

Supporting Information

Polyaromatic Hydrocarbon based 3D Coordination Polymeric Materials: Synergistic Effect of Nickel (II) Nitrate and Tetraalkynyl Anthracene Towards Electrocatalytic Hydrogen Production

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1. Synthesis and Methodology

Synthesis of Ni(OH)₂ nanoparticles

Nickel hydroxide nanoparticles were synthesized by treating 1 M Ni(NO₃)₂·6H₂O dissolved in 20 mL distilled water with 2 mL of 2 M NaOH solution dropwise. The precipitates were formed instantly and were washed with distilled water 5 × 10 minutes at 10,000 rpm to remove unreacted nitrate.

Method S1. Calculation of Faradaic efficiency

Charge passed in the CA experiment for HER= x C

$$\text{Theoretical amount of H}_2 = \frac{x C}{96485 \times 2C} \text{ mol} = y \text{ mmol}$$

$$\left(22.4 \frac{\text{mL}}{\text{mmol}} \times y \right) = z \text{ mL}$$

Amount of H₂ observed through eudiometric technique = a mL

$$\% \text{ of Faradaic efficiency} = \frac{\text{Experimentally observed volume of H}_2}{\text{Theoretical volume of H}_2} = \frac{a}{z} \times 100 = b \% \quad \dots (\text{S1})$$

Conversion of $E_{(Ag/AgCl)}$ to E_{RHE}

$$E_{RHE} = 0.222 + 0.0591(\text{pH}) + E_{Ag/AgCl}, \text{ pH} = 0.301 \quad \dots (\text{S2})$$

Method S2. Inductively coupled plasma-mass spectroscopy (ICP-MS):

Inductively coupled plasma-mass spectroscopy (ICP-MS) instrument (Make: Agilent, Model: 7850 ICP-MS, USA) was used for a quantitative analysis of Nickel % loading in **3D-CPM-a**. An initial acid hydrolysis of the material is done in 7 mL nitric acid + 3 mL distilled water in a microwave digester (Make: Milestone, Model: ETHOS EASY – advanced microwave digestion system, USA). After digestion, the solution was diluted upto 50 mL distilled water to get a stock solution. During analysis 1 mL was taken from the stock solution and diluted further by ten times.

Concentration of an element (metal) in the sample = 871.176 ppb

Dilution factor = 10

$$871.1 \times 10 = 8711 \text{ ppb} = \frac{8711 \text{ ppb}}{1000} = 8.711 \text{ mg/mL}$$

Total Volume of stock solution = 50 mL

$$\text{Total metal concentration} = 8.711 \text{ mg/mL} \times \frac{50 \text{ mL}}{1000} = 0.435 \text{ mg}$$

Amount of sample taken = 5 mg

$$\text{Mass \% of element} = \frac{0.435 \text{ mg}}{5 \text{ mg}} \times 100 = 8.71\%$$

$$\text{Mass \%} = \left(\frac{\left(\frac{(\text{Concentration of metal in ppb}) \times \text{Dilution factor}}{1000} \right) \left(\frac{\text{Total volume of sample in mL}}{1000} \right)}{(\text{Weight of sample taken in mg})} \right) \times 100 \quad \dots (\text{S3})$$

Table S1. Comparison of theoretical mass % of elements present in PPP and Fe₃O₄ PPP with mass % obtained from XPS and ICP-MS

Entry	Catalyst	Elements	Theoretical ^a (%)	Normalized ^a (%)	XPS ^b (%)	XPS ^c (%)	ICP-MS ^d (%)
1	3D-CPM-a	C	56	59	54	53	-
2		N	4	4	5	5	-
3		O	28	30	33	36	-
4		Ni	7	8	8	7	8.7

The theoretical mass % of elements was calculated from Chemdraw and was normalized only for C, N and O, ^b About 10 mg of sample was used for XPS analysis measured using PHI 5000 Versa Probe III instrument, ^c XPS analysis measured after 15 h of HER for **3D-CPM-a** using PHI 5000 Versa Probe III instrument ^d ICP-MS was used to detect the mass % of Ni in **3D-CPM-a** carried out in an Agilent, Model: 7850 ICP-MS instrument.

2. Characterizations

X-ray Diffraction Analysis

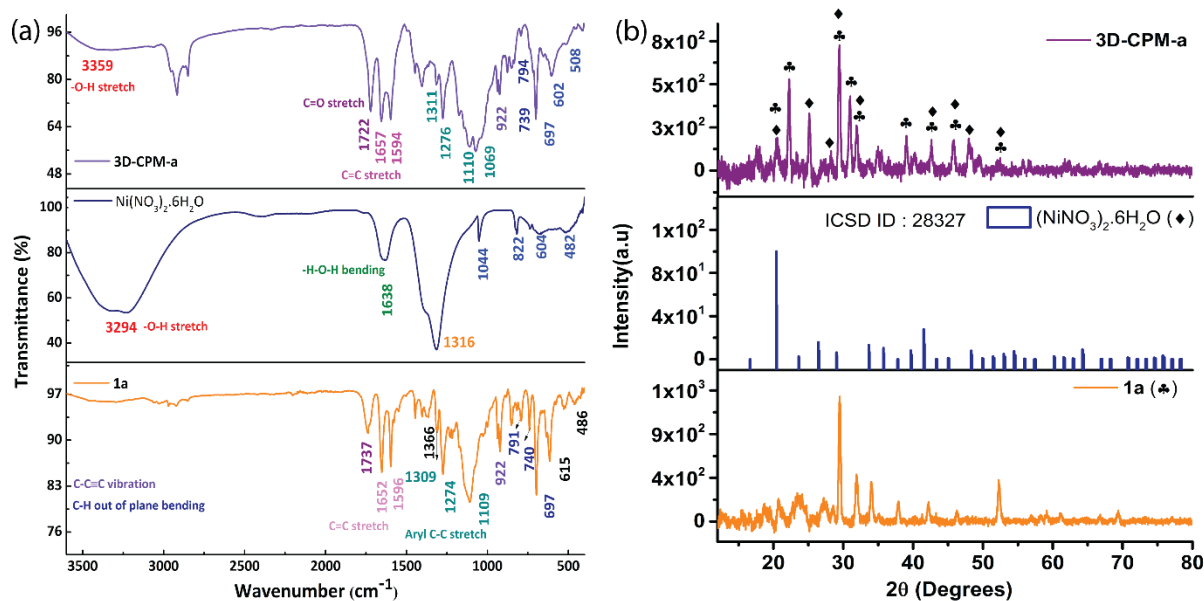


Figure S1 (a) Comparative FT-IR plot of **1a**, Ni(NO₃)₂·6H₂O and **3D-CPM-a** (b) Thin-film XRD of **1a**, Ni(NO₃)₂·6H₂O and **3D-CPM-a** carried out using a Rigaku SmartLab diffractometer utilizing Cu K α radiation ($\lambda = 1.541 \text{ \AA}$) at 40 kV and 125 mA. The 2θ angular region between 10° and 80° was explored at a scan rate of 5-10°/min in a continuous scan mode.

Electron Paramagnetic Resonance

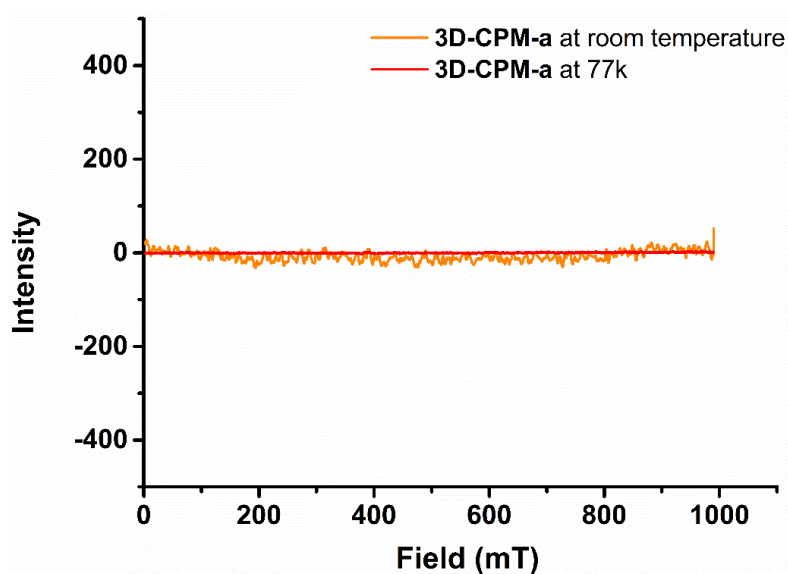


Figure S2 EPR spectrum of **3D-CPM-a** carried out in a JES-FA 200 ESR spectrometer at room temperature as well as in a liquid N_2 .

3. Electrochemical Studies

Cyclic Voltammetry for Activation of Working Electrode

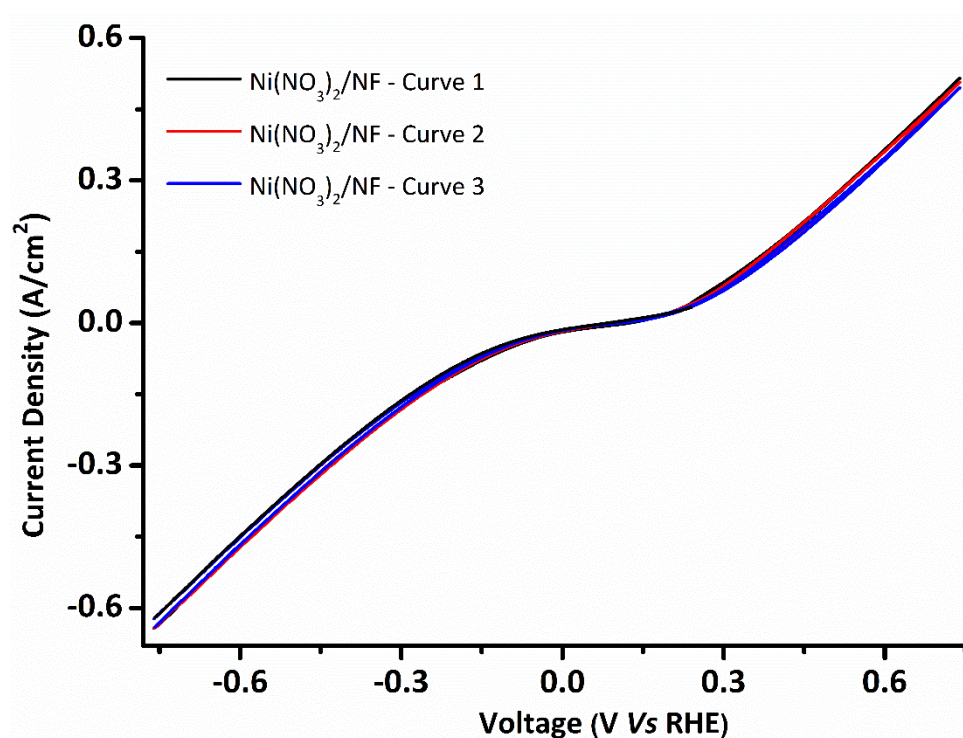


Figure S3 Cyclic voltammetry curves of $Ni(NO_3)_2/NF$ at $90^\circ C$ performed at 50 mV/s scan rate in a potential range of -0.76 V to 0.74 V Vs RHE

