Supporting Information

Interfacial engineering and chemical reconstruction into Mo/Mo₂C@CoO@NC heterostructure for promoting oxygen evolution reaction

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OER process

For OER in alkaline electrolyte (pH=14), since OH⁻ may act as an electron donor,

the overall reaction scheme of OER can be expressed as:

$$OH^- + * \to OH^* + e^- \tag{1}$$

$$OH^* + OH^- \to O^* + H_2O(l) + e^-$$
 (2)

$$O^* + OH^- \to OOH^* + e^- \tag{3}$$

$$OOH^* + OH^- \to O_2(g) + H_2O(l) + e^- + *$$
 (4)

where * represents the catalyst and active adsorption site, (l) and (g) represent the liquid and gas phases, and OH*, O*, and OOH* represent the adsorbed intermediates.

TOF calculation

To have better quantification of the activity of Mo/Mo₂C@CoO@NC electrocatalysts, the turnover frequency (TOF) value was calculated from the equation: [1]

$$TOF = (J^*A)/(4F^*m) \tag{5}$$

where J is the measured current density, A is the surface area of the working electrode, F is the Faraday constant (96485 C mol⁻¹), and m is the number of moles of active materials loaded on the working electrodes. The TOF was calculated by only taking the metal ions (10.51 wt% of cobalt and 43.37 wt% of molybdenum, Table S1) in the catalysts into consideration.



Figure S1. SEM images of MoO₃ nanoribbons.



Figure S2. Low-magnification (a) and high-magnification (b) SEM images of $MoO_3@ZIF-67$ heterogeneous nanoribbons.



Figure S3. SEM images of $Mo/Mo_2C@CoO@NC$ heterostructures.



Figure S4. XRD patterns of MoO₃@CoO_x catalysts.



Figure S5. XRD patterns of MoO₃@ZIF-67-P catalysts.



Figure S6. N 1s XPS spectra of Mo/Mo₂C@CoO@NC heterostructures.



Figure S7. O 1s XPS spectra of Mo/Mo₂C@CoO@NC heterostructures.



Figure S8. Low-magnification (a) and high-magnification (b) SEM images of $Mo/Mo_2C@CoO@NC$ heterostructures.



Figure S9. Elemental mapping images of Mo, Co, C, N, and O elements in Mo/Mo₂C@CoO@NC heterostructures detected by SEM.



Figure S10. Elemental mapping images of N element in Mo/Mo₂C@CoO@NC heterostructures detected by HAADF-STEM.



Figure S11. Low-magnification (a) and high-magnification (b-d) SEM images of $MoO_3@CoO_x$ catalysts.



Figure S12. Elemental mapping images of Mo, O, and Co elements in $MoO_3@CoO_x$ catalysts detected by SEM.



Figure S13. Low-magnification (a) and high-magnification (b-d) SEM images of MoO₃@ZIF-67-P catalysts.



Figure S14. OER LSV polarization curves of MoO₃@ZIF-67 heterogeneous

nanoribbons heat-treated at 700 °C, 800 °C, and 900 °C.



Figure S15. OER LSV polarization curves of Mo/Mo₂C@CoO@NC heterostructure

with 0.025 g, 0.05 g, and 0.075 g MoO₃.



Figure S16. SEM images of Mo/Mo₂C@CoO@NC heterostructure with (a) 0.025 g, (b) 0.05 g, and (c) 0.075 g MoO₃.



Figure S17. OER LSV polarization curves of Mo/Mo $_2$ C@CoO@NC heterostructure

prepared with stirring time of 0.5 h, 1 h, and 1.5 h.



Figure S18. SEM images of Mo/Mo₂C@CoO@NC heterostructure prepared with stirring time of (a) 0.5 h, (b) 1 h, and (c) 1.5 h.



Figure S19. OER LSV polarization curves of $MoO_3@ZIF-67$ heterogeneous nanoribbons heat-treated in different conditions.



Figure S20. ECSA of MoO₃-HT, ZIF-67-HT, Mo/Mo₂C@CoO@NC, and RuO₂.



Figure S21. TOF of Mo/Mo₂C@CoO@NC and RuO₂.



Figure S22. XRD patterns of $Mo/Mo_2C@CoO@NC$ heterostructures after chronoamperometry.



