Supplementary Information (SI) for Chemical Science.

Supplementary Information

Pd-Cu Dual Sites Turning H Adsorption for Efficient Electrocatalytic Hydrogenation of HMF

Materials and methods

1. Materials

$Cu(NO_3)_2·3H_2O$ (99 %), $PdCl_2$ (98 %), NaCl (99 %), $C_6H_{12}O_6$ (95 %), and $KHCO_3$ (99.5 %) were purchased from Aladdin. Purified water (ρ > 18 MΩ cm) was produced in the laboratory.

2. Synthesis of Pd/Cu@3DC catalysts

First, 18.3 g of NaCl, 0.469 g of glucose, $Cu(NO_3)_2·3H_2O$ and $PdCl_2$ in different ratios (n_{Cu}:n_{Pd} = 99:1, 97:3, 95:5) were dissolved in 60 mL of purified water with stirring. The solution was then freeze-dried at -20 °C for 20 h. The yellow-green powder obtained was calcined at 700 °C in an H_2/Ar atmosphere for 2 h at a ramp rate of 10 °C/min. The resulting product was washed three times with purified water to remove NaCl and dried overnight to obtain the Pd/Cu@3DC catalyst.

3. Material characterization

Scanning electron microscopy (SEM) measurements were performed using a Hitachi S4800 at 15 kV. Transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDS) and scanning transmission electron microscopy measurements were carried out using a JEM-F200 equipped with an EDS detector (at 200 kV) to analyze the microstructure of the samples. X-ray diffraction (XRD) patterns were obtained using a Bruker D8 with Cu Kα radiation, operated at 40 mA and 40 kV. X-ray photoelectron spectroscopy (XPS) was performed using an ESCALAB 250Xi with a standard Al Kα X-ray source, standard lens pattern, and an analyzer passing energy at 20 eV.

4. Electrochemical measurements

5 mg electrocatalyst was dispersed in 950 μL of anhydrous ethanol and 50 μL of 5 wt% Nafion solution by sonication for 30 min, and then the ink was dripped onto a 3 mm diameter L-shaped glassy carbon electrode with a loading of 0.42 mg cm^{-2}. All electrochemical tests were carried out at room temperature using a three-electrode setup on a CHI760E in an aqueous 0.5 M $KHCO_3$ solution saturated with N_2. An H-type electrolytic cell was used with an Ag/AgCl electrode as the reference electrode and a graphite rod as the counter electrode. At first, the samples were reduced by galvanostatic at 10 Ma for 10 min. All linear sweep voltammetry (LSV) tests were

performed at a scan rate of 5 mV s^{-1}. Electrochemical Impedance Spectroscopy (EIS) tests were performed over a frequency range from 10^6 to 0.05 Hz. For product testing, electrocatalyst ink was uniformly coated on carbon paper and used as the working electrode at constant current -0.90 V to -1.10 V (vs. Ag/AgCl) potentials. To evaluate the ECSA (electrochemically active surface area) in terms of the double-layer capacitance (C_{dl}) using the equation ECSA $=C_{\mathrm{dl}}/C_{\mathrm{s}}$, where C_{s} refers to the surface bilayer capacitance of the ideal at electrode (40 μF cm^{-2}, and cyclic voltammogram (CV) curves were collected in the non-faradaic region (-0.2 V~ -0.35 V vs. Ag/AgCl) at varied scan rates from 20 to 100 mV s^{-1}.

PEM test: the catalyst ink was sprayed on the carbon paper with a loading of 1 mg cm^{-2}. The proton exchange membrane (PEM)-based HMF hydrogenation electrolysis was performed on a single cell with serpentine flow fields (25 cm^{-2}). Titanium felt and carbon paper were taken as the anode and cathode, and Nafion 115 was used as the PEM. An aqueous 0.5 M $KHCO_3$ solution with or without 10 mM HMF flowed into the cathode or anode with a flow rate of 1 ml min^{-1} respectively.

5. Product analysis.

The substrates and products were analyzed by high-performance liquid chromatography (HPLC). For HPLC sample preparation, 20 μ L of electrolyte was collected in a sample vial before and after electrolysis and diluted with 980 μL of deionized water and filtered to obtain the HPLC sample. The HPLC is equipped with Ultimate XB-C18 column (4.6mm × 250mm ,5μm) and a UV-visible detector. The detector's wavelength was set to 230 nm. The chromatographic column was operated at 45 °C with isocratic elution of water and acetonitrile, and the flow rate was set at 0.6 mL min^{-1}, the ratio of water to acetonitrile was 85%:15%. HMF and BHMF eluted at around 8.8 min and 7.6 min, respectively, and 5-MF eluted at around 21.9 min.

HMF conversion (Conv.), product selectivity (Sel.), and FE were calculated by the following equations.

$$\text{Conv. (HMF) (\%)} = n\,(\text{HMF})_{\text{consumed}} / n\,(\text{HMF})_{\text{initial}} \times 100\% \quad (1)$$

$$\text{Sel. (\%)} = n\,(\text{BHMF})_{\text{formed}} / n\,(\text{HMF})_{\text{consumed}} \times 100\% \quad (2)$$

$$\text{FE (\%)} = n\,(\text{BHMF})_{\text{formed}} \times 2 \times F / Q_{\text{passed}} \times 100\% \quad (3)$$

where n is the molar amount of a component measured by HPLC, F is Faraday's constant (96485 C mol^{-1}), and Q is the charge recorded at the electrochemical workstation.

BHMF was extracted from the electrolyte with ethyl acetate three times and then removed the solvent using a rotary evaporator. The product was obtained after vacuuming dry.

6. The pseudo-first-order kinetic test.

The pseudo-first-order kinetic pattern for the electrochemical hydrogenation of HMF can be calculated by using Equation (1):

$$\ln\left(\frac{C_0}{C}\right) = kt \tag{1}$$

Wherein, C is the HMF concentration at different time (t) intervals ($mol \cdot L^{-1}$), and C_0 is the initial HMF concentration ($mol \cdot L^{-1}$), and k is the apparent pseudo-first-order reaction rate constant (min^{-1}), and t is the reaction time (min).

