

Integrated Cell Engineering and Scale-Up of a Non-PGM Bifunctional Electrocatalyst for Durable AEM Water Electrolysis

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Fig. S01. (a) Backscattered area of NCP-NS electrocatalyst, (b), (c), (d), (e) and (f) are elemental mapping of O, Ni, Cu, P and S elements.

Fig. S02. HRTEM analysis of the NCP-NS electrocatalyst, (a) HRTEM morphology image, (b) and (c) HRTEM with labeled d-spacing values.

Fig.S03. XPS characterization (a) High resolution spectra (survey scan) of NCP-NS electrocatalysts, (b) Ni (2p) (c) Cu (2p), (d) S (2p), and (e) P (2p).

Fig. S04. Nyquist plot for NCP-NS electrocatalyst at different temperature.

Fig. S05. Polarization curve of 13 cm² electrolyzer cell using benchmarked electrocatalyst pair (Pt/C || RuO₂) at different temperature.

Fig.S06. SEM analysis of NCP-NS electrocatalyst (a) & (b) before and (c) & (d) after durability

Fig.S07. XRD pattern for NCP-NS electrocatalyst before and after the durability test.

Table S01. Mass loading effects on electrolyzer cell using Sym. NCP-NS electrocatalyst.

Table S02. Effect of applied torque on electrochemical performance.

Table S03. Gasket thicknesses effects on electrochemical performance.

Table S04. ICR measurements of the cell components for various gasket thickness (at 0.1A).

Table S05. Flow rate effects on electrochemical impedance and performance.

Table S06. Temperature effects on electrochemical performance.

Table S07. Various non-platinum group metal-based bifunctional electrocatalyst performance comparison

