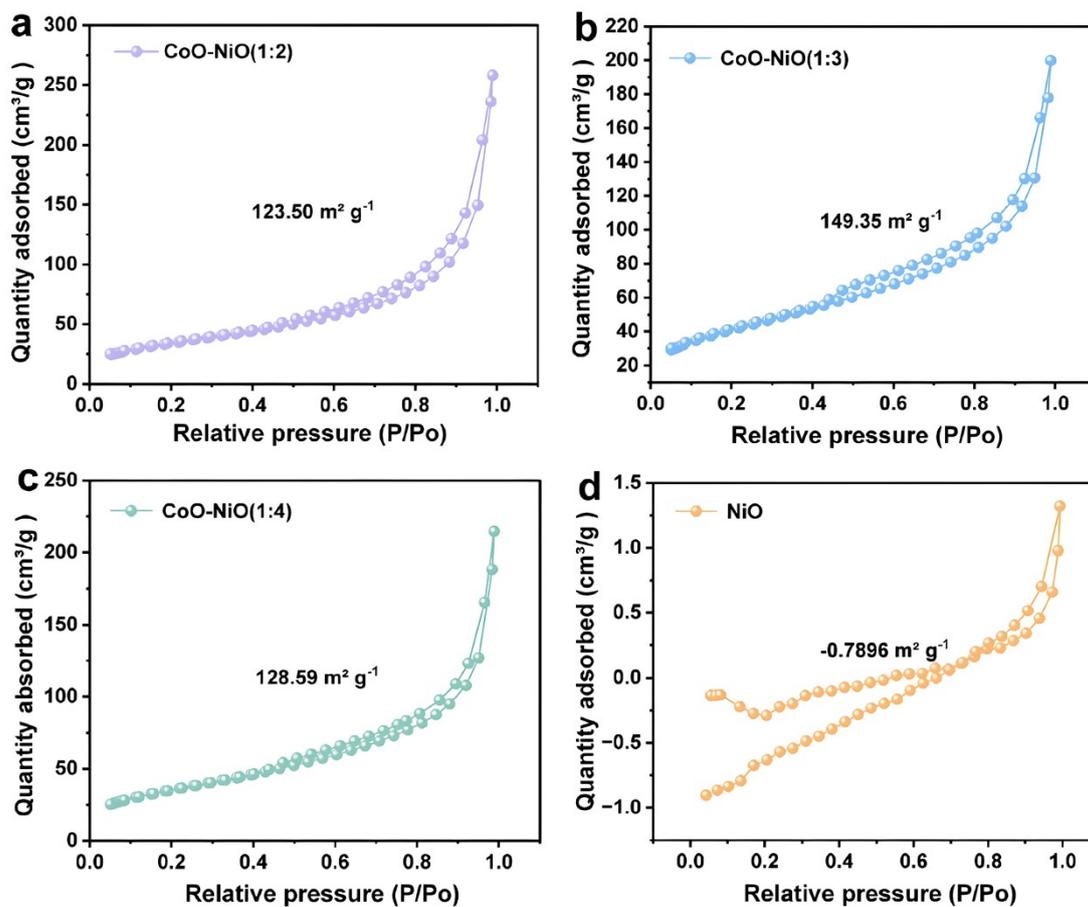


Fig. S7 N₂ adsorption-desorption isotherms of (a) CoO–NiO (1:2), (b) CoO–NiO (1:3), (c) CoO–NiO (1:4), (d) NiO.

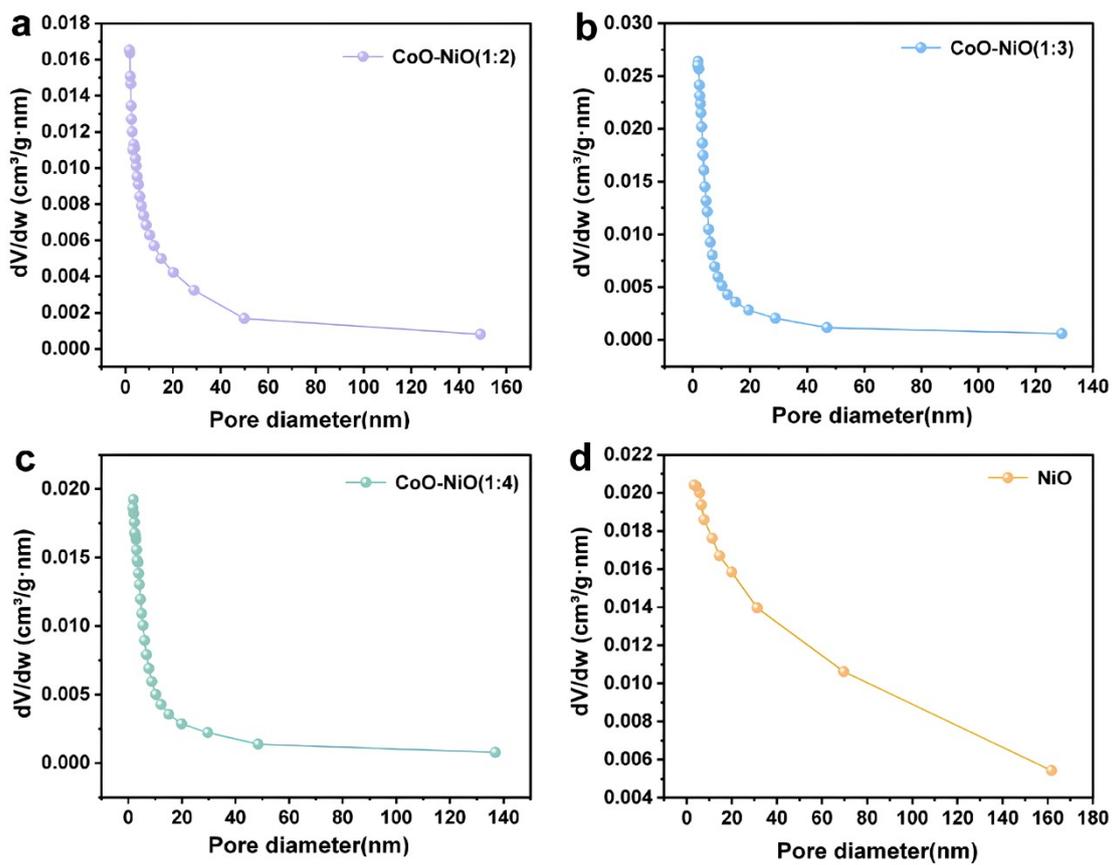


Fig. S8 Pore size distributions of (a) CoO–NiO (1:2), (b) CoO–NiO (1:3), (c) CoO–NiO (1:4), (d) NiO.

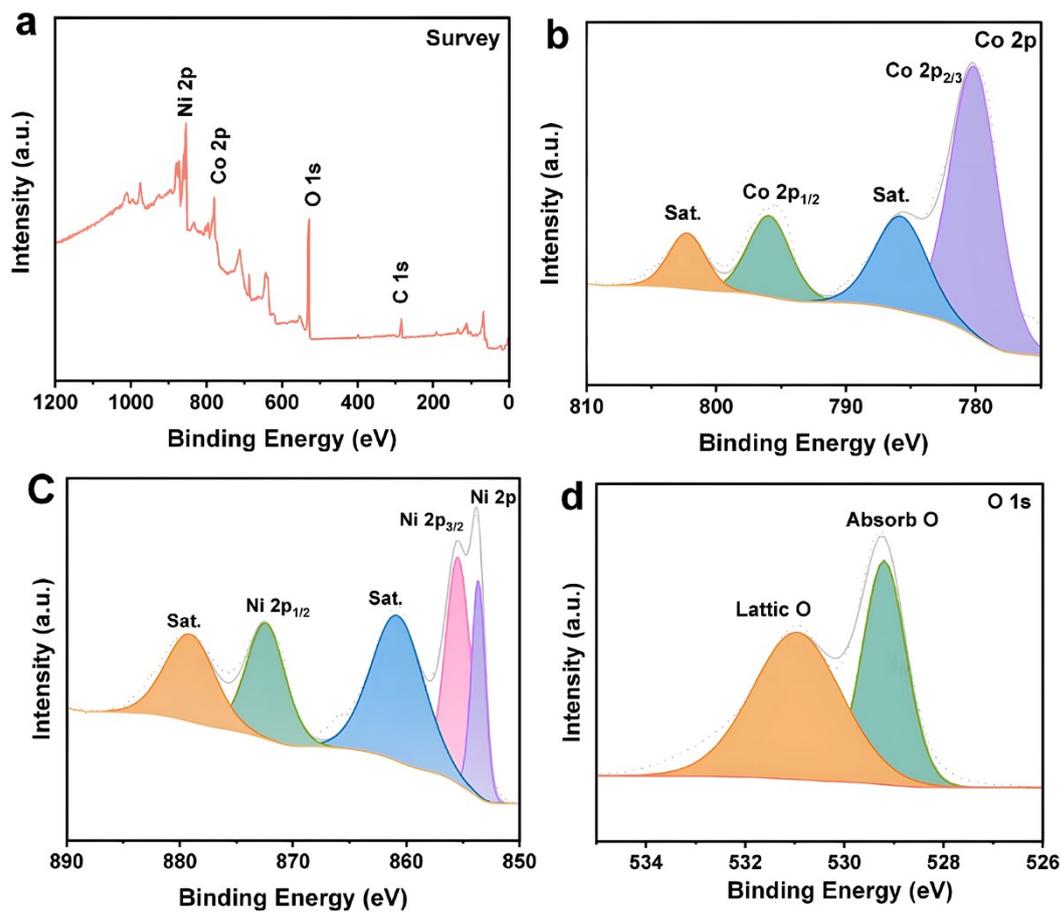


Fig. S9 (a) XPS survey spectrum of CoO–NiO (1:3). High-resolution XPS spectra of (b) Co 2p, (c) Ni 2p and (d) O 1s.

