Electronic Supplementary Information (ESI)

Platelike carbon-encapsulated nickel nanocrystals for efficient electrooxidation of 5-hydroxymethylfurfural

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Experimental Section

Materials and Chemicals

Choline chloride (ChCl), oxalic acid ($H_2C_2O_4$), potassium chloride (KCl) and nickel powder were purchased from Aladdin Chemistry Co., Ltd. Nickel chloride hexahydrate ($NiCl_2\ 6H_2O$) and Potassium hydroxide (KOH) were obtained from Sinopharm Chemical Regent Co., Ltd. 5-hydroxymethylfurfural (HMF), 2,5-furandicarboxylic acid (FDCA), 5-hydroxymethyl-2-furancarboxylic acid (HMFCA) and 5-formyl-2-furancarboxylic acid (FFCA) were purchased from Alfa-Aesar. 2,5-diformylfuran (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. Nickel foam was purchased from Suzhou Sinero Technology Co., Ltd. Nafion 115 membrane was purchased from Wuhan GaossUnion technology Co., Ltd.

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

The deep eutectic solvent (DES) was synthesized according to the previous literature.[1] Specifically, the colorless and transparent (ChCl/OA) DES was obtained by mixing equimolar amounts of choline chloride and oxalic acid, followed by magnetic stirring at 80 ℃.

Synthesis of platelike carbon-encapsulated nickel nanocrystals (Ni@C)

In a typical procedure, 100.0 mg $NiCl_2\ 6H_2O$ were added in 1 mL of ChCl/OA DES and subjected the solution to ultrasonic treatment at 50 ℃ until a uniformly

dispersed solution was obtained. Then, the above solution was transferred to a microwave oven for microwave heating at 100 W for 15 s to achieve the Ni-based precursors. Subsequently, the precursors was recovered, washed with ethanol and dried under vacuum oven.

Then, the dried precursors were put in a quartz tube of the tube furnace and heat-treated at 450 ℃ for 2 h with 10 °C min^{-1} in N_2 atmosphere to achieve the platelike Ni@C. The platelike Ni@C was washed by water and ethanol, and then dried in the vacuum oven. The achieved product was labeled as Ni@C-450 (for convenience, we labeled Ni@C achieved at various pyrolysis temperature as Ni@C-X, where X represented pyrolysis temperature).

In order to make comparisons, Ni@C-400 and Ni@C-500 were prepared by adjusting the pyrolysis temperature to 400 ℃ and 500 ℃, using the same preparation method as Ni@C-450.

Characterizations

The X-ray diffraction (XRD) pattern was characterized on the Rigaku SmartLab 9 KW X-ray diffractometer. Transmission electron microscopy (TEM) was performed on the JEM-1400 microscope. High-resolution transmission electron microscopy (HRTEM) and energy-dispersive X-ray (EDX) were tested on the FEI Talos F200x. X-ray photoelectron spectroscopy (XPS) measurements were carried out using the Thermo Fisher ESCALAB XI. Thermogravimetric (TG) analysis was performed using the TGA/DSC3+ analyzer. Nitrogen adsorption-desorption experiments were

conducted on the micropolitics ASAP 2460. High-performance liquid chromatography (HPLC) analysis was performed using the Agilent G7114A system.

Electrochemical Measurements

CHI760E electrochemical workstation was used for electrochemical tests. A catalyst suspension was created by combining 5.0 mg of the as-prepared catalyst with 20 μL of a 5 wt% Nafion solution, along with 100 μL of ethanol and 80 μL of deionized water, followed by sonication. Subsequently, 200 μL of the catalyst ink was casted on a carbon cloth (1×1 cm^2) to establish a working electrode. Pt foil and saturated Ag/AgCl electrode were utilized as counter electrode and reference electrode. For control, nickel foam (1×1 cm^2) was also used as the electrode for the HMF electrooxidation study. The potentials in this experiment were referenced to the reversible hydrogen electrode (RHE):

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

The linear sweep voltammetry (LSV) was performed at 10 mV s^{-1} in 10 mL 1.0 M KOH electrolyte (with and without 10 mM HMF). Cyclic voltammetry (CV) used to measure the electrochemical double-layer capacitance (C_{dl}) , which was carried out in 1 M KOH electrolyte (10 mM HMF) at 40, 50, 60, 70, 80 and 90 mV s^{-1}, with no Faraday processes occurring in the potential window. Electrochemical impedance spectroscopy (EIS) was conducted from 1 Hz to 100 kHz. HMF electrolysis at constant potential (1.34 V) was performed with a two-compartment cell separated by a Nafion 115 membrane. The electrooxidation of HMF occurred in the anode chamber containing 10 mL electrolyte (1 M KOH with 10 mM HMF).

Products analysis

High-performance liquid chromatography (HPLC) with a 4.6 mm × 250 mm Zorbax SB-C18 5 μm column and a UV-Vis detector (265 nm) was applied to deterimine the concentrations of the components. In the constant potential electrolysis test (1.34 V), 10 μL of the electrolyte was taken out and diluted to 500 μL by ultrapure water. Then, a 10 μL volume of the diluted electrolyte was injected into the HPLC for analysis at 30 ℃. 30% methanol with 70% ammonium formate aqueous solution (5 mM) was used as the eluent. Calibration curves for HPLC were achieved by standard solution.

HMF conversion, FDCA yield and Faraday efficiency (FE) were achieved by the below equations:

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

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

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

wherein Q is total transferred charge, F is Faraday constant (96485 C mol^{-1}) and n is the mole number of reactant.

Density functional theory (DFT) Calculation

The Vienna Ab-initio Simulation Package (VASP) was employed to conduct all Density Functional Theory (DFT) calculations.[2,3] The Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional with Grimme D3 dispersion correction, employing the generalized gradient approximation (GGA) method, was utilized in this study.[4,5] The projected augmented wave (PAW) method was utilized to describe core-valence

interactions in all DFT calculations.[6] The energy cutoff for plane wave expansions was set to 450 eV, and the 1×1×1 Monkhorst-Pack grid k-points were used to sample the Brillouin zone integration for structural optimization. 15 Å vacuum was applied to both the upper and lower surfaces of the model to eliminate image interactions. Structural optimization was carried out with energy and force convergence criteria setting at 1.0×10^{-5} eV and 0.02 eV $Å^{-1}$, respectively.

The adsorption energy of HMF was calculated according to the following equation:

$$E_{ads} = E_{ad/sub} - E_{ad} - E_{sub}$$

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.

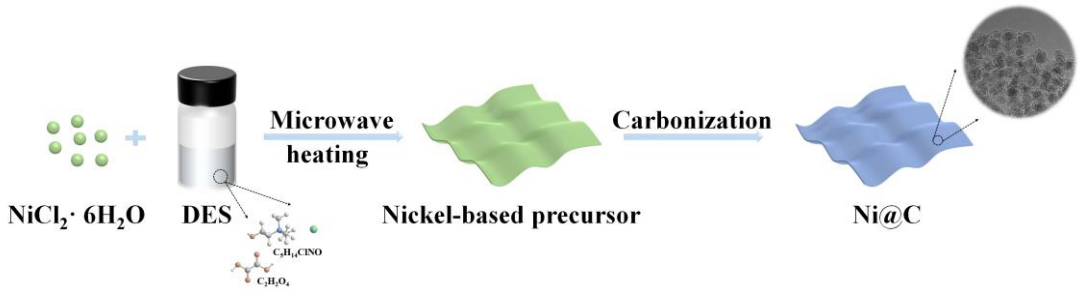

Fig. S1 Schematic diagram of platelike Ni@C synthesis.

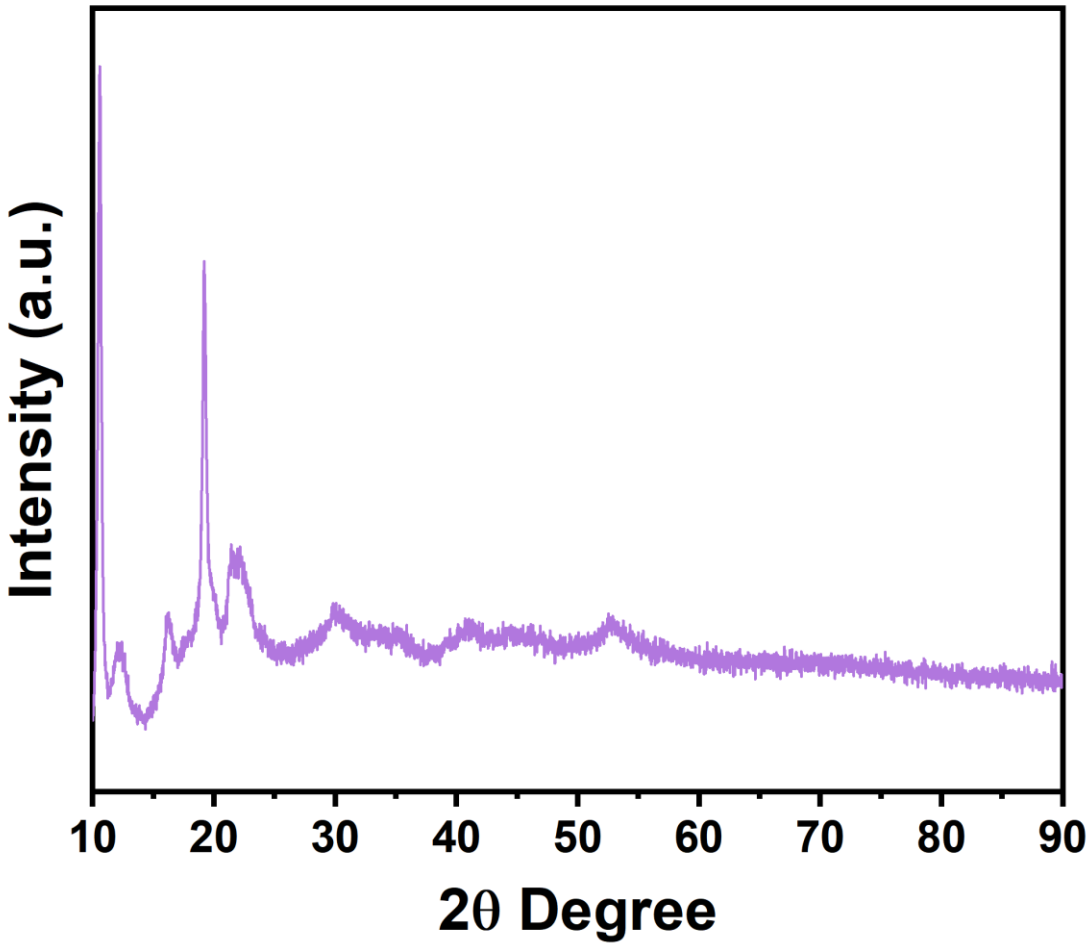

Fig. S2 XRD pattern of the Ni precursors obtained after microwave heating 1 mL ChCl/OA DES with 100.0 mg $NiCl_2$ $6H_2O$.

