

Construction of a Highly Efficient MoS₂-Based Composite Electrocatalyst for the Oxygen Evolution Reaction

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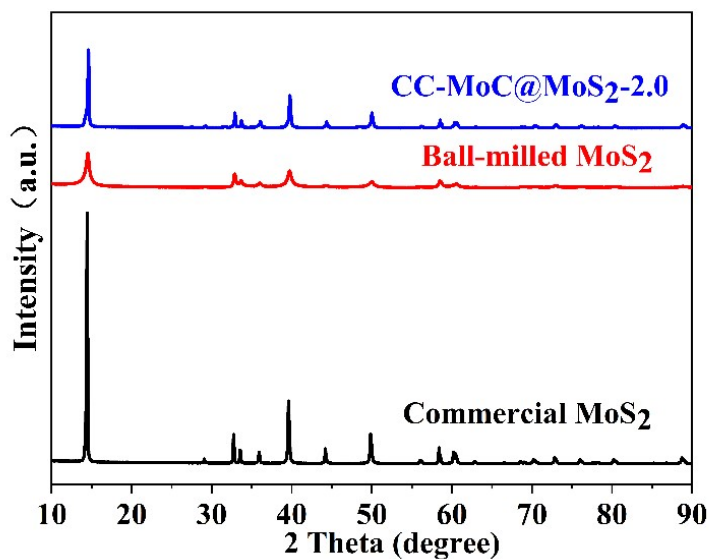


Fig. S1 XRD patterns of commercial MoS₂, BM-MoS₂ and CC-MoC@MoS₂-2.0.

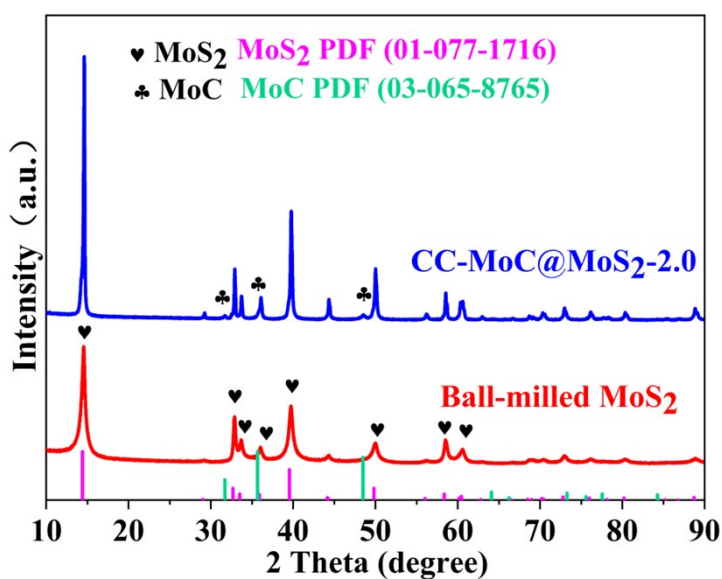


Fig. S2 XRD patterns of BM-MoS₂ and CC-MoC@MoS₂-2.0.

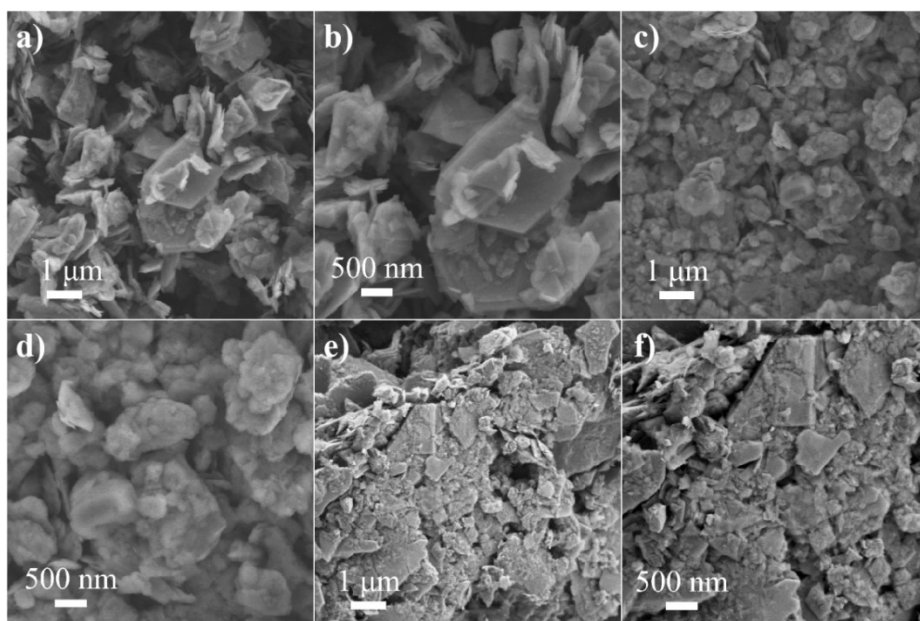


Fig. S3 SEM images of (a, b) commercial MoS₂, (c, d) BM-MoS₂, and (e, f) CC-MoC@MoS₂-2.0.