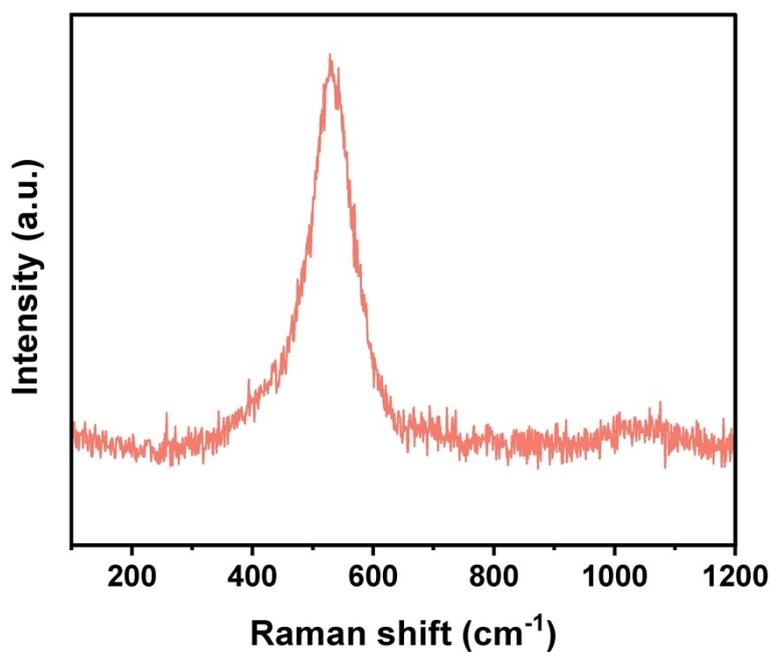


Fig. S10 Raman spectrum of CoO–NiO (1:3)

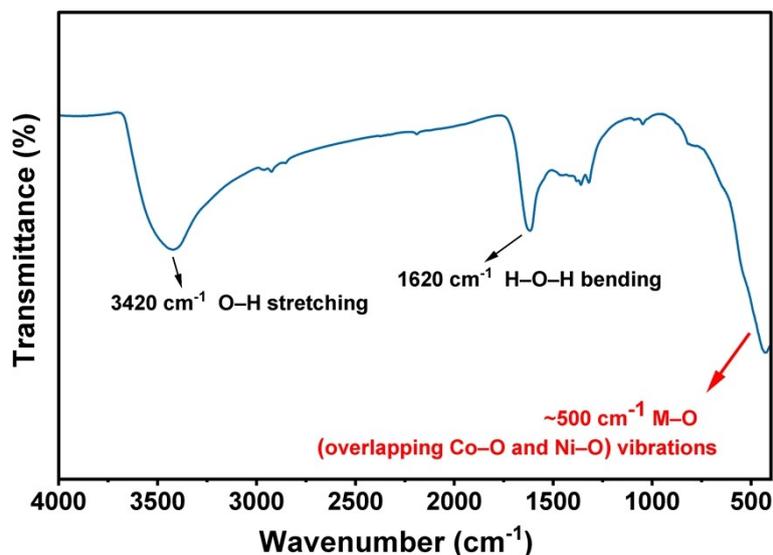


Fig. S11 Fourier transform infrared (FTIR) spectrum of CoO–NiO (1:3)

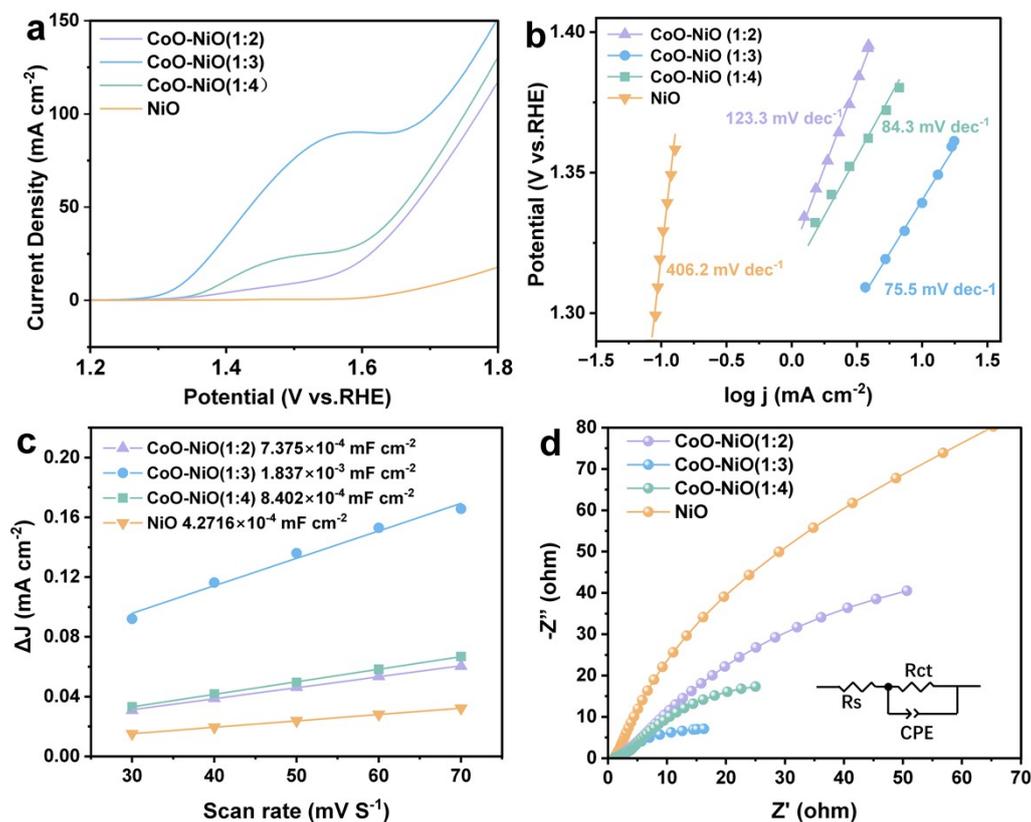


Fig. S12 (a) LSV curves, (b) Tafel plots, (c) electrochemical double layer capacitance (C_{dl}) of CoO–NiO (1:2), CoO–NiO (1:3), CoO–NiO (1:4), NiO in 1.0 M KOH solution with 10 mM HMF and (d) electrochemical impedance spectra of different catalysts at 1.35 V, along with the corresponding equivalent circuit.

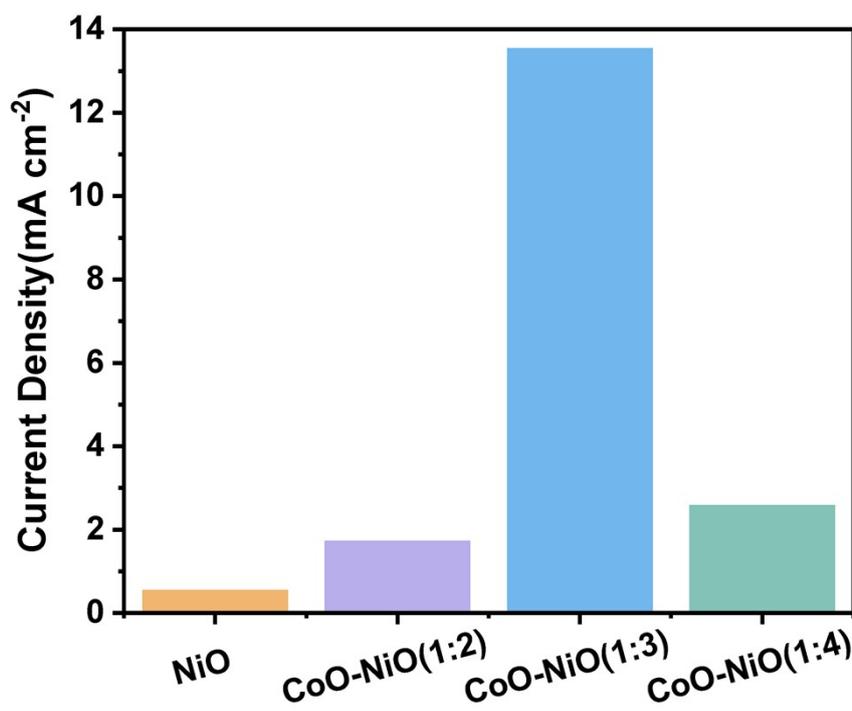


Fig. S13 Corresponding current densities at 1.35 V in 1.0 M KOH with 10 mM HMF.

