

Supporting Information

Synthesis of Mo₂C nanoparticles on N -doped carbon as electrocatalyst for efficient electrocatalytic hydrogen evolution

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Characterization

X-ray powder diffraction (XRD, Rigaku Smartlab 9kW, Cu K α , $\lambda=1.5406 \text{ \AA}$) was used to characterize the phase purities of the prepared materials. Field emission scanning electron microscopy (FESEM) technique was applied for characterizing the morphologies and structure of the fabricated catalysts (Thermo Fisher Scientific FIB-SEM GX4 electron microscope at 10 kV and 43 pA operating currents). Transmission electron microscopy (TEM, Thermo Fischer, Talos F200x, 200 kV) was employed for the characterization of the morphologies, sizes, lattice fringes and distribution of elements of the samples. Raman spectra were measured in the range of 2000-800 cm^{-1} using an Invia Raman microscope (Invia Microscope, Renishaw, excitation: 532 nm). Thermogravimetric analysis (TGA, METTLER TOLEDO) was conducted with a heating rate of 10 $^{\circ}\text{C min}^{-1}$ in oxygen. X-ray photoelectron spectra (XPS) data were obtained using an ESCALAB 250 instrument (Thermo Fischer, EACALAB 250Xi). The surface areas and pore size distributions of the samples were acquired using a nitrogen adsorption/desorption apparatus (Quantachrome, autosorb IQ-C).

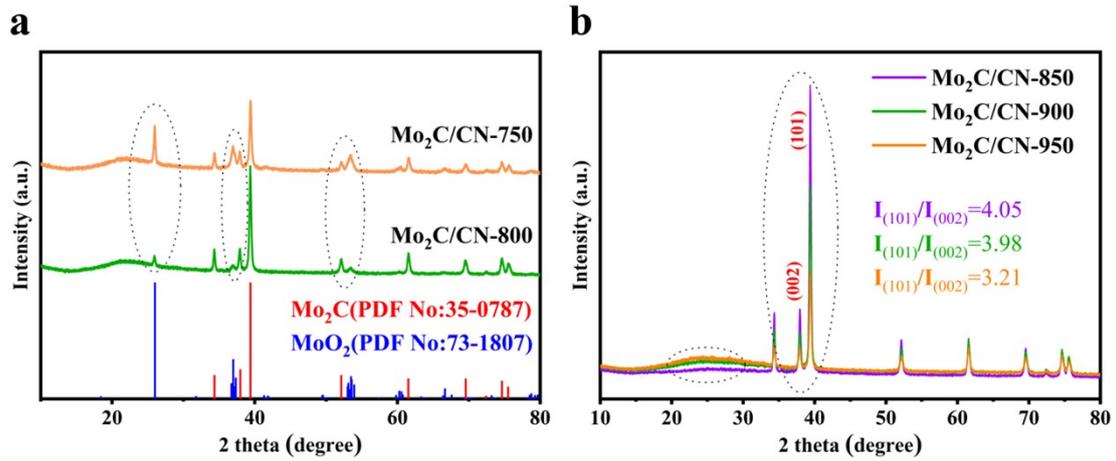


Figure S1. (a) XRD pattern of $\text{Mo}_2\text{C}/\text{CN-750}$ and $\text{Mo}_2\text{C}/\text{CN-800}$, (b) XRD pattern of $\text{Mo}_2\text{C}/\text{CN-850}$, $\text{Mo}_2\text{C}/\text{CN-900}$ and $\text{Mo}_2\text{C}/\text{CN-950}$.

