

Supplementary Information

Controllable Synthesis of Molybdenum-Based Electrocatalysts for Hydrogen Evolution Reaction

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Table S1. Structural parameters and particle sizes for molybdenum-based compounds.

	Lattice plane	2 θ , degree	D ₁ , nm	\bar{D} , nm	D ₂ , nm
MoO ₂ /C	(111)	26.13	7.43	8.49	8.3
	(211)	37.08	8.84		
	(312)	49.54	9.21		
MoC/C	(111)	36.39	3.64	3.26	3.2
	(200)	42.27	2.74		
	(220)	61.31	3.41		
Mo ₂ C/C	(002)	38.04	3.16	3.0	2.5
	(101)	39.58	3.06		
	(110)	61.86	2.67		

D1: Particle sizes calculated from XRD patterns for Mo composite catalysts; D : Average particle sizes; D2: Particle sizes obtained from TEM images.

Table S2. Comparison of the HER performance of molybdenum compounds reported in literature in acid media.

Catalysts	Tafel slope mV dec ⁻¹	j_0 mA cm ⁻²	η_{10} mV	Electrolyte	Refs
Bulk Mo ₂ C	56	1.3*10 ⁻³	210	1 M H ₂ SO ₄	1
Np-Mo ₂ C NWS	53	1.4*10 ⁻³	130	0.5 M H ₂ SO ₄	2
Mo ₂ C/CNT	55.2	1.4*10 ⁻²	152	0.1 M HClO ₄	3
Mo ₂ C/GCS	62.6	1.25*10 ⁻²	200	0.5 M H ₂ SO ₄	4
Mo ₂ C/CNT-GR	58	6.2*10 ⁻²	130	0.5 M H ₂ SO ₄	5
Mo ₂ C-RGO	54		130	0.5 M H ₂ SO ₄	6
Mo ₂ C-NCNT	71	0.115	147	0.5 M H ₂ SO ₄	7
MoC _x	53	2.3*10 ⁻²	142	0.5 M H ₂ SO ₄	8
MoO ₂ /RGO	68		310	0.5 M H ₂ SO ₄	9
MoS ₂ /MoO ₂	76		240	0.5 M H ₂ SO ₄	10
MoC-G	88	2.6*10 ⁻²	221	0.5 M H ₂ SO ₄	11
MoC@NC	68	1.7*10 ⁻²	210	0.5 M H ₂ SO ₄	12
MoO ₂ /C	107.1	0.05	246	0.5 M H ₂ SO ₄	This
MoC/C	91.1	0.13	179	0.5 M H ₂ SO ₄	
Mo ₂ C/C	75.1	0.36	135	0.5 M H ₂ SO ₄	work

Table S3. Comparison of the HER performance of molybdenum compounds reported in literature in alkaline media.

Catalysts	Tafel slope mV dec ⁻¹	j_0 mA cm ⁻²	η_{10} mV	Electrolyte	Refs
MoC _x	59	2.9×10^{-2}	151	1M KOH	8
NiMo ₂ C/NF	36.8	0.51	47	6M KOH	10
Mo ₂ C	58		176	1M KOH	13
nanoparticle					
Mo ₂ C	45	1.1×10^{-2}	130	1M KOH	14
nanorad					
Ni-MoO ₂			257	1M KOH	7
MoO ₂ /C	88.0	0.05	184	1M KOH	This
MoC/C	75.1	0.14	138	1M KOH	
Mo ₂ C/C	62.2	0.25	96	1M KOH	work