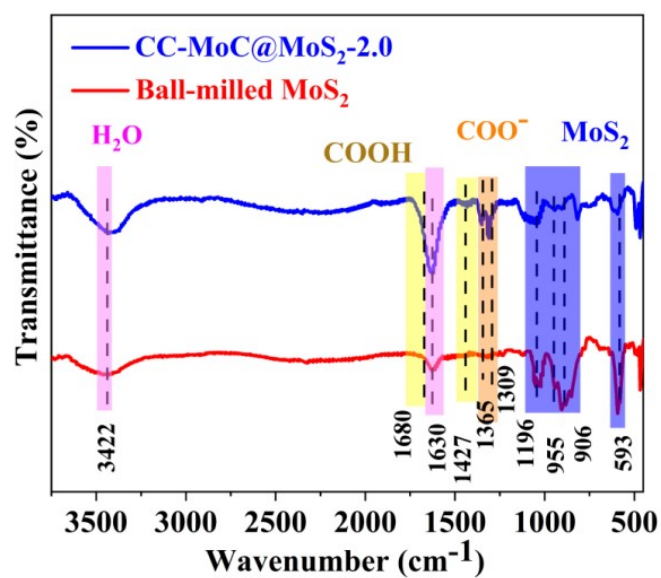


Fig. S4 FTIR spectra of BM-MoS₂ and CC-MoC@MoS₂-2.0.

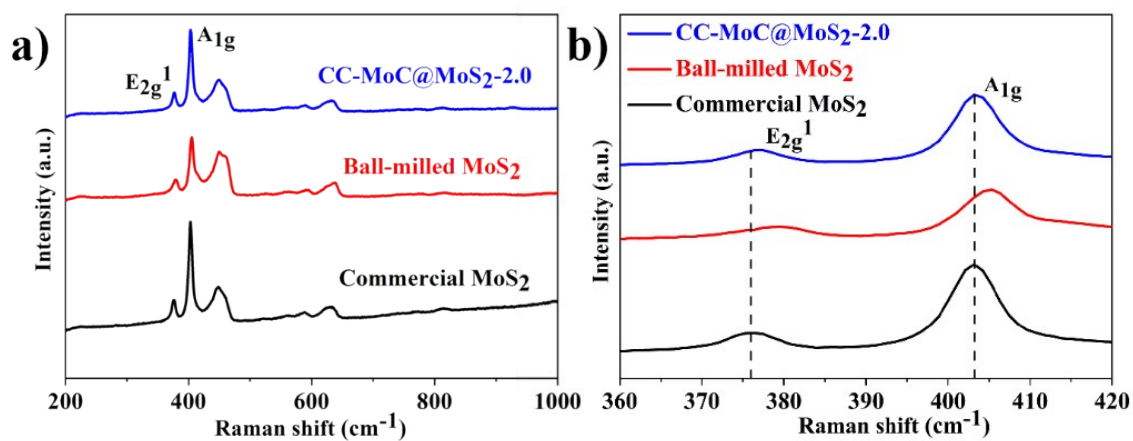


Fig. S5 Raman spectra of commercial MoS₂, BM-MoS₂ and CC-MoC@MoS₂-2.0.