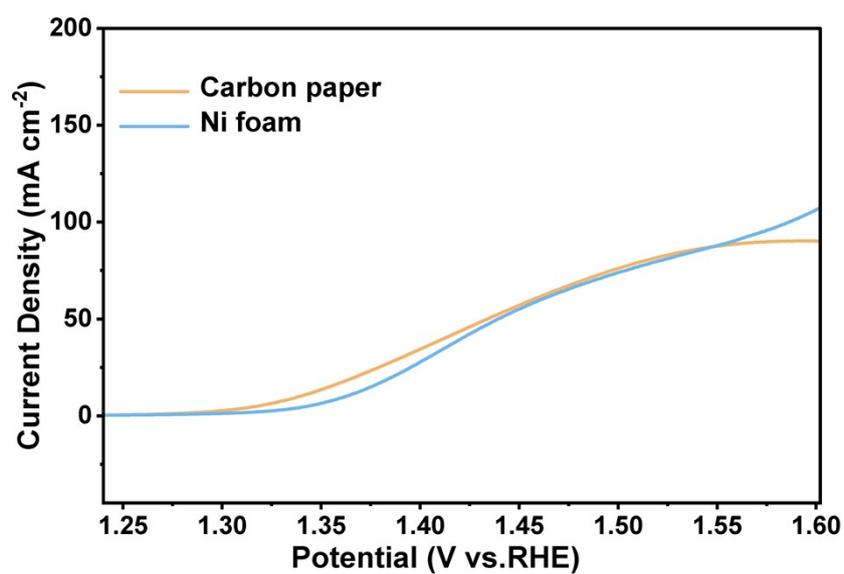


Fig. S14 LSV curves of CoO–NiO (1:3) deposited on carbon paper and nickel foam

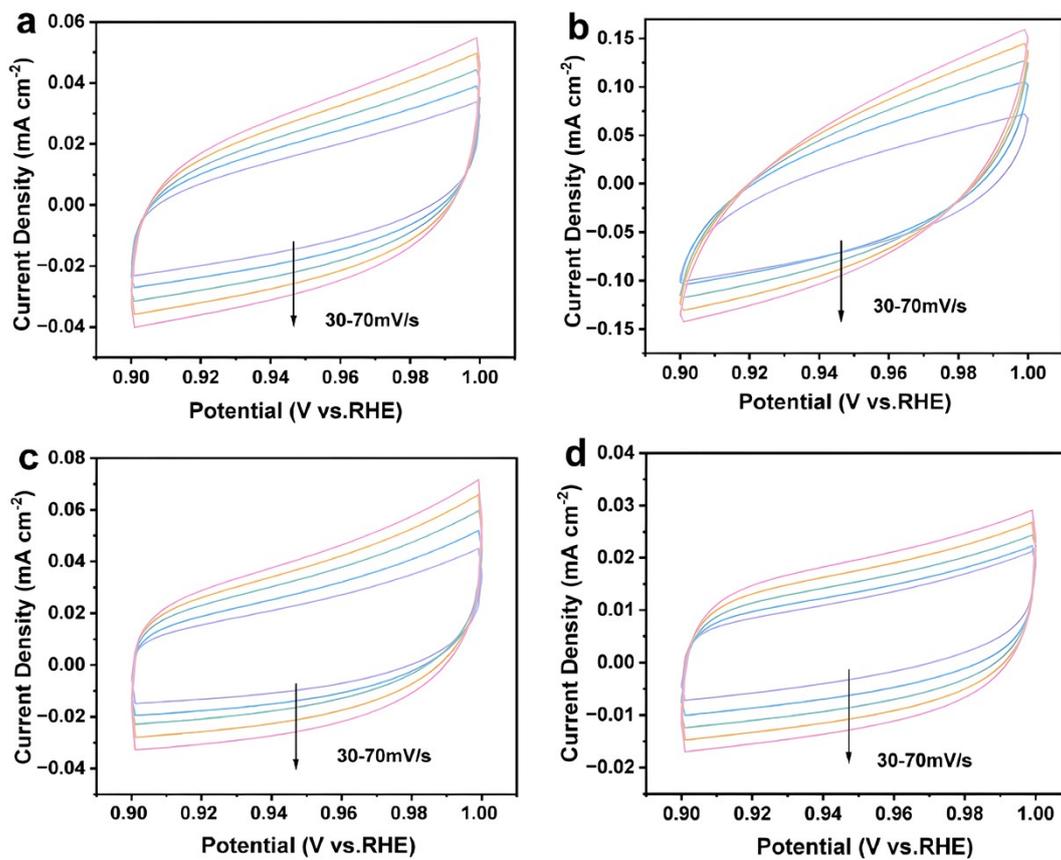


Fig. S15 Cyclic voltammograms of (a) CoO–NiO (1:2), (b) CoO–NiO (1:3), (c) CoO–NiO (1:4) and (d) NiO at different scan rates from 0.90 to 1.00 V vs. RHE.

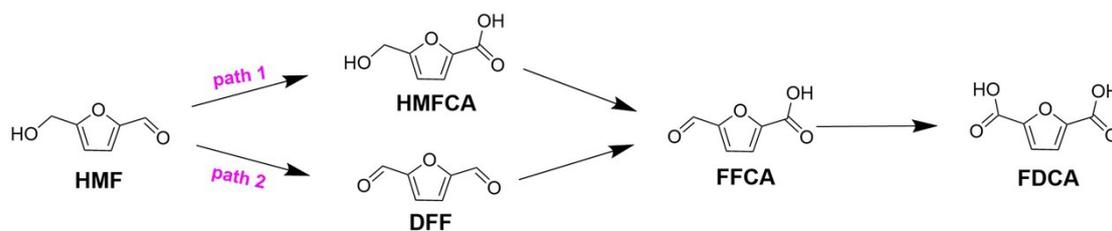


Fig. S16 Possible pathways for the oxidation of HMF to FDCA.

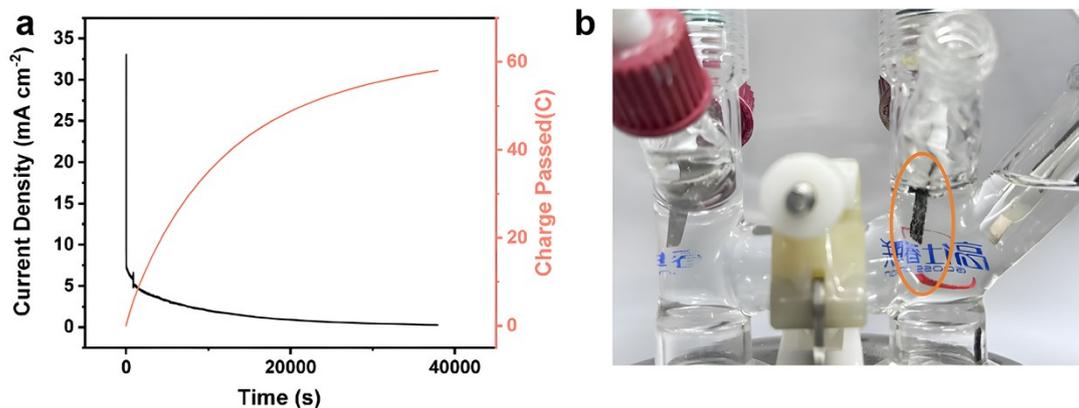


Fig. S17 (a) Corresponding current change and the accumulated charges over time for the chronoamperometry test of CoO–NiO (1:3) at 1.3 V in 1.0 M KOH with 10 mM HMF. (b) Oxygen generated from the electrode surface at 1.4 V.

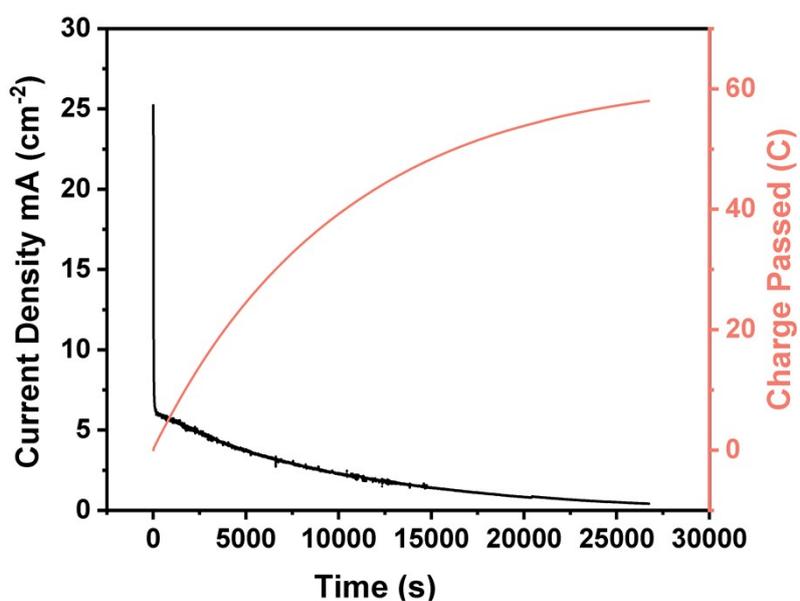


Fig. S18 Corresponding current change and the accumulated charges over time for the chronoamperometry test of CoO–NiO (1:3) at 1.35 V for 7.6 h in 1.0 M KOH solution with 10 mM HMF.(10 mL)



Fig. S19 Color change of the recovered electrolyte before and after reaction.

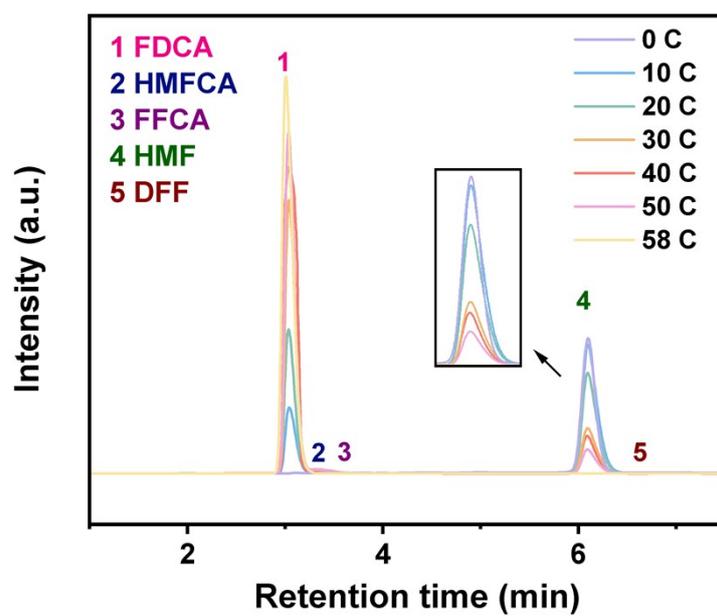


Fig. S20 HPLC chromatograms.