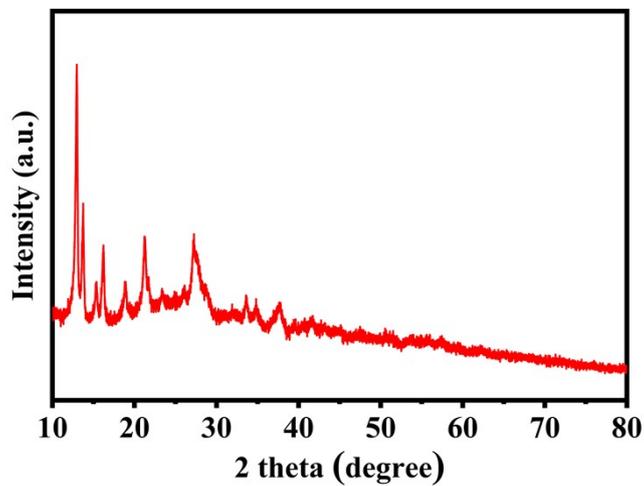


Figure S2. XRD pattern of Mo-ZIF.

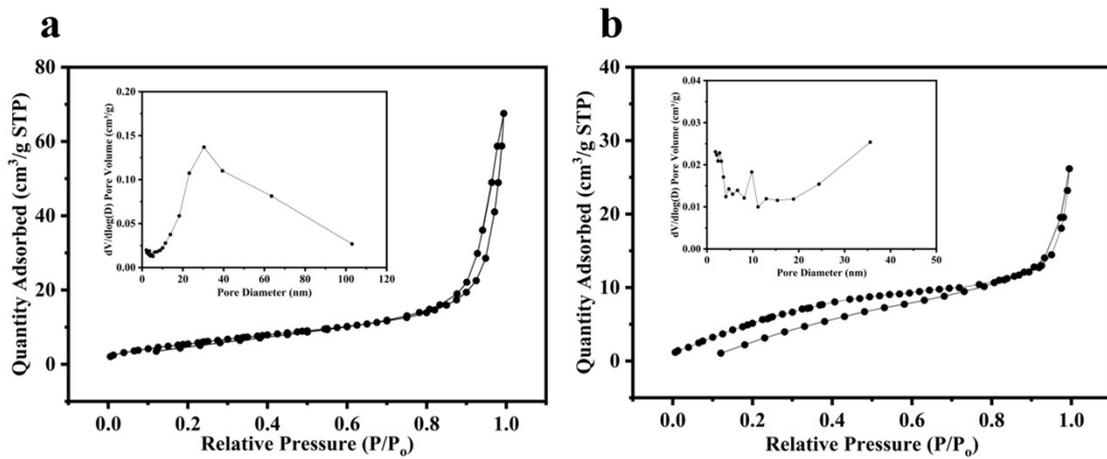


Figure S3. N_2 adsorption/desorption isotherms curve, the insets displaying the pore size distribution of (a)

$\text{Mo}_2\text{C}/\text{CN-900}$ and (b) $\text{Mo}_2\text{C}/\text{CN-950}$.