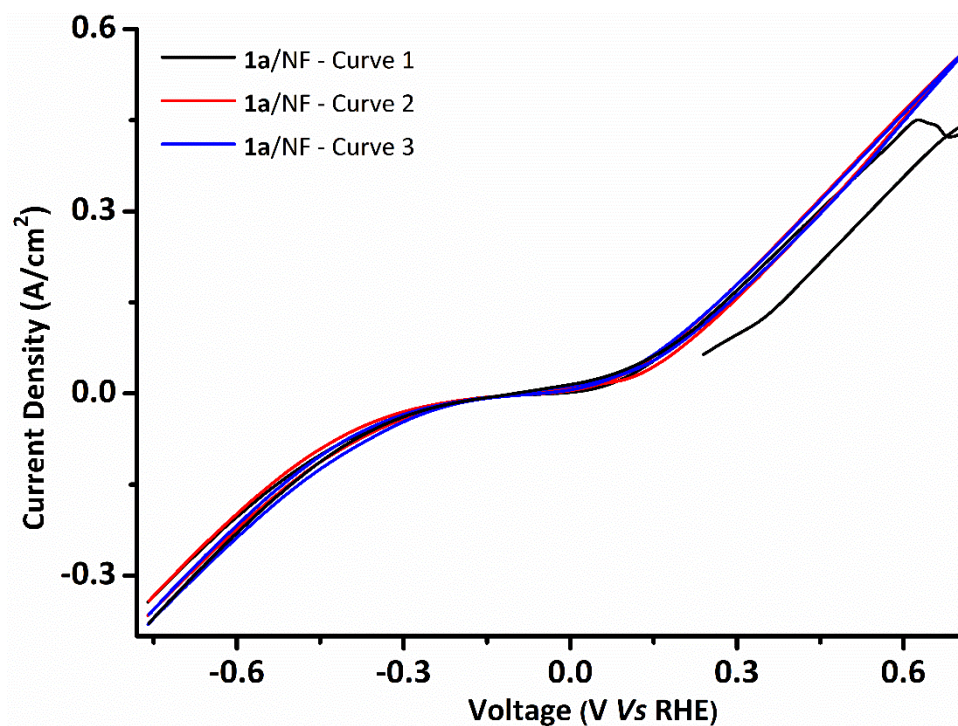


Figure S4 Cyclic voltammety curves of 1a/NF at 90°C performed at 50 mV/s scan rate in a potential range of -0.76 V to 0.74 V Vs RHE

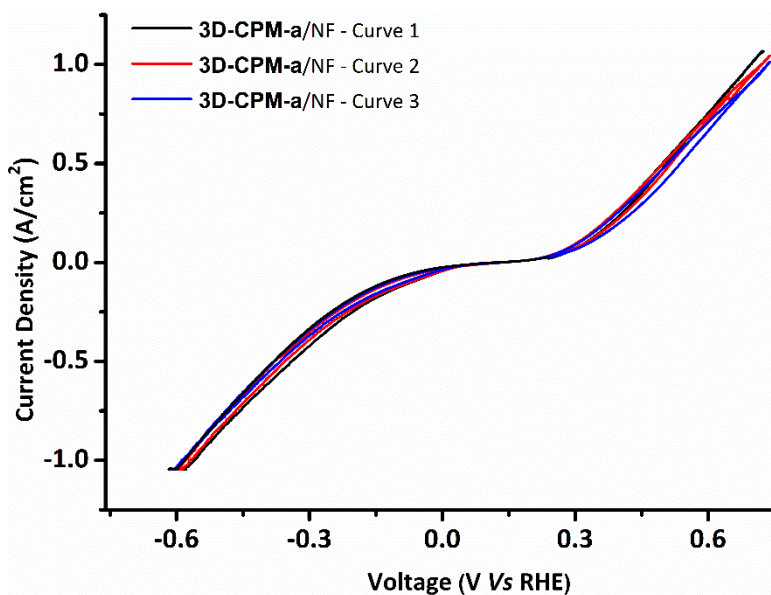


Figure S5 Cyclic voltammety curves of 3D-CPM-a/NF at 90°C performed at 50 mV/s scan rate in a potential range of -0.76 V to 0.74 V Vs RHE

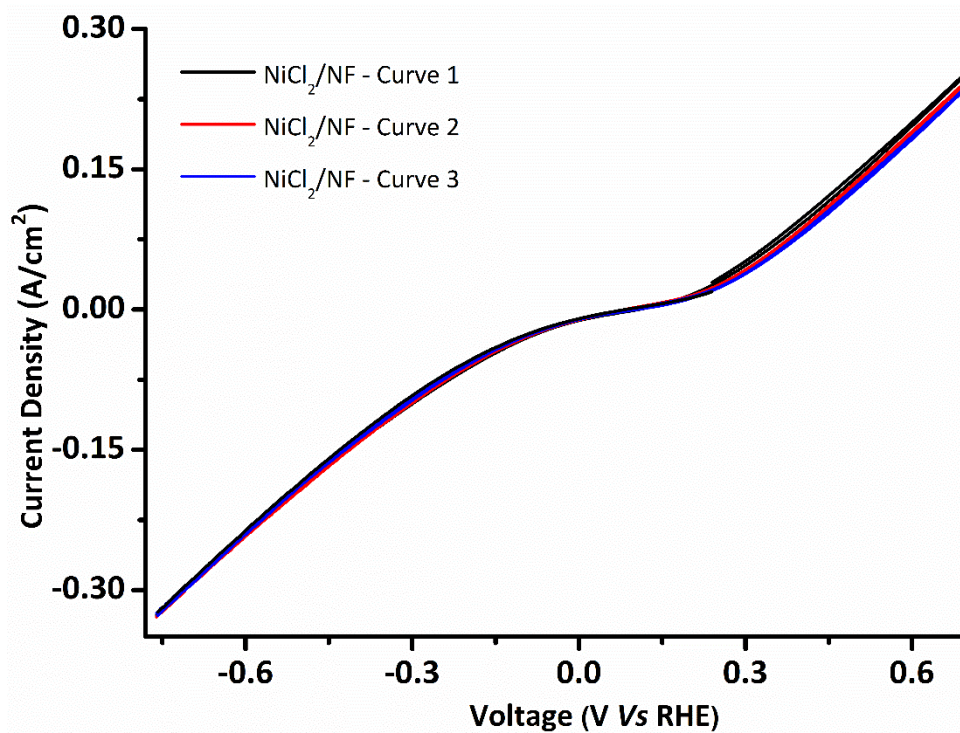


Figure S6 Cyclic voltammetry curves of NiCl₂/NF at 90°C performed at 50 mV/s scan rate in a potential range of -0.76 V to 0.74 V Vs RHE

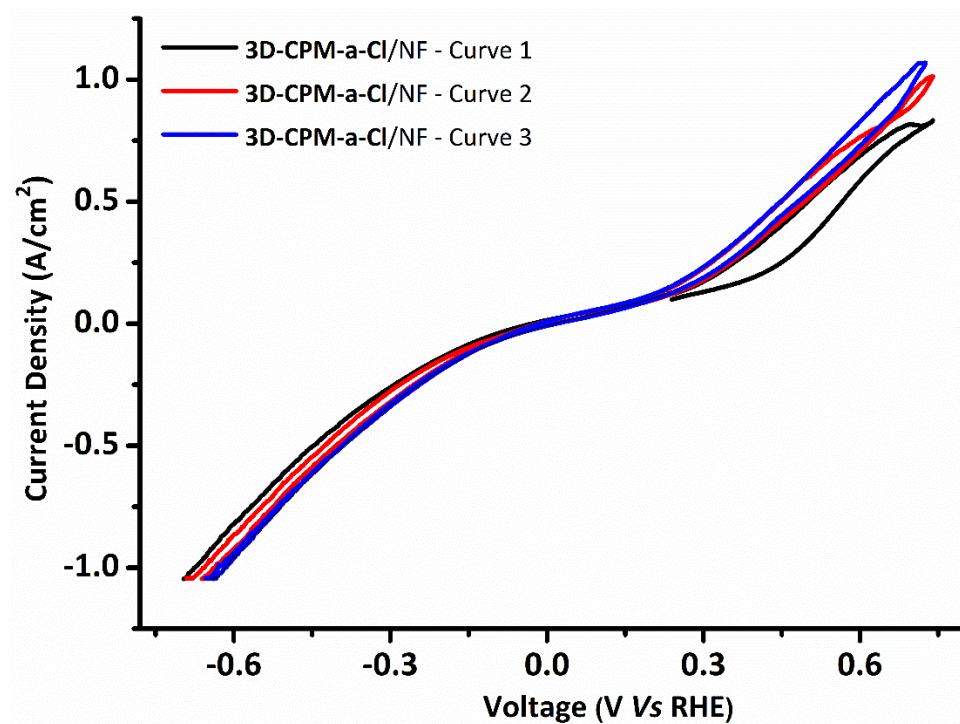


Figure S7 Cyclic voltammetry curves of 3D-CPM-a-Cl/NF at 90°C performed at 50 mV/s scan rate in a potential range of -0.76 V to 0.74 V Vs RHE

Linear Sweep Voltammetry for HER

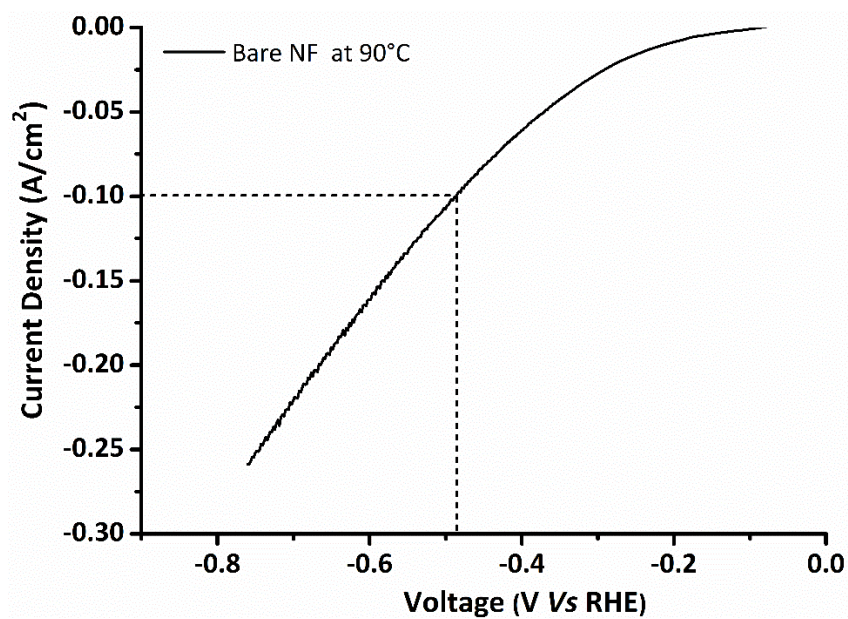


Figure S8 Linear sweep voltammetric plot for HER in 0.5 M H₂SO₄ using bare NF at 90°C performed at 10 mV/s.