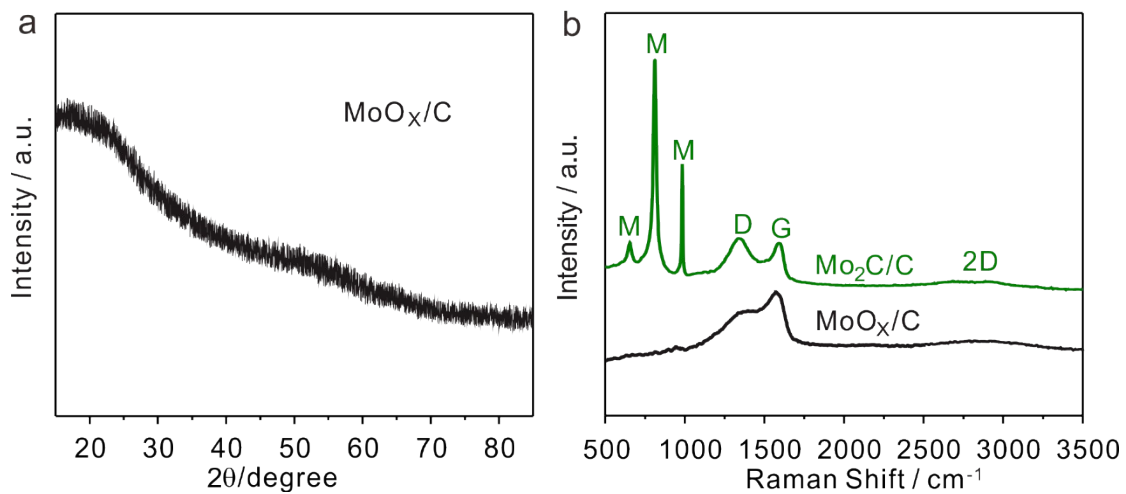


Figure S1. (a) XRD pattern of solvothermal product; (b) Raman spectra of solvothermal product and $\text{Mo}_2\text{C}/\text{C}$ nanocatalyst.

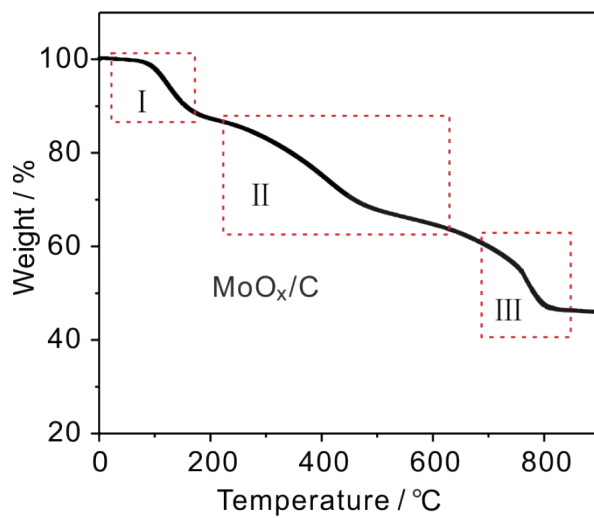


Figure S2. Thermo gravimetric analysis (TGA) of solvothermal product tested under flowing N_2 atmosphere.

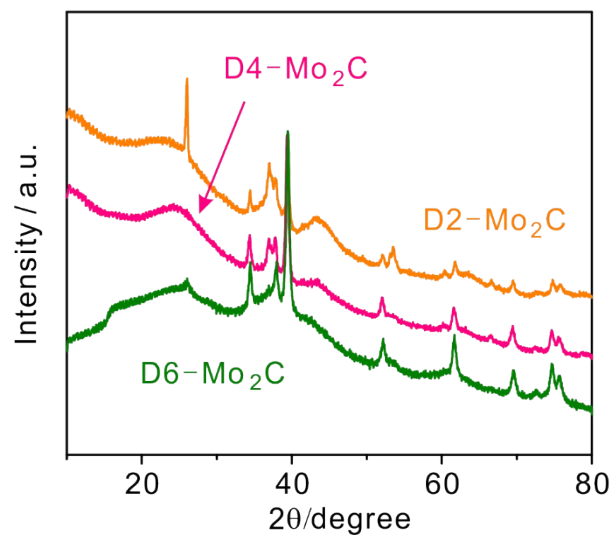


Figure S3. Powder XRD patterns of D2-Mo₂C, D4-Mo₂C and D6-Mo₂C.