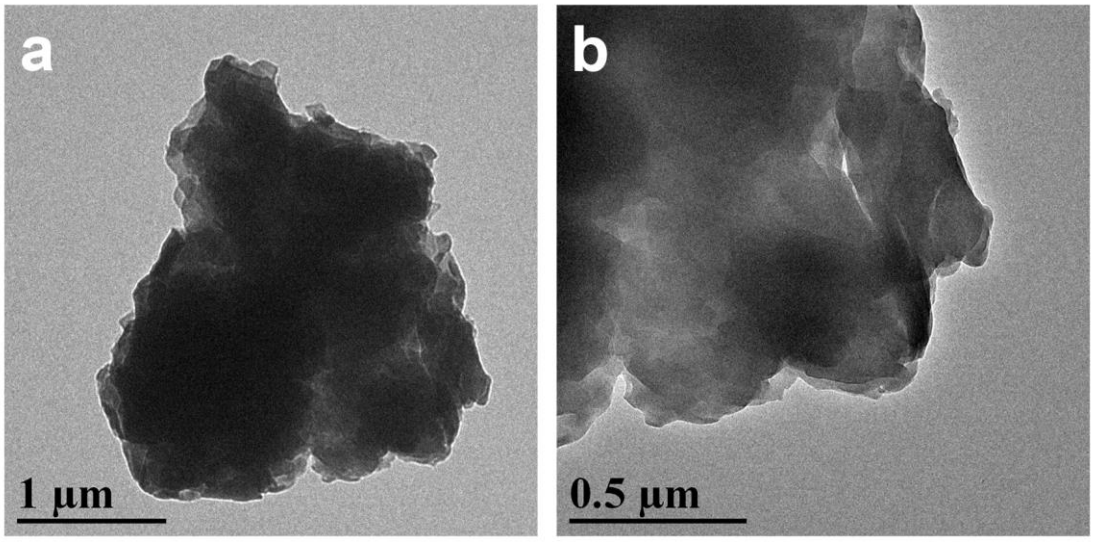

Fig. S3 Low- and high- magnification TEM images of the Ni precursor obtained after microwave heating 1 mL ChCl/OA DES with 100.0 mg $NiCl_2$ $6H_2O$. The precursor will be used for synthesizing platelike Ni@C.

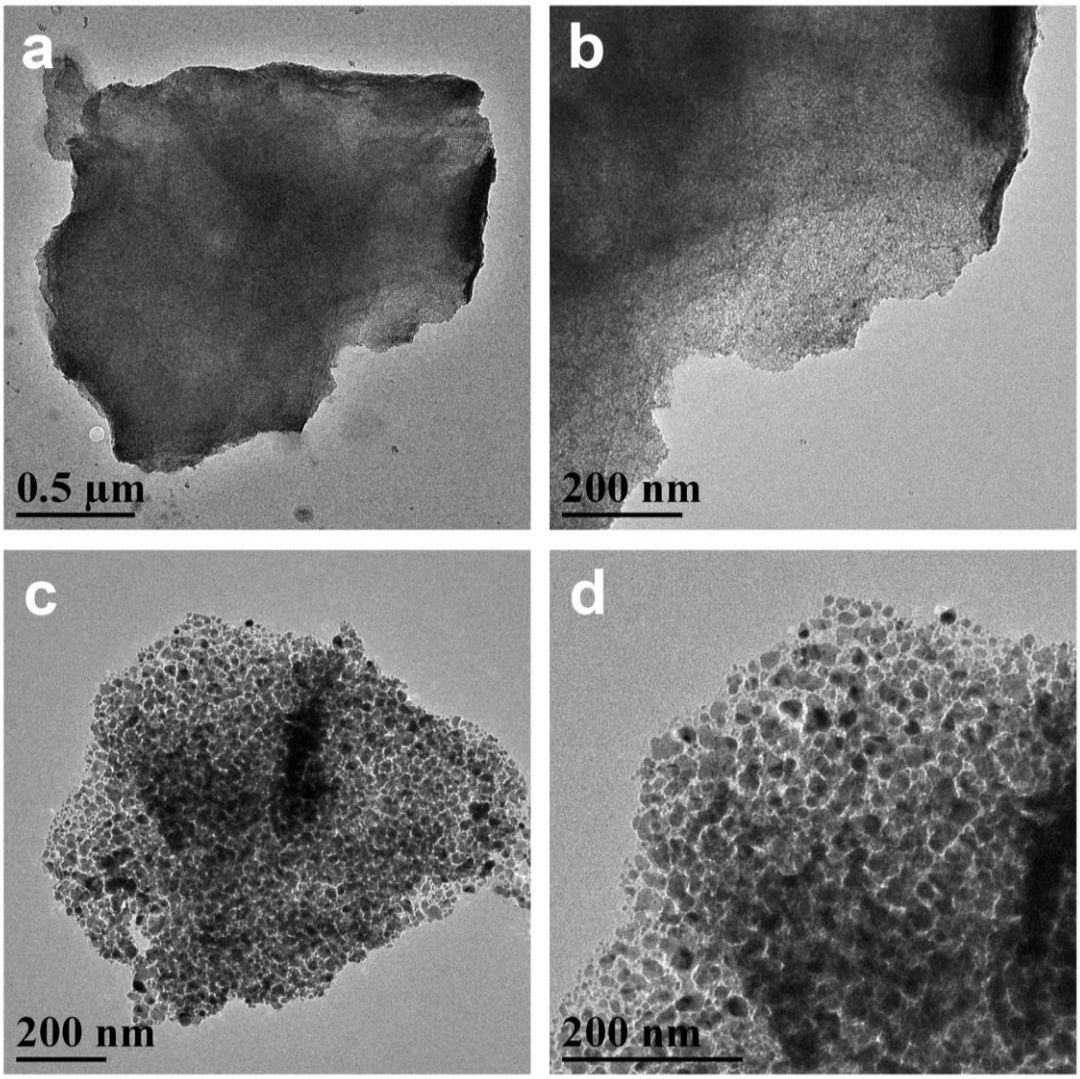

Fig. S4 TEM images of (a, b) Ni@C-400, (c, d) Ni@C-500.

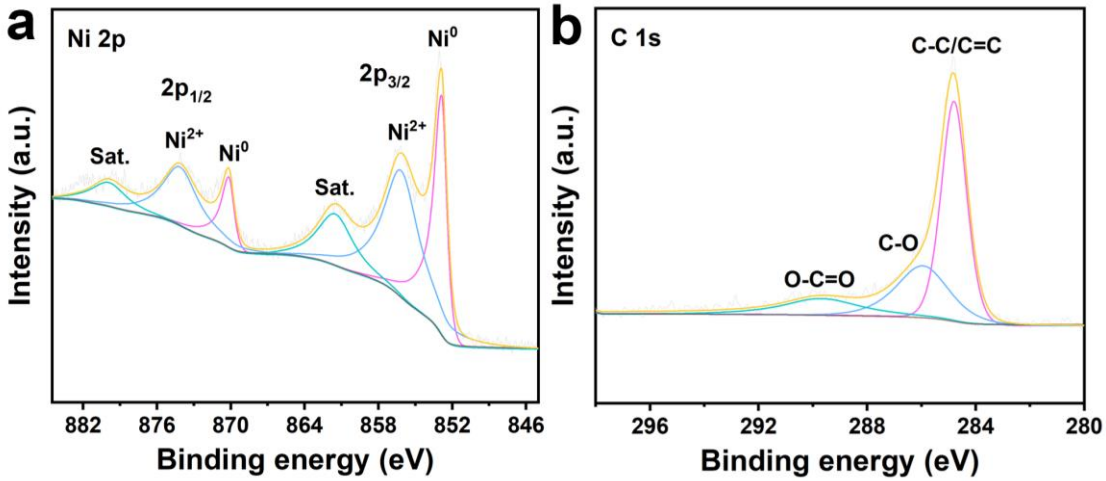

Fig. S5 XPS spectra of the Ni@C-450: (a) Ni 2p, (b) C 1s.

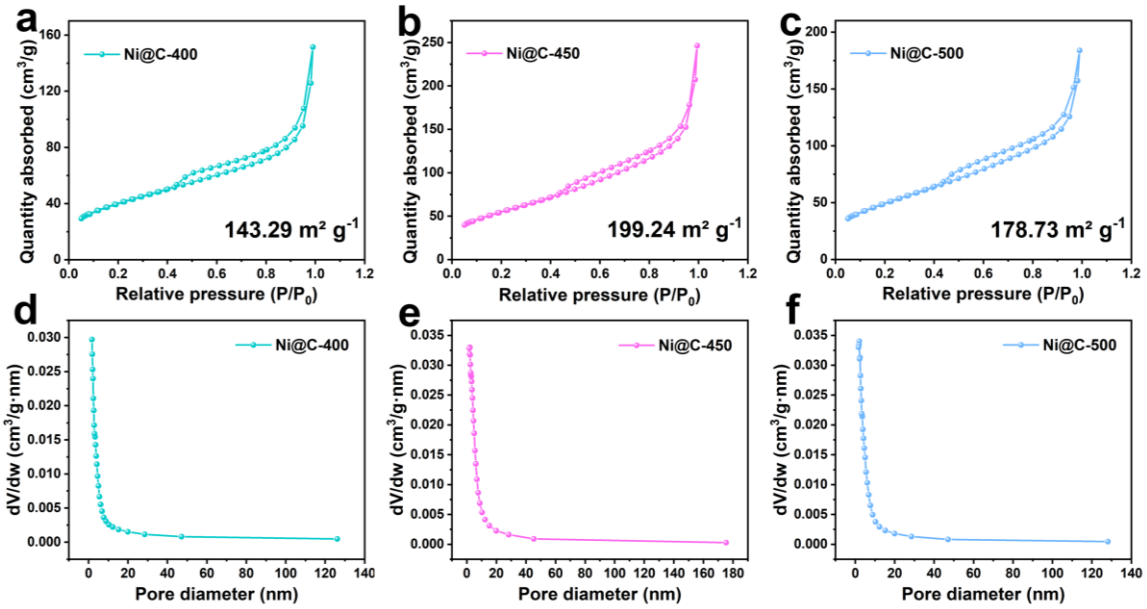

Fig. S6 N_2 adsorption-desorption isotherms of (a) Ni@C-400, (b) Ni@C-450, (c) Ni@C-500. Pore size distributions of (d) Ni@C-400, (e) Ni@C-450, (f) Ni@C-500.