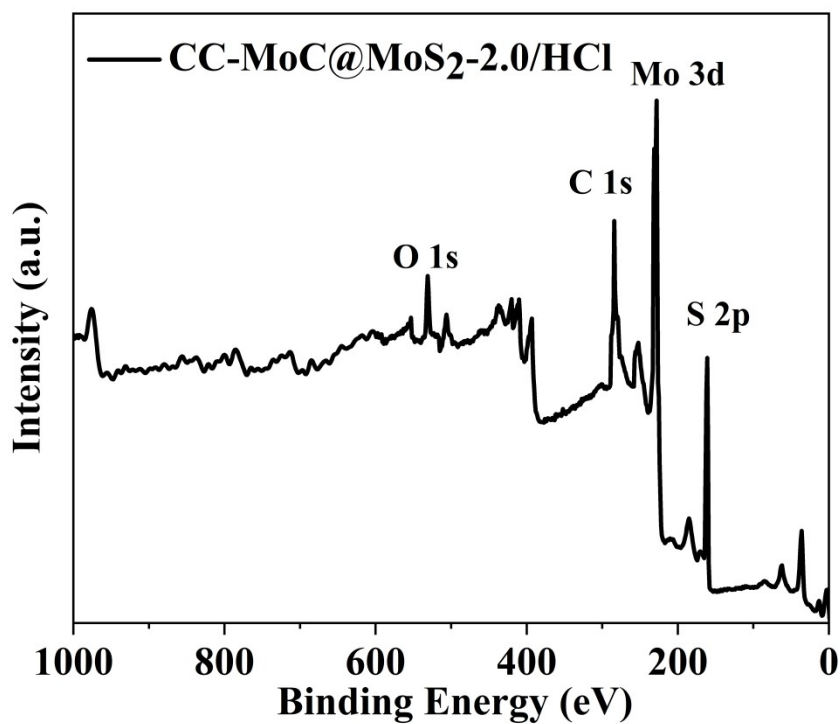


Fig. S6 XPS survey scan of CC-MoC@MoS₂-2.0 after treatment in 1.0 M HCl. The S/Mo ratio is 1.7.

Table S1: Elemental composition (mole %) of BM-MoS₂ and CC-MoC@MoS₂-2.0 before and after treatment in 1.0 M HCl.

	Mo	S	C	O	S/Mo
Ball-milled MoS ₂	24.94%	50.28%	1.60%	23.18%	2.0
CC-MoC@MoS ₂ -2.0	28.51%	40.24%	10.71%	20.54%	1.4
CC-MoC@MoS ₂ -2.0 after HCl treatment	26.98%	45.87%	11.37%	15.78%	1.7

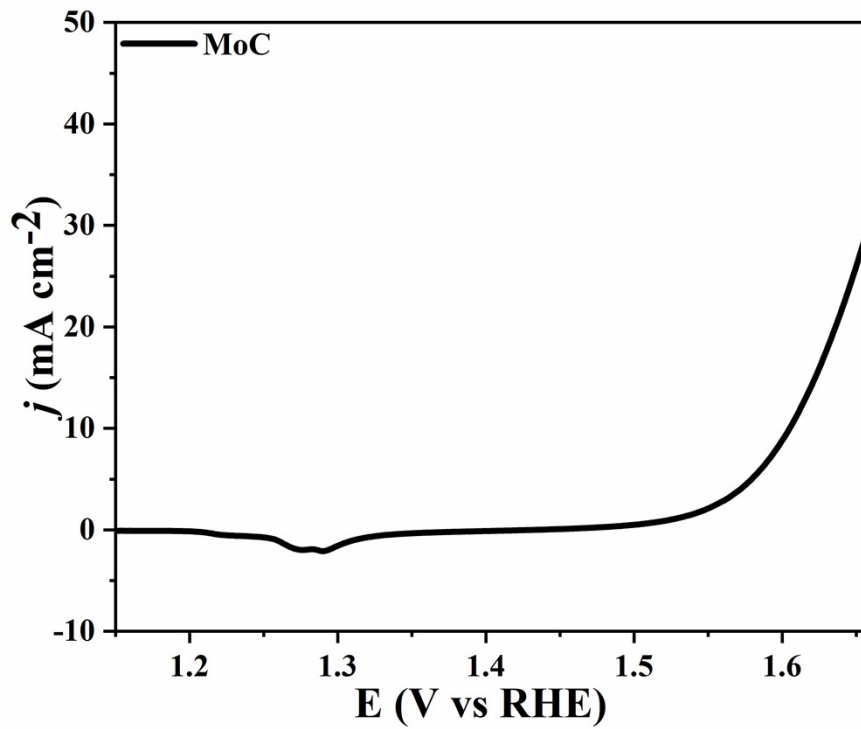


Fig. S7 LSV curves of MoC supported on nickel foam for OER.