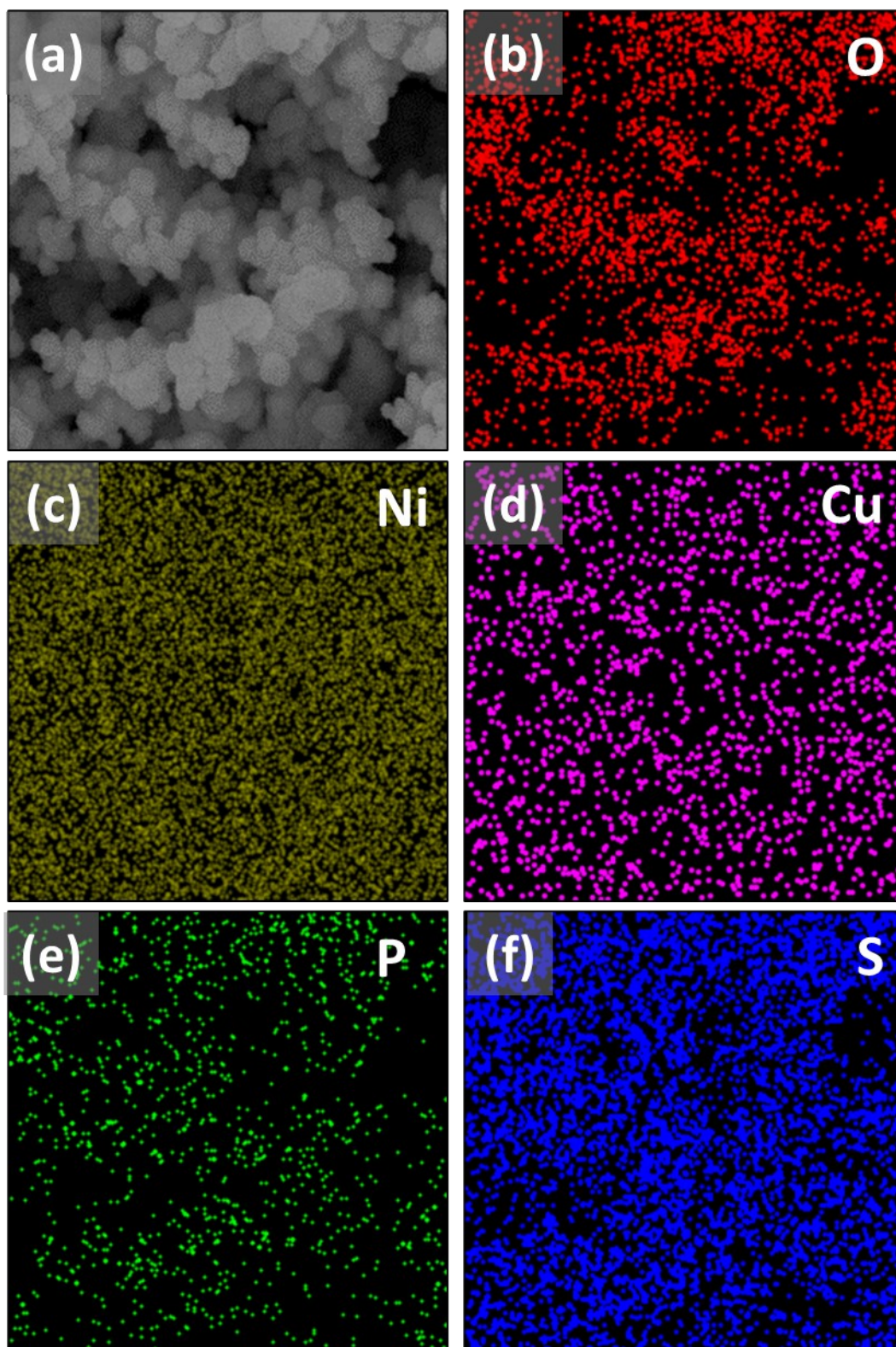


Fig. S01. (a) Backscattered area of NCP-NS electrocatalyst, (b), (c), (d), (e) and (f) are elemental mapping of O, Ni, Cu, P and S elements.

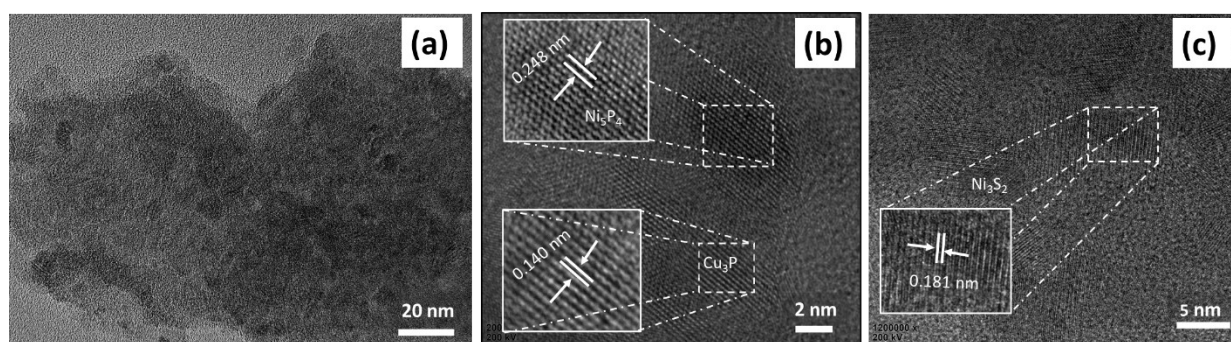


Fig. S02. HRTEM analysis of the NCP-NS electrocatalyst, (a) HRTEM morphology image, (b) and (c) HRTEM with labeled d-spacing values.