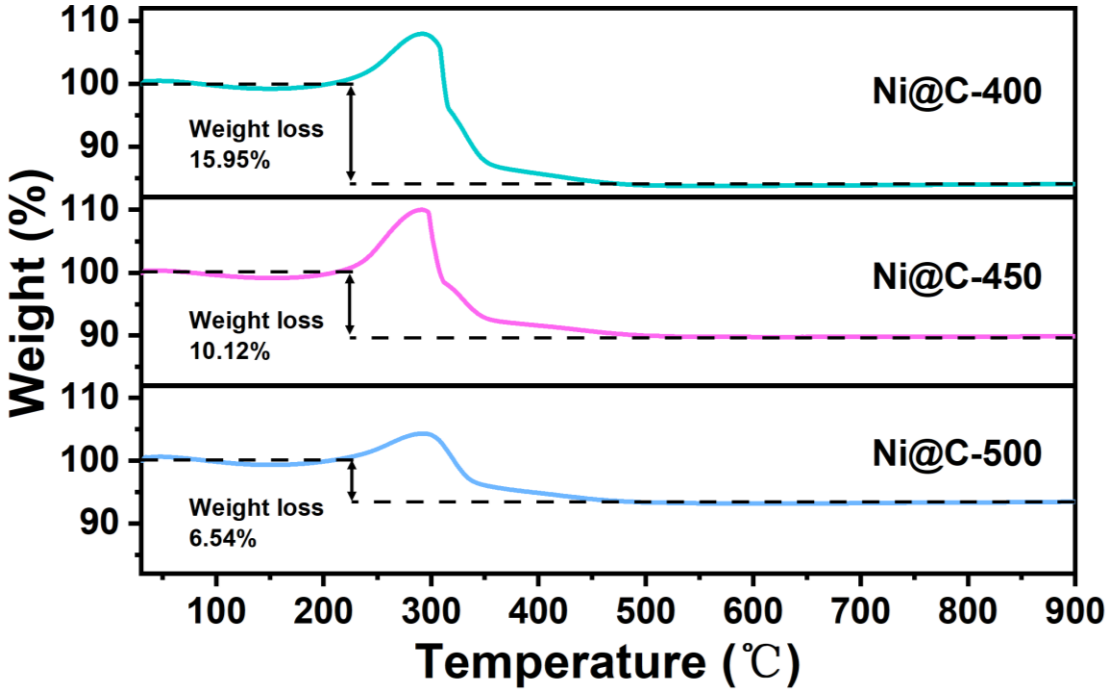

Fig. S7 TG curves of the Ni@C-400, Ni@C-450 and Ni@C-500. Based on the weight loss in TG result, the proportions of carbon in Ni@C-400, Ni@C-450 and Ni@C-500 were calculated to be 33.95%, 29.37% and 26.56%, respectively.

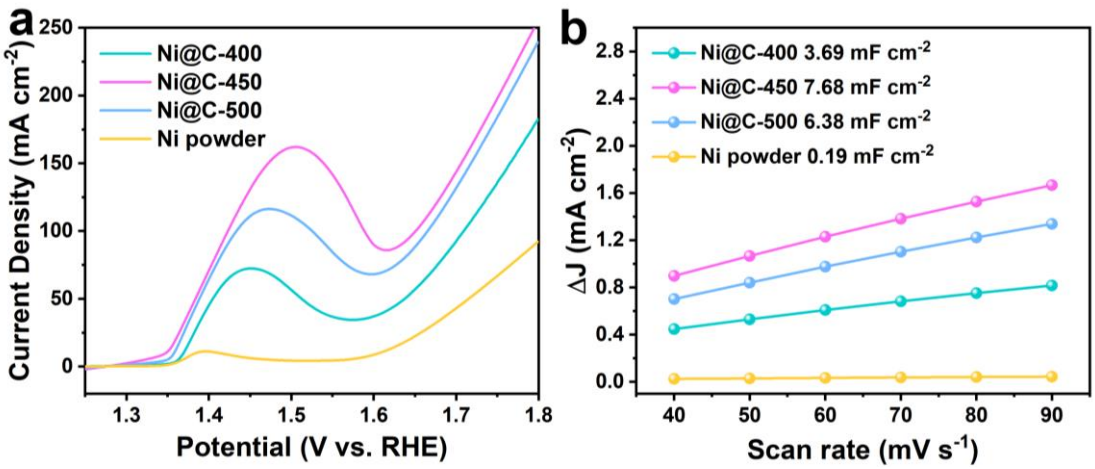

Fig. S8 (a) LSV curves and (b) C_{dl} of Ni powder, Ni@C-400, Ni@C-450 and Ni@C-500 in 1.0 M KOH with 10 mM HMF.

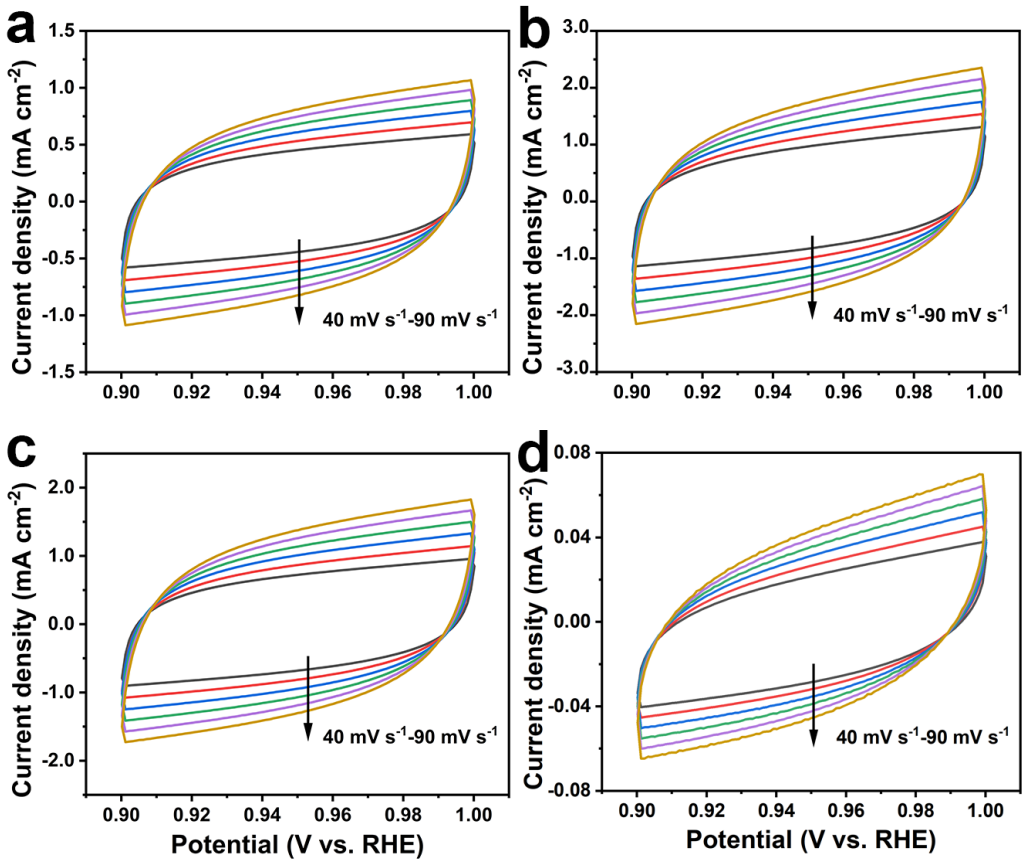

Fig. S9 Cyclic voltammograms of (a) Ni@C-400, (b) Ni@C-450, (c) Ni@C-500, (d) Ni powder at different scan rates.

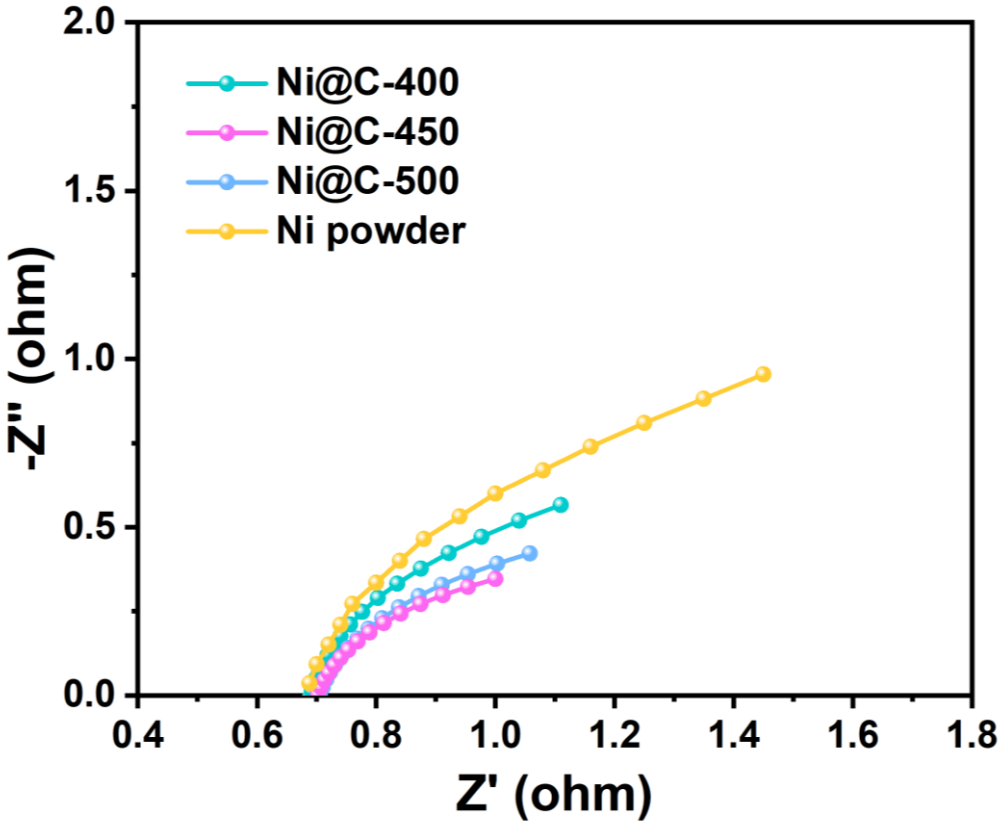

Fig. S10 Nyquist plots of Ni@C-400, Ni@C-450, Ni@C-500 and Ni powder at 1.34 V.

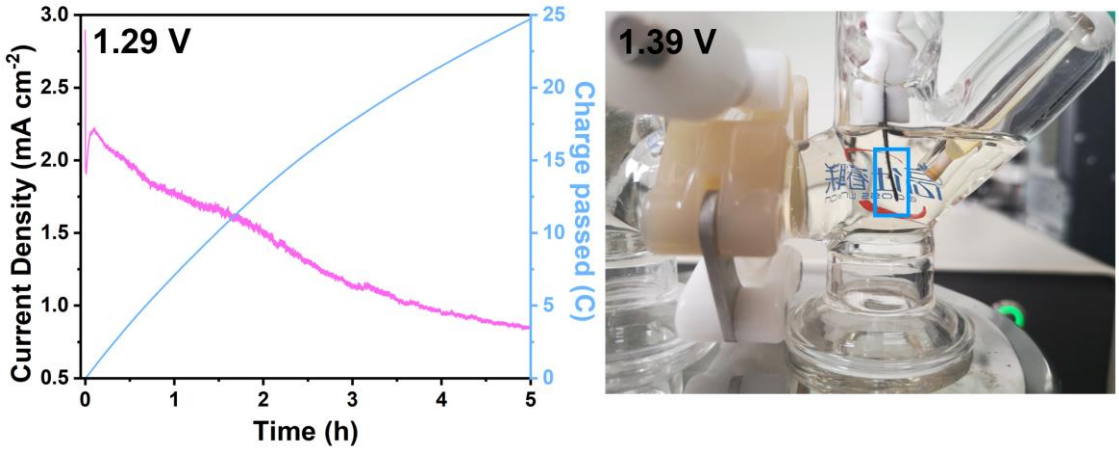

Fig. S11 (a) Corresponding current change and the accumulated charges over time of the chronoamperometry test of Ni@C-450 at 1.29 V in 1.0 M KOH with 10 mM HMF. (b) Oxygen generated from the electrode surface at 1.39 V.