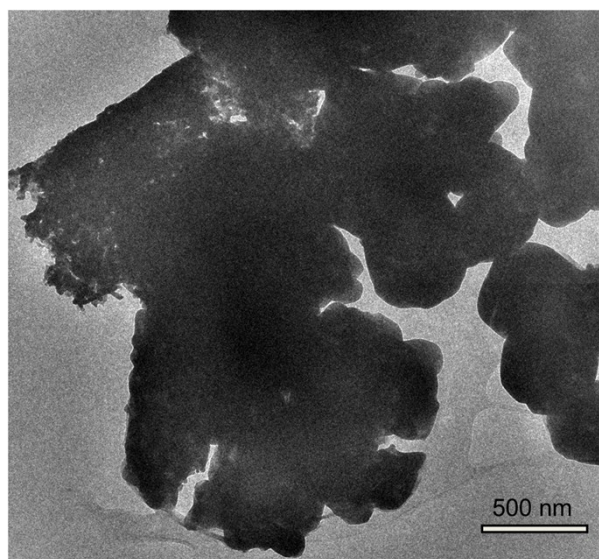


Figure S4. TEM images of D4-Mo₂C

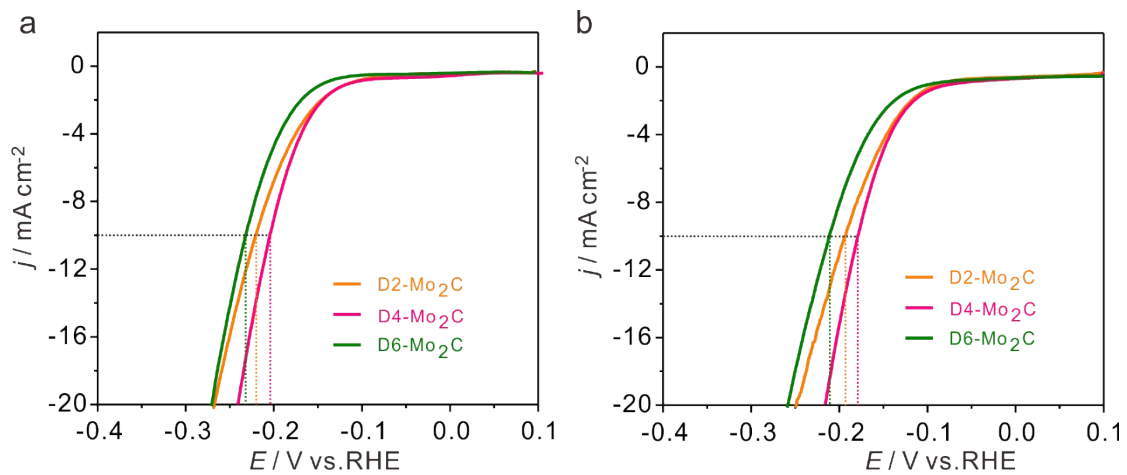


Figure S5. Polarization curves of D2-Mo₂C, D4-Mo₂C and D6-Mo₂C in 0.5 M H₂SO₄ solution (a) and 1 M KOH solution (b).

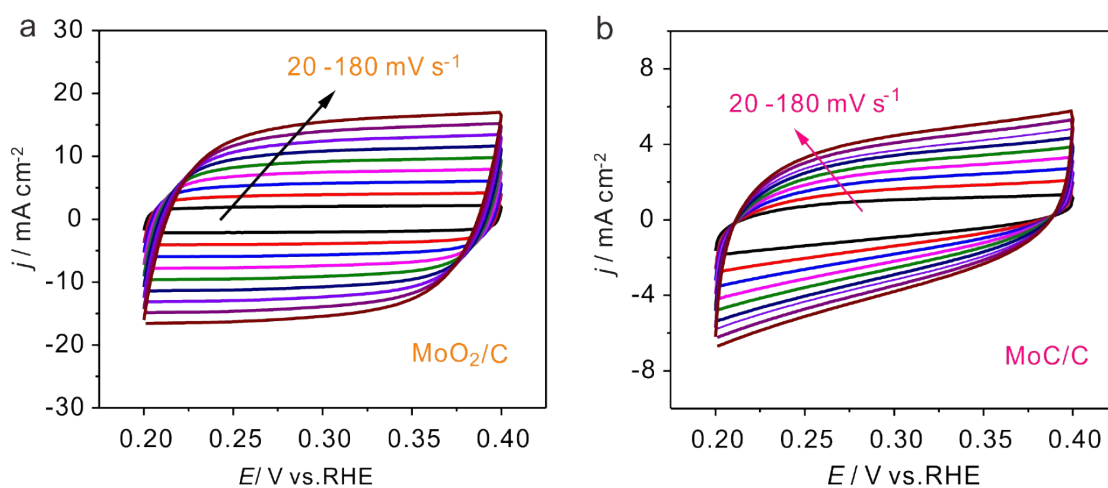


Figure S6. Cyclic voltammograms (CVs) of MoO₂/C (a) and MoC/C (b) in 0.5 M H₂SO₄ solution between 0.2 V and 0.4 V at scan rates ranging from 20 to 180 mV s^{-1} .