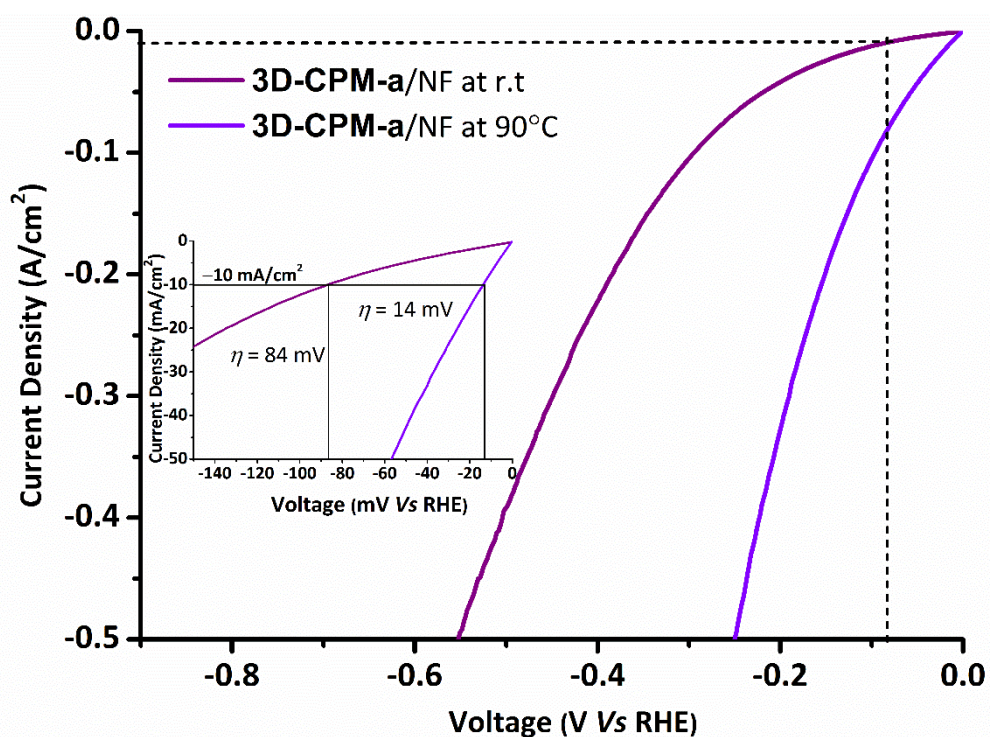


Figure S9 Linear sweep voltammetric plot for HER in 0.5 M H₂SO₄ using 3D-CPM-a/NF at room temperature and at 90°C performed at 10 mV/s.

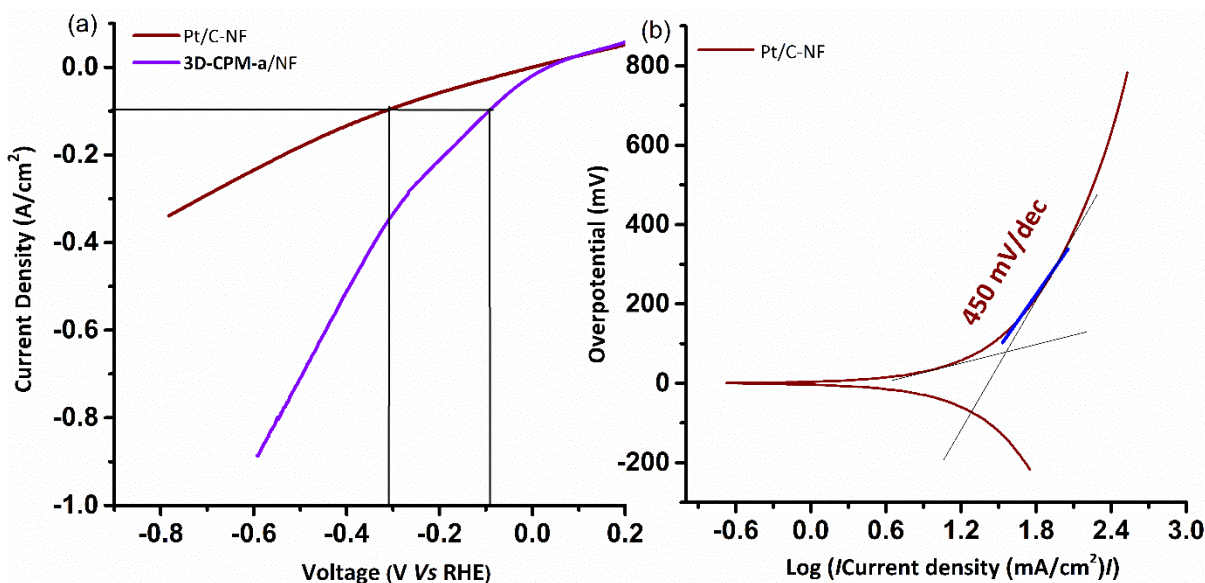


Figure S10 (a) Linear sweep voltammetric plot for HER in 0.5 M H₂SO₄ using 3D-CPM-a/NF in comparison with Pt/C on NF at 90°C performed at 10 mV/s (b) Tafel plot for Pt/C (40 wt% Pt) at 90°C in 0.5 M H₂SO₄.

4. Determination of Faradaic Efficiency

A eudiometric technique was used to quantify the hydrogen generated during the reaction and the hydrogen was collected in a water column through water displacement technique. In this respect, chronoamperometry experiment was run with 3D-CPM-a/NF (activated) for 0.6 hours at a constant potential of -0.16 V Vs RHE. The Faradaic efficiency was calculated according to method S1

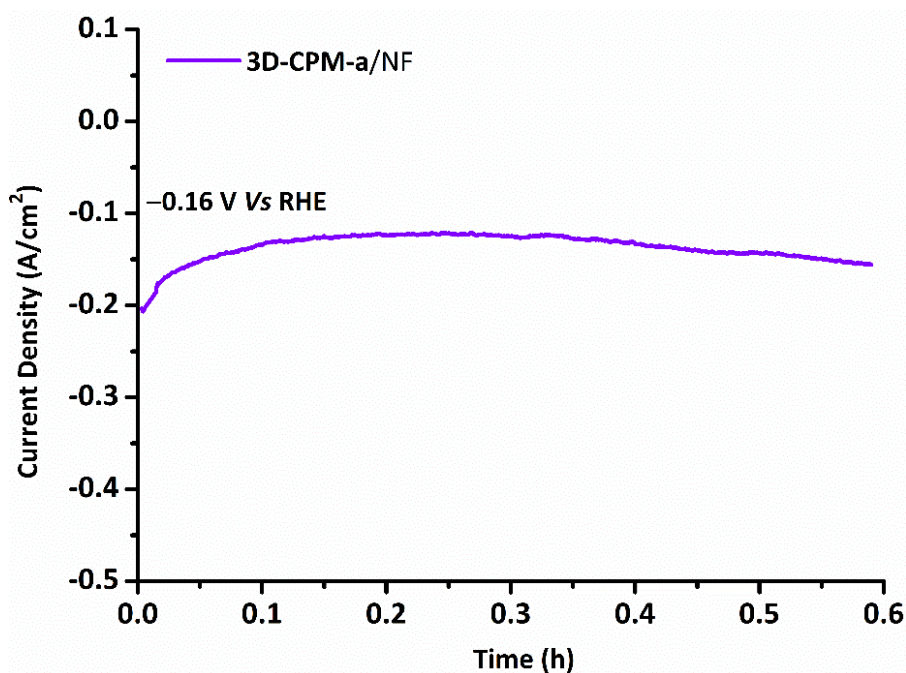


Figure S11 Chronoamperometric plot for HER in 0.5 M H₂SO₄ using 3D-CPM-a/NF at constant potential of -0.160 V Vs RHE at 90°C for 2200 s on an activated NF.

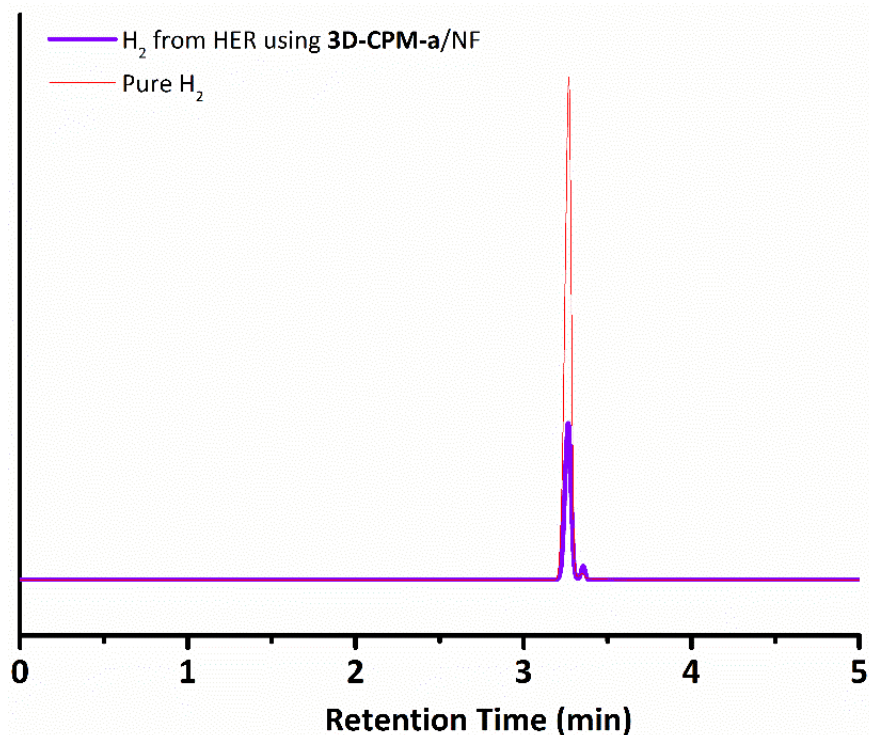


Figure S12 GC-FID file analysis of H₂ evolved from HER using **3D-CPM-a/NF** at constant potential of -0.160 V Vs RHE at 90°C for 2200 s on an activated NF. Fresh sample of pure H₂ was also injected as reference sample.