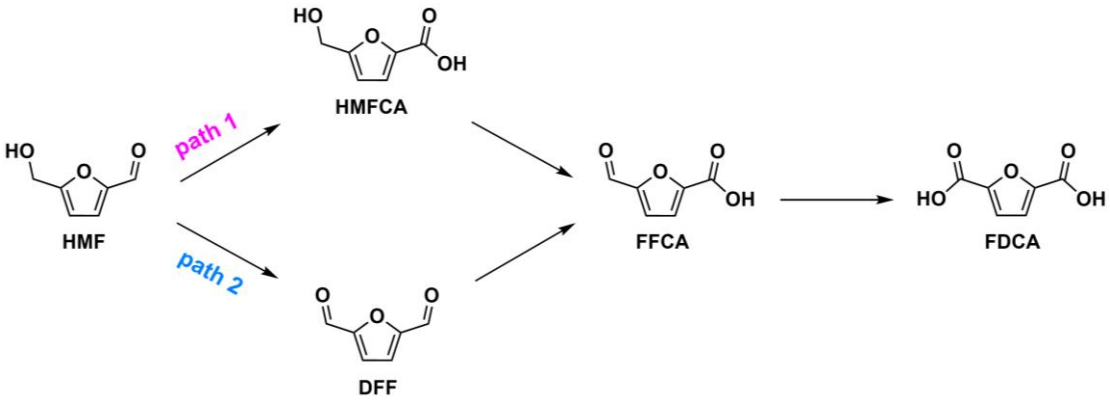

Fig. S12 Possible pathways for the oxidation of HMF to FDCA.

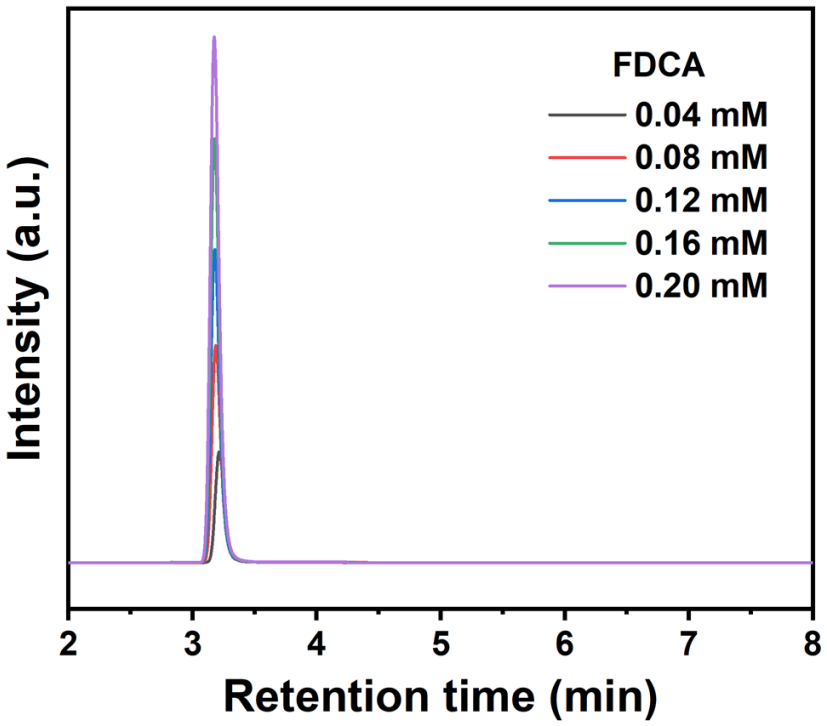

Fig. S13 HPLC traces of different concentrations of FDCA standard substance.

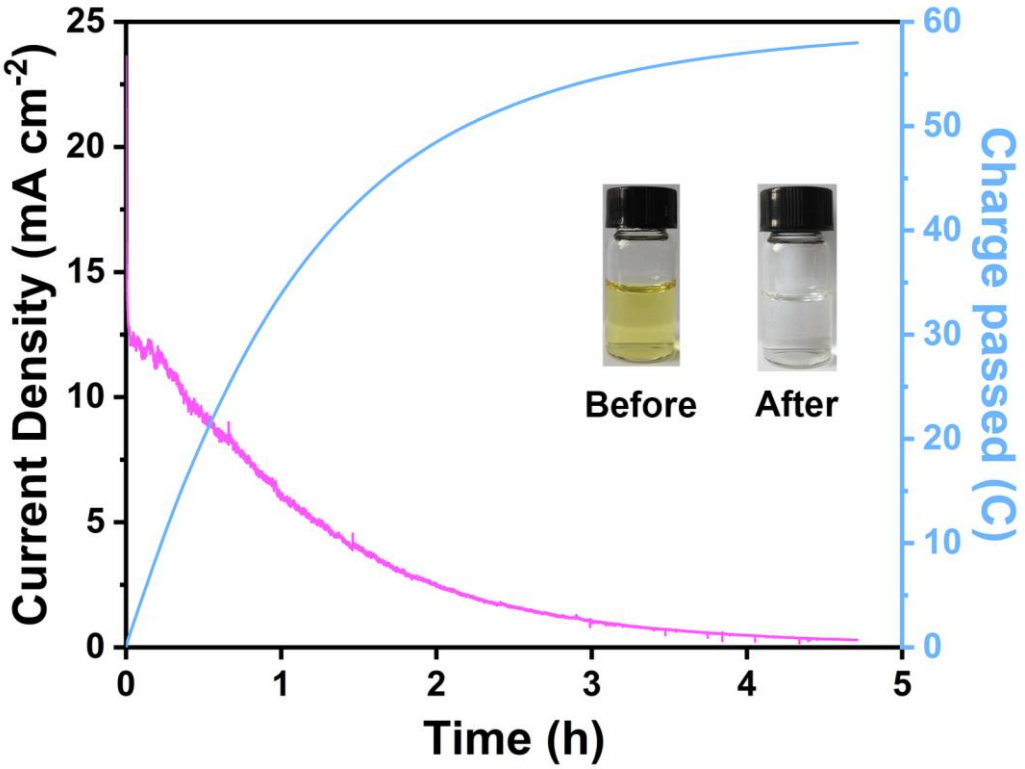

Fig. S14 Corresponding current change and the accumulated charges over time of the chronoamperometry test of Ni@C-450 at 1.34 V in 1.0 M KOH electrolyte with 10 mM HMF (insets: color change of the electrolyte before and after electrolysis).

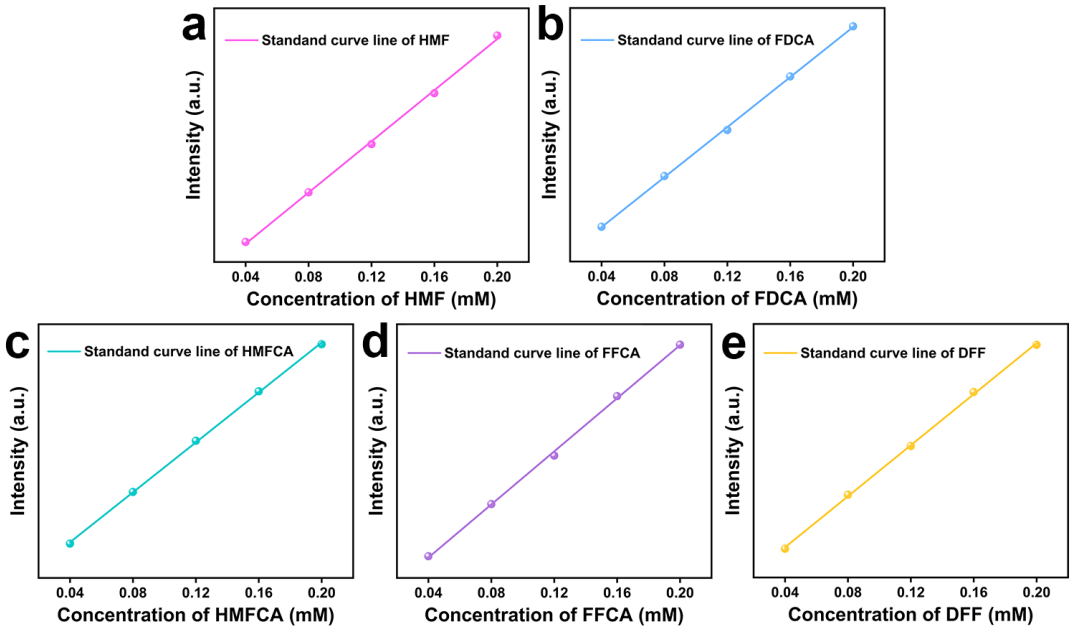

Fig. S15 Standard curves of the HPLC for (a) HMF, (b) FDCA, (c) HMFCA, (d) FFCA, (e) DFF.