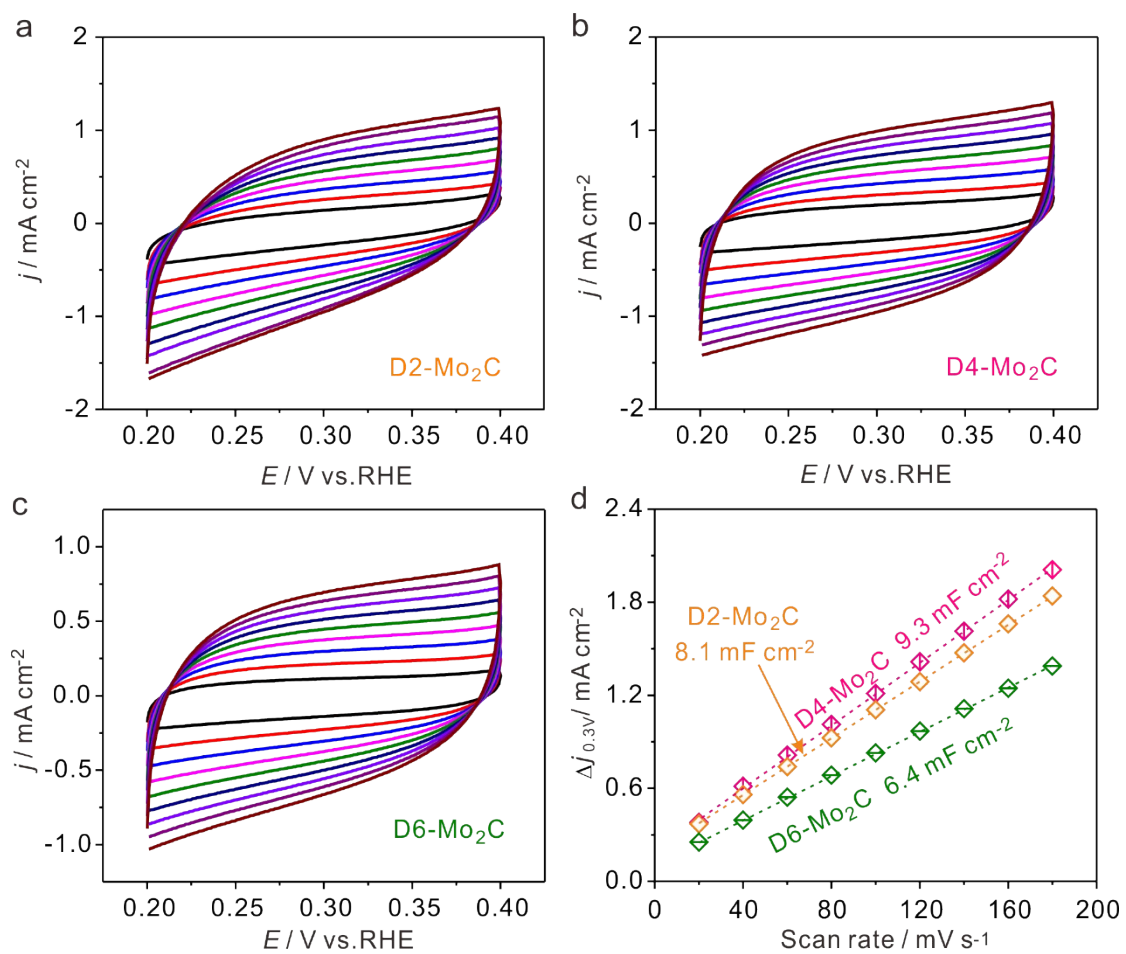


Fig S7. Cyclic voltammograms (CVs) of D2-Mo₂C (a), D4-Mo₂C (b) and D6-Mo₂C (c) in 0.5 M H₂SO₄ solution between 0.2 V and 0.4 V at scan rates ranging from 20 to 180 mV s^{-1} ; (d) Capacitive current at 0.3 V as a function of scan rate ($\Delta j_0 = j_a - j_c$).

