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磷化镍@镍-氮-碳双功能催化剂电还原 CO₂-H₂O 制合成气

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Engineering of Bifunctional Nickel Phosphide@Ni-N-C Catalysts for Selective Electroreduction of CO₂-H₂O to Syngas

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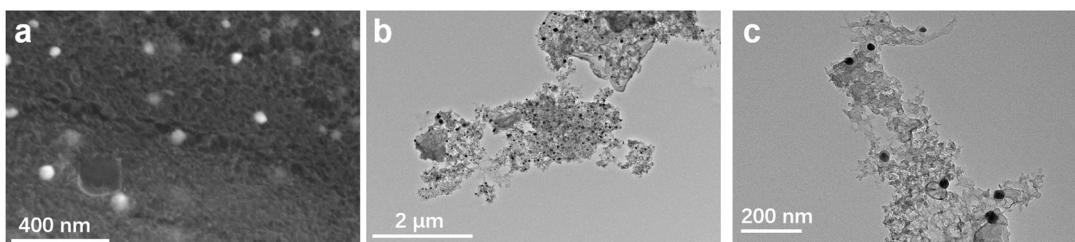


Fig. S1 (a) SEM and (b, c) TEM images of P/Ni-4@Ni-N-C.

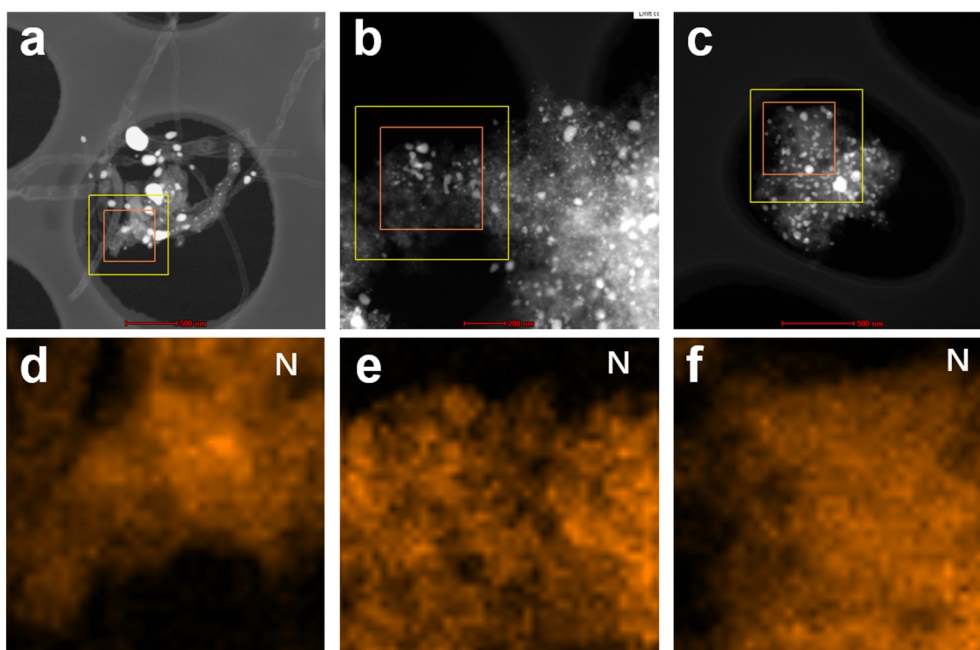


Fig. S2 HAADF-STEM images of (a) P/Ni-0@Ni-N-C, (b) P/Ni-4@Ni-N-C, (c) P/Ni-10@Ni-N-C and EDX element mapping of N in (d) P/Ni-0@Ni-N-C, (e) P/Ni-4@Ni-N-C, (f) P/Ni-10@Ni-N-C.