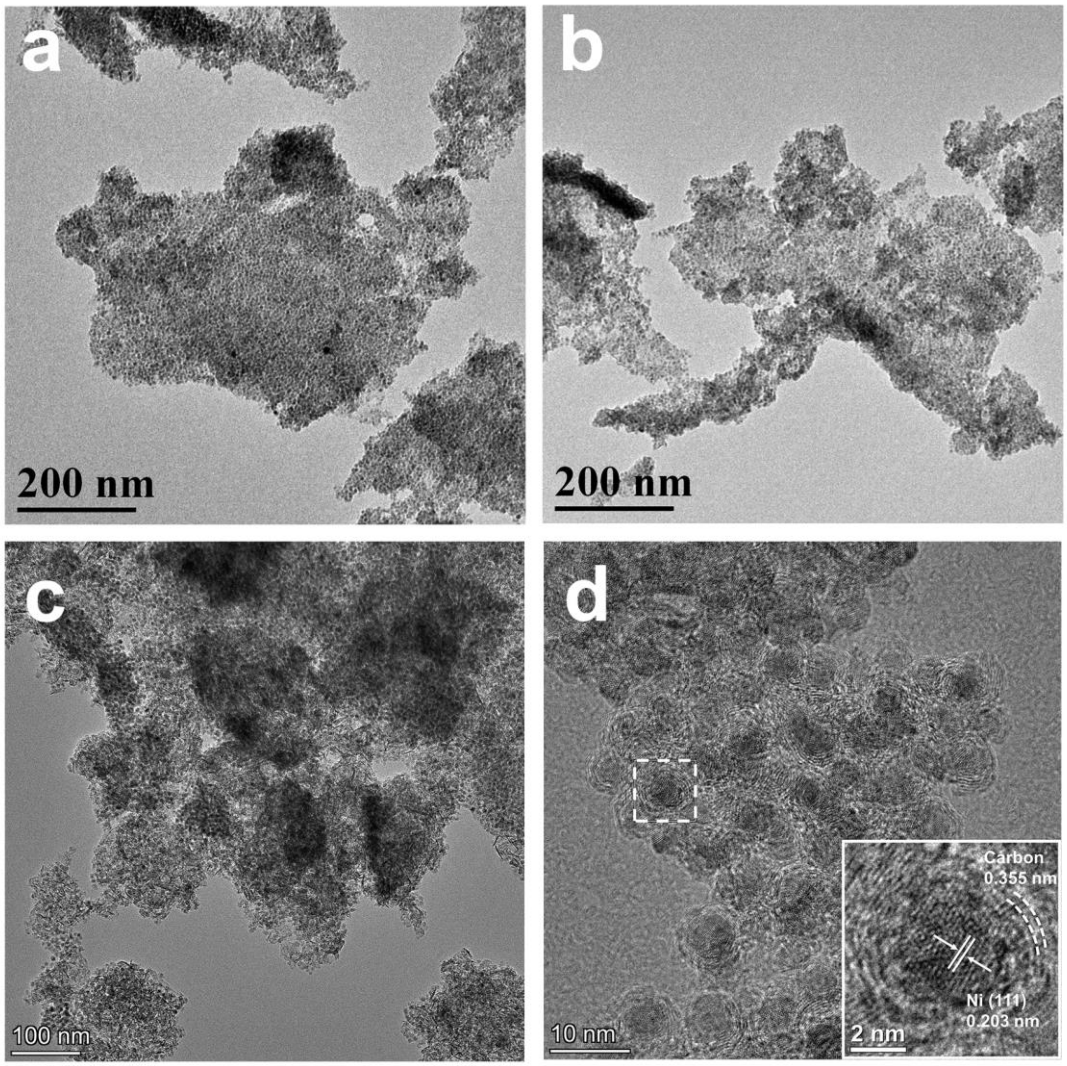

Fig. S16 (a, b) TEM images of Ni@C-450 after catalysis. (c, d) HRTEM images of Ni@C-450 after catalysis (The marked area represented the inserted HRTEM image).

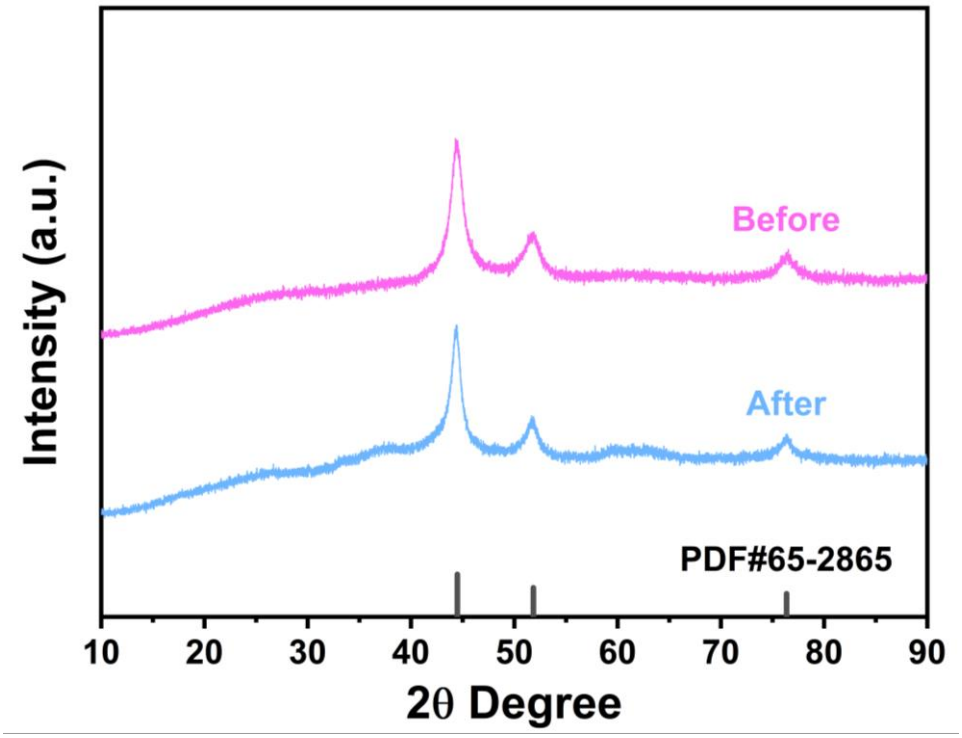

Fig. S17 XRD patterns of Ni@C-450 before and after electrolysis.

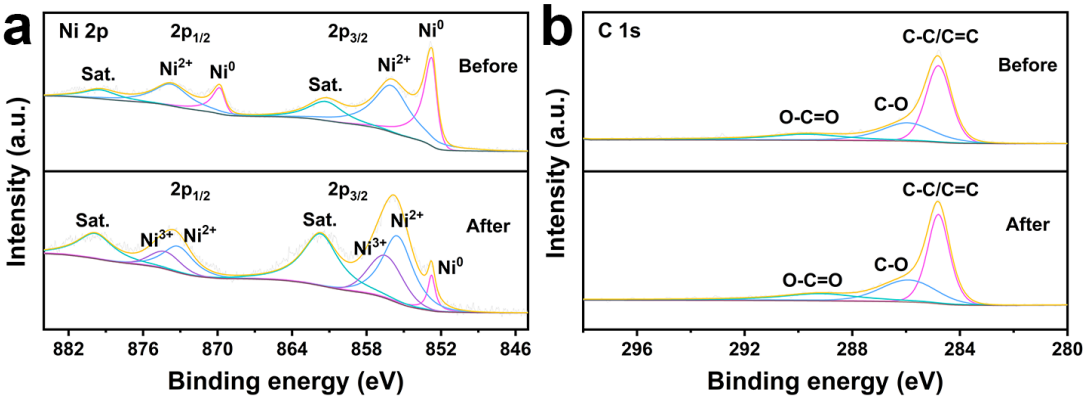

Fig. S18 XPS spectra of Ni@C-450 before and after electrolysis: (a) Ni 2p, (b) C 1s.

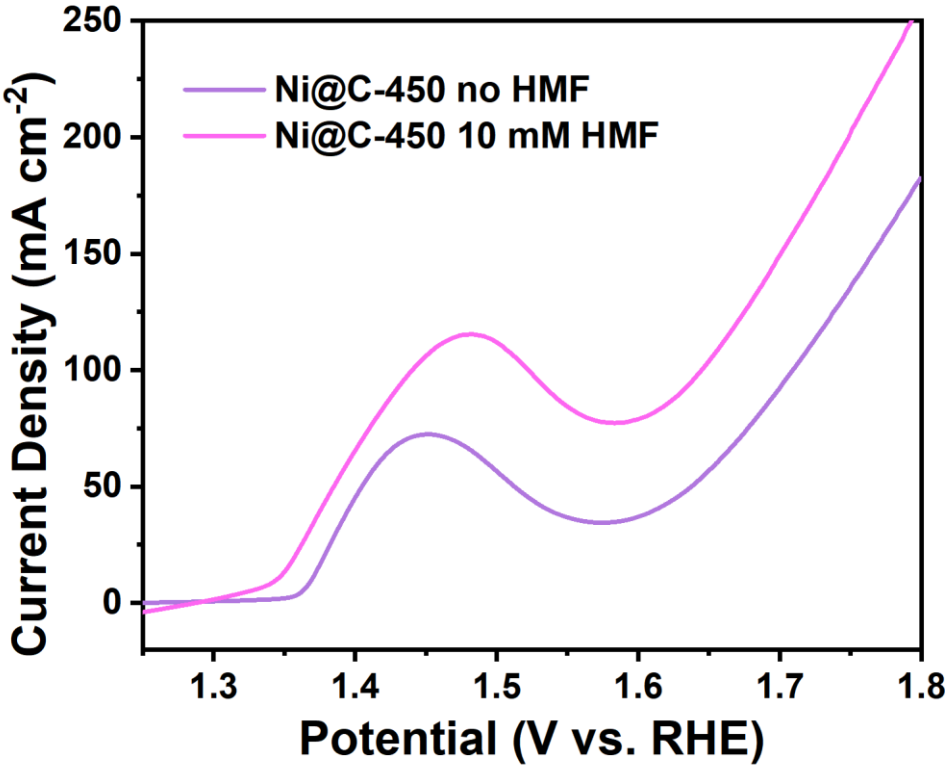

Fig. S19 LSV curves of Ni@C-450 in 1.0 M KOH electrolyte with and without 10 mM HMF after catalysis.

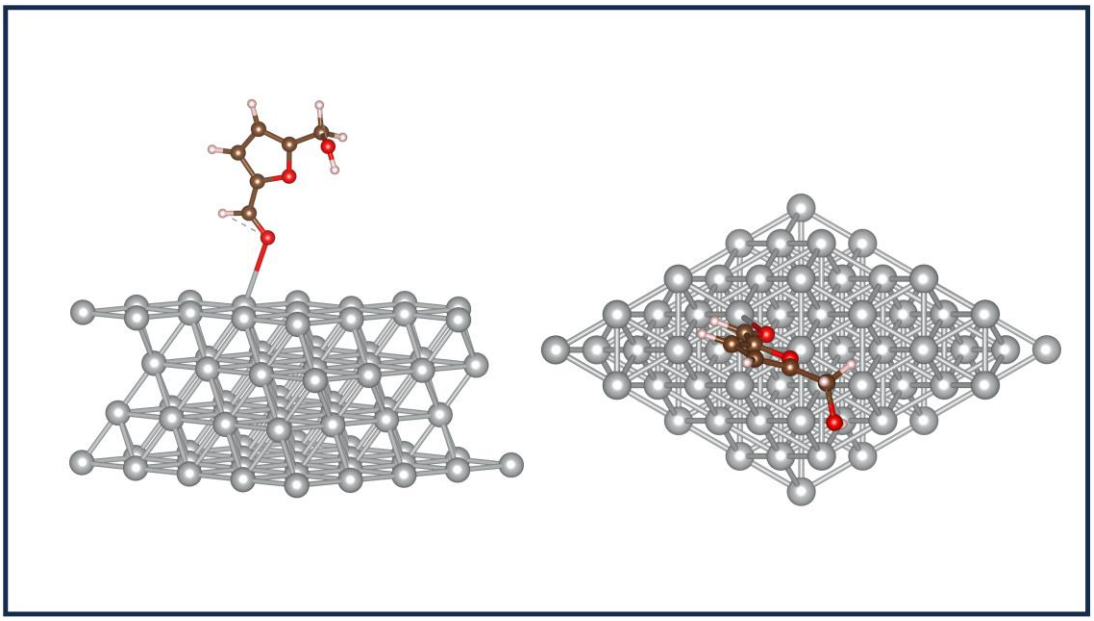

Fig. S20 Side and top views of an optimized structure of HMF on Ni.