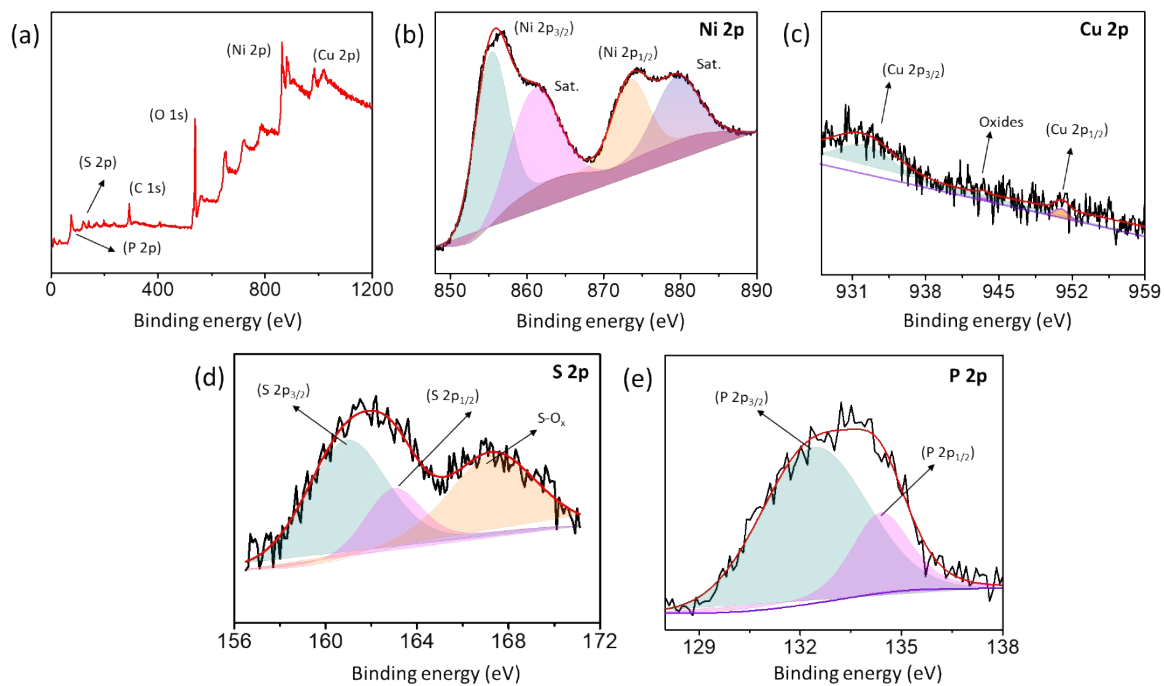


Fig. S03. XPS characterization, (a) High resolution spectra (survey scan) of NCP-NS electrocatalysts, (b) Ni (2p) (c) Cu (2p), (d) S (2p), (e) P (2p).

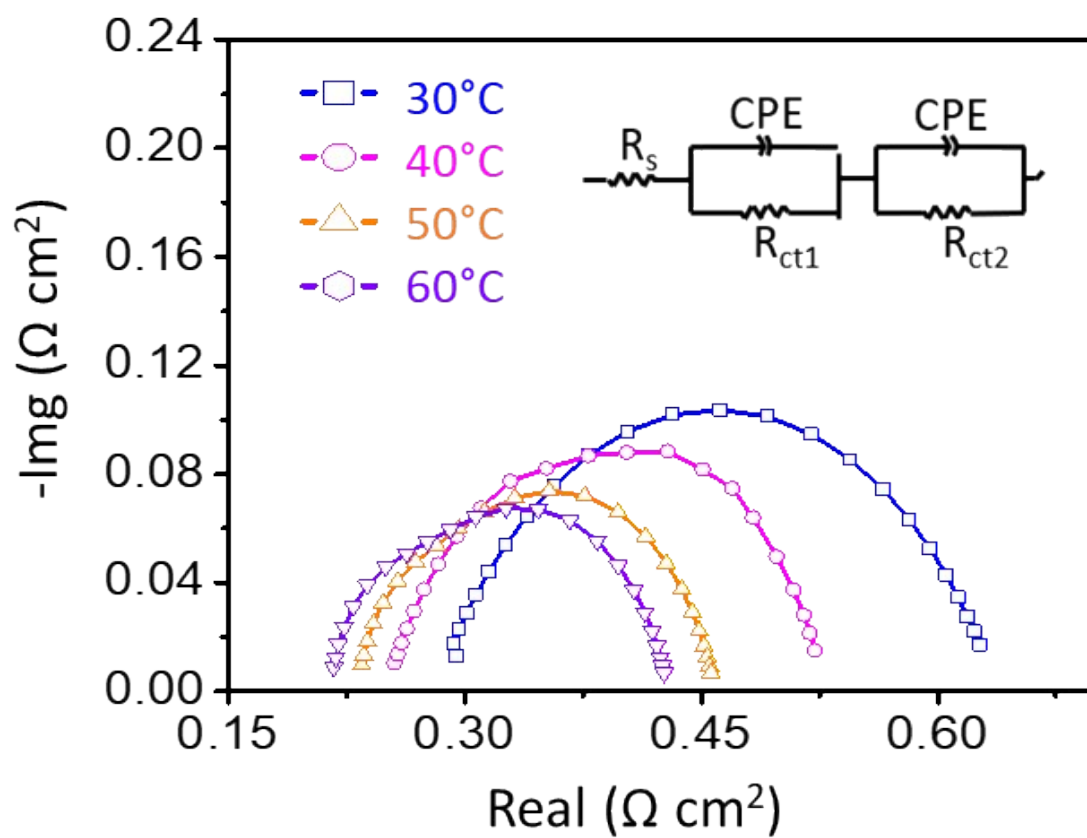


Fig. S04. Nyquist plot for NCP-NS electrocatalyst at different temperature.