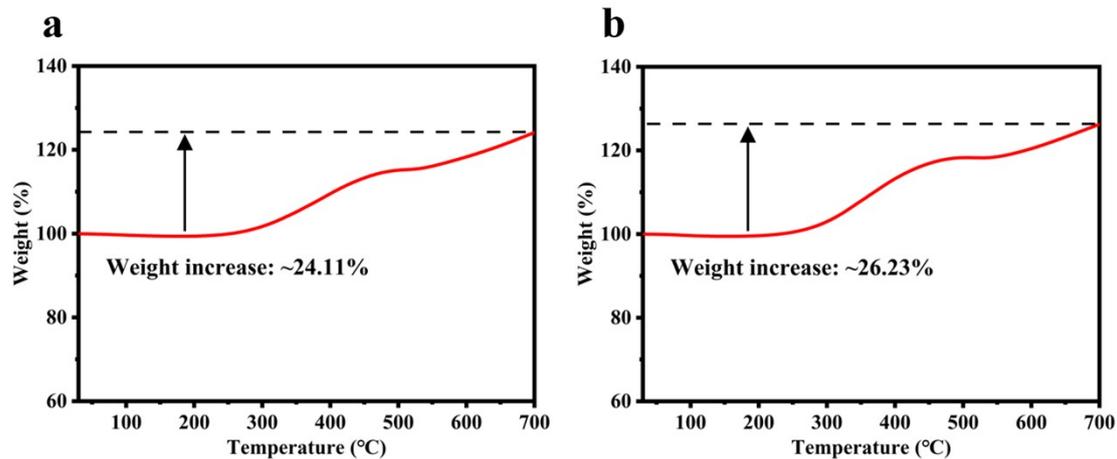


Figure S4. TGA curve of (a) Mo₂C/CN-900 and (b) Mo₂C/CN-950.

TGA of Mo₂C/CN-T catalysts was tested under oxygen atmosphere from room temperature to 700°C. It's assumed that there is no residual of carbon under 700°C, the residual mass is determined to be MoO₃ according to the XRD examination of the residual after TG process. Accordingly, the Mo₂C content was calculated from the following equation:

$$\text{Mass\% (Mo}_2\text{C)} = \frac{\text{residual mass}}{2 \times M(\text{MoO}_3)} \times \frac{M(\text{Mo}_2\text{C})}{\text{Mass}_{\text{Original}}} = \frac{\text{residual mass (\%)}}{2 \times M(\text{MoO}_3)} \times M(\text{Mo}_2\text{C})$$

Where M represents the molar weight.

Table S1. residual mass (%) and Mass% (Mo₂C) of Mo₂C/CN-T.

Samples	residual mass (%)	Mass% (Mo ₂ C)
Mo ₂ C/CN-850	122.89%	87%
Mo ₂ C/CN-900	124.11%	87.9%
Mo ₂ C/CN-950	126.23%	89.4%

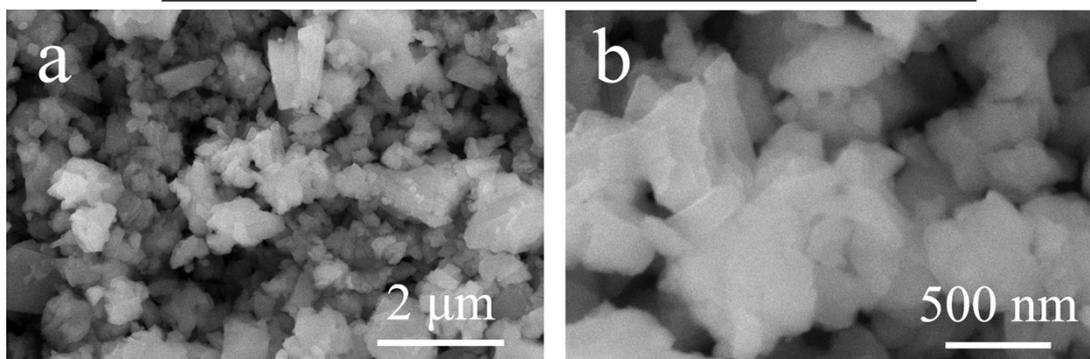


Figure S5. (a) and (b) FESEM images of Mo-ZIF.