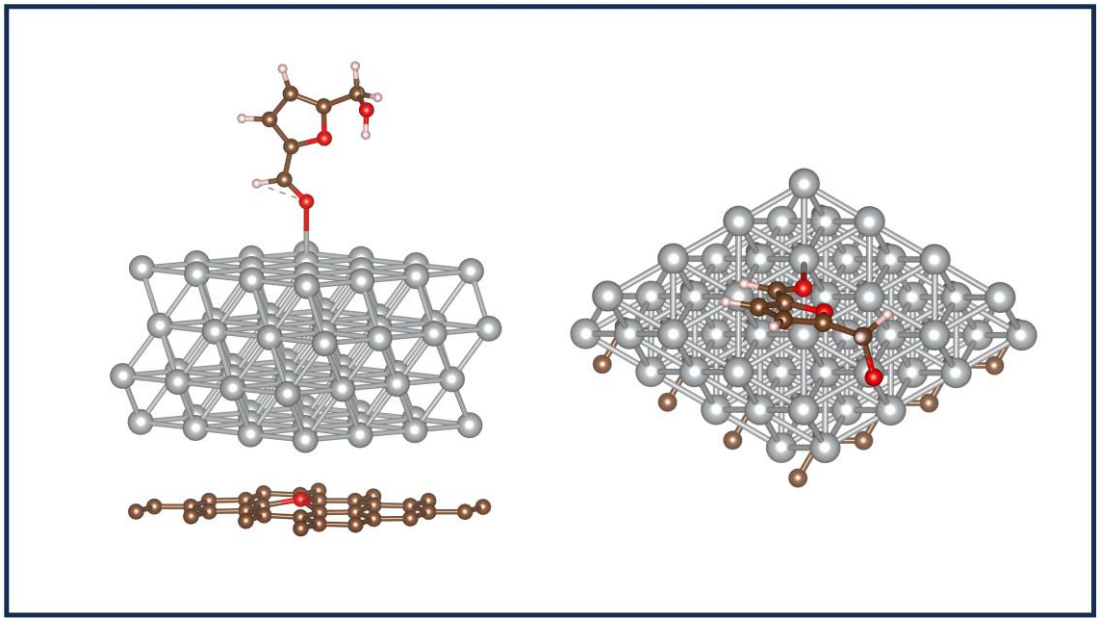

Fig. S21 Side and top views of an optimized structure of HMF on Ni@C-450.

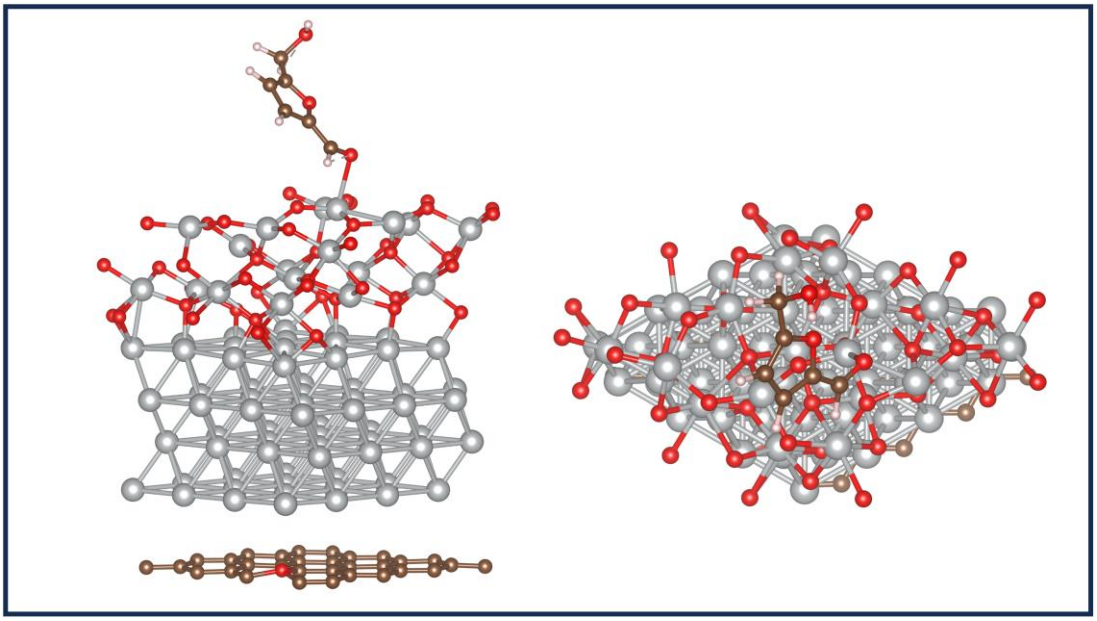

Fig. S22 Side and top views of an optimized structure of HMF on NiO-Ni@C-450.

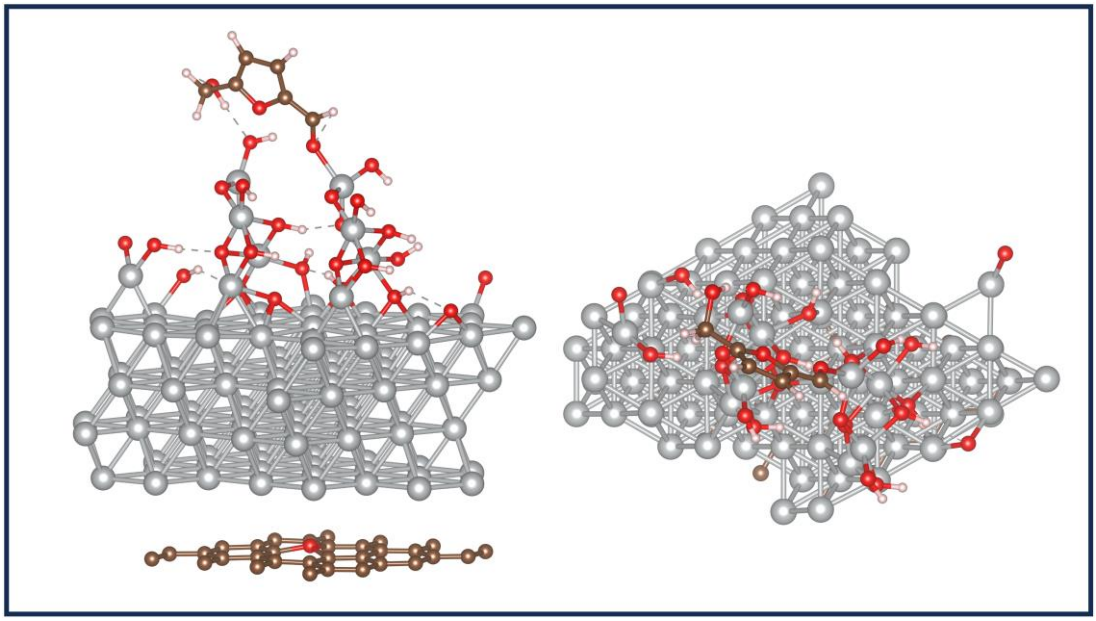

Fig. S23 Side and top views of an optimized structure of HMF on NiOOH-Ni@C-450.

Table S1 Recently reported high performance electrocatalytic HMF catalysts.

Catalysts	C_{HMF} (mM)	Potential (V *vs.* RHE)	Conversion (%)	FDCA Yield (%)	FE (%)	Reference
Ni@C-450	**10**	**1.34**	**100**	**97.7**	**97.4**	**This work**
FeCoNi-S@NF	10	1.45	95.68	94.83	94.71	7
MoO_2-FeP@C	10	1.424	99.4	98.6	97.8	8
$Ni_3S_2/MoS_2/NiMoO_4$	10	1.393	99.2	96.7	96.5	9
$NF@Co_3O_4/CeO_2$	10	1.40	98.0	94.5	97.5	10
NiVCo-LDHs	10	1.376	~	99.7	97.0	11
Mn-$5Ni_2P$	10	1.43	100	98.0	97.8	12
Co_3O_4-NiO-500	10	1.45	96.95	83.33	89.47	13
NiS_x/Ni_2P	10	1.46	~100	98.5	95.1	14
$NiSe_2$-$NiMoO_4$	10	1.50	98.0	96.5	95.6	15
NiO-N/C	10	1.473	99	84	96	16
$Ni(OH)_2$/CB	10	~	~100	98.1	~	17
NiO-CFP	10	1.43	82.4	79.7	61.0	18

Table S2 Adsorption energy of HMF on different surfaces.

Adsorbed sites	**$E_{ad/sub}$**	**E_{ad}**	**E_{sub}**	**E_{ads}**
Ni	-447.612	-351.971	-95.363	-0.27742
Ni@C-450	-741.360	-645.648	-95.363	-0.34948
NiO-Ni@C-450	-1017.076	-921.331	-95.363	-0.38184
NiOOH-Ni@C-450	-960.044	-863.832	-95.363	-0.84888

*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 S3 Unit-cell and position parameters of the optimized model for the adsorption of HMF on Ni.

		Ni	
a (Å)		9.82920	
b (Å)		9.82920	
c (Å)		36.01913	
α (deg)		90.0	
β (deg)		90.0	
γ (deg)		60.0	
Atom Coordinates	***x***	***y***	***z***
Ni1	0.00000	0.00000	0.41644
Ni2	0.83333	0.08333	0.47215
Ni3	0.08333	0.83333	0.47215
Ni4	0.08333	0.08333	0.47215
Ni5	0.83333	0.83333	0.47215
Ni6	0.00000	0.25000	0.41644
Ni7	0.25000	0.00000	0.41644
Ni8	0.25000	0.25000	0.41644
Ni9	0.83333	0.33333	0.47215
Ni10	0.00000	0.75000	0.41644
Ni11	0.25000	0.50000	0.41644
Ni12	0.25000	0.75000	0.41644
Ni13	0.00000	0.50000	0.41644
Ni14	0.83333	0.58333	0.47215
Ni15	0.08333	0.33333	0.47215
Ni16	0.08333	0.58333	0.47215
Ni17	0.33333	0.83333	0.47215
Ni18	0.50000	0.25000	0.41644
Ni19	0.75000	0.00000	0.41644
Ni20	0.75000	0.25000	0.41644
Ni21	0.50000	0.00000	0.41644
Ni22	0.33333	0.08333	0.47215
Ni23	0.58333	0.83333	0.47215

Ni24	0.58333	0.08333	0.47215
Ni25	0.50000	0.50000	0.41644
Ni26	0.33333	0.58333	0.47215
Ni27	0.58333	0.33333	0.47215
Ni28	0.58333	0.58333	0.47215
Ni29	0.33333	0.33333	0.47215
Ni30	0.50000	0.75000	0.41644
Ni31	0.75000	0.50000	0.41644
Ni32	0.75000	0.75000	0.41644
Ni33	0.66667	0.66667	0.52785
Ni34	0.50027	0.75013	0.58435
Ni35	0.75042	0.49992	0.58439
Ni36	0.75011	0.75002	0.58447
Ni37	0.50050	0.49997	0.58441
Ni38	0.66667	0.91667	0.52785
Ni39	0.91667	0.66667	0.52785
Ni40	0.91667	0.91667	0.52785
Ni41	0.50018	-0.00010	0.58427
Ni42	0.66667	0.41667	0.52785
Ni43	0.91667	0.16667	0.52785
Ni44	0.91667	0.41667	0.52785
Ni45	0.66667	0.16667	0.52785
Ni46	0.50039	0.24956	0.58450
Ni47	0.75011	0.99991	0.58440
Ni48	0.75045	0.24980	0.58436
Ni49	0.00018	0.49990	0.58420
Ni50	0.16667	0.91667	0.52785
Ni51	0.41667	0.66667	0.52785
Ni52	0.41667	0.91667	0.52785
Ni53	0.16667	0.66667	0.52785
Ni54	-0.00008	0.75009	0.58435
Ni55	0.25030	0.49998	0.58495
Ni56	0.25000	0.75029	0.58435
Ni57	0.16667	0.16667	0.52785

Ni58	0.00024	0.24989	0.58444
Ni59	0.25008	0.00008	0.58443
Ni60	0.25006	0.24989	0.58433
Ni61	0.00005	0.00007	0.58433
Ni62	0.16667	0.41667	0.52785
Ni63	0.41667	0.16667	0.52785
Ni64	0.41667	0.41667	0.52785
C1	0.54048	0.41681	0.77644
C2	0.43823	0.37520	0.79185
C3	0.33870	0.37993	0.76279
C4	0.38621	0.42336	0.73096
C5	0.66919	0.43675	0.79259
C6	0.32511	0.44608	0.69343
H1	0.43580	0.34555	0.82079
H2	0.24297	0.35493	0.76469
H3	0.65960	0.43612	0.82297
H4	0.65349	0.55176	0.78415
H5	0.22354	0.42535	0.69100
H6	0.84616	0.32295	0.75782
O1	0.51018	0.44635	0.73934
O2	0.82477	0.31235	0.78372
O3	0.37520	0.48415	0.66640

Table S4 Unit-cell and position parameters of the optimized model for the adsorption of HMF on Ni@C-450.