7. BHMF separation and polymerization

At the end of the reaction, the water in the electrolyte is removed in a rotary evaporator at a 65°C. The remaining solid was washed 5 times with ethyl acetate. Finally, the BHMF was recrystallized from the solution by removing the ethyl acetate.

Poly(2,5-furandimethylene succinate) (PFS) was synthesized via a modified method from a literature.[1] At first, BHF (1.5 g), SA (1.38 g), and N,N-dimethyl-4-aminopyridine (4.28 g) were dissolved in 20 mL anhydrous dichloroethane under N_2 atmosphere. Then, N,N′-diisopropylcarbodiimide (4.43 g) was slowly dropped into the above solution. After stirring at room temperature for 24 h, the solvent evaporated. Purification by precipitation (chloroform → excess methanol) afforded the product as a yellow solid.

8. Theory calculations

Density functional theory (DFT) calculations were carried out by using the Vienna ab initio simulation package (VASP)[2-4]. Projector-augmented wave (PAW) pseudopotentials[5, 6] were adopted with an energy cutoff of 450 eV. The generalized gradient approximation with the function of Perdew−Burke−Ernzerhof (GGA-PBE)[7] was applied to describe the exchange-correlation function. The convergence criterion of the residual Hellmann-Feynman force and energy during structure optimization were set to 0.02 eV $Å^{-1}$ and 10^{-5} eV, respectively. The Brillouin zone was built with the 2×2×1 Monkhorst-Pack grid k-points for all models in the structural optimization and Denser k-point meshes (4×4×1) were used for density of states (DOS) calculations. The vacuum space of 20 Å was adopted above the surfaces to avoid periodic interactions. The impact of van der Waals interactions was evaluated using the DFT-D2 semi-empirical force field method[8].

The adsorption energy of Pd/Cu-H is calculated as follows:

$$E_a = E_{Pd/Cu\text{-}H} - E_{Pd/Cu} - n/2E_{H2}$$

Where $E_{Pd/Cu\text{-}H}$ is the energy of the whole system, $E_{Pd/Cu}$ is the energy of Pd/Cu structure, and E_{H2} is the energy of H_2 molecule.

The Gibbs free energy is given as follow:

$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S$$

where ΔE, ΔE_{ZPE} and $T\Delta S$ denote total energy from DFT calculations, zero-point energy and entropic contributions (at 298 K), respectively.

9. Techno-economic analysis (TEA)

To evaluate the economic potential of the BHMF electrosynthesis by the proposed HMFRR process, a TEA was performed based on the recently reported model.

Assumptions:

(1) The electrolyzer cost, anticipated service life of the electrolyzer, electricity cost and working time were 920 \$ m^{-2}, 20 years, and 350 day per year, respectively. [9]

(2) The electricity price was considered to be 0.03 \$ kWh^{-1}.[10]

(3) The balance of plant factor and maintenance factor were 0.35 and 0.025, respectively. [9]

(4) Separation equipment: Evaporator *2: 700000 \$; Vacuum filter: 7000 \$; Dryer *2: 24000 \$; Condenser: 36000 \$.[11]

(5) The maintenance factor were 2 in the $KHCO_3$ system.

(6) HMF price: 217.24 \$ kg^{-1}; BHMF price: 1336.91 \$ kg^{-1}; O_2 price: 0.05 \$ kg^{-1}. [12]

(7) The daily productivity of BHMF was assumed to be 1000 kg day^{-1}.

Calculation processes:

(1) The $KHCO_3$ system:

1) The base case scenario based on the flow cell experiments in 0.5 M $KHCO_3$ system: FE_{BHMF} of 91%, $productivity_{BHMF}$ of 250 μmol cm^{-2} h^{-1}, current density of 2.4 mA cm^{-2}, and cell voltage of -2.4 V.

2) After calculation, it can be seen that for every 1 kg of BHMF produced, the mass of HMF consumed were 1.16 kg. The FE of the cathode OER was assumed to be 100% and the mass of O_2 produced was 0.15 kg.

3) The energy consumption was calculated as:

$$\begin{aligned} & Energy\ consumption \\ & = 1000\frac{kg}{day} \times \frac{mol}{128.13g} \times 2e^- \times 96485\frac{C}{mol} \times \frac{1}{91\%} \times \frac{h}{3600s} \times 2.4V \\ & \approx 1103.33\frac{kWh}{day} \end{aligned}$$

4) The required total current was calculated as:

$$Total\ current = 1103.33\frac{kWh}{day} \times \frac{1000W}{kW} \times \frac{day}{24h} \times \frac{1}{2.4V} \approx 19155.03A$$

5) The needed electrolyzer area was calculated as:

$$Electrolyzer\ area = 19155.03A \times \frac{cm^2}{2.4mA} \times \frac{1000mA}{A} \times \frac{m^2}{10000cm^2} \approx 798.13m^2$$

6) Capital costs:

i. Electrolyzer:

$$\begin{aligned} & Electrolyzer\ cost \\ & = 798.13m^2 \times 920\frac{\$}{m^2} \times \frac{1}{20year} \times \frac{year}{350day} \times \frac{day}{ton_{BHMF}} \approx 104.90 \end{aligned}$$

ii. Separation equipment:

$$\begin{aligned} & Separation\ equipment\ cost \\ & = (700000\$ + 7000\$ + 24000\$ + 36000\$) \times \frac{1}{20year} \times \frac{year}{350day} \\ & \times \frac{day}{ton_{BHMF}} \approx 109.57\ \$\ ton_{BHMF}^{-1} \end{aligned}$$

iii. Balance of plant:

$$Balance\ of\ plant\ cost = (104.90 + 109.57)\ \$\ ton_{BHMF}^{-1} \times 0.35 \approx 75.06\$\ ton_{BHMF}^{-1}$$