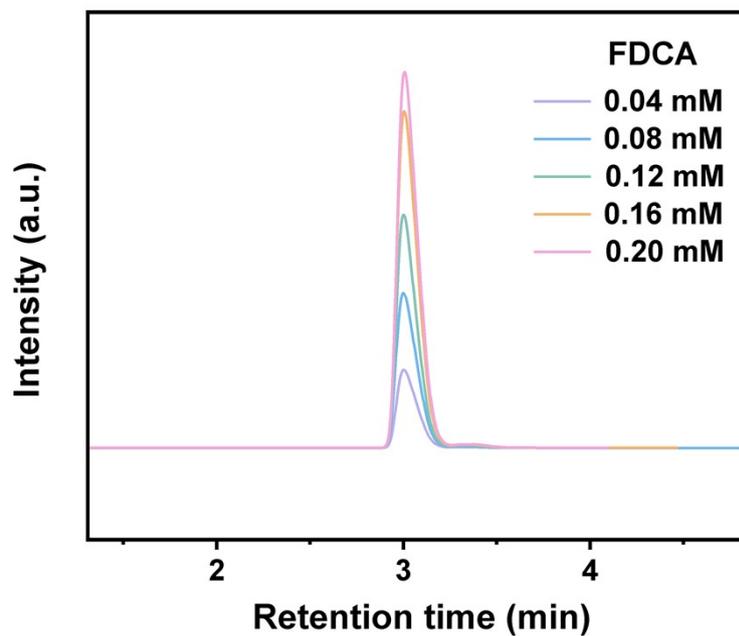


Fig. S21 HPLC traces of different concentrations of FDCA standard substance.

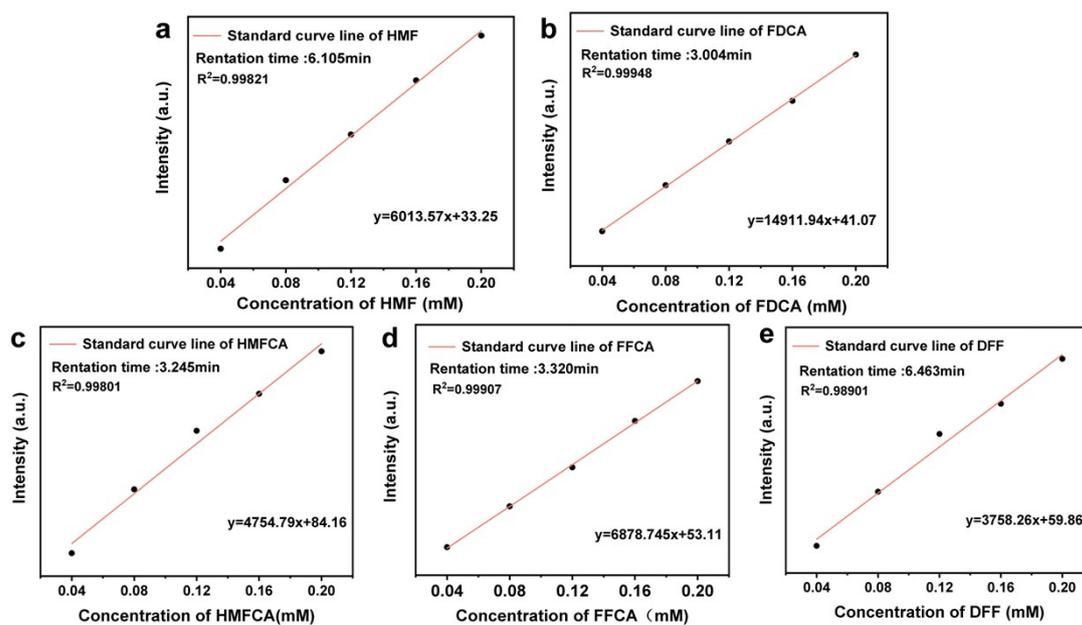


Fig. S22 Standard curves of the HPLC for (a) HMF, (b) FDCA, (c) HMFCA, (d) FFCA and (e) DFF.

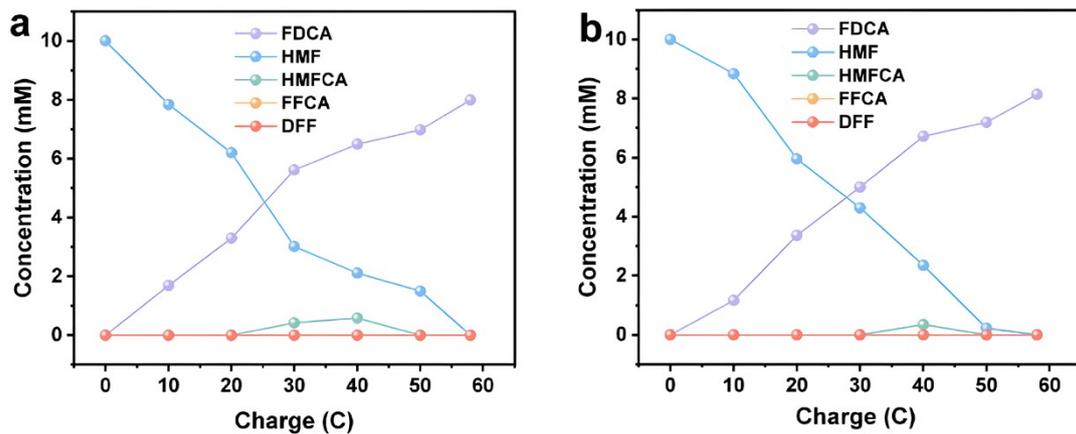


Fig. S23 Concentration change of HMF and oxidation product during electrooxidation process (a) CoO–NiO (1:2), (b) CoO–NiO (1:4).

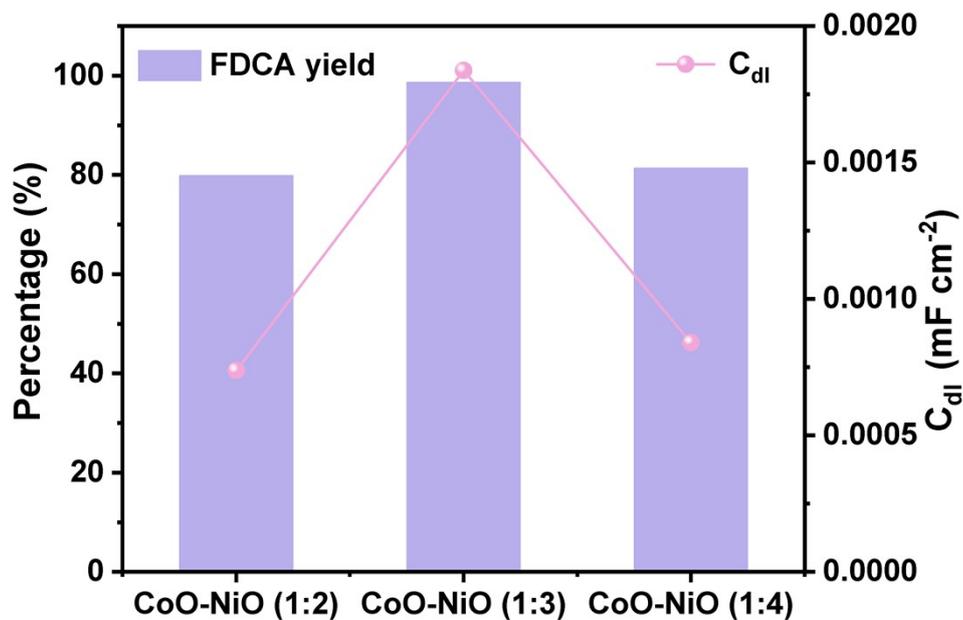


Fig. S24 FDCA yield and C_{dl} of the CoO–NiO (1:2, 1:3,1:4).

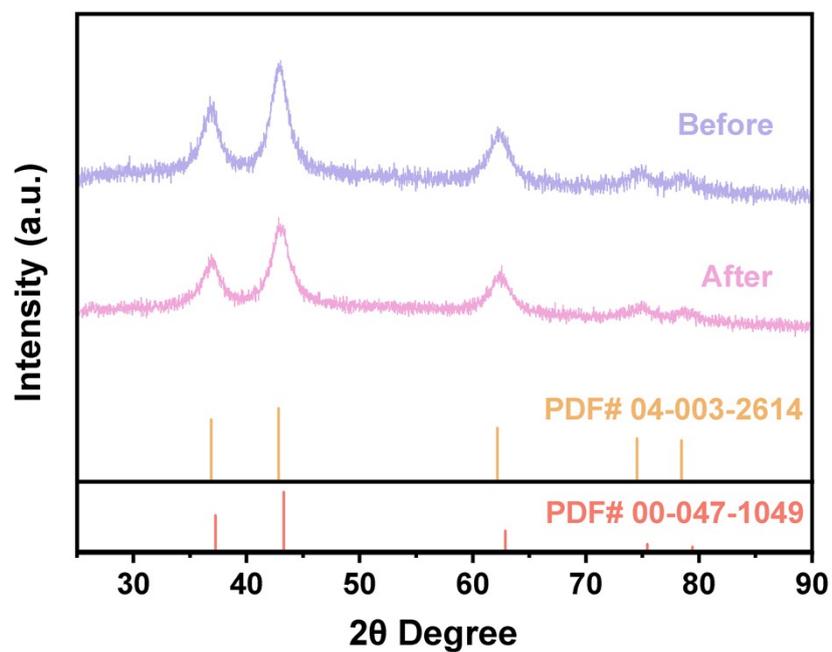


Fig. S25 XRD patterns of CoO–NiO (1:3) before and after four electrolysis cycles.