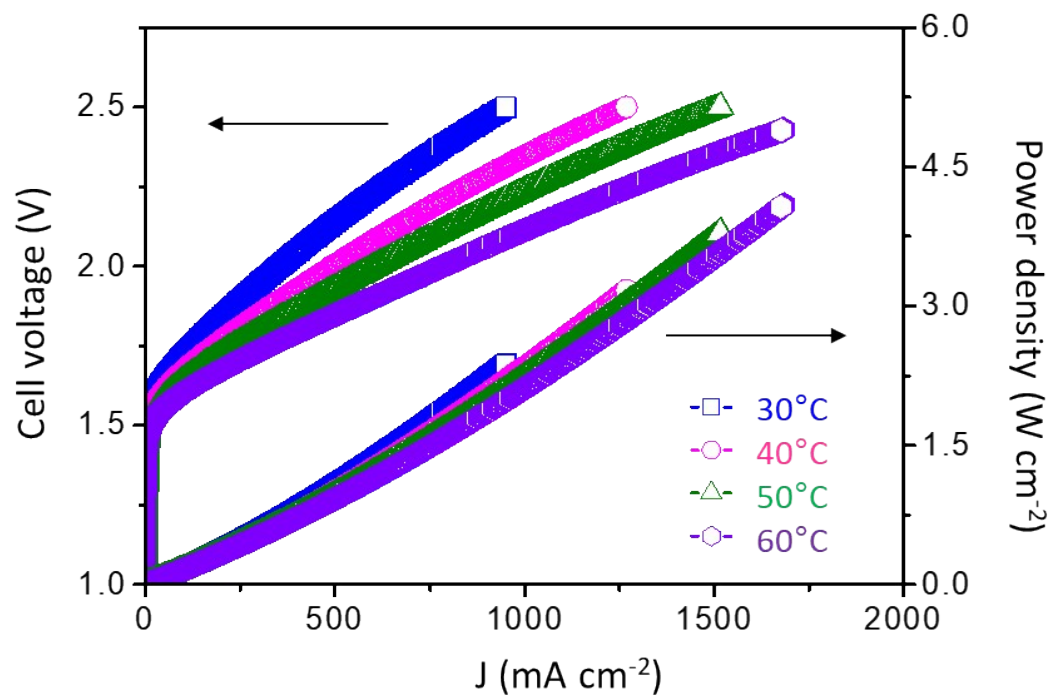


Fig. S05. Polarization curve of 13 cm² electrolyzer cell using benchmarked electrocatalyst pair (Pt/C || RuO₂) at different temperature.