Figure S23. TEM images of $Mo/Mo_2C@CoO@NC$ heterostructures after chronoamperometry.

 Table S1. Element contents in Mo/Mo2C@CoO@NC heterostructure detected by XPS

 technique.

Samples	Mo (At.%)	Co (At.%)	N (At.%)	C (At.%)	O (At.%)
Mo/Mo ₂ C@CoO@NC	11.66	4.6	25.96	24.62	33.16
	Mo (wt.%)	Co (wt.%)	N (wt.%)	C (wt.%)	O (wt.%)
	43.37	10.51	14.09	11.46	20.57

Table S2. Electrocatalytic performances toward OER of Mo/Mo₂C@CoO@NC and

Electrocatalysts	Loading (mg cm ⁻²)	OER η (mV) @10 mA cm ⁻²	Electrolyte	Ref.
ACTP5@Co,N-800	0.30	374	0.1 M KOH	[2]
CoV ₂ O ₆	0.23	360	1 M KOH	[3]
BP-CN-c	0.50	350	1 M KOH	[4]
MnSAC	0.10	350	0.1 M KOH	[5]
CoNi ₄₀ -MOFNs@MXene	0.20	346	1 M KOH	[6]
GNiPy350N	-	320	1 M KOH	[7]
CoFe PBA@CoP/NF	-	312	1 M KOH	[8]
Fe-Co-CN/rGO-700	0.25	308	1 M KOH	[9]
Mo ₂ C/Co@NC	1.00	308	1 M KOH	[10]
CoSA/N,S-HCS	1.50	306	1 M KOH	[11]
LC-CoOOH NAs/CFC	-	294	1 M KOH	[12]
P-Co ₃ O ₄	0.30	290	1 M KOH	[13]
Vo-MnCo ₂ O ₄	0.40	290	1 M KOH	[14]
FeNi ₂ S ₄ NPs/CB	0.10	290	1 M KOH	[15]
FeNi-Mo ₂ C/C	0.07	288	1 M KOH	[16]
NiFeP/MXene	0.25	286	1 M KOH	[17]

recently advanced non-noble-based OER electrocatalysts.

Ni/Ni ₂ P@N-CNF	0.25	285	1 M KOH	[18]
P ₃₀ -doped Fe/NF	-	284	1 M KOH	[19]
Co/CoO@COF	0.26	278	1 M KOH	[20]
NiCo _{2-x} Fe _x O ₄	0.50	274	1 M KOH	[21]
$Fe_{0.4}Co_{0.6}Se_2$		270	1 M KOH	[22]
Co-MOF-NK	1.00	268	1 M KOH	[23]
$Co_2P@Ti_3C_2T_x$	5.70	267	1 M KOH	[24]
NiCo LDH-TPA	2.00	267	1 M KOH	[25]
Co(OH) ₂ /NiMo CA@CC	-	267	1 M KOH	[26]
NiFe _{0.2} -O _x H _y	0.20	263	1 M KOH	[27]
Fe-Co-O/Co@NC-mNS/NF	-	257	1 M KOH	[28]
NiFeLDH-Bir	2.50	258	6 M KOH	[29]
NiFe-MOF/G	0.30	258	1 M KOH	[30]
NiFeLa-LDH/v-MXene	-	255	1 M KOH	[31]
FeNi-LDH-V ₂ C MXene	0.35	250	1 M KOH	[32]
NiPS _{3-x} Se _x	1.00	250	1 M KOH	[33]
Co-C@NiFe LDH	0.82	249	1 M KOH	[34]
NiFe LDH/NF-IH	-	246	1 M KOH	[35]
FeS ₂ @MXene	1.00	240	1 M KOH	[36]
Fe-CoP	-	237	1 M KOH	[37]
Ni ₈ Fe ₂ -MI/OH	0.26	229	1 M KOH	[38]
(Ni _x Fe _{1-x}) ₂ P@pc/PG	2.40	220	1 M KOH	[39]
a-LNFBPO@Ni	3.00	215	1 M KOH	[40]
Mo/Mo ₂ C@CoO@NC	0.20	215	1 M KOH	This work
CIF:FeNiMo-II	1.00	203	1 M KOH	[41]
Ni _{0.9} Fe _{0.1} -MOF	0.20	198	1 M KOH	[42]

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