7) Operating costs:

i. Electricity:

$$Electricity = 1103.33\frac{kWh}{day} \times 0.03\frac{\$}{kWh} \times \frac{day}{ton_{BHMF}} \approx 33.10\ \$\ ton_{BHMF}^{-1}$$

ii. Separation:

$$Separation = 33.10\ \$\ ton_{BHMF}^{-1} \times 2 \approx 66.20\ \$\ ton_{BHMF}^{-1}$$

iii. Maintenance of electrolyzer:

$$798.13m^2 \times 920\frac{\$}{m^2} \times 0.025 \times \frac{year}{350day} \times \frac{day}{ton_{BHMF}} \approx 52.45\ \$\ ton_{BHMF}^{-1}$$

iv. Maintenance of separation equipment:

$$157.35\frac{\$}{ton_{BHMF}} \times \frac{ton_{BHMF}}{day} \times \frac{365day}{year} \times 20year \times 0.025 \times \frac{year}{350day} \times \frac{day}{ton_{BHMF}} \approx 82.05\ \$\ ton_{BHMF}^{-1}$$

8) Material costs:

HMF:

$$1.16\frac{kg_{HMF}}{kg_{BHMF}} \times 217.24\frac{\$}{kg_{HMF}} \times \frac{1000kg_{BHMF}}{ton_{BHMF}} \approx 251998.40\ \$\ ton_{BHMF}^{-1}$$

9) Catalyst and membrane replacement cost. The electrolyzer uses Platinised titanium felts as the anode and 3% Pd-Cu@3DC as the cathode. The cost of Pd is significantly higher at \$37 per gram, compared to Cu, which cost \$0.006 per gram. Therefore, Pd cost dominates the overall catalyst cost. For this analysis, we considered a catalyst loading of 2 mg cm^{-2}, which is the typical cathode loading for this work. This results in a catalyst unit area cost of \$46 m^{-2}. The cost of the membrane is estimated to be \$180 m^{-2}, based on a previous study. [13]

$$Catalyst\ and\ membrane\ cost = \frac{226\frac{\$}{m^2} \times 798.13m^2}{350\frac{day}{year} \times 1\frac{ton_{BHMF}}{day} \times 5\ year}$$

$$\approx 103.07\$\ ton_{BHMF}^{-1}$$

10) Total cost:

$$Total\ cost$$
$$= (104.90 + 109.57 + 75.06 + 33.10 + 66.20 + 52.45 + 82.05$$
$$+ 103.07)\ \$\ ton_{BHMF}^{-1} \approx 252624.80\ \$\ ton_{BHMF}^{-1}$$

11) Revenue (except BHMF):

O$_2$:
$$0.15\frac{kg_{O2}}{kg_{BHMF}} \times 0.05\frac{\$}{kg_{O2}} \times \frac{1000kg_{BHMF}}{ton_{BHMF}} \approx 7.5\ \$\ ton_{BHMF}^{-1}$$

12) BHMF levelized cost:

$$BHMF\ levelized\ cost\ = (252624.80 - 7.5)\ \$\ ton_{BHMF}^{-1} \approx 252617.30\ \$\ ton_{BHMF}^{-1}$$

Calculation of Net Present Value

Assumptions:

i. . 38.9% Income tax

ii. 10% Nominal Interest Rate[9]

In year zero, the facility is built, hence the cumulative present value:

$$Year\ 0\ cumulative\ value$$
$$=-\ Fixed\ Capital\ Investment - \ (Working\ Capital\ +\ Startu$$
$$=-\left(798.13m^2 \times 920\frac{\$}{m^2}\right) - (355940\$ + 40000\$)$$
$$-\left(\left(798.13m^2 \times 920\frac{\$}{m^2}\right) + (700000\$ + 7000\$ + 24000\$ + 360\right.$$
$$\times 0.35 - \left(1103.33\frac{kWh}{day} \times 0.05\frac{\$}{kWh}\right) - \left(1103.33\frac{kWh}{day} \times 0.05\frac{\$}{kW}\right.$$
$$\times 2 - \left(226\frac{\$}{m^2} \times 798.13m^2\right) \approx\ -2207270.34\ \$$$

$$Year\ 1\ depreciation$$
$$=\ Fixed\ Capital\ Investment\ \times\ depriciation\ rate = \left(798.13m\right.$$
$$\times 1.35 \times 0.05 \approx 101336.37\$$$

$$Yearly\ profit$$
$$=\ (Product\ income\ - operating\ cost)\ \times\ 350\ days = \left(1336.\right.$$
$$\times 350\ days \approx 75355420\ \$\ year^{-1}$$

$$Year\ 1\ net\ earnings$$
$$=\ (Net\ Profit - Year\ 1\ deprication) \times\ (1 - Income\ tax) =$$
$$(75355420\$ - 101336.37\$) \times (1 - 0.389) \approx 45980245.10\ \$$$

$$
\begin{aligned}
&Year\ 1\ discounted\ cash\ flow \\
&\qquad = Year\ 1\ net\ Earnings\ + Year\ 1\ depriciation\ = 45980245.10\ \$ \\
&\qquad + 101336.37\$ \approx 46081581.50\$
\end{aligned}
$$

$$
Year\ 1\ cash\ flow\ = Year\ 1\ discounted\ cash\ flow \times \frac{1}{(1 + Interest\ Rate)^{time}}
$$

$$
= 46081581.50\$ \times \frac{1}{(1 + 0.1)^{1}} = 41892346.80\$
$$

$$
\begin{aligned}
&Year\ 1\ cumulative\ present\ value \\
&\qquad = Year\ 0\ cumulative\ value\ +\ Year\ 1\ cash\ flow \\
&\qquad = -\ 2207270.34\ \$ + 41892346.80\$ \approx 39685076.40\$
\end{aligned}
$$

10. In situ ATR-SEIRAS tests

In situ ATR-SEIRAS tests were performed on PerkinElmer Spectrum 3 provided by Hefei in situ technology Co., Ltd. China. Au-coated Si pillar with 3%Pd-Cu@3DC catalysts coating was as working electrode, while a platinum wire and an Ag/AgCl were used as the counter and reference electrodes, respectively. The potential was applied to the working electrode ranged from -0.7 to -1.7 V. At the same time, infrared spectra were acquired within the wave number range of 4000-1000 at a spectral resolution of 4 cm^{-1}.