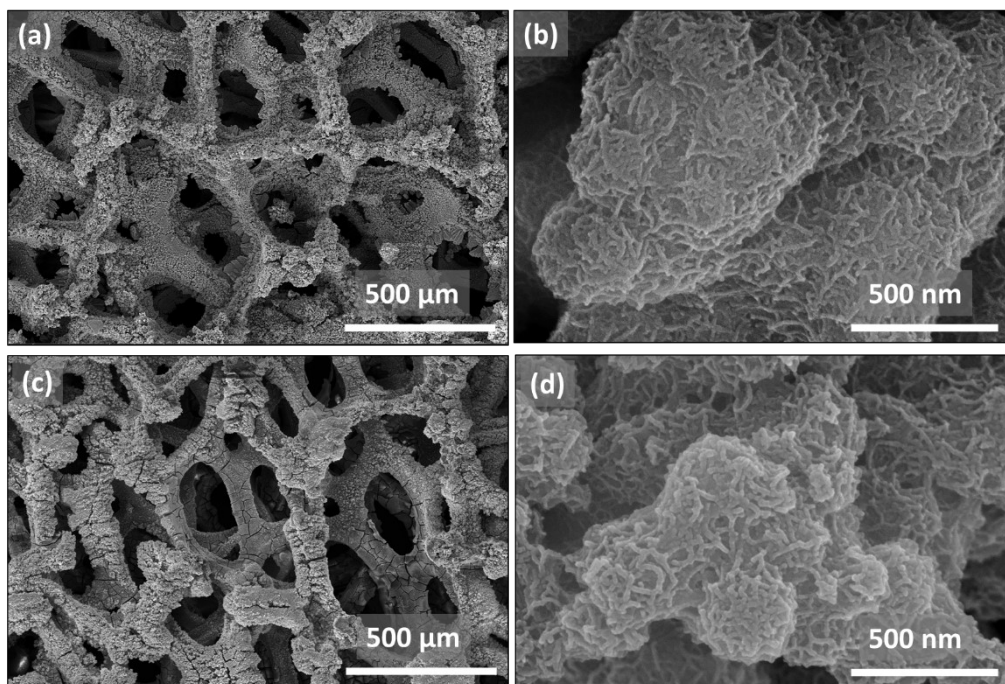


Fig. S06. FESEM images of NCP-NS electrocatalyst before and after the durability test: (a) and (b) Before durability, and (c) and (d) after durability.

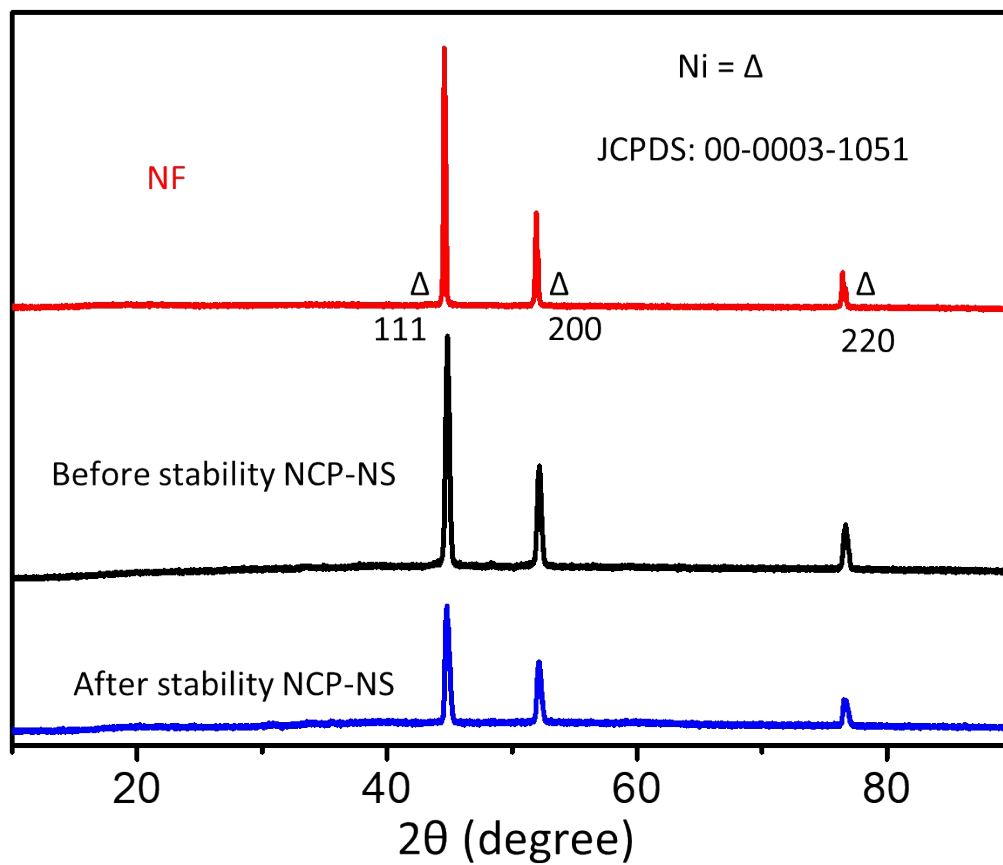


Fig. S07. XRD pattern for NCP-NS electrocatalyst before and after the durability test.

Table S01. Mass loading effects on electrolyzer cell using Sym. NCP-NS electrocatalyst.

MLD (mg cm ⁻²)	J ₂ (mA cm ⁻²)	R _s (mΩ cm ²)	Total R _{ct} (mΩ cm ²)
03	231	365	745
07	344	350	420
10	396	320	350
13	408	310	335

Table S02. Effect of applied torque on electrochemical performance.

Torque (Nm)	J_2 (mA cm ⁻²)	R_s (mΩ cm ²)	Total R_{ct} (mΩ cm ²)
01	396	293	365
02	412	290	354
03	426	291	349
04	439	289	340

Table S03. Gasket thicknesses effects on electrochemical performance.