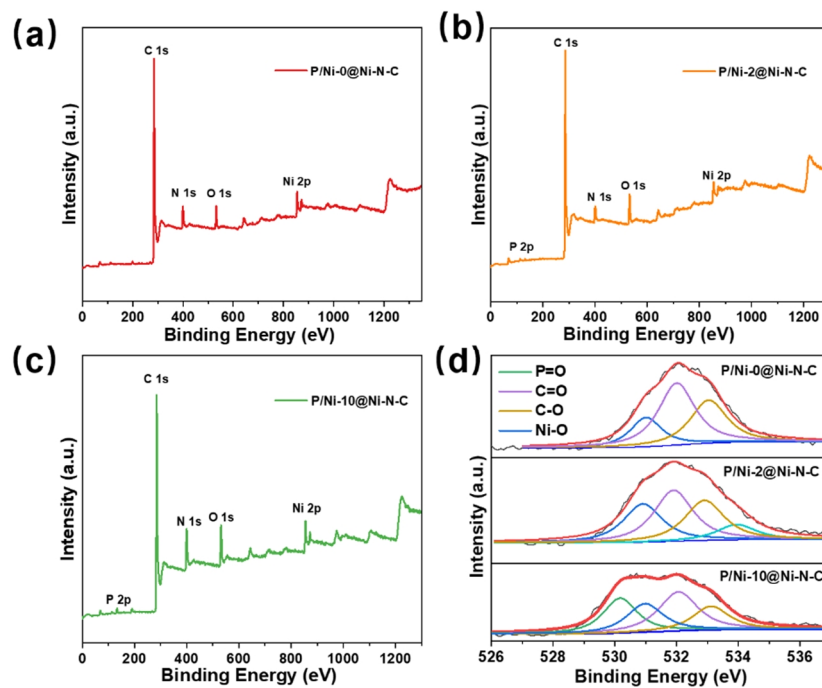


Fig. S3 XPS survey spectra of (a) P/Ni-0@Ni-N-C, (b) P/Ni-2@Ni-N-C, (c) P/Ni-10@Ni-N-C and (d) O 1s spectra of P/Ni-x@Ni-N-C ($x = 0, 4, 10$).

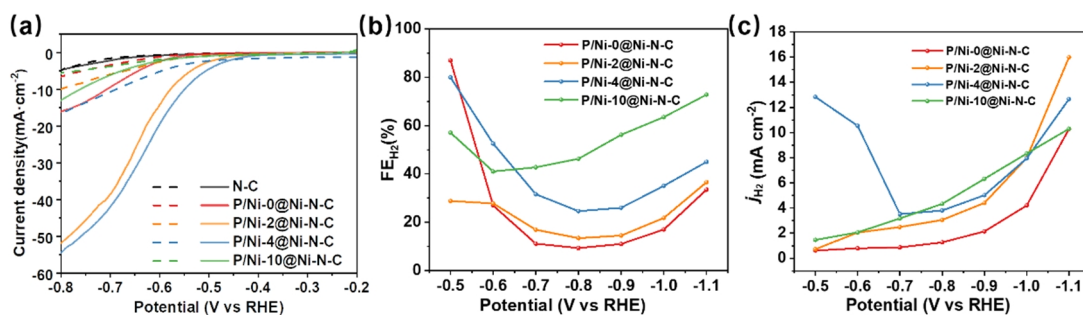


Fig. S4 (a) LSV curves of N-C and P/Ni-*x*@Ni-N-C in Ar (dash) and CO₂ (solid) saturated 0.5 mol·L⁻¹ KHCO₃ solutions (all curves were reported with iR compensation). loading amount: 0.85 mg cm⁻² on glassy carbon electrode, scan rate: 5 mV s⁻¹. (b) H₂ Faradaic efficiency and (c) H₂ partial current density of P/Ni-*x*@Ni-N-C at different potentials.

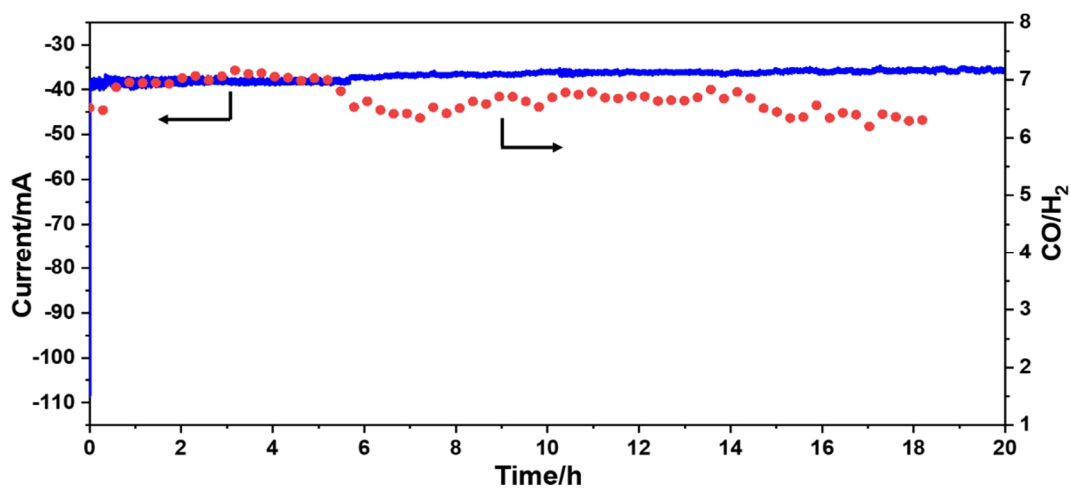


Fig. S5 Stability of P/Ni-2@Ni-N-C at -0.8 V.