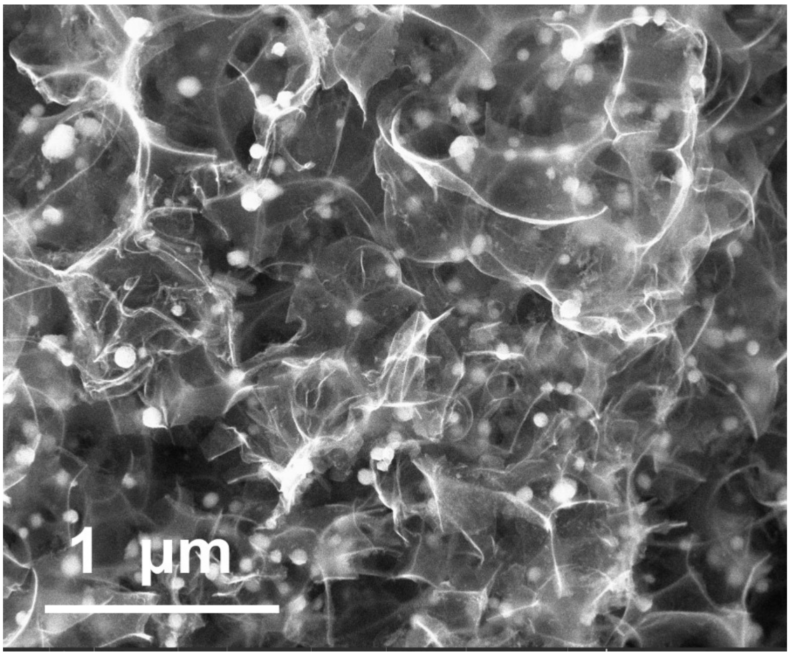

Figure S1 SEM image of 3%Pd-Cu@3DC

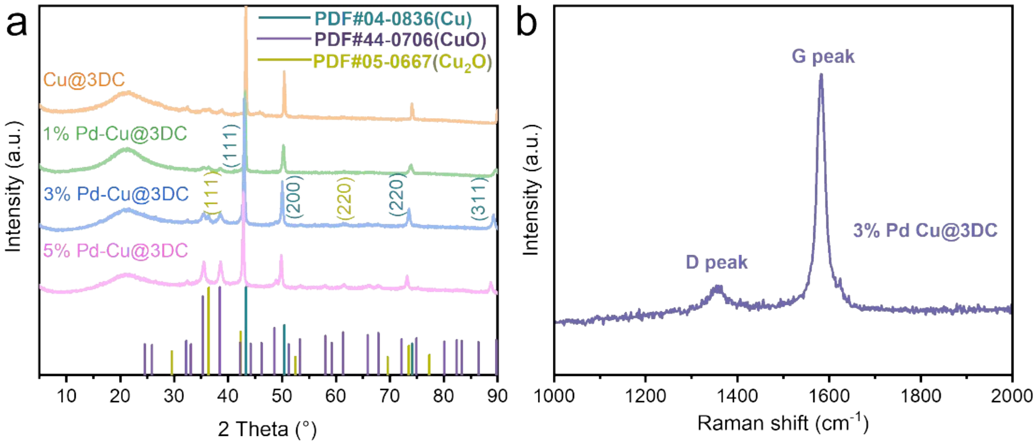

Figure S2 (a) XRD and (b) Raman patterns of the samples

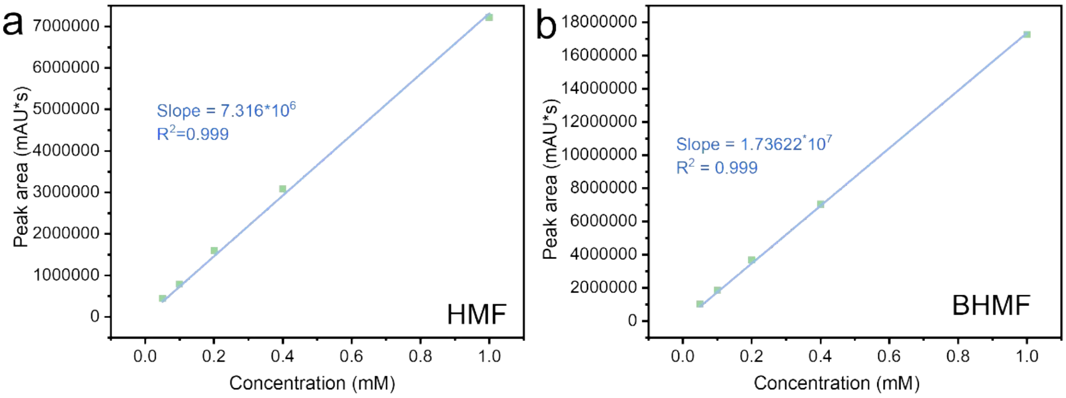

Figure S3 HPLC analysis standard curves of (a) HMF and (b)BHMF

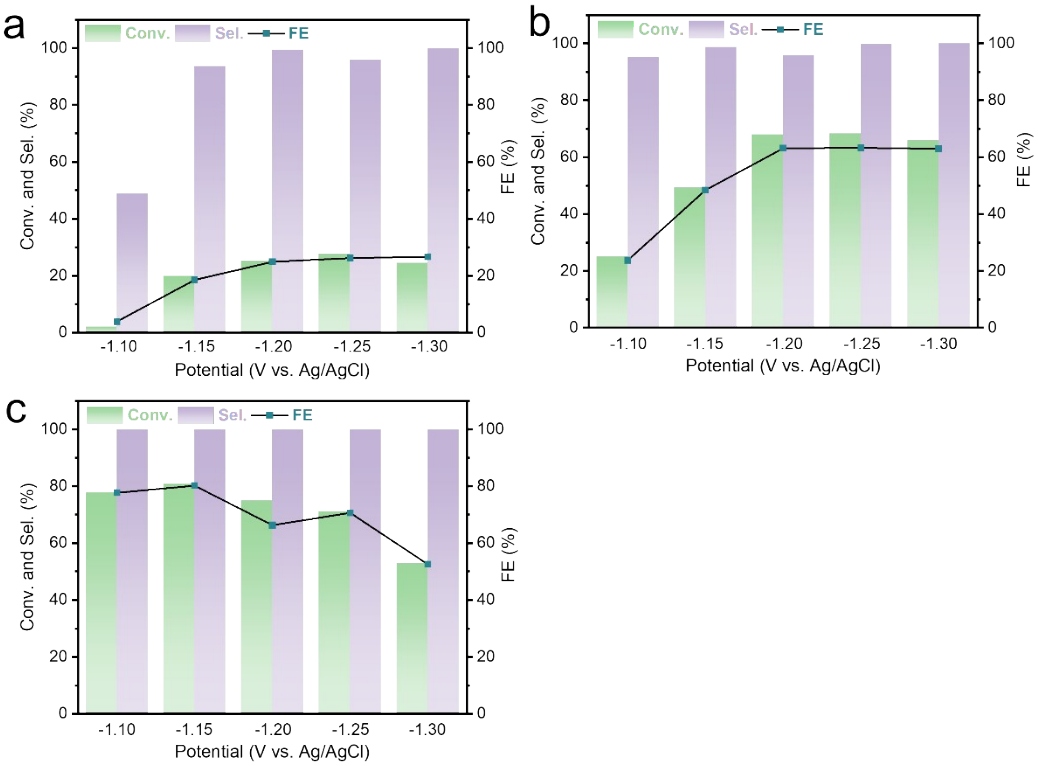