Gasket thickness (μm)	J_2 (mA cm^{-2})	R_s ($\text{m}\Omega \text{ cm}^{-2}$)	Total R_{ct} ($\text{m}\Omega \text{ cm}^{-2}$)
700	172	804	720
600	269	503	470
500	368	317	352
400	440	312	350
300	407	307	410

Table S04. ICR measurements of the cell components for various gasket thickness (at 0.1A).

Gasket thickness (μm)	Resistance ($\text{m}\Omega$)			
	Endplate	Gasket	Electrodes	Overall
700	0.28	300	130	430
400	0.28	4.92	0.5	5.70

Table S05. Flow rate effects on electrochemical impedance and performance

Flow rate (mL min ⁻¹ cm ⁻²)	J ₂ (mA cm ⁻²)	R _s (mΩ cm ²)	Total R _{ct} (mΩ cm ²)	Cell Temp. (°C)
0.50	434	300	420	30 ± 2
1.00	495	295	345	30 ± 2
1.50	448	305	346	30 ± 2
2.00	443	307	352	30 ± 2
2.50	415	300	452	30 ± 2

Table S06. Temperature effects on electrochemical performance

Temperature (°C)	J_2 (mA cm ⁻²)	R_s (mΩ cm ²)	Total R_{ct} (mΩ cm ²)
30	496	295	335
40	601	250	290
50	807	230	200
60	1010	210	180

Table S07. Various non-platinum group metal-based bifunctional electrocatalyst performance comparison

Electrocatalysts	Material synthesis temp. (°C)	MEA size (cm ²)	Electrolyzer Operating temp. (°C)	Activity J ₂ (mA cm ⁻²)	Reference number
Co ₆₅ Fe ₃₅ O _x H _y	30	1	50	605	1
LDHQDs/NiCoP	400	1	80	574	2
NiCo(OH) ₂	140	2	30	~170	3
g-CN/NCF	800	5	70	~450	4
SmNi _{0.02} Fe-LDH	160	5	60	900	5
MoS ₂ -Ni ₃ S ₂	220	4	30	~50	6
NiFeS@Ti ₃ C ₂	160	25	50	800	7
NiFeLDH/Ni ₄ Mo	30	1	30	100@1.68	8
FCPWP	200	25	50	425@1.85	9
NCP-NS	30	13	60	1012	Our work

Energy efficiency calculation:¹⁰

Applied Current = 13.15 A (1012 mA cm⁻²) and corresponding voltage = 2.0 V

Power (W) = Current (A) × Cell voltage (V)

Power (W) = 13.15 A × 2 = 26.3 W (0.0263 kW)

Hydrogen production = 106 mL/min @ 60 °C (333.15 K) and 1 atm pressure.

Volume to mass conversion based on Ideal gas law: V = 27.32 L/mol @ 60 °C

However, $n = \frac{0.106 \text{ L/min}}{27.32 \text{ L/mol}} = 0.0039 \text{ mol/min}$

Conversion into g/min: Molar mass of hydrogen = 2.016 g/mol

Hydrogen production (g/min) = 0.0039 mol/min × 2.016 g/mol = 0.0078 g/min

Hydrogen production (g/h) = 0.469

Hydrogen production (kg/h) = 0.00047

$$\text{Specific energy consumption (kWhkg}^{-1}\text{)} = \frac{\text{Power consumed (kW)}}{\text{Hydrogen production (kg/h)}}$$

$$\text{Specific energy consumption (kWhkg}^{-1}\text{)} = \frac{0.0263 \text{ (kW)}}{0.00047 \text{ (kg/h)}}$$

$$\text{Specific energy consumption (kWhkg}^{-1}\text{)} = 55.96 \text{ kWhkg}^{-1}$$

$$\text{Energy efficiency (kWhkg}^{-1}\text{)} = \frac{\text{Theoretical energy consumption based on HHV (39.4 kWh/kg)}}{\text{Experimental energy consumption (}\frac{\text{kWh}}{\text{kg}}\text{)}} \times 100$$

$$\text{Energy efficiency (kWhkg}^{-1}\text{)} = \frac{(39.4 \text{ kWhkg}^{-1})}{(55.96 \text{ kWhkg}^{-1})} \times 100$$

$$\text{Energy efficiency (kWhkg}^{-1}\text{)} = 70.41 \%$$

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