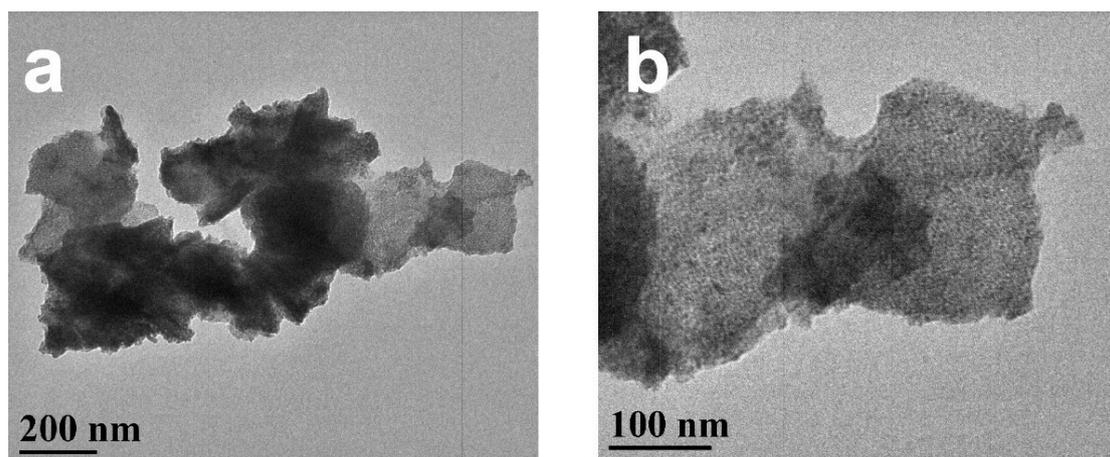


Fig. S26 TEM images of CoO–NiO (1:3) after four electrolysis cycles.

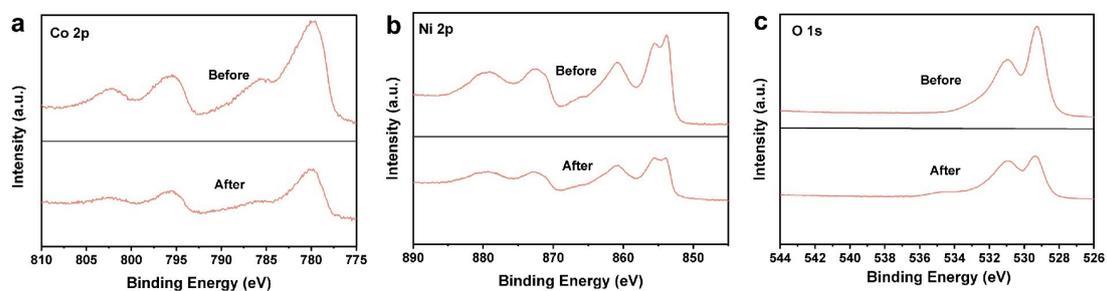


Fig. S27 XPS spectra of (a) Co 2p, (b) Ni 2p, (c) O 1s of CoO–NiO (1:3) before and after four electrolysis cycles.

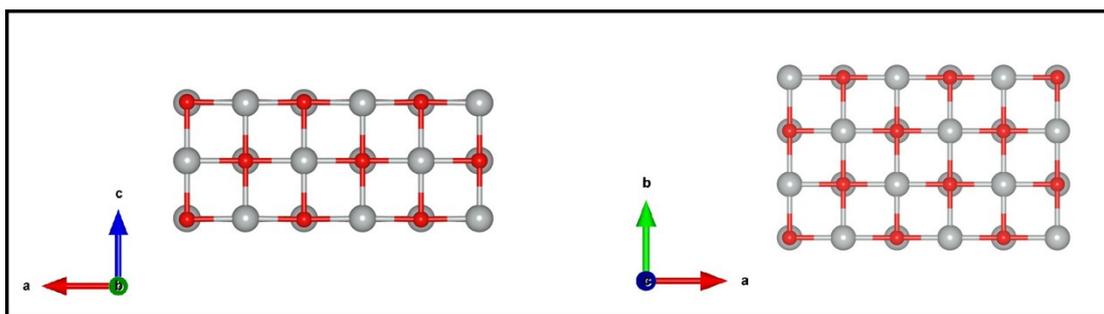


Fig. S28 Side and top views of an optimized structure for the NiO

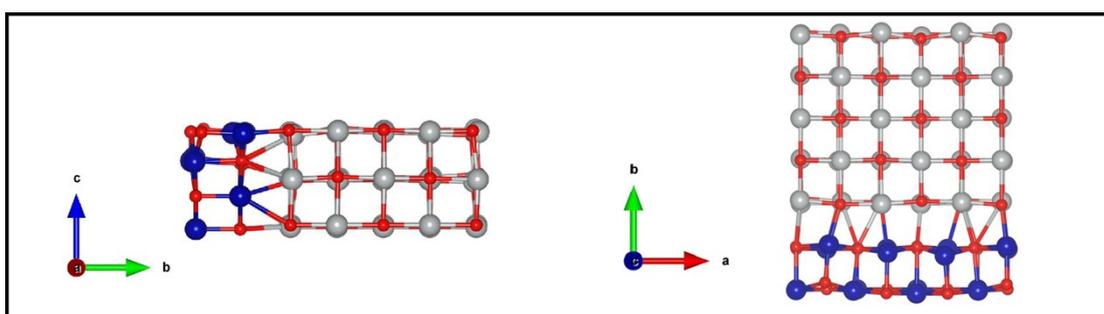


Fig. S29 Side and top views of an optimized structure for the CoO–NiO (1:3).

Table S1 ICP-OES analysis of catalysts

catalysts	CoO–NiO(1:2)	CoO–NiO(1:3)	CoO–NiO(1:4)
Co/Ni atomic ratio (ICP-OES)	1:1.7	1:2.5	1:3.3

Table S2 ECSA values of catalysts

catalysts	CoO–NiO(1:2)	CoO–NiO(1:3)	CoO–NiO(1:4)	NiO
ECSA (cm ²)	0.018	0.046	0.021	0.011

Table S3 Rct of catalysts

catalysts	CoO–NiO(1:2)	CoO–NiO(1:3)	CoO–NiO(1:4)	NiO
Rct (Ω)	181.2	53.19	74.67	2751

Table S4 Recently reported electrocatalysts for HMF conversion.

Catalysts	C _{HMF} (mM)	Potential (V vs. RHE)	Conver- -sion (%)	FDCA Yield (%)	FE (%)	Cycles (FDCA yield%)
CoO–NiO (This work)	10	1.35	100	98.7	98.5	4 (>97)
Ni/CoO ⁹	50	1.45	100	96.82	92.14	5 (~94.9)
NCO-0.75 ¹⁰	10	1.5	100	96.05	93.78	25 (95.65)
Ni(OH) ₂ - NiOOH/NiFeP ¹¹	10	1.435	-	99.4	94.62	3 (>90)
NiCo ₂ O ₄ ¹²	5	1.5	99.6	90.8	87.5	3 (>80)
Mn-5Ni ₂ P ¹³	10	1.43	100	98	97.8	4 (>90)
NiCo ₂ O ₄ -CFP ¹⁴	10	1.43	-	94.3	89.6	4 (85)

NiVCo-LDHs ¹⁵	10	1.376	-	99.7	97.0	10 (86.5-97.8)
NiCoMn-LDHs ¹⁶	1	1.50	100	91.7	-	4 (>85)
NiO-N/C ¹⁷	10	1.437	99	84	96	6 (~60)
Co ₃ O ₄ /NF ¹⁸	10	1.43	100	96.7	96.5	10(>95)
Co ₃ O ₄ -NiO-500 ¹⁹	10	1.45	96.95	83.33	89.47	6 (~80)
P-Co ₃ O ₄ -NBA@NF ²⁰	10	1.636	100	96.9	97.0	30 (~90)

Table S5 HMF catalysis at 1.35V: four cycles

Cycle	Conversion (%)	FDCA Yield(%)	FE (%)
1	100	98.7	98.5
2	100	98.3	98.1
3	100	97.6	97.4
4	100	97.3	97.1

Table S6 Adsorption energy of HMF on different surfaces

Adsorbed sites	$E_{ad/sub}$	E_{sub}	E_{ad}
NiO	-471.10972	-375.1938	-0.85
CoO-NiO	-733.54017	-637.46213	-1.01

*Where $E_{ad/sub}$, E_{ad} , and E_{sub} are the total energies of the optimized adsorbate/substrate system, the adsorbate in the gas phase, and the clean substrate, respectively