Figure S4 Potential-dependent activity profiles of (a) Cu@3DC, (b) 1%Pd-Cu@3DC, (c) 5%Pd-Cu@3DC

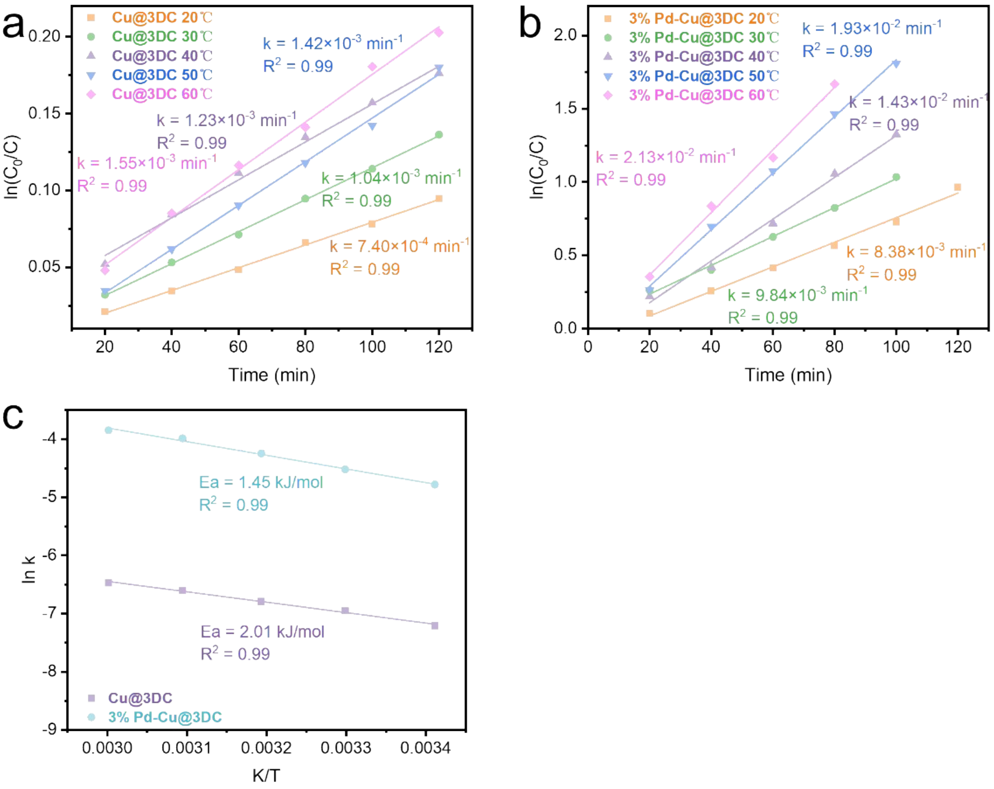

Figure S5 $\ln(C_0/C) \sim t$ plots at different temperatures for (a) Cu@3DC and (b) 3%Pd-Cu@3DC. (c) Arrhenius plots.

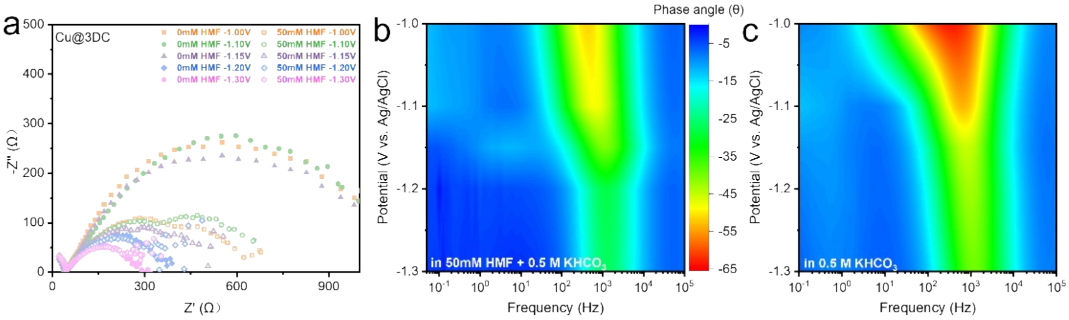

Figure S6 EIS characterization of Cu@3DC, (d) Nyquist and (e-f) Bode plots.