Table S1 Atom contents of surface Ni, P, N elements tested by XPS.

| Sample | Surface element content (atomic fraction/%) | | |
|----------------|---|------|-------|
| | Ni | P | N |
| P/Ni-0@Ni-N-C | 1.37 | – | 6.84 |
| P/Ni-2@Ni-N-C | 1.07 | 0.34 | 5.07 |
| P/Ni-10@Ni-N-C | 1.2 | 1.56 | 10.41 |

Table S2 Comparison of electrocatalytic activity of different samples for CO₂RR.

| Catalyst | Electrolyte | Potential/(V vs RHE) | j_{CO} /(mA cm ⁻²) | FE _{CO} /% | Ratio (CO/H ₂) | Ref. |
|---|---|------------------------|----------------------------------|---------------------|----------------------------|-----------|
| CuO/Co ₃ O ₄ | 0.1 mol·L ⁻¹ KHCO ₃ | -0.9 V | 5.2 | 34.5 | 0.5 | 1 |
| CoNi-NC | 0.5 mol·L ⁻¹ KHCO ₃ | -0.5 – -1.0 V | 5–35 | 46–53 | 0.8–1.3 | 2 |
| CdS _x Se _{1-x} (x = 0–1) | 0.1 mol·L ⁻¹ KHCO ₃ | -1.2 V | 4–21.9 | 19–81 | 0.25–4 | 3 |
| Co ₃ O ₄ -CDots-C ₃ N ₄ | 0.5 mol·L ⁻¹ KHCO ₃ | -0.3 – -0.8 V | 0.05–3.2 | 10–89 | 0.25–14.3 | 4 |
| Co-HNC | 0.1 mol·L ⁻¹ KHCO ₃ | -0.8 V | 2.6 | 35 | 0.54 | 5 |
| AuCu/CNT | 0.5 mol·L ⁻¹ KHCO ₃ | -0.4 V | 0.05–1.4 | 5–94 | 0.05–19 | 6 |
| Zn-Co@N-C | 0.5 mol·L ⁻¹ KHCO ₃ | -0.8 V | 2 | 20 | 0.25 | 7 |
| Cu ₂ O cubes | 0.1 mol·L ⁻¹ KHCO ₃ | -0.6 – -0.8 V | 3.7–5.2 | 32–45 | 0.15–0.7 | 8 |
| ZnCu alloy | 0.1 mol·L ⁻¹ CsHCO ₃ | -0.9 V | ~6.3 | 44–80 | 0.8–4 | 9 |
| CF | 0.1 mol·L ⁻¹ KHCO ₃ | -0.9 V | 5–17.5 | 20–60 | 0.25–1.5 | 10 |
| Co _{0.75} Ni _{0.25} /N-CNFs | 0.5 mol·L ⁻¹ NaHCO ₃ | -0.9 V | 11.4 | 85 | 5.7 | 11 |
| Co@CoNC | 0.1 mol·L ⁻¹ KHCO ₃ | -0.3 – -0.8V | 0.05–4.2 | 10–62 | 0.15–2 | 12 |
| F/P- γ -In ₂ Se ₃ /CP | 30% (w) [Bmim]PF ₆ /65% (w) MeCN/5% (w) H ₂ O | -1.8 – -2.3 V (vs SCE) | 1–54 | 20–96.5 | 1/3–24 | 13 |
| Rate-aligned electrocatalyst (Au substrate 3d Co, Ni, Fe) | 0.1 mol·L ⁻¹ KHCO ₃ | -0.8 | 33.8 | 62.5 | 1.7 | 14 |
| Fe-N-C | 0.5 mol·L ⁻¹ NaHCO ₃ | -0.5 – -0.8 V | 3.8–6.25 | 50–78 | 1–4 | 15 |
| P/Ni-x@Ni-N-C | 0.5 mol·L ⁻¹ KHCO ₃ | -0.9 V | 5–27.5 | 38–91 | 0.7–8.1 | This work |

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