Table S7 Bader charge analysis of CoO–NiO

#	X	Y	Z	CHARGE	MIN DIST	ATOMIC VOL
1	1.9237	3.3691	3.522	7.859	0.9105	9.5085
2	2.0333	3.5905	6.3699	7.9756	0.8641	49.3734
3	0.4414	1.3683	2.0347	8.178	0.9425	62.7523
4	0.4165	1.3244	5.1755	7.8121	0.8444	9.5742
5	4.8991	3.3691	3.522	7.8029	0.8996	9.0818
6	4.9238	3.1774	6.3587	8.1948	0.8774	48.1506
7	3.4167	1.3683	2.0347	8.1195	0.9425	59.4195
8	3.2437	1.299	5.2664	7.8656	0.8459	9.8231
9	7.8744	3.3691	3.522	7.8359	0.9063	9.2999
10	7.7492	3.0359	6.3678	8.089	0.8326	58.7185
11	6.3921	1.3683	2.0347	8.0471	0.9425	51.207
12	6.3522	1.1583	5.1145	7.9073	0.8644	9.8389
13	10.8497	3.3691	3.522	7.8942	0.9105	9.6665
14	10.7943	3.5031	6.3527	7.9382	0.8965	58.3752
15	9.3674	1.3683	2.0347	8.1638	0.9425	68.859
16	9.3899	1.2998	5.0693	7.8612	0.852	9.3512
17	1.9291	1.3683	3.5222	7.0455	0.9527	10.2075
18	1.8477	1.7099	6.5442	6.9503	0.8482	61.5007
19	0.4361	3.3691	2.0345	6.9598	0.9593	41.0973
20	0.4112	3.4805	5.0852	7.0849	0.891	10.2636
21	4.9044	1.3683	3.5222	7.0154	0.9527	10.546
22	4.8684	1.1683	6.4173	7.0218	0.8973	39.1783
23	3.4114	3.3691	2.0345	6.907	0.9593	46.5324
24	3.4741	3.3845	4.9919	7.092	0.895	9.7609
25	7.8797	1.3683	3.5222	7.0286	0.9527	10.1897
26	7.8929	1.1483	6.4194	6.994	0.9056	50.0922
27	6.3867	3.3691	2.0345	6.8576	0.9593	53.1008
28	6.3821	3.4908	4.983	7.1006	0.8873	9.8648
29	10.8551	1.3683	3.5222	7.0526	0.9527	9.9996
30	10.8083	1.6186	6.4116	6.9061	0.874	37.3132
31	9.362	3.3691	2.0345	6.9476	0.9593	48.7983

32	9.1989	3.4283	5.1437	7.0768	0.84	10.1391
33	2.5078	5.6308	2.1382	6.9422	0.893	33.9846
34	2.5963	5.584	6.483	7.0811	0.9503	35.2697
35	4.5509	7.725	2.1394	6.9906	0.9759	32.8342
36	4.5933	7.7994	6.4358	6.9654	0.9336	30.8605
37	2.625	7.7653	4.3477	7.0366	0.9456	9.118
38	4.6097	5.6819	4.1963	7.0186	0.9173	9.3752
39	6.5942	5.6331	2.1405	6.9352	0.972	34.8176
40	6.6081	5.7406	6.4903	6.9883	0.9561	37.2243
41	8.6374	7.7272	2.1419	7.0199	0.9698	34.319
42	8.5806	7.731	6.4752	7.0237	0.9412	34.9455
43	6.5852	7.7357	4.2675	7.0806	0.9757	9.4032
44	8.5584	5.7716	4.2363	7.0432	0.9632	9.3957
45	2.5078	9.8174	2.1382	7.0235	0.893	33.0613
46	2.6138	9.8445	6.4597	7.0659	0.9573	33.7356
47	4.5509	11.9115	2.1394	7.0032	0.9756	32.8076
48	4.6113	11.8663	6.4253	7.0226	0.9563	32.9129
49	2.5906	11.9239	4.2728	7.0887	0.977	9.3355
50	4.5911	9.815	4.2346	7.0562	0.9358	9.1392
51	6.5942	9.8194	2.1405	7.059	0.9719	32.6229
52	6.591	9.8281	6.4149	7.0463	0.9751	31.0417
53	8.6374	11.9136	2.1419	7.0679	0.9697	34.2465
54	8.5494	11.8803	6.4445	7.0071	0.9726	33.5852
55	6.5928	11.8658	4.2084	6.972	0.9653	8.6632
56	8.5782	9.8319	4.2831	7.0936	0.9439	9.3163
57	2.5078	14.0034	2.1382	7.0075	0.8931	31.2373
58	2.6287	13.8993	6.3596	6.9852	0.9429	32.3343
59	4.5755	13.8622	4.183	6.9936	0.9167	9.7889
60	6.5942	14.0057	2.1405	7.0647	0.972	31.491
61	6.5723	13.7995	6.2653	6.9821	0.9187	29.0809
62	8.6064	13.9378	4.3203	7.0243	0.9505	9.6932
63	10.6091	5.6347	2.2196	7.0071	0.9528	30.0726
64	10.5547	5.5552	6.4895	7.1016	0.9218	39.8895
65	0.6509	7.7312	2.2233	7.0386	0.8805	28.4031
66	0.6347	7.7717	6.6202	7.0482	0.9248	51.4635

67	10.5582	7.7684	4.3909	7.0373	0.9525	9.0831
68	0.6643	5.8894	4.3185	7.0075	0.9143	9.1925
69	10.6091	9.8211	2.2196	7.1253	0.9528	29.0262
70	10.5462	9.84	6.5092	7.0947	0.9406	36.3256
71	0.6509	11.9175	2.2233	7.0347	0.8808	27.7534
72	0.6285	11.9157	6.5129	7.0328	0.9698	36.0835
73	10.5715	11.9267	4.325	7.0247	0.9661	8.9764
74	0.6341	9.8812	4.3784	7.109	0.9753	9.3396
75	10.6091	14.0073	2.2196	7.075	0.9528	28.4832
76	10.5155	13.8425	6.4678	6.9069	0.8966	39.0422
77	0.6177	14.1247	4.5211	7.0462	0.9188	9.5762
78	2.6614	5.7088	4.3217	9.0355	0.909	9.1932
79	4.6058	7.7388	4.2668	8.9124	0.9208	8.482
80	2.5078	7.724	2.1382	8.9633	0.8941	44.0738
81	2.6256	7.7551	6.4467	8.939	0.9265	36.3879
82	4.5509	5.6321	2.1394	9.0039	0.9362	42.6498
83	4.6281	5.6043	6.3936	9.2121	0.8978	45.7637
84	6.5709	5.6057	4.3246	8.9248	0.8865	8.7829
85	8.5662	7.774	4.2634	8.8902	0.8997	8.2836
86	6.5942	7.7262	2.1405	8.9539	0.9355	42.4761
87	6.5764	7.741	6.4158	8.9923	0.905	37.5259
88	8.6374	5.6341	2.1419	8.9639	0.884	44.4677
89	8.5839	5.7049	6.2591	9.0817	0.9133	33.8642
90	2.6139	9.8497	4.309	8.9158	0.9143	8.4108
91	4.583	11.8962	4.2639	8.9064	0.9216	8.3547
92	2.5078	11.9103	2.1382	9.0131	0.8937	41.7327
93	2.6368	11.9243	6.3869	8.9295	0.9329	35.2102
94	4.5509	9.8184	2.1394	9.0273	0.9749	40.2937
95	4.6001	9.8221	6.3965	9.0059	0.9255	38.8493
96	6.5855	9.8061	4.2511	8.8516	0.8902	8.1899
97	8.5893	11.9256	4.2944	8.8448	0.9321	8.1161
98	6.5942	11.9126	2.1405	8.9669	0.9314	38.9033
99	6.5774	11.8653	6.3459	8.9431	0.8827	37.6224
100	8.6374	9.8205	2.1419	8.992	0.8839	43.7168
101	8.5664	9.8286	6.4002	8.9896	0.9156	35.5781

102	2.5759	14.0338	4.2492	9.0056	0.876	9.2069
103	4.5509	14.0044	2.1394	9.157	0.9252	44.0225
104	4.6289	14.1063	6.4401	8.9824	0.8939	50.4342
105	6.6028	13.9058	4.1855	8.9847	0.9084	8.9039
106	8.6374	14.0067	2.1419	9.1828	0.884	46.5058
107	8.5189	14.0978	6.4083	8.955	0.8682	42.9015
108	10.5592	5.7142	4.2863	9.0789	0.9179	9.2425
109	0.6447	7.8352	4.3242	8.8175	0.8717	7.9594
110	10.6091	7.7279	2.2196	8.8909	0.8687	38.7549
111	10.5546	7.7806	6.47	8.9499	0.9219	38.3049
112	0.6509	5.638	2.2233	8.9513	0.8799	38.7071
113	0.6077	5.7904	6.3034	9.0782	0.8835	26.5203
114	10.5566	9.8578	4.3333	8.9017	0.9204	8.2836
115	0.629	11.9805	4.3683	8.9124	0.8852	8.5134
116	10.6091	11.9142	2.2196	8.887	0.8687	35.7819
117	10.5236	11.9193	6.4396	8.9868	0.9196	38.2269
118	0.6509	9.8244	2.2233	8.9962	0.8798	36.5171
119	0.6333	9.8546	6.4711	8.8769	0.8891	36.8352
120	10.5819	14.0721	4.2774	8.9703	0.8925	9.0544
121	0.6509	14.0106	2.2233	9.2392	0.8798	41.1651
122	0.6183	13.979	6.52	8.9734	0.9133	51.8185

Table S8 Unit-cell and position parameters of NiO optimization model.