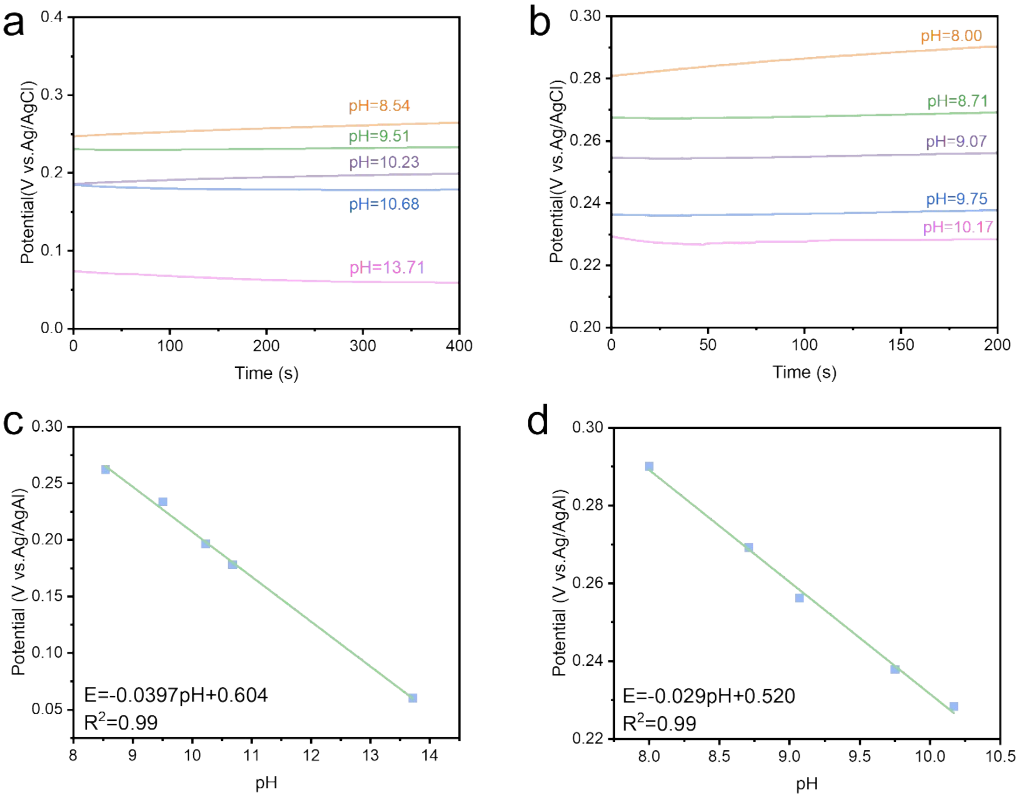

Figure S7 pH measurements at electrode surface of 3%Pd-Cu@3DC and Cu@3DC. (a-b) Open circuit potential (OCP) of 3%Pd-Cu@3DC and Cu@3DC electrode at different pH values. (c-d) Derived standard curve of OCP vs solution pH.

The measurements were performed in 0.5 M $KHCO_3$. The pH values of the solution were adjusted by adding KOH. Measurements of pH on the electrode surface of (a) 3%Pd-Cu@3DC and (d) Cu@3DC with loading mass of 0.16 mg cm^{-2} at increased anodic potentials. Pt foil was used as the counter electrode, and Ag/AgCl was used as the reference electrode.

Test conditions: in 0.5 M $KHCO_3$ with the working electrode rotating at a speed of 1600 rpm and scan rate of 1 mV s^{-1}.

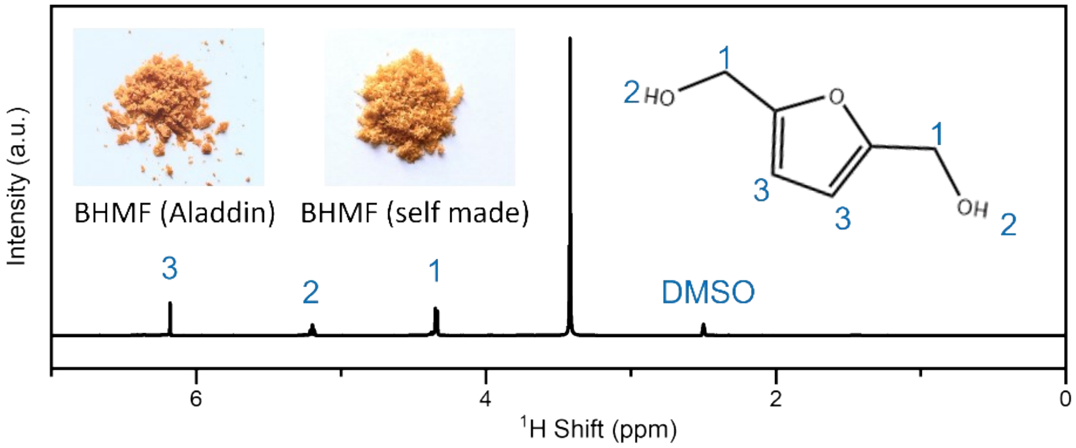

Figure S8 H NMR analysis of BHMF. (Insert: BHMF photograph)