5. Mechanistic Studies

Electrochemical Active Surface Area

The electrochemical active surface area (ECSA) of **1a/NF**, Ni(NO₃)₂/NF, **3D-CPM-a-Cl/NF** and **3D-CPM-a/NF** was measured by performing cyclic voltammetry in a non-faradaic region (0.04 V to 0.24 V Vs RHE) at varied scan rates of 100 mV/s to 500 mV/s in 0.5 M H₂SO₄ as the electrolyte at 90°C. Across an open-circuit voltage/centre voltage of 0.215 V for **1a/NF** and Ni(NO₃)₂/NF and 0.065 V for **3D-CPM-a-Cl/NF** and **3D-CPM-a/NF**, a current density vs scan rate plot was generated for all the four catalysts. The slope of the linear plot obtained, represents the double layer capacitance (C_{dl}) for varied catalysts.

The electrochemical active area was determined using the formula

$$ECSA = C_{dl} / C_s$$

where C_s is considered as 0.04 mF/cm² for 0.5 M H₂SO₄ electrolyte.

Determination of ECSA

Catalysts	C _{dl} (mF)	ECSA (cm ²)
1a/NF	9	225
Ni(NO ₃) ₂ /NF	4.5	113
3D-CPM-a-Cl/NF	47	1200
3D-CPM-a/NF	90	2300

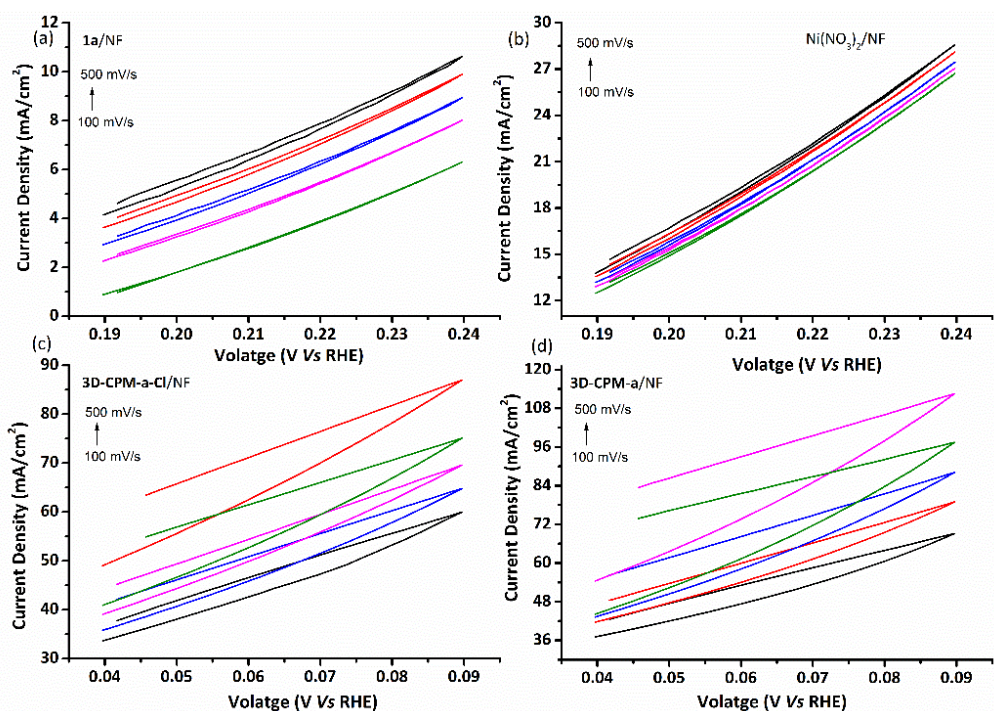


Figure S13 CV curves of (a) **1a/NF** (b) $\text{Ni}(\text{NO}_3)_2/\text{NF}$ (c) **3D-CPM-a-Cl/NF** and (d) **3D-CPM-a/NF** in 0.5 M H_2SO_4 at different scan rates in a non-faradaic region with potential range of 0.04 V to 0.24 V Vs RHE.

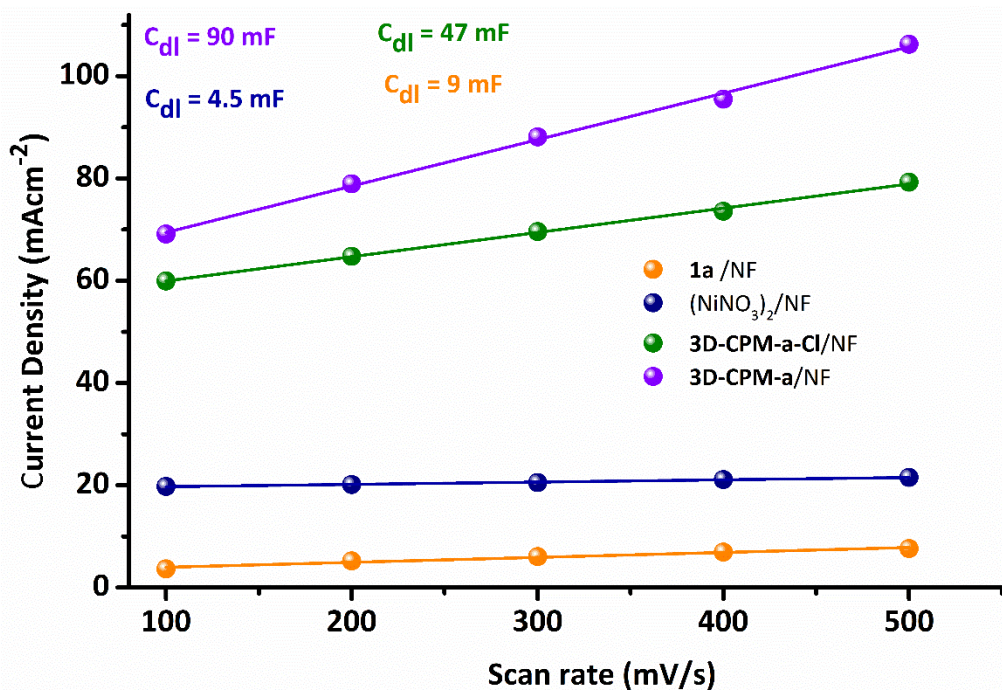


Figure S14 Linear fitting of capacitive currents Vs scan rates to estimate C_{dl} for **1a/NF**, $\text{Ni}(\text{NO}_3)_2/\text{NF}$, $\text{NiCl}_2\text{-1a/NF}$ and **3D-CPM-a/NF** in 0.5 M H_2SO_4 at different scan rates in a non-faradaic region with potential range of 0.04 V to 0.24 V Vs RHE.

6. Post Catalytic Characterizations

Field Emission Scanning Electron Microscopy

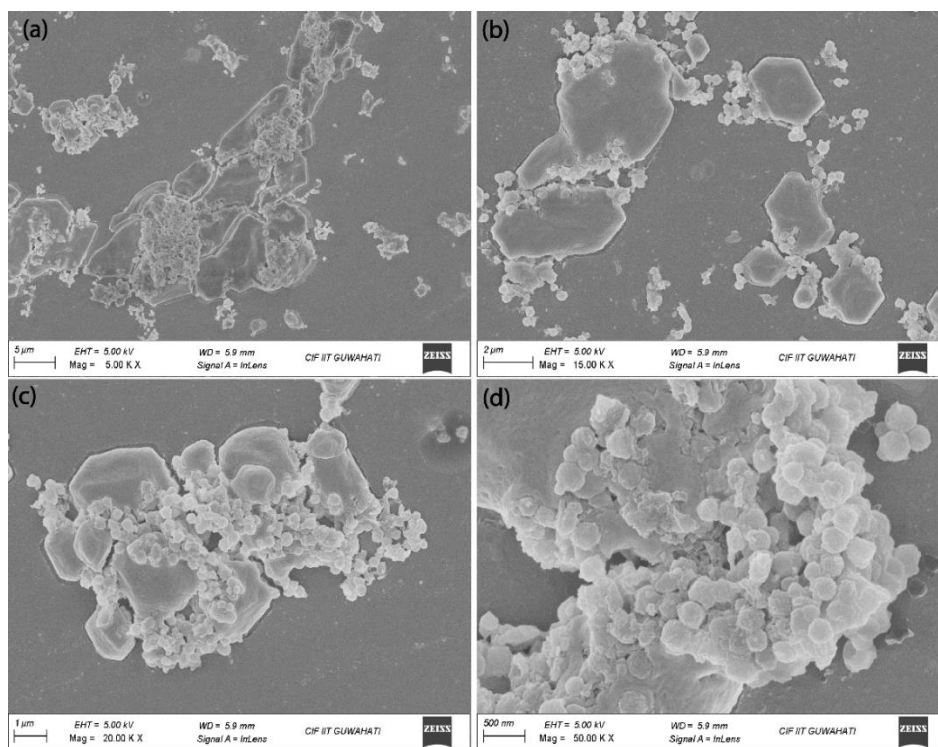


Figure S15 Post catalytic FESEM images of **3D-CPM-a** taken in a magnification range of 5 KX -50 KX in a Zeiss Sigma 300 instrument.