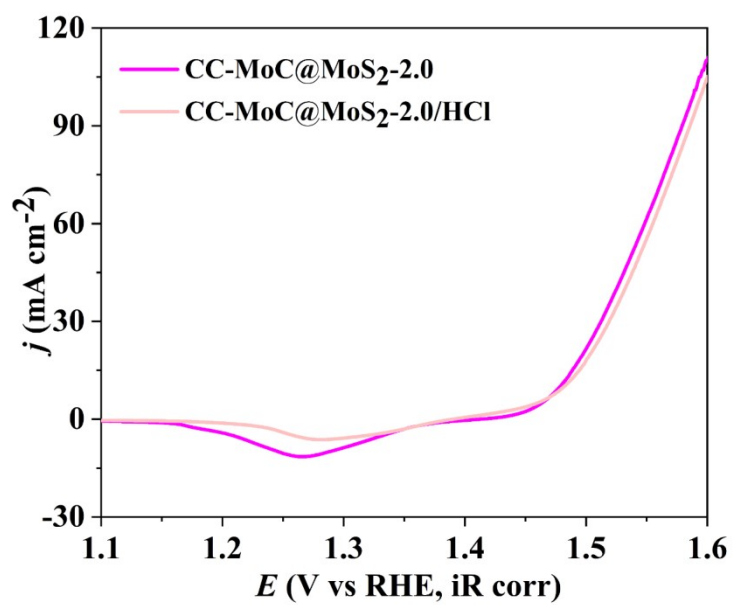


Fig. S8 LSV curves of CC-MoC@MoS₂-2.0 before and after acid treatment (1.0 M HCl).

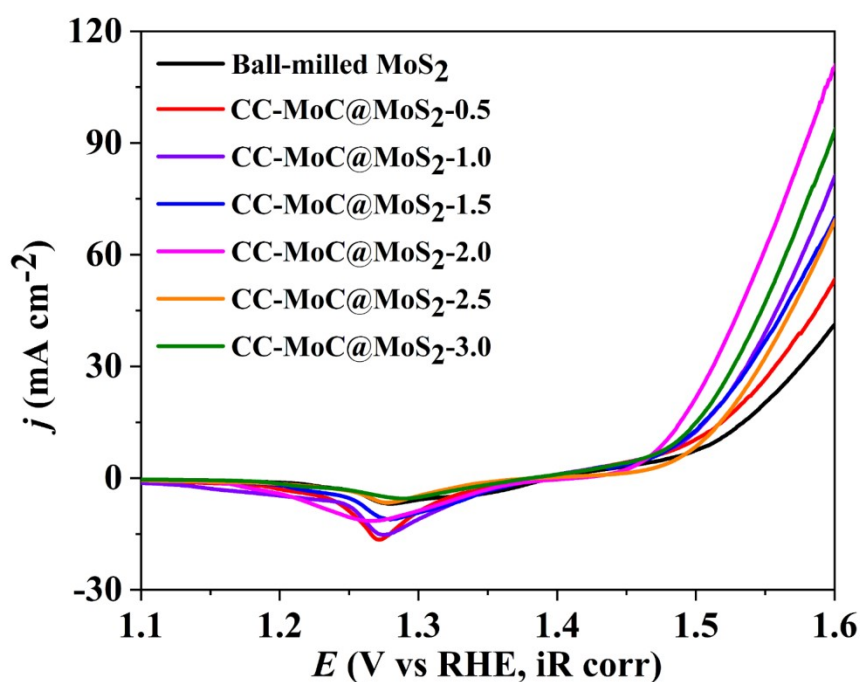


Fig. S9 OER polarization curves of BM-MoS₂, CC-MoC@MoS₂-0.5, CC-MoC@MoS₂-1.0, CC-MoC@MoS₂-1.5, CC-MoC@MoS₂-2.0, CC-MoC@MoS₂-2.5 and CC-MoC@MoS₂-3.0.

Table S2: Comparison of the OER performance of CC-MoC@MoS₂-2.0 with that of reported electrocatalysts (in 1M KOH).

Catalysts	η_{10} (mV)	Tafel slope (mV dec ⁻¹)	C_{dl} (mF cm ⁻²)	R_{ct} (Ω)	Refs
CC-MoC@MoS ₂ -2.0	248	47.09	4.02	0.716	This work
Fe ₃ O ₄ /CoO CNTs	270	59	30.07	17.5	[1]
Fe ₅ Co ₄ Ni ₂₀ Se ₃₆ B _x	279.8	59.5	3.25	1.586	[2]
p Ni _{0.7} Co _{0.3} Se ₂ Ns	258	42.3	0.04	32.8	[3]
Fe-NiO _x NT	310	49	22.73	14.4	[4]
Ni ₂ P NPs	290	47	0.176	1.8	[5]
Co-Ni-Fe ₅₁₁ Ns	288	43	0.475	/	[6]
MnO ₂ -CoP ₃	288	65	0.091	/	[7]
Fe ₃ C@NCNTs-NCNFs	284	56	28.2	/	[8]
Fe ₃ O ₄ -Co ₃ S ₄ NS	260	56	63.2	/	[9]