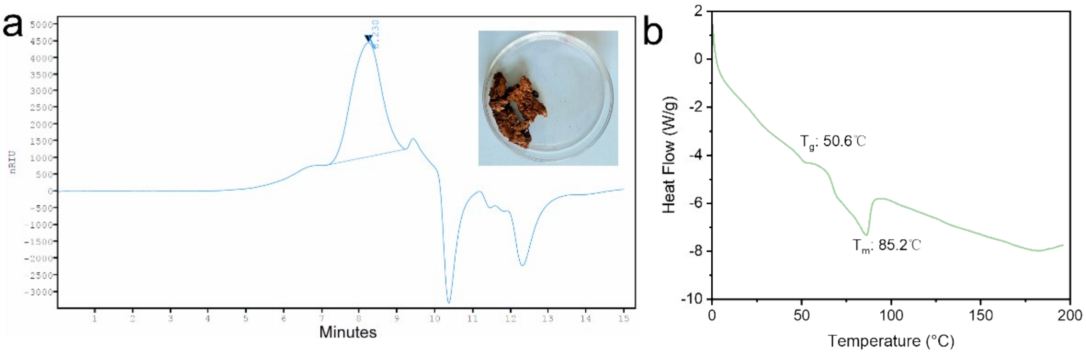

Figure S9 (a) GPC and (b) DSC characterization of PFS

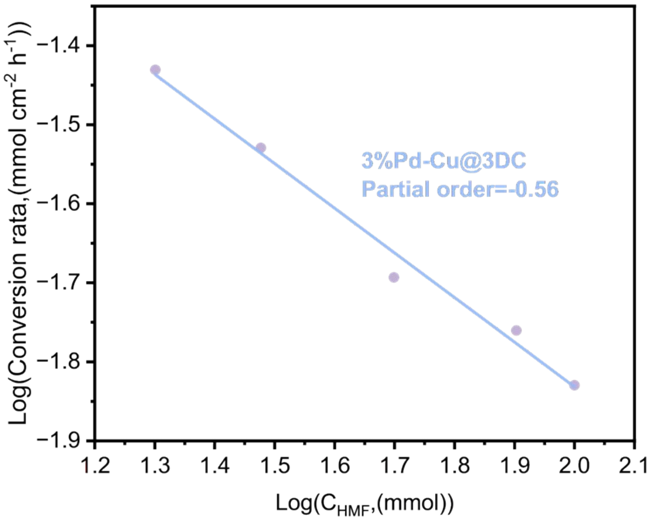

Figure S10. The conversion rate for the electrochemical reduction of HMF over 3%Pd-Cu@3DC as a function of HMF content in the 0.5 M $KHCO_3$ solution. Reaction condition: −1.15 V (vs. Ag/AgCl), all tests control the conversion of HMF

<15%, error bars represented three independent tests.

Note: As shown in our work, competitive adsorption between HMF and H_2O is involved in the 3%Pd-Cu@3DC. According to the Lopez-Ruiz's work,[14] the rate expression for Langmuir−Hinshelwood (L-H) competitive adsorption follows as:

$$r_{LH} = \frac{k_T \times K_{sub} \times [sub] \times (K_{H^+} \times a_{H_3O^+})^2}{(1 + K_{sub} \times [sub] + K_{H^+} \times a_{H_3O^+})^3} \qquad \text{(S1)}$$

Wherein, k_T is the kinetic constant of the hydrogenation step, K_{sub} is the adsorption equilibrium constant of the sub, [sub] is the concentration of substrate, K_{H^+} is the adsorption equilibrium constant of H_3O^+, and aH_3O^+ is the activity of H_3O^+.

The expression in our cases could follow:

$$r_{LH} = \frac{k_T \times K_{HMF} \times [HMF] \times (K_{H_2O} \times a_{H_2O})^2}{(1 + K_{HMF} \times [HMF] + K_{H_2O} \times a_{H_2O})^3} \qquad \text{(S2)}$$

k_T is the kinetic constant of the hydrogenation step, K_{HMF} is the absorption equilibrium constant of sub, [HMF] is the concentration of substrate, $K_{H_2O}$is the absorption equilibrium constant of H_2O, and a_{H_2O} is the activity of H_2O.

With the increased HMF bulk concentration, K_{HMF}×[HMF]>1 and the expression could be simplified as:

$$r_{LH} = \frac{k_T \times (K_{H_2O} \times a_{H_2O})^2}{(K_{HMF} \times [HMF])^2} \qquad \text{(S3)}$$

Accordingly, equation S3 reflects the L-H mechanism with competitive adsorption between HMF and H_2O, which predicts a negative order with an elevation of HMF concentration.

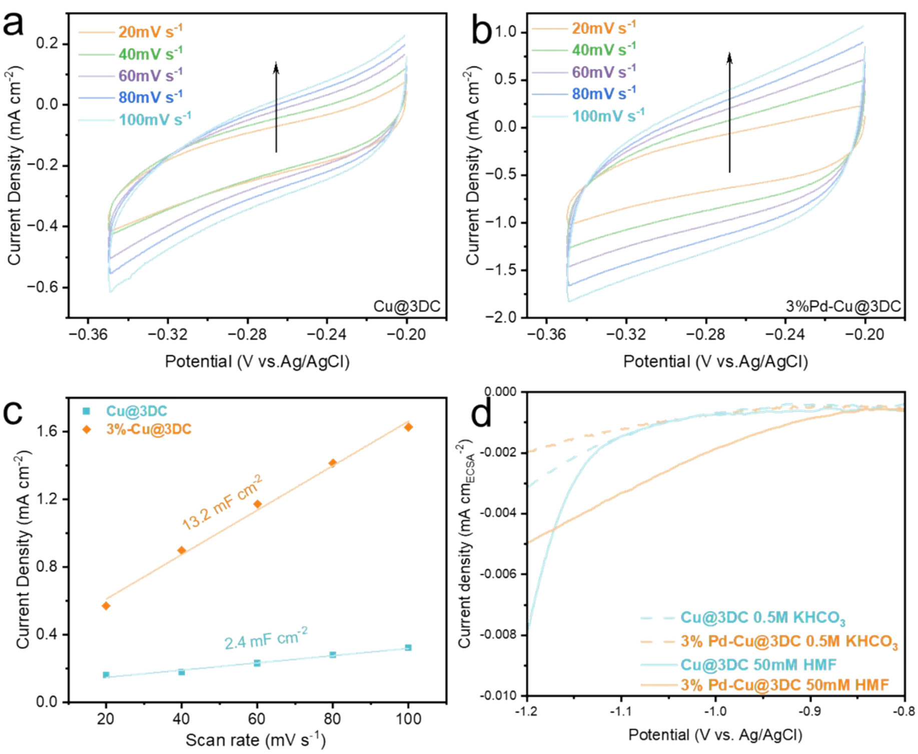

Figure S11. Cyclic voltammograms (CVs) of (a) Cu@3DC and (b)3%Pd- Cu@3DC. (c) C_{dl} curves. (d) LSV curves of the current density normalized by ECSA.