X-ray Photoelectron Spectroscopy

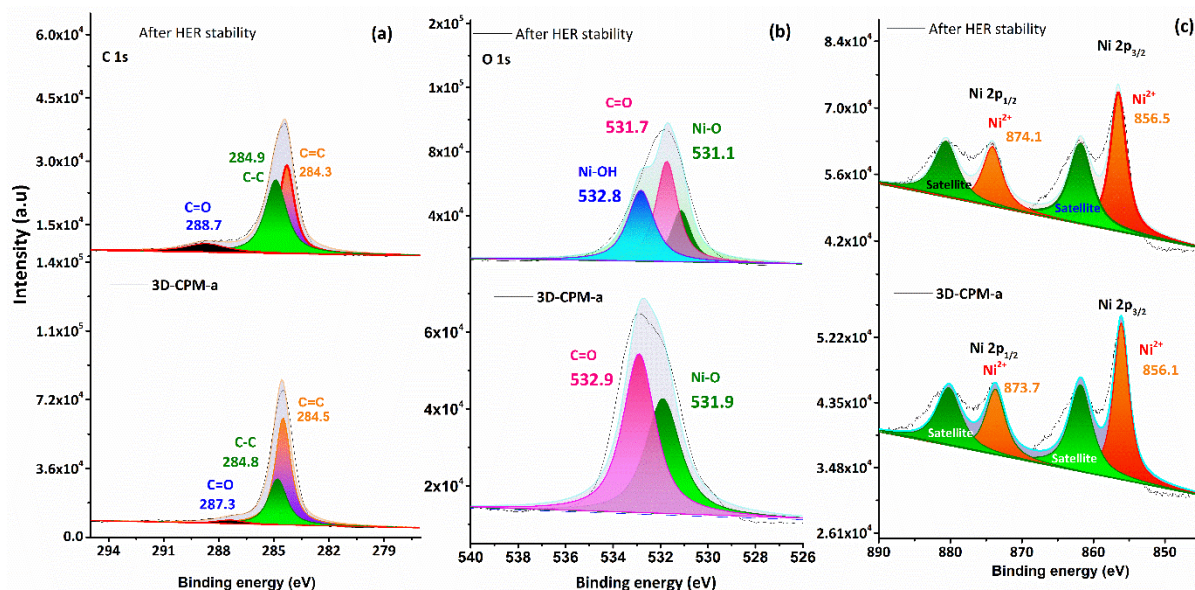


Figure S16 Comparison of XPS analysis of **3D-CPM-a** before and after HER (a) high resolution C1s spectra (b) high resolution O1s spectra and (c) high resolution Ni 2p spectra.

7. Control Studies

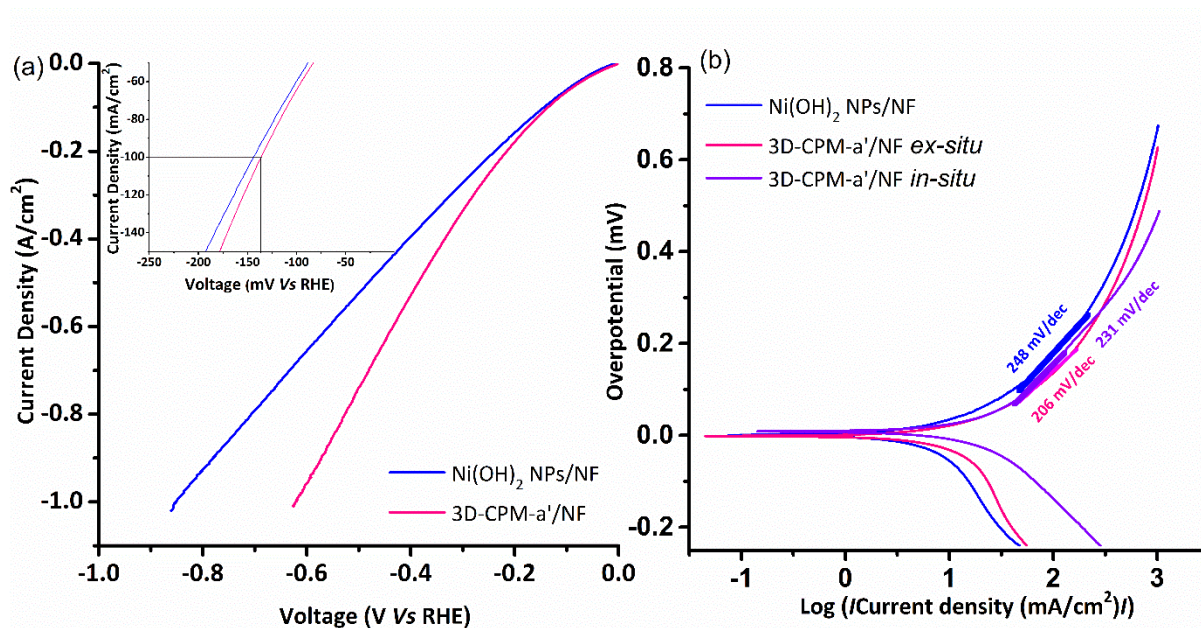


Figure S17 (a) Linear sweep voltammetric plot for HER in 0.5 M H_2SO_4 using $\text{Ni}(\text{OH})_2$ NPs/NF and **3D-CPM-a'** (*ex-situ*) at 90°C performed at 10 mV/s. The LSV plot is an average of 2 runs for each catalyst, (b) Tafel plots for $\text{Ni}(\text{OH})_2$ NPs/NF and **3D-CPM-a'** (*ex-situ* and *in-situ*).

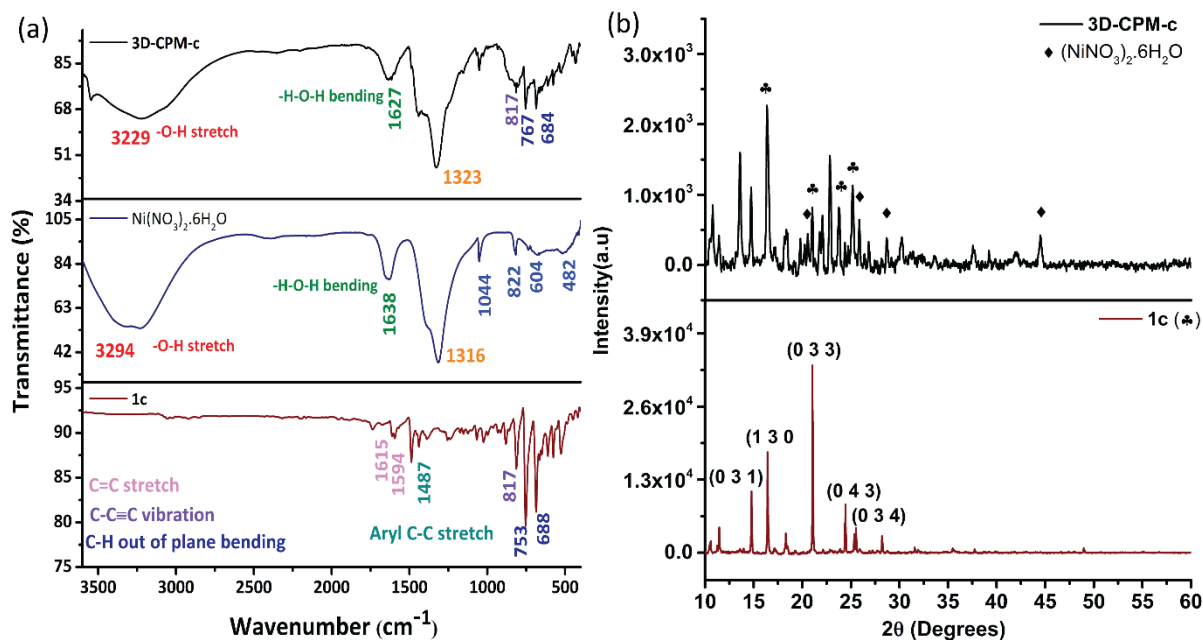


Figure S18 (a) A comparative FT-IR plot of **1c**, $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and **3D-CPM-c** (b) *p*-XRD of **1c** and **3D-CPM-c** carried out using a Rigaku SmartLab diffractometer utilizing $\text{Cu K}\alpha$ radiation ($\lambda = 1.541 \text{ \AA}$) at 40 kV and 125 mA. The 2θ angular region between 10° and 60° was explored at a scan rate of $10^\circ/\text{min}$ in a continuous scan mode.

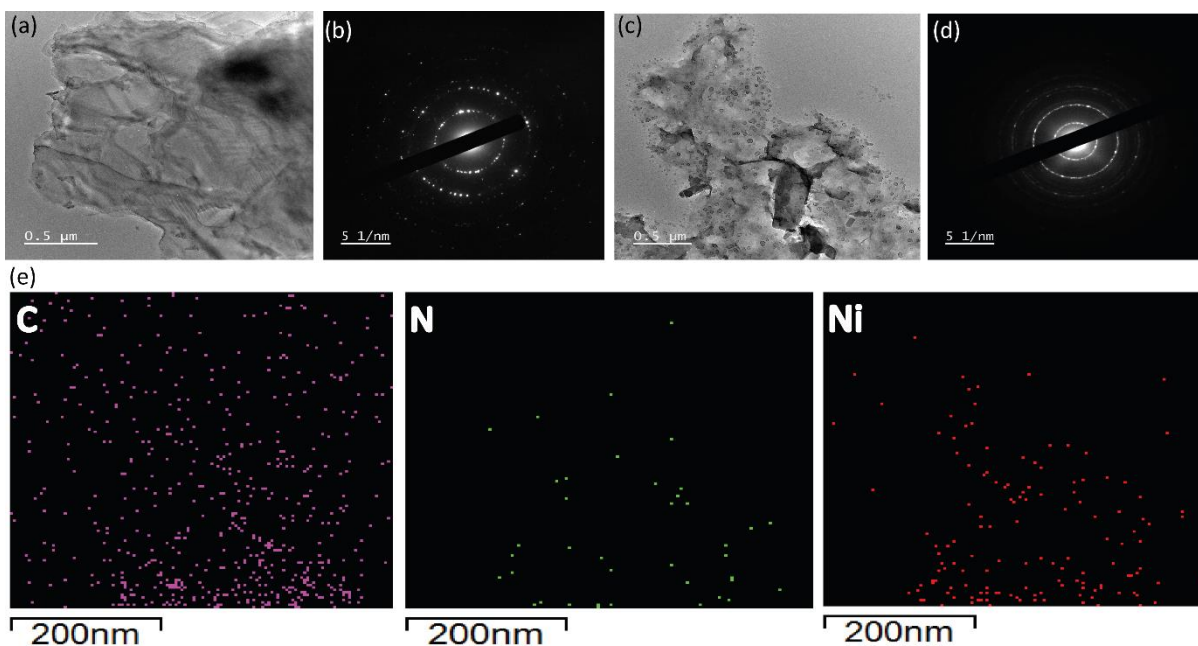


Figure S19 (a) FETEM image of **1c** at 500 nm (b) SAED of **1c** at 5 nm (c) FETEM image of **3D-CPM-c** at 500 nm (d) SAED of **3D-CPM-c** at 5nm taken in a JEOL Model 2100F instrument after drop-casting on a Cu-grid and drying at 70°C for overnight. (e) TEM elemental mapping of **3D-CPM-c**.