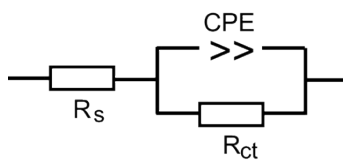


Figure S8. Electrical Equivalent circuit models for fitting the EIS response on Mo-based catalysts, where R_s is the solution resistance, R_{ct} represents the charge transfer resistance, and the double layer capacitance is represented by the elements CPE.

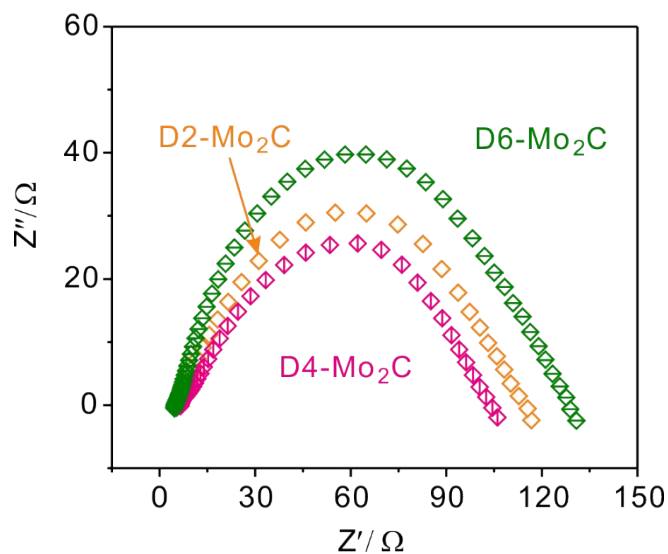


Figure S9. Nyquist plots of D2-Mo₂C, D4-Mo₂C and D6-Mo₂C recorded at 150 mV in 0.5 M H₂SO₄ solution.

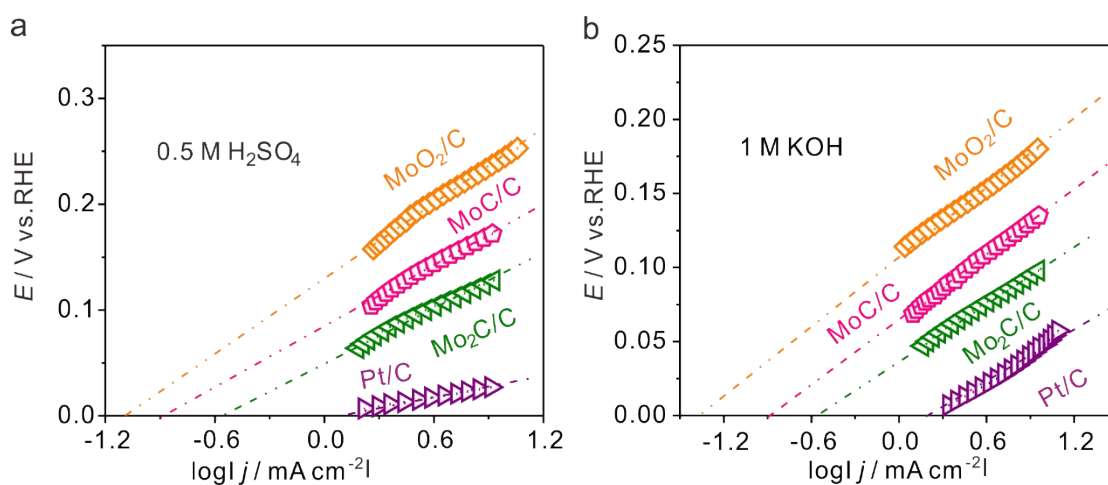


Figure S10. Tafel plots and the corresponding exchange current density of MoO₂/C, MoC/C, Mo₂C/C and Pt/C in 0.5 M H₂SO₄ (a) and 1 M KOH solution (b).

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