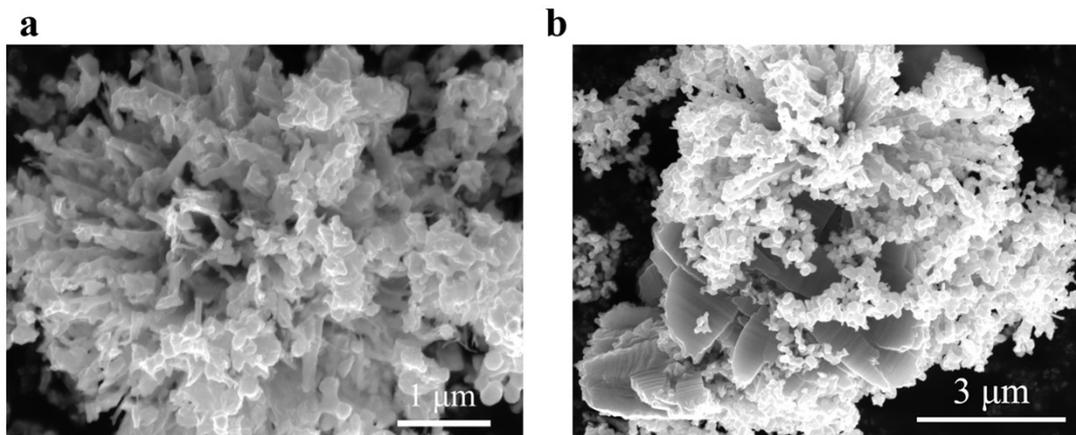


Figure S6. SEM images of (a) Mo₂C/CN-900 and (b) Mo₂C/CN-950.

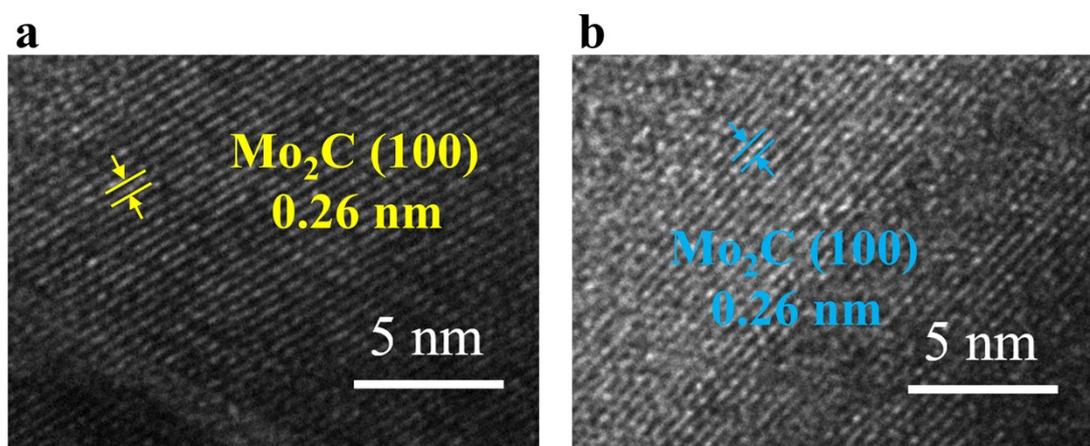


Figure S7. HRTEM images of (a) Mo₂C/CN-900 and (b) Mo₂C/CN-950.

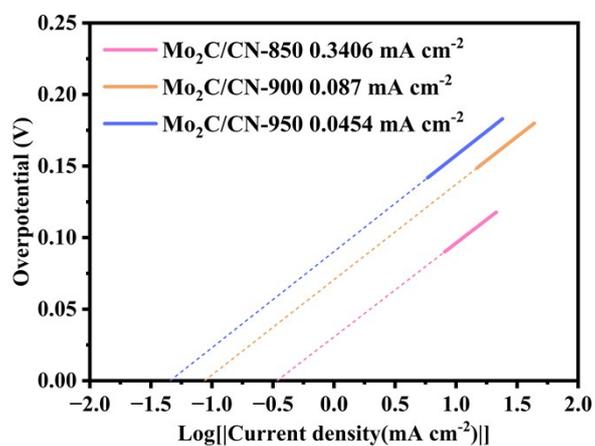


Figure S8. Exchange current density of Mo₂C/CN-850, Mo₂C/CN-900 and Mo₂C/CN-950 in 0.5 M H₂SO₄ solution.