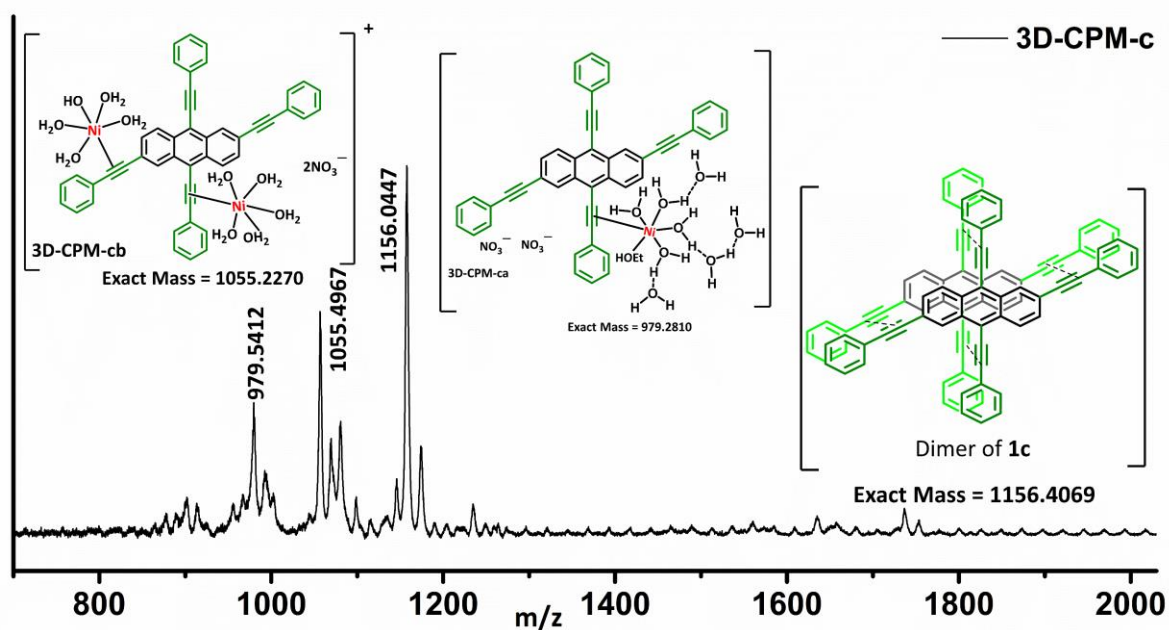


Figure S20 MALDI analysis of **3D-CPM-c** performed using sinapic acid as MATRIX and ethanol + water (1:1) as solvents.

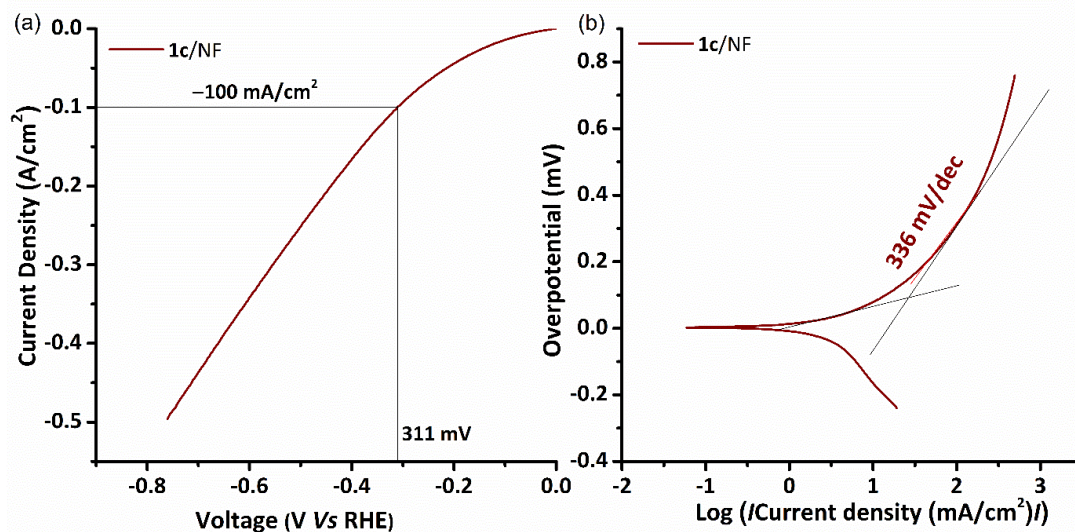


Figure S21 (a) Linear sweep voltammetric plot for HER in 0.5 M H₂SO₄ using 1c/NF at 90°C performed at 10 mV/s. The LSV plot is an average of 2 runs, (b) Tafel plot for 1c/NF at 90°C.

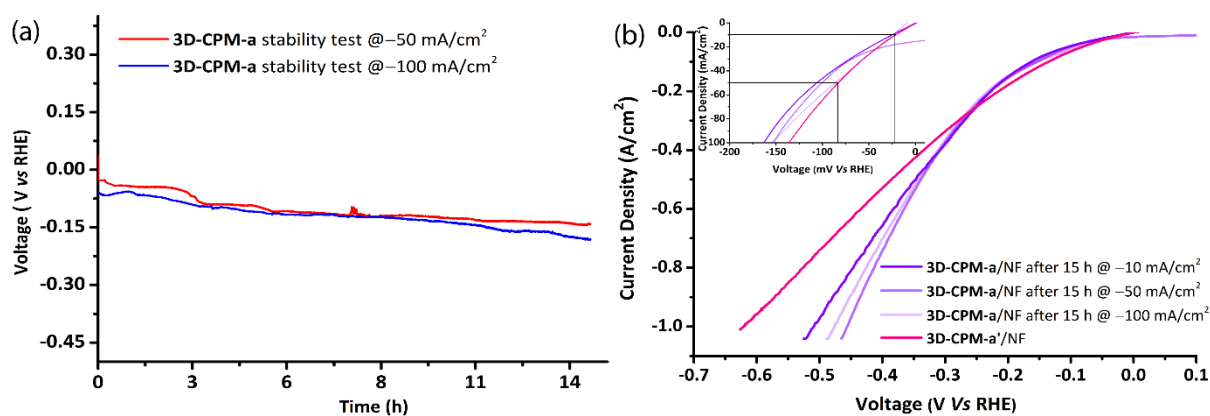


Figure S22 (a) V-t response of 3D-CPM-a at -50 mA/cm² and -100 mA/cm² for 15 h. (b) Comparative linear sweep voltammetric plot for 3D-CPM-a after chronopotentiometry at varied current densities for 15 h in comparison to 3D-CPM-a'/NF 90°C performed at 10 mV/s.

Table S2. Comparative HER performances of *ex-situ* and *in-situ* generated 3D-CPM-a' with Ni(OH)₂ nanoparticles

Current Density (mA/cm ²)	η (mV) of 3D-CPM-a' ex-situ	η (mV) of 3D-CPM-a' in-situ	η (mV) of Ni(OH) ₂ /NF
-10	21 ± 0.1	19 ± 4	34 ± 2
-50	82 ± 3	84 ± 11	114 ± 3
-100	137 ± 4	155	174 ± 1

8. DFT Studies

Table S3. Calculated Mulliken charges in eV for the hydrogen binding sites

Mulliken Charges (eV)			
	*3D-CPM-a	*3D-CPM-a_1H	*3D-CPM-a_2H
O	-0.33	-0.21	-0.28
Ni	-0.05	-0.03	-0.15

Energies of the optimized geometries:

Structures	Energy (a.u.)
*3D-CPM-a	-1972.1141
*3D-CPM-a_1H	-1972.6822
*3D-CPM-a_2H	-1973.2525
*3D-CPM-a + H ₂	-1973.2854
H ₂	-1.1652
H	-0.5826

Coordinates of the Optimized Geometries:

*3D-CPM-a:

C	31.387610742	25.925232415	27.750152808
C	30.281066180	26.708284071	27.940065357
C	30.380321255	28.126827727	28.059960353
C	31.681602308	28.734958999	27.954490502
C	32.810486975	27.900822807	27.764722977
C	32.691302005	26.516914782	27.664647652
C	29.228925690	28.934385060	28.260329151
C	31.815850496	30.161378705	28.038019197
C	30.673080901	30.958886538	28.334941797
C	29.372400572	30.346575953	28.443552419

C	28.254100671	31.159258013	28.745260263
H	27.278375517	30.687895097	28.856927050
C	28.377134270	32.533529315	28.944674665
C	29.673336961	33.134276700	28.826074833
C	30.771173751	32.368096875	28.526722218
H	31.297892437	24.841630061	27.679335906
H	29.293314063	26.253741550	28.016387291
H	33.795727143	28.361261058	27.706729661
H	29.773477315	34.206346439	28.994144177
H	31.756064491	32.829451931	28.448414204
C	27.941499139	28.353774764	28.242928297
C	26.817231101	27.872316658	28.165036434
C	25.505562717	27.379408465	27.972887225
C	24.914679631	26.433976737	28.848041621
C	24.732964697	27.847038325	26.880319898
C	23.609491163	26.005152630	28.660644769
H	25.497474973	26.060218491	29.690133949
C	23.446101485	27.377138949	26.664637091
H	25.167945169	28.582905251	26.203831423
C	22.841373389	26.452069987	27.554969375
H	23.153563969	25.305410502	29.361743462
H	22.872748480	27.757990894	25.818441171
C	21.438130372	26.040327011	27.418635708
O	20.755924340	25.738405506	28.476990417
C	27.238239852	33.295443698	29.292948670
C	26.224435228	33.902774788	29.614297427
C	25.020808695	34.500540054	30.042890837
C	24.923756996	35.878035563	30.363355667
C	23.860223670	33.699132691	30.192071714
C	23.749961446	36.409377214	30.873981558
H	25.793584402	36.521188826	30.234982644