		Ni@C-450	
a (Å)		9.82920	
b (Å)		9.82920	
c (Å)		36.01913	
α (deg)		90.0	
β (deg)		90.0	
γ (deg)		60.0	
Atom Coordinates	***x***	***y***	***z***
C1	0.89141	0.92628	0.32118
C2	0.97513	0.00988	0.31986
C3	0.89194	0.17663	0.31902
C4	0.72418	0.26035	0.32022
C5	0.64857	0.42331	0.31969
C6	0.38853	0.68328	0.32032
C7	0.22553	0.75893	0.32055
C8	0.22525	0.00991	0.31876
C9	0.14185	0.17668	0.31844
C10	0.97511	0.26004	0.31842
C11	0.89191	0.42663	0.31906
C12	0.72415	0.51071	0.32024
C13	0.64231	0.67709	0.32203
C14	0.47594	0.75896	0.32068
C15	0.3918	0.92676	0.31951
C16	0.14188	0.92671	0.31931
C17	0.39179	0.17666	0.31952
C18	0.47541	0.0099	0.32019
C19	0.14088	0.67717	0.32192
C20	0.22547	0.51079	0.32057
C21	0.38848	0.42338	0.32034
C22	0.47592	0.26032	0.32068
C23	0.64231	0.17581	0.32199

C24	0.72539	0.00966	0.32167
C25	0.97484	0.76019	0.32161
C26	0.6427	0.92626	0.32136
C27	0.72539	0.76019	0.32169
C28	0.8914	0.67752	0.3212
C29	0.97508	0.51021	0.3199
C30	0.14183	0.42665	0.31935
C31	0.22524	0.26006	0.31878
Ni1	0.17379	0.91249	0.51785
Ni2	0.42374	0.66282	0.51811
Ni3	0.42374	0.91253	0.51793
Ni4	0.17347	0.66288	0.51803
Ni5	0.00704	0.74579	0.57441
Ni6	0.25674	0.49602	0.57465
Ni7	0.25697	0.7455	0.57553
Ni8	0.25694	0.99576	0.57456
Ni9	0.00672	0.24586	0.57468
Ni10	0.00673	0.49597	0.57449
Ni11	0.2567	0.24602	0.57462
Ni12	0.00692	0.99583	0.57438
Ni13	0.17384	0.41276	0.51785
Ni14	0.4237	0.41261	0.51814
Ni15	0.17366	0.16274	0.51799
Ni16	0.42376	0.1628	0.51793
Ni17	0.00792	0.99553	0.40592
Ni18	0.50672	0.24611	0.57471
Ni19	0.50729	0.99562	0.406
Ni20	0.75753	0.24559	0.40599
Ni21	0.75775	0.99546	0.40569
Ni22	0.5081	0.2456	0.40571
Ni23	0.3407	0.82898	0.46224
Ni24	0.09046	0.57929	0.46222
Ni25	0.09044	0.32923	0.46238
Ni26	0.84049	0.57907	0.46231

Ni27	0.00804	0.49493	0.40593
Ni28	0.34054	0.07914	0.46244
Ni29	0.25808	0.745	0.40604
Ni30	0.00818	0.74512	0.4054
Ni31	0.84026	0.3292	0.46225
Ni32	0.25777	0.24539	0.40609
Ni33	0.25774	0.99527	0.40609
Ni34	0.00774	0.24539	0.40608
Ni35	0.84067	0.829	0.46194
Ni36	0.09042	0.07913	0.46237
Ni37	0.09044	0.8291	0.46221
Ni38	0.84044	0.07903	0.46232
Ni39	0.25815	0.49533	0.40605
Ni40	0.59059	0.82904	0.46224
Ni41	0.59057	0.07923	0.46223
Ni42	0.50771	0.49537	0.40713
Ni43	0.67373	0.16258	0.51806
Ni44	0.92357	0.41271	0.51793
Ni45	0.92356	0.1628	0.51792
Ni46	0.67384	0.41265	0.51805
Ni47	0.50705	0.99625	0.57446
Ni48	0.92357	0.91259	0.51775
Ni49	0.92366	0.66282	0.51774
Ni50	0.67387	0.91261	0.51768
Ni51	0.50669	0.49601	0.57475
Ni52	0.75709	0.7464	0.57447
Ni53	0.75668	0.49633	0.57467
Ni54	0.50693	0.74612	0.57463
Ni55	0.67378	0.66288	0.51804
Ni56	0.75772	0.7452	0.40574
Ni57	0.7575	0.49537	0.40594
Ni58	0.50806	0.74481	0.40574
Ni59	0.34068	0.32909	0.46224
Ni60	0.59063	0.57941	0.46267

Ni61	0.59056	0.32878	0.46269
Ni62	0.34018	0.57934	0.46274
Ni63	0.75702	0.99616	0.57455
Ni64	0.75669	0.24618	0.57463
O1	0.47543	0.50988	0.32769
C1	0.50176	0.57233	0.75782
C2	0.41701	0.50532	0.77094
C3	0.32808	0.49994	0.74046
C4	0.36371	0.56388	0.71028
C5	0.62259	0.60354	0.77409
C6	0.30916	0.5889	0.67221
H1	0.42028	0.46457	0.79917
H2	0.24756	0.45449	0.74035
H3	0.62031	0.59567	0.80446
H4	0.59607	0.72349	0.76663
H5	0.22344	0.54918	0.66628
H6	0.7808	0.48485	0.73581
O1	0.46988	0.60884	0.72103
O2	0.77932	0.48914	0.76285
O3	0.35133	0.64858	0.64777

Table S5 Unit-cell and position parameters of the optimized model for the adsorption of HMF on NiO-Ni@C-450.

	NiO-Ni@C-450		
a (Å)	9.82920		
b (Å)	9.82920		
c (Å)	36.01913		
α (deg)	90.0		
β (deg)	90.0		
γ (deg)	60.0		
Atom Coordinates	***x***	***y***	***z***
C1	0.1471	0.51367	0.04633
C2	0.48093	0.84744	0.04393
C3	0.39752	0.01403	0.04449
C4	0.23077	0.09759	0.04505
C5	0.14709	0.26491	0.04634
C6	0.98108	0.34757	0.04683
C7	0.89839	0.51364	0.04651
C8	0.98108	0.59704	0.04682
C9	0.898	0.76319	0.04714
C10	0.73162	0.84771	0.04583
C11	0.64417	0.01076	0.04548
C12	0.48116	0.09817	0.04571
C13	0.39657	0.26456	0.04707
C14	0.7311	0.59728	0.04533
C15	0.64748	0.76405	0.04467
C16	0.23053	0.34757	0.04675
C17	0.64749	0.51414	0.04465
C18	0.39757	0.51409	0.04445
C19	0.23082	0.59726	0.04501
C20	0.14763	0.76401	0.04417
C21	0.97987	0.84773	0.04536
C22	0.64422	0.27066	0.04546
C23	0.48122	0.34632	0.04569

C24	0.90426	0.0107	0.04484
C25	0.39754	0.76406	0.04359
C26	0.23081	0.84742	0.04357
C27	0.14761	0.01401	0.0442
C28	0.97984	0.0981	0.04539
C29	0.898	0.26447	0.04717
C30	0.73163	0.34634	0.04583
C31	0.48094	0.5973	0.0439
Ni1	0.84632	0.1668	0.18781
Ni2	0.75312	0.34086	0.29813
Ni3	0.59637	0.91647	0.18739
Ni4	0.76375	0.33219	0.13089
Ni5	0.01319	0.08275	0.13109
Ni6	0.01341	0.33258	0.13089
Ni7	0.92947	0.25026	0.24318
Ni8	0.00974	0.08465	0.29838
Ni9	0.17925	0.75018	0.24306
Ni10	0.75889	0.08127	0.29531
Ni11	0.92957	0.49999	0.24282
Ni12	0.17935	0.2502	0.24289
Ni13	0.17926	0.49998	0.24289
Ni14	0.76674	0.58209	0.30248
Ni15	0.92954	0.00003	0.2432
Ni16	0.17927	0.00009	0.24307
Ni17	0.84625	0.91617	0.18783
Ni18	0.00733	0.33393	0.29664
Ni19	0.59587	0.16673	0.18789
Ni20	0.0499	0.091	0.36839
Ni21	0.01336	0.83203	0.30039
Ni22	0.84278	0.9122	0.4391
Ni23	0.14393	0.48078	0.4128
Ni24	0.42486	0.46852	0.38071
Ni25	0.5397	0.56084	0.46376
Ni26	0.92942	0.74996	0.2432

Ni27	0.09335	0.76294	0.37477
Ni28	0.18925	0.85333	0.44872
Ni29	0.84321	0.21889	0.42952
Ni30	0.01474	0.5847	0.2979
Ni31	0.77715	0.60008	0.45263
Ni32	0.03472	0.37774	0.35991
Ni33	0.51112	0.24665	0.44759
Ni34	0.76485	0.76037	0.37609
Ni35	0.4239	0.0932	0.3743
Ni36	0.73047	0.09668	0.36736
Ni37	0.54931	0.90117	0.43817
Ni38	0.42015	0.78336	0.38012
Ni39	0.72517	0.43807	0.36874
Ni40	0.22824	0.14826	0.44476
Ni41	0.76341	0.08275	0.13228
Ni42	0.84628	0.41643	0.18738
Ni43	0.5098	0.58509	0.30401
Ni44	0.76349	0.83231	0.29843
Ni45	0.26361	0.58291	0.13107
Ni46	0.67945	0.75018	0.24308
Ni47	0.67939	0.99999	0.24328
Ni48	0.42953	0.00015	0.243
Ni49	0.26446	0.5846	0.2998
Ni50	0.51347	0.83452	0.30267
Ni51	0.25652	0.09164	0.30181
Ni52	0.2634	0.83599	0.30001
Ni53	0.84626	0.66661	0.18738
Ni54	0.50578	0.33375	0.30257
Ni55	0.50962	0.08382	0.29812
Ni56	0.25961	0.33844	0.29818
Ni57	0.42917	0.25027	0.24318
Ni58	0.67943	0.49991	0.24307
Ni59	0.67944	0.25021	0.24326
Ni60	0.42948	0.49987	0.243