NiO			
	a (Å)	12.55900	
	b (Å)	8.37270	
	c (Å)	21.00660	
	α (deg)	90.0000	
	β (deg)	90.0000	
	γ (deg)	90.0000	
Atom Coordinates	x	y	z
Ni1	0.10511	0.17211	0.22765
Ni2	0.27176	0.42215	0.22764
Ni3	0.10512	0.42212	0.12886
Ni4	0.10512	0.42212	0.32644
Ni5	0.27176	0.17213	0.12886
Ni6	0.27176	0.17214	0.32642
Ni7	0.43842	0.17214	0.22764
Ni8	0.60511	0.42211	0.22765
Ni9	0.43844	0.42213	0.12885
Ni10	0.43844	0.42213	0.32644
Ni11	0.60512	0.17212	0.12886
Ni12	0.60512	0.17212	0.32644
Ni13	0.77176	0.17215	0.22764
Ni14	0.93842	0.42214	0.22764
Ni15	0.77176	0.42213	0.12886
Ni16	0.77176	0.42214	0.32642
Ni17	0.93844	0.17213	0.12885
Ni18	0.93844	0.17213	0.32644
Ni19	0.10511	0.67211	0.22765
Ni20	0.27176	0.92215	0.22764
Ni21	0.10512	0.92212	0.12886
Ni22	0.10512	0.92212	0.32644
Ni23	0.27176	0.67213	0.12886

Ni24	0.27176	0.67214	0.32642
Ni25	0.43842	0.67214	0.22764
Ni26	0.60511	0.92211	0.22765
Ni27	0.43844	0.92213	0.12885
Ni28	0.43844	0.92213	0.32644
Ni29	0.60512	0.67212	0.12886
Ni30	0.60512	0.67212	0.32644
Ni31	0.77176	0.67215	0.22764
Ni32	0.93842	0.92214	0.22764
Ni33	0.77176	0.92213	0.12886
Ni34	0.77176	0.92214	0.32642
Ni35	0.93844	0.67213	0.12885
Ni36	0.93844	0.67213	0.32644
O1	0.10508	0.17213	0.12718
O2	0.10509	0.17214	0.32809
O3	0.27176	0.42211	0.1272
O4	0.27176	0.42209	0.32807
O5	0.10507	0.42214	0.22764
O6	0.27175	0.17217	0.22764
O7	0.43843	0.17213	0.12719
O8	0.43843	0.17214	0.32809
O9	0.60508	0.42213	0.12718
O10	0.60509	0.42214	0.32809
O11	0.43848	0.42211	0.22764
O12	0.60507	0.17214	0.22764
O13	0.77176	0.17211	0.1272
O14	0.77176	0.17209	0.32807
O15	0.93844	0.42213	0.12719
O16	0.93843	0.42214	0.32809
O17	0.77175	0.42217	0.22764
O18	0.93848	0.17211	0.22764
O19	0.10508	0.67213	0.12718
O20	0.10509	0.67214	0.32809
O21	0.27176	0.92211	0.1272
O22	0.27176	0.92209	0.32807

O23	0.10507	0.92214	0.22764
O24	0.27175	0.67217	0.22764
O25	0.43843	0.67213	0.12719
O26	0.43843	0.67214	0.32809
O27	0.60508	0.92213	0.12718
O28	0.60509	0.92214	0.32809
O29	0.43848	0.92211	0.22764
O30	0.60507	0.67214	0.22764
O31	0.77176	0.67211	0.1272
O32	0.77176	0.67209	0.32807
O33	0.93844	0.92213	0.12719
O34	0.93843	0.92214	0.32809
O35	0.77175	0.92217	0.22764
O36	0.93848	0.67211	0.22764

Table S9 Unit-cell and position parameters of CoO–NiO (1:3) optimization model.

CoO–NiO (1:3)			
	a (Å)	11.90130	
	b (Å)	15.00000	
	c (Å)	19.46300	
	α (deg)	90.0000	
	β (deg)	90.0000	
	γ (deg)	90.0000	
Atom Coordinates	x	y	z
Co1	0.16164	0.22461	0.18096
Co2	0.17085	0.23937	0.32728
Co3	0.03709	0.09122	0.10454
Co4	0.035	0.08829	0.26591
Co5	0.41164	0.22461	0.18096
Co6	0.41372	0.21183	0.32671
Co7	0.28709	0.09122	0.10454
Co8	0.27255	0.0866	0.27059
Co9	0.66164	0.22461	0.18096
Co10	0.65112	0.2024	0.32717
Co11	0.53709	0.09122	0.10454
Co12	0.53374	0.07722	0.26278
Co13	0.91164	0.22461	0.18096
Co14	0.90699	0.23354	0.3264
Co15	0.78709	0.09122	0.10454
Co16	0.78898	0.08665	0.26046
O1	0.16209	0.09122	0.18097
O2	0.15525	0.11399	0.33624
O3	0.03664	0.22461	0.10453
O4	0.03455	0.23203	0.26127
O5	0.41209	0.09122	0.18097
O6	0.40907	0.07789	0.32972
O7	0.28664	0.22461	0.10453
O8	0.29191	0.22563	0.25648

O9	0.66209	0.09122	0.18097
O10	0.6632	0.07655	0.32982
O11	0.53664	0.22461	0.10453
O12	0.53626	0.23272	0.25602
O13	0.91209	0.09122	0.18097
O14	0.90816	0.10791	0.32943
O15	0.78664	0.22461	0.10453
O16	0.77294	0.22855	0.26428
O17	0.21072	0.37539	0.10986
O18	0.21815	0.37227	0.3331
O19	0.38239	0.515	0.10992
O20	0.38595	0.51996	0.33067
O21	0.22057	0.51768	0.22339
O22	0.38733	0.37879	0.21561
O23	0.55407	0.37554	0.10998
O24	0.55524	0.38271	0.33347
O25	0.72575	0.51515	0.11005
O26	0.72098	0.5154	0.3327
O27	0.55332	0.51571	0.21926
O28	0.71911	0.38477	0.21766
O29	0.21072	0.65449	0.10986
O30	0.21962	0.6563	0.3319
O31	0.38239	0.7941	0.10992
O32	0.38746	0.79109	0.33013
O33	0.21767	0.79492	0.21954
O34	0.38577	0.65433	0.21757
O35	0.55407	0.65463	0.10998
O36	0.5538	0.65521	0.32959
O37	0.72575	0.79424	0.11005
O38	0.71836	0.79202	0.33112
O39	0.55396	0.79105	0.21622
O40	0.72078	0.65546	0.22006
O41	0.21072	0.93356	0.10986
O42	0.22088	0.92662	0.32675
O43	0.38446	0.92415	0.21492

O44	0.55407	0.93371	0.10998
O45	0.55223	0.91996	0.32191
O46	0.72315	0.92919	0.22197
O47	0.89142	0.37565	0.11404
O48	0.88685	0.37035	0.33343
O49	0.05469	0.51541	0.11423
O50	0.05333	0.51811	0.34014
O51	0.88715	0.51789	0.2256
O52	0.05582	0.39263	0.22188
O53	0.89142	0.65474	0.11404
O54	0.88614	0.656	0.33444
O55	0.05469	0.7945	0.11423
O56	0.05281	0.79438	0.33463
O57	0.88826	0.79512	0.22221
O58	0.05328	0.65875	0.22496
O59	0.89142	0.93382	0.11404
O60	0.88356	0.92283	0.33231
O61	0.0519	0.94165	0.23229
Ni1	0.22362	0.38059	0.22205
Ni2	0.387	0.51592	0.21923
Ni3	0.21072	0.51493	0.10986
Ni4	0.22062	0.51701	0.33123
Ni5	0.38239	0.37547	0.10992
Ni6	0.38887	0.37362	0.3285
Ni7	0.55212	0.37372	0.22219
Ni8	0.71977	0.51827	0.21905
Ni9	0.55407	0.51508	0.10998
Ni10	0.55258	0.51607	0.32964
Ni11	0.72575	0.37561	0.11005
Ni12	0.72126	0.38033	0.32159
Ni13	0.21963	0.65664	0.22139
Ni14	0.38509	0.79308	0.21908
Ni15	0.21072	0.79402	0.10986
Ni16	0.22155	0.79495	0.32815
Ni17	0.38239	0.65456	0.10992

Ni18	0.38652	0.65481	0.32865
Ni19	0.55335	0.65374	0.21842
Ni20	0.72171	0.79504	0.22065
Ni21	0.55407	0.79417	0.10998
Ni22	0.55266	0.79102	0.32605
Ni23	0.72575	0.6547	0.11005
Ni24	0.71979	0.65524	0.32884
Ni25	0.21644	0.93558	0.21832
Ni26	0.38239	0.93363	0.10992
Ni27	0.38894	0.94042	0.33089
Ni28	0.5548	0.92705	0.21505
Ni29	0.72575	0.93378	0.11005
Ni30	0.7158	0.93986	0.32926
Ni31	0.88723	0.38095	0.22023
Ni32	0.05417	0.52235	0.22217
Ni33	0.89142	0.51519	0.11404
Ni34	0.88685	0.51871	0.33242
Ni35	0.05469	0.37587	0.11423
Ni36	0.05106	0.38603	0.32387
Ni37	0.88701	0.65719	0.22264
Ni38	0.05285	0.7987	0.22444
Ni39	0.89142	0.79428	0.11404
Ni40	0.88424	0.79462	0.33086
Ni41	0.05469	0.65496	0.11423
Ni42	0.05321	0.65697	0.33248
Ni43	0.88914	0.93814	0.21977
Ni44	0.05469	0.93404	0.11423
Ni45	0.05195	0.93194	0.335

Table S10 Unit-cell and position parameters of the optimized model for the adsorption of HMF on NiO

HMF@NiO			
a (Å)	12.55900		
b (Å)	8.37270		
c (Å)	21.00660		
α (deg)	90.0000		
β (deg)	90.0000		
γ (deg)	90.0000		
Atom Coordinates	x	y	z
Ni1	0.10511	0.17211	0.22765
Ni2	0.27176	0.42215	0.22764
Ni3	0.10512	0.42212	0.12886
Ni4	0.10512	0.42212	0.32644
Ni5	0.27176	0.17213	0.12886
Ni6	0.27176	0.17214	0.32642
Ni7	0.43842	0.17214	0.22764
Ni8	0.60511	0.42211	0.22765
Ni9	0.43844	0.42213	0.12885
Ni10	0.43844	0.42213	0.32644
Ni11	0.60512	0.17212	0.12886
Ni12	0.60512	0.17212	0.32644
Ni13	0.77176	0.17215	0.22764
Ni14	0.93842	0.42214	0.22764
Ni15	0.77176	0.42213	0.12886
Ni16	0.77176	0.42214	0.32642
Ni17	0.93844	0.17213	0.12885
Ni18	0.93844	0.17213	0.32644
Ni19	0.10511	0.67211	0.22765
Ni20	0.27176	0.92215	0.22764
Ni21	0.10512	0.92212	0.12886
Ni22	0.10512	0.92212	0.32644