C	22.695797211	34.231960726	30.714803841
H	23.904308113	32.647560158	29.909483583
C	22.619980852	35.590407075	31.113013694
H	23.718418163	37.471007861	31.131595701
H	21.819002678	33.594610920	30.814213531
C	21.408349318	36.115428859	31.737576952
O	21.143566749	37.364868560	31.809650921
C	33.072922055	30.745355160	27.781768672
C	33.824741850	25.691006453	27.496029369
C	34.782657818	24.941599334	27.369200020
C	35.897333989	24.078726496	27.267729722
C	37.207516551	24.564755410	27.475210330
C	35.732174793	22.700077897	27.002289214
C	38.300237676	23.709551073	27.428156224
H	37.349538205	25.621645966	27.699933096
C	36.827667799	21.848210346	26.975096756
H	34.727581039	22.310672788	26.834462167
C	38.132805631	22.333705176	27.187406413
H	39.294535829	24.109951782	27.625976635
H	36.690842124	20.782128090	26.792956981
C	39.270441277	21.366431332	27.166940790
O	38.997202319	20.126399877	27.646033403
C	34.183926736	31.165671058	27.477344978
C	35.473799111	31.576234567	27.069866073
C	36.233030457	30.756780488	26.202728027
C	36.048109169	32.802960742	27.486205476
C	37.502390432	31.138192888	25.782632055
H	35.796285467	29.825081538	25.840245433
C	37.321447715	33.166849990	27.077604137
H	35.479425409	33.456135173	28.148587311
C	38.090124630	32.341756248	26.224038724

H	38.028080598	30.502561133	25.071887086
H	37.758187910	34.107344125	27.411934906
C	39.436547015	32.818081263	25.795535640
O	39.672010451	34.131422818	25.854902159
C	40.284280624	21.456335896	26.060882896
C	41.113764629	22.578953679	25.881281888
C	40.422273080	20.376875432	25.166916997
C	42.053267450	22.614264383	24.850106493
H	41.051136477	23.412774574	26.579439473
C	41.362780339	20.414534181	24.135936360
H	39.769801326	19.510597710	25.282288150
C	42.183413166	21.533894170	23.970745043
H	42.698389622	23.487879328	24.737513649
H	41.446475805	19.569168126	23.450477201
H	42.917523707	21.564850228	23.164748115
C	20.755607027	26.011680601	26.120019955
C	21.432551751	25.677423211	24.926851732
C	19.370085367	26.276867420	26.055876052
C	20.747109362	25.616382418	23.715277821
H	22.495166573	25.435650520	24.961799694
C	18.691957670	26.221807922	24.841713140
H	18.845446788	26.556922140	26.969936051
C	19.376425954	25.893364511	23.665172215
H	21.283067483	25.343576040	22.805247826
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H	40.993262307	18.958127075	29.255503664
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C	39.748321399	25.123359183	30.674850729
C	40.607654575	23.310093800	32.037352063
C	40.827657268	25.917810528	31.062396945
H	39.010781995	25.510902044	29.971810881
C	41.679414600	24.113523303	32.431804999
H	40.507612077	22.289062742	32.408889405
C	41.790325160	25.421080236	31.946410558
H	40.918146999	26.927787834	30.664448696
H	42.425060444	23.720411502	33.124371328
H	42.626085684	26.050191115	32.255091994
C	19.432086897	30.229365007	31.359524627
C	19.762966450	31.350422100	30.573278718
C	18.121962100	30.141316977	31.873226069
C	18.822598247	32.345860304	30.310346894
H	20.754943672	31.420537206	30.125691995
C	17.184513766	31.140718969	31.615094337
H	17.848997126	29.277714724	32.480440982
C	17.530091353	32.246725351	30.832006657
H	19.101120866	33.199327298	29.690915776
H	16.178375740	31.056316778	32.028629848
H	16.797975744	33.029185343	30.630817525
C	39.759594833	28.751004482	28.288414427
C	38.902555234	28.193244062	27.317794840
C	41.104588435	28.328356961	28.323706979
C	39.378043930	27.234449011	26.422227944
H	37.877674307	28.554390449	27.234793912
C	41.569468936	27.352525747	27.444566630
H	41.774492652	28.773980372	29.060168800
C	40.706758021	26.800442441	26.490061673
H	38.709633792	26.822799874	25.665622550

H	42.607122060	27.020851106	27.502133690
H	41.066164152	26.040860209	25.794593605
C	21.690344229	38.827722269	34.955294018
C	20.880405096	37.675931030	35.062903151
C	21.452018243	39.872085891	35.870879955
C	19.885250590	37.572150741	36.039030794
H	20.989633464	36.861230814	34.350060371
C	20.462471929	39.763223231	36.850228535
H	22.055377486	40.774474255	35.800442698
C	19.670250871	38.616484999	36.942278238
H	19.272688327	36.670032119	36.076943449
H	20.307857237	40.589318427	37.546495450
H	18.890751484	38.540613708	37.701220360
Ni	40.614026149	33.308971907	26.980882323
O	42.134011287	34.664687561	27.597763492
H	42.911589556	34.252990253	27.114705582
O	41.694811270	31.610352450	27.514238313
H	41.503336292	31.004326578	26.760852451
H	41.959243405	35.510231640	27.148340530
H	41.233361472	31.169402158	28.312118860
O	43.879195232	33.017321082	26.349273494
H	43.541680752	32.906666433	25.438853947
O	39.982710851	33.466202444	29.230775659
H	40.755580085	33.918501179	29.613469221
H	43.392846260	32.321507955	26.848632863
H	40.036304100	32.529500508	29.548198003
Ni	21.815406160	38.866689326	32.142437163
O	24.015515462	41.192660517	31.321814555
H	23.215530566	40.875464897	30.843584033
O	19.379179120	41.530941386	31.408982469
H	19.704225272	42.278638102	31.939817009

H	24.710276099	40.572898074	31.038069756
H	19.297449146	40.779785916	32.044443841
O	21.423920262	40.180718134	30.326032616
H	20.643532992	40.767600834	30.560296722
O	19.726296451	39.086444472	32.695351997
H	19.681553439	38.827390362	33.643474665
H	21.160005809	39.640030080	29.561211758
H	19.621883609	38.236084058	32.190545570
Ni	20.549541444	26.784780346	29.900190247
O	17.334489704	27.405085116	30.140503551
H	18.176044330	27.703841465	30.571522228
O	19.884570966	25.201897811	30.924633636
H	19.526029384	25.548853010	31.764081963
O	17.922848156	24.838086501	29.223772957
H	18.561246286	24.942199660	28.488114905
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H	21.556108265	29.031027499	29.587371113
H	21.943020636	28.179511934	28.326394379
H	19.076850721	24.900574848	30.374476693
H	17.582297312	25.758180642	29.382856701
H	16.998587077	28.197171548	29.689218307
Ni	40.033194254	21.035592195	28.637471120
O	38.181577501	19.084715660	30.587512282
H	37.838774194	18.847389325	29.706852512
O	40.783489914	19.461016538	29.845408397
H	40.922114830	18.792794908	29.118276607
O	40.663872198	18.072049278	27.467863567
H	40.026501493	18.800297890	27.224890544
O	41.598088926	22.156133894	29.280670114
H	42.089506013	21.471866795	29.779171835
H	41.290235560	22.777161548	29.978936349

H	41.397624798	18.177513337	26.838856904
H	38.143505239	20.075459640	30.586118194
H	39.931303344	19.166753339	30.282226427
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C	31.547862812	28.823605174	28.015703827
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C	32.629575908	26.641433743	27.737131346
C	29.085945953	28.950816508	28.270333383
C	31.637774270	30.252702733	28.099806309
C	30.468719444	31.017806265	28.367334245
C	29.187302728	30.365552300	28.459299646
C	28.043378455	31.142633311	28.752931461
H	27.082389811	30.640922744	28.858699869
C	28.122462421	32.519207567	28.954895796
C	29.397428822	33.163977481	28.838045440
C	30.520460247	32.431526908	28.549720455
H	31.286241824	24.927201487	27.686796572
H	29.232261074	26.274021570	27.992229210
H	33.678355278	28.514670145	27.828114027
H	29.462133170	34.238988664	29.003030441
H	31.491482656	32.922481132	28.477187083
C	27.812531118	28.338656466	28.232791883
C	26.699512157	27.834476479	28.138794085
C	25.407655066	27.295528123	27.930547287
C	24.818709231	26.376016036	28.833264915

C	24.654297694	27.682534425	26.792814173
C	23.533896438	25.897345204	28.628776137
H	25.386145037	26.060947145	29.708883480
C	23.384408792	27.173292401	26.567895640
H	25.088639301	28.394842728	26.091157924
C	22.778917174	26.276888921	27.486818416
H	23.079631960	25.217141419	29.349990991
H	22.824538129	27.503723878	25.692530270
C	21.383692747	25.843232206	27.349425594
O	20.701287719	25.531860120	28.404319530
C	26.958117775	33.236526873	29.309680814
C	25.924954352	33.801240843	29.646566060
C	24.724052868	34.377932398	30.107212068
C	24.626333477	35.755036876	30.427846930
C	23.575554752	33.567270774	30.301145264
C	23.466584475	36.273816596	30.977556088
H	25.490339584	36.400186285	30.274782861
C	22.423289853	34.091157835	30.859936288
H	23.620394962	32.513621100	30.026186402
C	22.347548907	35.452660185	31.250729934
H	23.429065482	37.332485102	31.252868752
H	21.556763872	33.445652634	30.991575856
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C	32.886360416	30.860674174	27.863080510
C	33.789571263	25.849985604	27.588489835
C	34.767357249	25.126601664	27.466309539
C	35.880550832	24.267885477	27.339538814
C	37.193464914	24.737714890	27.562772918
C	35.707214036	22.905280770	27.004158302
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C	36.797850256	22.052985186	26.926919109
H	34.700226240	22.530799696	26.818846316
C	38.106374801	22.523225897	27.152954084
H	39.282601743	24.276259269	27.640794565
H	36.660757215	20.997787640	26.692021962
C	39.234678437	21.552612173	27.068226699
O	38.905508846	20.265853833	27.324221395
C	34.003669375	31.261641482	27.559636404
C	35.294185725	31.634782312	27.121730041
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C	35.932820994	32.819634872	27.560448791
C	37.242819983	31.167418576	25.727391184
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C	37.195534030	33.154202796	27.101007340
H	35.419712182	33.464879639	28.273902367
C	37.888848686	32.336768495	26.179491070
H	37.714775585	30.540055852	24.972648673
H	37.682827823	34.064535728	27.447329665
C	39.225192457	32.791276448	25.705007621
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C	40.333470697	21.790966128	26.070402666
C	41.274865295	22.826879230	26.201878737
C	40.434662932	20.931216993	24.960680824
C	42.282060948	22.997989616	25.251159821
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C	42.374328344	22.136436691	24.153062538
H	43.015300424	23.796642775	25.379642673
H	41.504396128	20.425216840	23.158353220