Ni61	0.76298	0.583	0.13115
Ni62	0.01322	0.83297	0.13114
Ni63	0.42935	0.75013	0.24314
Ni64	0.76379	0.83298	0.13086
Ni65	0.51384	0.08271	0.13119
Ni66	0.09613	0.66641	0.18746
Ni67	0.34613	0.41648	0.18736
Ni68	0.34611	0.66652	0.18752
Ni69	0.01344	0.58285	0.13083
Ni70	0.26344	0.83277	0.13123
Ni71	0.51344	0.58265	0.13123
Ni72	0.51346	0.83278	0.13124
Ni73	0.09595	0.91659	0.1874
Ni74	0.09637	0.41638	0.18709
Ni75	0.51377	0.33238	0.13119
Ni76	0.59623	0.66652	0.18759
Ni77	0.26373	0.08232	0.13107
Ni78	0.09618	0.16645	0.18746
Ni79	0.34614	0.91661	0.18752
Ni80	0.34615	0.16667	0.18737
Ni81	0.59639	0.41636	0.18739
Ni82	0.26387	0.33251	0.13054
O1	0.43542	0.1093	0.45712
O2	0.27503	0.72466	0.40304
O3	0.66013	0.70308	0.41202
O4	0.642	0.3165	0.38759
O5	0.02283	0.84405	0.46285
O6	0.9805	0.68505	0.40421
O7	0.38937	0.758	0.46526
O8	0.35634	0.34875	0.4054
O9	0.74172	0.80221	0.4639
O10	0.84856	0.86085	0.34199
O11	0.91328	0.03979	0.39512
O12	0.37314	0.97052	0.40752

O13	0.51001	0.583	0.35647
O14	0.48353	0.4198	0.46817
O15	0.82772	0.17021	0.33017
O16	0.5418	0.84805	0.3519
O17	0.19689	0.1591	0.3516
O18	0.52877	0.16977	0.34214
O19	0.92802	0.2965	0.38627
O20	0.106	0.35668	0.44121
O21	0.0811	0.08525	0.44732
O22	0.7531	0.42673	0.45366
O23	0.82386	0.55915	0.35333
O24	0.13979	0.46548	0.33744
O25	0.13547	0.89254	0.34274
O26	0.73113	0.09726	0.05284
O27	0.73489	0.12821	0.45501
O28	0.68395	0.96398	0.39962
C1	0.36219	0.48377	0.61269
C2	0.44805	0.32193	0.614
C3	0.56936	0.27446	0.58731
C4	0.55096	0.41049	0.57127
C5	0.22191	0.60133	0.63369
C6	0.63548	0.43312	0.54144
H1	0.42396	0.24726	0.63176
H2	0.65877	0.15575	0.5799
H3	0.16738	0.53929	0.64715
H4	0.13553	0.68939	0.6146
H5	0.73067	0.32228	0.52918
H6	0.34314	0.61431	0.67565
O1	0.42413	0.53904	0.58685
O2	0.25636	0.68931	0.66028
O3	0.60428	0.56333	0.52916

Table S6 Unit-cell and position parameters of the optimized model for the adsorption of HMF on NiOOH-Ni@C-450.

	NiOOH-Ni@C-450		
a (Å)	9.82920		
b (Å)	9.82920		
c (Å)	36.01913		
α (deg)	90.0		
β (deg)	90.0		
γ (deg)	60.0		
Atom Coordinates	***x***	***y***	***z***
C1	0.89141	0.92628	0.04077
C2	0.22524	0.26006	0.03838
C3	0.14183	0.42665	0.03894
C4	0.8914	0.67752	0.04079
C5	0.72539	0.76019	0.04128
C6	0.6427	0.92626	0.04095
C7	0.97484	0.76019	0.0412
C8	0.72539	0.00966	0.04126
C9	0.64231	0.17581	0.04158
C10	0.47592	0.26032	0.04028
C11	0.38848	0.42338	0.03993
C12	0.22547	0.51079	0.04016
C13	0.14088	0.67717	0.04151
C14	0.47541	0.0099	0.03978
C15	0.39179	0.17666	0.03911
C16	0.97508	0.51021	0.0395
C17	0.3918	0.92676	0.0391
C18	0.97513	0.00988	0.03945
C19	0.89194	0.17663	0.03861
C20	0.72418	0.26035	0.03981
C21	0.14188	0.92671	0.0389
C22	0.38853	0.68328	0.03991
C23	0.22553	0.75893	0.04014

C24	0.64857	0.42331	0.03929
C25	0.14185	0.17668	0.03804
C26	0.97511	0.26004	0.03802
C27	0.89191	0.42663	0.03865
C28	0.72415	0.51071	0.03983
C29	0.64231	0.67709	0.04162
C30	0.47594	0.75896	0.04028
C31	0.22525	0.00991	0.03835
H1	0.89641	0.57016	0.40484
H2	0.52211	0.83192	0.45552
H3	0.15541	0.82542	0.36525
H4	0.3941	0.67917	0.34912
H5	0.62178	0.87564	0.38223
H6	0.57977	0.13174	0.45565
H7	0.0941	0.26807	0.38163
H8	0.08617	0.72094	0.49774
H9	0.0927	0.18073	0.44952
H10	0.89741	0.55647	0.34624
H11	0.4186	0.52945	0.405
H12	0.59109	0.22724	0.38626
Ni1	0.76181	0.48647	0.29342
Ni2	0.49368	0.75323	0.29306
Ni3	0.75772	0.7452	0.12533
Ni4	0.67378	0.66288	0.23763
Ni5	0.67387	0.91261	0.23727
Ni6	0.50626	0.49381	0.29684
Ni7	0.92366	0.66282	0.23734
Ni8	0.92357	0.91259	0.23734
Ni9	0.50323	0.99643	0.29849
Ni10	0.67384	0.41265	0.23764
Ni11	0.92356	0.1628	0.23751
Ni12	0.7575	0.49537	0.12553
Ni13	0.74695	0.75038	0.2947
Ni14	0.50806	0.74481	0.12534

Ni15	0.55144	0.58478	0.45608
Ni16	0.59063	0.57941	0.18226
Ni17	0.59056	0.32878	0.18228
Ni18	0.34018	0.57934	0.18233
Ni19	0.75202	0.99701	0.2939
Ni20	0.75596	0.24231	0.29331
Ni21	0.39565	0.21467	0.34812
Ni22	0.85791	0.33072	0.42049
Ni23	0.92357	0.41271	0.23752
Ni24	0.35967	0.29902	0.42356
Ni25	0.06266	0.58204	0.44933
Ni26	0.64811	0.61345	0.37493
Ni27	0.88666	0.24747	0.34639
Ni28	0.19495	0.54565	0.36953
Ni29	0.34068	0.32909	0.18184
Ni30	0.67373	0.16258	0.23765
Ni31	0.09044	0.8291	0.1818
Ni32	0.59057	0.07923	0.18183
Ni33	0.51147	0.24246	0.29237
Ni34	0.00792	0.99553	0.12552
Ni35	0.42376	0.1628	0.23753
Ni36	0.17366	0.16274	0.23759
Ni37	0.4237	0.41261	0.23773
Ni38	0.17384	0.41276	0.23745
Ni39	0.50771	0.49537	0.12673
Ni40	0.25742	0.23664	0.29346
Ni41	0.50729	0.99562	0.1256
Ni42	0.01235	0.48464	0.29121
Ni43	0.25019	0.99872	0.2941
Ni44	0.23775	0.75713	0.29624
Ni45	0.25617	0.49135	0.29333
Ni46	0.99606	0.7526	0.29357
Ni47	0.17347	0.66288	0.23762
Ni48	0.42374	0.91253	0.23752

Ni49	0.42374	0.66282	0.23771
Ni50	0.17379	0.91249	0.23745
Ni51	0.01041	0.24153	0.29239
Ni52	0.75753	0.24559	0.12558
Ni53	0.99691	0.00353	0.29578
Ni54	0.75775	0.99546	0.12528
Ni55	0.25815	0.49533	0.12564
Ni56	0.84044	0.07903	0.18191
Ni57	0.09042	0.07913	0.18196
Ni58	0.84067	0.829	0.18153
Ni59	0.00774	0.24539	0.12567
Ni60	0.25774	0.99527	0.12568
Ni61	0.25777	0.24539	0.12569
Ni62	0.84026	0.3292	0.18184
Ni63	0.59059	0.82904	0.18183
Ni64	0.25808	0.745	0.12563
Ni65	0.00818	0.74512	0.12499
Ni66	0.3407	0.82898	0.18184
Ni67	0.09046	0.57929	0.18181
Ni68	0.5081	0.2456	0.12531
Ni69	0.84049	0.57907	0.1819
Ni70	0.00804	0.49493	0.12552
Ni71	0.34054	0.07914	0.18204
Ni72	0.09044	0.32923	0.18197
O1	0.79132	0.59465	0.33591
O2	0.80627	0.55243	0.41167
O3	0.42423	0.39307	0.32965
O4	0.72776	0.3807	0.37672
O5	0.21925	0.72874	0.35122
O6	0.50243	0.6373	0.33667
O7	0.23049	0.33557	0.37936
O8	0.07124	0.5821	0.32708
O9	0.5096	0.76876	0.47482
O10	0.98486	0.22489	0.4588

O11	0.56363	0.83767	0.36752
O12	0.00498	0.6963	0.49031
O13	0.49922	0.63809	0.41011
O14	0.53306	0.17149	0.39105
O15	0.02599	0.22046	0.38557
O16	0.0219	0.63336	0.40349
O17	0.18195	0.38458	0.45062
O18	0.47543	0.50988	0.04729
O19	0.69718	0.39103	0.45259
O20	0.33232	0.50317	0.40905
O21	0.47052	0.19526	0.46397
C1	0.20214	0.43084	0.5678
C2	0.28852	0.39299	0.60041
C3	0.41999	0.41096	0.5933
C4	0.40674	0.46036	0.55672
C5	0.05195	0.43889	0.55658
C6	0.50033	0.49751	0.53333
H1	0.2593	0.35595	0.62611
H2	0.51396	0.39137	0.61223
H3	0.02235	0.37613	0.57738
H4	0.06986	0.37814	0.52964
H5	0.61052	0.48495	0.54473
H6	0.9366	0.64417	0.53199
O1	0.27311	0.47218	0.54137
O2	0.9241	0.59671	0.55515
O3	0.45706	0.54394	0.50094

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