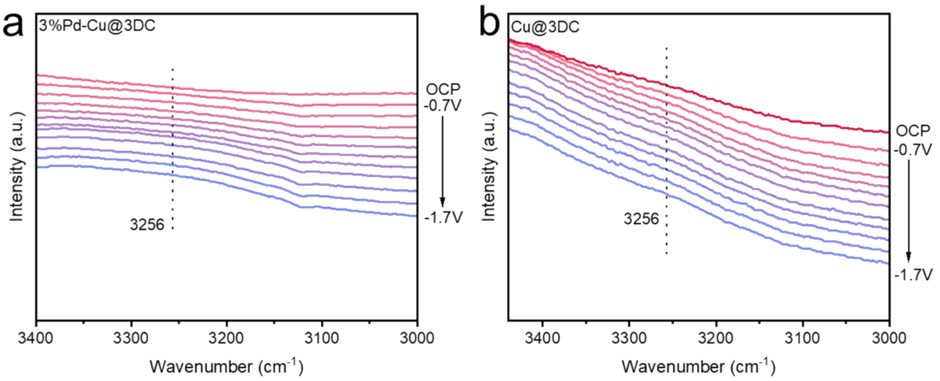

Figure S12 In situ ATR-SEIRAS spectroscopy recorded on (a) 3%Pd-Cu@3DC and (b) Cu@3DC.

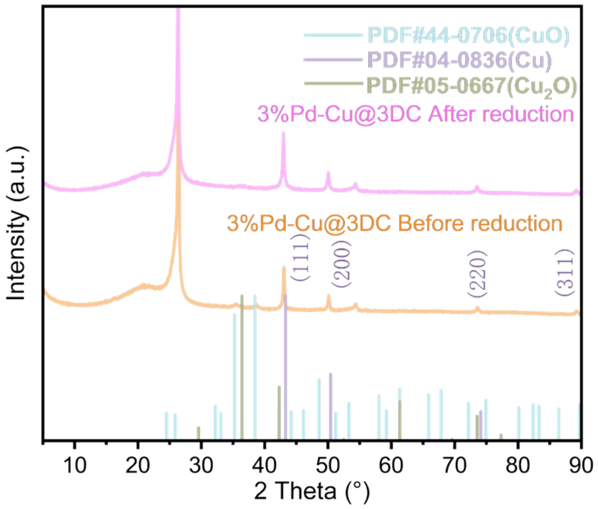

Figure S13 XRD patterns of 3% Pd-Cu@3DC before and after reduction.

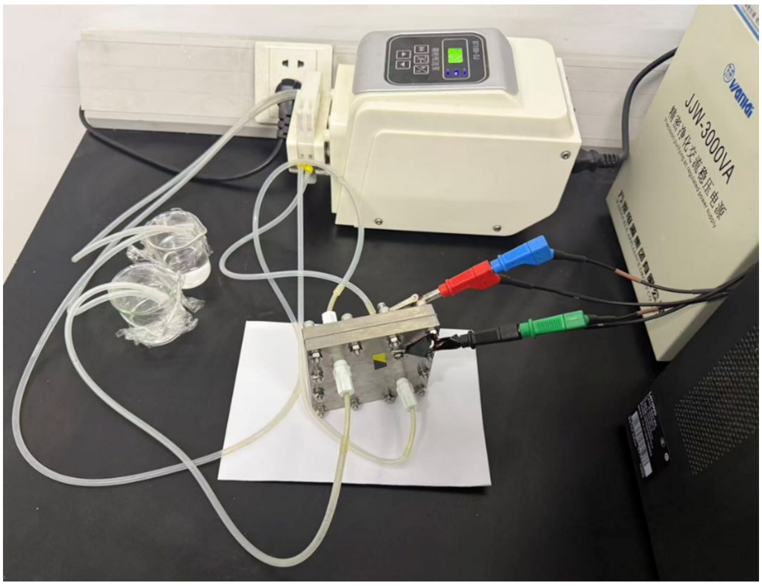

Figure S14 Photograph of the PEM flow reactor for the continuous electroreduction of HMF to BHMF

Table S1 Performance comparison with catalyst in literature

Catalyst	**Con.**	**Sel.**	**FE**	**Total cycle time**	**BHMF Yield (%)**	**Ref.**
Pt-Cu	--	94%	90%	10h	--	10.1016/j.jechem.2025.02.010
Ru_1Cu SAA	87%	97%	85%	4h	84	10.1002/ange.202209849
$Cu(OH)_2ER/CF$	92%	90%	92%	10h	83	10.1016/j.jechem.2023.05.003
Ag_1Cu_1/PA	93%	94%	62%	12h	87	10.1016/j.ijhydene.2022.06.211
$CuFeO_x/CF$	90%	93%	98%	15h	90	10.1002/cssc.202401278
Pd Nps/XC-72	--	90%	50%	8 cycles	--	10.1002/adma.202307799
RhCu-CTAB	75%	~100%	74%	26h	75	10.1002/anie.202407121
3%Pd-Cu@3DC	97%	99%	97%	31h	96	**This work**

Table S2 GPC test results of PFS

sample	**M_n**	**M_v**	**M_z**	**M_{z+1}**	**polydispersity**
PFS	10861	19364	31992	46475	1.782893

Reference

1. Zeng, C.; Seino, H.; Ren, J.; Hatanaka, K.; Yoshie, N., Bio-Based Furan Polymers with Self-Healing Ability. *Macromolecules* **2013,** *46* (5), 1794-1802.

2. Blöchl, P. E., Projector augmented-wave method. Physical Review B 1994, 50 (24), 17953-17979.

3. Kresse, G.; Joubert, D., From ultrasoft pseudopotentials to the projector augmented-wave method. Physical Review B 1999, 59 (3), 1758-1775.

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