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C	20.690701882	25.802738733	26.055153431
C	21.346511182	25.424739178	24.863374536
C	19.308229958	26.088321526	26.002510900
C	20.641499468	25.331414465	23.665451770
H	22.406725732	25.171249336	24.891063838
C	18.611296555	26.004947641	24.800683120
H	18.801409311	26.404461309	26.915057172
C	19.273418691	25.623679572	23.626925328
H	21.159443440	25.020483537	22.756961479
H	17.546798594	26.242314941	24.774215130
H	18.725120608	25.553653526	22.686719941
C	40.128900386	31.977860481	24.829749346
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H	39.681194564	30.022871181	25.674937612
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C	42.118761649	30.578036256	23.361990959
H	41.413133775	28.823877973	24.414439820
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C	18.788051348	35.445552989	32.522267489
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H	21.621373565	33.743620482	33.369818997
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H	19.963923549	32.389909871	34.614960768
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H	17.547662963	32.992139266	34.538305005
C	29.750819387	26.188496202	31.430044749
C	28.930230853	27.271239181	31.650620142
C	29.444823218	28.591479305	31.800349103
C	30.860958353	28.783661475	31.679592199
C	31.679354409	27.660067984	31.466560263
C	31.164602246	26.367431346	31.350655517
C	28.596796719	29.714388924	32.061680177
C	31.433746481	30.104474244	31.776332868
C	30.591030842	31.218676119	32.075922495
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C	28.900401823	33.418016646	32.706493494
C	30.305292656	33.603309824	32.527609127
C	31.113755458	32.533971759	32.222813435
H	29.331974639	25.187808742	31.323466436
H	27.851053528	27.132495342	31.717344478
H	32.754273173	27.804041646	31.391135801
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H	32.186811815	32.678562469	32.091142522
C	27.214424033	29.556733954	32.147002111
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H	21.747695951	31.234552978	32.325105839
C	20.353826323	28.923849388	31.640431280
O	19.858324231	27.718195566	31.439057310
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C	26.171116402	37.581893374	33.074853914
C	25.066663612	35.867233608	34.380354954
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C	23.980008029	36.711880785	34.565135292
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C	23.924875617	37.979288139	33.945871114
H	25.068273141	39.391624307	32.768342655
H	23.156231219	36.370389765	35.187670954
C	22.695818799	38.820062839	33.949412808
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C	33.107852575	24.629935385	31.046443904
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C	37.108009453	23.186916908	30.897879019

H	37.531361811	25.015975308	32.001028682
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C	38.485809313	22.718935303	30.862863507
O	38.801501882	21.526880812	30.529199232
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C	35.330407393	30.085315183	30.855177240
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C	36.218095631	31.196058542	30.854084227
C	37.111584485	28.725444207	29.891424164
H	35.175179912	27.962063621	30.398414364
C	37.502918169	31.075892416	30.370529617
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C	37.983365915	29.847087994	29.842857403
H	37.462034384	27.749840448	29.556011449
H	38.143048783	31.955127058	30.348157058
C	39.322986499	29.773695734	29.296896802
O	40.202128577	30.664815971	29.570336912
C	39.601221922	23.624106302	31.269699067
C	39.741570375	24.933371521	30.772654482
C	40.587475551	23.126597368	32.148532440
C	40.827270652	25.722986377	31.152542398
H	39.005187233	25.321356590	30.069085998
C	41.665888397	23.925355411	32.536645677
H	40.477088144	22.112882511	32.537599881
C	41.788370549	25.226881447	32.038902114
H	40.924468953	26.729090599	30.745495441
H	42.407429931	23.532420553	33.233842081
H	42.629736939	25.851839232	32.340432773
C	19.414448864	30.051888850	31.441863620
C	19.744707088	31.178926659	30.663269362
C	18.099652382	29.952475794	31.941490402

C	18.798092608	32.165441795	30.390630374
H	20.741197486	31.260921293	30.227558274
C	17.155483022	30.942735188	31.672398080
H	17.827800854	29.085082036	32.544227242
C	17.499896399	32.053165451	30.894869928
H	19.072694568	33.022676198	29.774290499
H	16.145963122	30.849546200	32.076589956
H	16.762955172	32.829117549	30.686476627
C	39.737288661	28.680168542	28.378937725
C	38.878518702	28.153383411	27.392985583
C	41.074459381	28.234125901	28.418737787
C	39.344556627	27.199903463	26.486849912
H	37.858957402	28.529955551	27.311632174
C	41.527482255	27.262936315	27.528354193
H	41.746337604	28.657265424	29.166544450
C	40.663861399	26.741365530	26.558276729
H	38.673773646	26.809397117	25.721469841
H	42.558094527	26.910660696	27.589844074
H	41.014062233	25.980662805	25.859452526
C	21.626609868	38.672226749	34.995119931
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C	21.237192291	39.812646551	35.723924735
C	19.865300947	37.416311884	36.126704645
H	21.165876158	36.584075943	34.640538601
C	20.175248718	39.758632359	36.627313900
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H	19.326737251	36.476862303	36.261475110
H	19.888819818	40.657652198	37.175353266
H	18.645679224	38.522611166	37.534095182
Ni	40.521997798	33.214035181	27.077759947

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O	41.618481686	31.505909795	27.566142675
H	41.404469481	30.899761033	26.819978655
H	41.933283082	35.391725124	27.263184969
H	41.187382412	31.067007826	28.383169414
O	43.816984312	32.880806225	26.442669901
H	43.503711755	32.793399732	25.521722764
O	39.975060548	33.365618265	29.321704489
H	40.765539125	33.814148122	29.672379604
H	43.297966530	32.191100063	26.918785333
H	40.027555422	32.431677759	29.648648900
Ni	21.868492142	38.814747844	32.191480421
O	24.153573508	41.154619848	31.029142908
H	23.407932231	40.951109508	30.437056022
O	20.013274812	41.305982214	32.492341789
H	20.801477061	41.246970025	33.074108466
H	23.797700884	40.885776641	31.901440884
H	19.444739149	40.551750783	32.810948609
O	21.281792743	40.020064095	30.616546613
H	20.692584992	40.636105568	31.185750237
O	18.661796166	38.955976078	33.173945597
H	18.657461329	38.835805467	34.143069504
H	20.699473295	39.590360321	29.966213128
H	19.346703089	38.316608172	32.877128018
Ni	20.504570811	26.639432935	29.951622663
O	17.322589928	27.132432896	30.245543483
H	18.152477367	27.474533274	30.666073774
O	19.917716061	25.043713384	31.000495205
H	19.551110468	25.386594886	31.838232110
O	17.971504869	24.593595033	29.314612825

H	18.596116169	24.714625717	28.569927134
O	21.118962360	28.279657968	28.980590403
H	21.478502651	28.894835582	29.660056176
H	21.874080672	28.061416298	28.389952295
H	19.120704224	24.700673187	30.458683050
H	17.603908440	25.502618335	29.475161407
H	16.926042268	27.910406317	29.819532659
Ni	39.936484906	20.937165233	28.735331048
O	38.336306298	18.943274523	31.166557205
H	37.650771315	18.511792186	30.629684287
O	40.667136576	19.251819347	29.796058115
H	40.739631039	18.617010676	29.028533268
O	40.554311766	18.063788559	27.345753134
H	39.963860617	18.834714930	27.116268163
O	41.604447601	21.866681956	29.488193995
H	41.975592616	21.078670203	29.937841508
H	41.361348900	22.469983283	30.226155357
H	41.336576521	18.180467105	26.780231830
H	38.234550961	19.912466669	30.979075071
H	39.891965622	18.942857351	30.347847231
H	24.608080919	41.885352219	35.239176334
H	24.202177202	41.518929030	34.721556727

9. Literature Survey

Table S4 State-of-the-art in electrochemical hydrogen evolution reaction from Ni-based electrocatalysts depicting best reported overpotentials.

Entry	Catalyst	Electrolyte	Overpotential (mV Vs RHE)	Current density (mA/cm ²)	Tafel slope (mV/dec)	References
1	a-Co/c-Ni@CP-600s	1 M KOH	41	-10	41.3	[1]
2	CoSe ₂ @NiFe-LDH/NF	1 M KOH	227	-50	64.5	[2]
3	Ru-NiAlEO-P/CFP	1 M KOH	60	-10	64.6	[3]
4	Te-Cu ₂ O/NiMo	1 M KOH	140	-10	136.7	[4]
5	NiCoW/Ti ₃ C ₂ MXene	1 M KOH	107	-100	19.6	[5]
6	Ni(OH) ₂ (NHCo)	1 M KOH	73	-10	85	[6]
7	NiIr(OH) ₂ -EO	1 M KOH	69	-100	40	[7]
8	(Pt@Ni(OH) ₂ -NF	1 M KOH	53	-100	27	[8]
9	N-doped 3D porous Ni/C	1 M KOH	94	-100	52	[9]
10	Ni-Mo Alloy Nanosheet	1 M KOH	35	-10	45	[10]
11	NiMo alloy nanowire	1 M KOH	98	-400	43	[11]
12	Pt/Ni ASs	1 M KOH	28	-10	48	[12]
Coordination Polymers						
13	[Ni ₂ (cis-1,4 chdc) ₂ (4,4'-bpy) ₃ (H ₂ O) ₂]	1 M KOH	427	-10	361	[13]
14	W-doped Ni C ₃ S ₃ N ₃	1 M KOH	88	-10	30	[14]
15	Mo-doped Ni C ₃ S ₃ N ₃	1 M KOH	116	-10	89	[15]
16	Co _{1/3} Ni _{2/3} -DHBQ s	1 M KOH	177	-10	119	[16]
17	(NiCP-1/GCE)	0.5 M H ₂ SO ₄	632	-10	159	[17]
18	2D Ni-CP	1 M KOH	266	-10	186	[18]
19	3D-CPM-a	0.5 M H ₂ SO ₄	94 ± 14	-100	55	This work

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