Ni23	0.27176	0.67213	0.12886
Ni24	0.27176	0.67214	0.32642
Ni25	0.43842	0.67214	0.22764
Ni26	0.60511	0.92211	0.22765
Ni27	0.43844	0.92213	0.12885
Ni28	0.43844	0.92213	0.32644
Ni29	0.60512	0.67212	0.12886
Ni30	0.60512	0.67212	0.32644
Ni31	0.77176	0.67215	0.22764
Ni32	0.93842	0.92214	0.22764
Ni33	0.77176	0.92213	0.12886
Ni34	0.77176	0.92214	0.32642
Ni35	0.93844	0.67213	0.12885
Ni36	0.93844	0.67213	0.32644
O1	0.10508	0.17213	0.12718
O2	0.10509	0.17214	0.32809
O3	0.27176	0.42211	0.1272
O4	0.27176	0.42209	0.32807
O5	0.10507	0.42214	0.22764
O6	0.27175	0.17217	0.22764
O7	0.43843	0.17213	0.12718
O8	0.43843	0.17214	0.32809
O9	0.60508	0.42213	0.12718
O10	0.60509	0.42214	0.32809
O11	0.43848	0.42211	0.22764
O12	0.60507	0.17214	0.22764
O13	0.77176	0.17211	0.1272
O14	0.77176	0.17209	0.32807
O15	0.93843	0.42213	0.12718
O16	0.93843	0.42214	0.32809
O17	0.77175	0.42217	0.22764
O18	0.93848	0.17211	0.22764
O19	0.10508	0.67213	0.12718
O20	0.10509	0.67214	0.32809
O21	0.27176	0.92211	0.1272

O22	0.27176	0.92209	0.32807
O23	0.10507	0.92214	0.22764
O24	0.27175	0.67217	0.22764
O25	0.43843	0.67213	0.12718
O26	0.43843	0.67214	0.32809
O27	0.60508	0.92213	0.12718
O28	0.60509	0.92214	0.32809
O29	0.43848	0.92211	0.22764
O30	0.60507	0.67214	0.22764
O31	0.77176	0.67211	0.1272
O32	0.77176	0.67209	0.32807
O33	0.93843	0.92213	0.12718
O34	0.93843	0.92214	0.32809
O35	0.77175	0.92217	0.22764
O36	0.93848	0.67211	0.22764
O37	0.549169	0.411107	0.477504
O38	0.270853	0.52477	0.486156
O39	0.823427	0.517826	0.467187
H1	0.73853	0.309217	0.471459
H2	0.648684	0.774146	0.46668
H3	0.428655	0.759829	0.470605
H4	0.357661	0.326323	0.517649
H5	0.346258	0.345104	0.433629
H6	0.215201	0.497339	0.455824
C1	0.459094	0.502019	0.476208
C2	0.634882	0.514309	0.473613
C3	0.598125	0.669823	0.470424
C4	0.485141	0.661911	0.472362
C5	0.355778	0.413952	0.478311
C6	0.739399	0.442535	0.470976

Table S11 Unit-cell and position parameters of the optimized model for the adsorption of HMF on CoO–NiO (1:3)

HMF@CoO–NiO (1:3)			
a (Å)			11.90130
b (Å)			15.00000
c (Å)			19.46300
α (deg)			90.0000
β (deg)			90.0000
γ (deg)			90.0000
Atom Coordinates	x	y	z
Co1	0.16164	0.22461	0.18096
Co2	0.17085	0.23937	0.32728
Co3	0.03709	0.09122	0.10454
Co4	0.03499	0.08829	0.26591
Co5	0.41164	0.22461	0.18096
Co6	0.41372	0.21183	0.32671
Co7	0.28709	0.09122	0.10454
Co8	0.27255	0.0866	0.27059
Co9	0.66164	0.22461	0.18096
Co10	0.65112	0.2024	0.32717
Co11	0.53709	0.09122	0.10454
Co12	0.53374	0.07722	0.26278
Co13	0.91164	0.22461	0.18096
Co14	0.90699	0.23354	0.3264
Co15	0.78709	0.09122	0.10454
Co16	0.78898	0.08665	0.26046
O1	0.16209	0.09122	0.18097
O2	0.15525	0.11399	0.33624
O3	0.03664	0.22461	0.10453
O4	0.03455	0.23203	0.26127
O5	0.41209	0.09122	0.18097
O6	0.40907	0.07789	0.32972

O7	0.28664	0.22461	0.10453
O8	0.29191	0.22563	0.25648
O9	0.66209	0.09122	0.18097
O10	0.6632	0.07655	0.32982
O11	0.53664	0.22461	0.10453
O12	0.53626	0.23272	0.25603
O13	0.91209	0.09122	0.18097
O14	0.90817	0.10791	0.32943
O15	0.78664	0.22461	0.10453
O16	0.77294	0.22855	0.26428
O17	0.21072	0.37539	0.10986
O18	0.21815	0.37227	0.3331
O19	0.38239	0.515	0.10992
O20	0.38595	0.51996	0.33067
O21	0.22057	0.51769	0.22339
O22	0.38733	0.37879	0.21561
O23	0.55407	0.37554	0.10998
O24	0.55525	0.38271	0.33347
O25	0.72575	0.51515	0.11005
O26	0.72098	0.5154	0.3327
O27	0.55332	0.51571	0.21926
O28	0.71911	0.38477	0.21766
O29	0.21072	0.65449	0.10986
O30	0.21962	0.6563	0.3319
O31	0.38239	0.7941	0.10992
O32	0.38746	0.79109	0.33013
O33	0.21767	0.79493	0.21954
O34	0.38577	0.65433	0.21757
O35	0.55407	0.65463	0.10998
O36	0.5538	0.65521	0.32959
O37	0.72575	0.79424	0.11005
O38	0.71836	0.79202	0.33112
O39	0.55396	0.79105	0.21622
O40	0.72078	0.65546	0.22007
O41	0.21072	0.93356	0.10986

O42	0.22088	0.92662	0.32676
O43	0.38446	0.92415	0.21492
O44	0.55407	0.93371	0.10998
O45	0.55223	0.91996	0.32191
O46	0.72315	0.92919	0.22197
O47	0.89142	0.37565	0.11404
O48	0.88685	0.37035	0.33343
O49	0.05469	0.51541	0.11423
O50	0.05333	0.51811	0.34014
O51	0.88715	0.51789	0.2256
O52	0.05581	0.39263	0.22188
O53	0.89142	0.65474	0.11404
O54	0.88614	0.656	0.33444
O55	0.05469	0.7945	0.11423
O56	0.05281	0.79438	0.33463
O57	0.88826	0.79512	0.22222
O58	0.05328	0.65875	0.22496
O59	0.89142	0.93382	0.11404
O60	0.88356	0.92283	0.33231
O61	0.0519	0.94165	0.23229
O62	0.605632	0.572856	0.485298
O63	0.547496	0.798785	0.445245
O64	0.512138	0.346027	0.490397
Ni1	0.22362	0.38059	0.22205
Ni2	0.387	0.51592	0.21923
Ni3	0.21072	0.51493	0.10986
Ni4	0.22062	0.51701	0.33123
Ni5	0.38239	0.37547	0.10992
Ni6	0.38887	0.37362	0.3285
Ni7	0.55212	0.37372	0.22219
Ni8	0.71977	0.51827	0.21905
Ni9	0.55407	0.51508	0.10998
Ni10	0.55258	0.51607	0.32964
Ni11	0.72575	0.37561	0.11005
Ni12	0.72126	0.38033	0.32159

Ni13	0.21963	0.65665	0.22139
Ni14	0.38509	0.79308	0.21908
Ni15	0.21072	0.79402	0.10986
Ni16	0.22155	0.79495	0.32815
Ni17	0.38239	0.65456	0.10992
Ni18	0.38652	0.65481	0.32865
Ni19	0.55335	0.65374	0.21842
Ni20	0.72171	0.79504	0.22065
Ni21	0.55407	0.79417	0.10998
Ni22	0.55266	0.79102	0.32605
Ni23	0.72575	0.6547	0.11005
Ni24	0.71979	0.65524	0.32884
Ni25	0.21644	0.93558	0.21832
Ni26	0.38239	0.93363	0.10992
Ni27	0.38894	0.94042	0.33089
Ni28	0.5548	0.92705	0.21505
Ni29	0.72575	0.93378	0.11005
Ni30	0.7158	0.93986	0.32926
Ni31	0.88723	0.38095	0.22023
Ni32	0.05417	0.52235	0.22217
Ni33	0.89142	0.51519	0.11404
Ni34	0.88685	0.51871	0.33242
Ni35	0.05469	0.37587	0.11423
Ni36	0.05106	0.38603	0.32387
Ni37	0.88702	0.65719	0.22264
Ni38	0.05285	0.7987	0.22444
Ni39	0.89142	0.79428	0.11404
Ni40	0.88424	0.79462	0.33086
Ni41	0.05469	0.65496	0.11423
Ni42	0.05321	0.65697	0.33248
Ni43	0.88914	0.93814	0.21977
Ni44	0.05469	0.93404	0.11423
Ni45	0.05195	0.93194	0.335
C1	0.546145	0.650168	0.486744
C2	0.528217	0.5033	0.488369

C3	0.421234	0.538666	0.492001
C4	0.43251	0.632755	0.491071
C5	0.612447	0.7343	0.482778
C6	0.571689	0.412958	0.486291
H1	0.582074	0.857375	0.450593
H2	0.693491	0.72124	0.456933
H3	0.630663	0.759791	0.534843
H4	0.366146	0.682344	0.492195
H5	0.344423	0.499732	0.493998
H6	0.664945	0.408528	0.480442

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