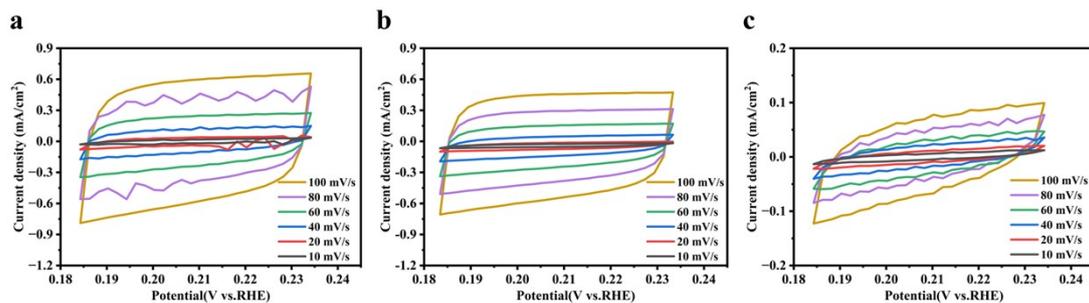


Figure S9. Cyclic voltammograms curves in 0.5 M H₂SO₄ solution. (a) Mo₂C/CN-850, (b) Mo₂C/CN-900, (c) Mo₂C/CN-950.

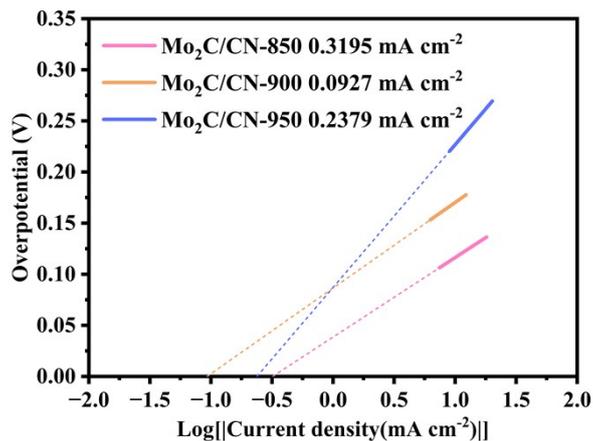


Figure S10. Exchange current density of Mo₂C/CN-850, Mo₂C/CN-900 and Mo₂C/CN-950 1 M KOH solution.

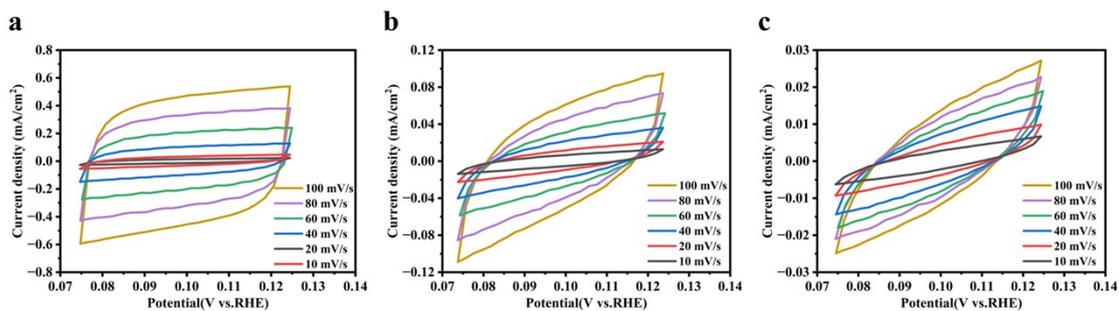


Figure S11. Cyclic voltammograms curves in 1 M KOH solution. (a) Mo₂C/CN-850, (b) Mo₂C/CN-900, (c) Mo₂C/CN-950.

Table S2. EIS fitting parameters for acidic and alkaline media.

Samples	Acidic media		Alkaline media	
	Solution resistance(R_s)/ Ω	Charge transfer resistance(R_{ct})/ Ω	Solution resistance(R_s)/ Ω	Charge transfer resistance(R_{ct})/ Ω
Mo ₂ C/CN-850	4.662	9.852	5.897	2.812
Mo ₂ C/CN-900	4.96	12.84	5.938	6.563
Mo ₂ C/CN-950	4.517	20.44	6.219	22.68