NiFeMn LDH	262	47	2.466	/	[10]
Co, Nb-MoS ₂ /TiO ₂	260.1	65	23.7	0.77	[11]
CoP/CN@MoS ₂	289	69	94.7	17	[12]
CoO _x -MoC/NC	330	89.8	257	/	[13]
Co ₉ S ₈ -CuS-FeS	300	79	1.51	26	[14]
Ag@CoOOH	256	64.6	/	2.9	[15]
Carboxyl coordinated Ni/Co	258	76.5	/	/	[16]
Co ₆ Mo ₆ C ₂ -NC-rGO	260	50	42	9	[17]

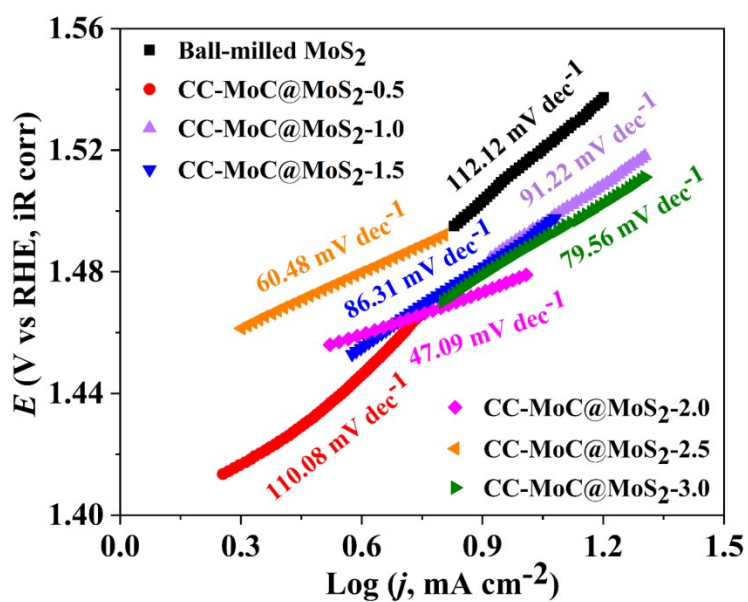


Fig. S10 Tafel slopes of BM-MoS₂, CC-MoC@MoS₂-0.5, CC-MoC@MoS₂-1.0, CC-MoC@MoS₂-1.5, CC-MoC@MoS₂-2.0, CC-MoC@MoS₂-2.5 and CC-MoC@MoS₂-3.0.

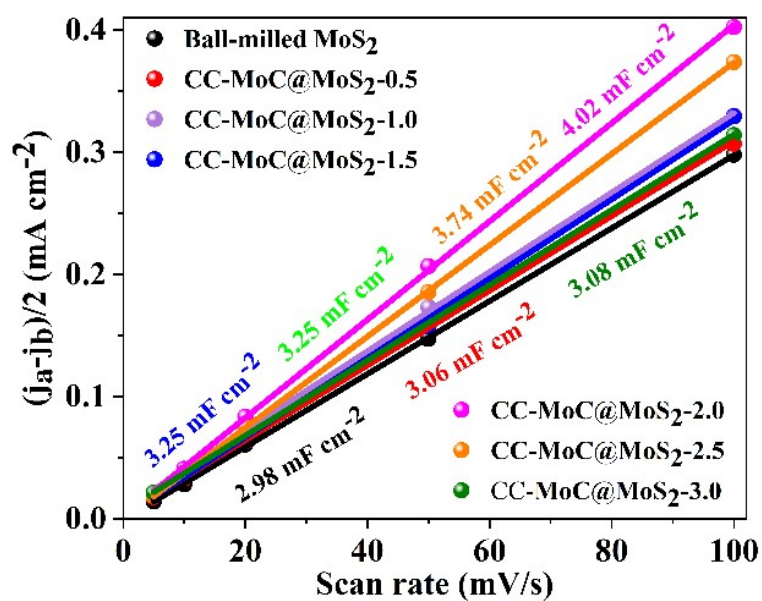


Fig. S11 C_{dl} of BM-MoS₂, CC-MoC@MoS₂-0.5, CC-MoC@MoS₂-1.0, CC-MoC@MoS₂-1.5, CC-MoC@MoS₂-2.0, CC-MoC@MoS₂-2.5 and CC-MoC@MoS₂-3.0.

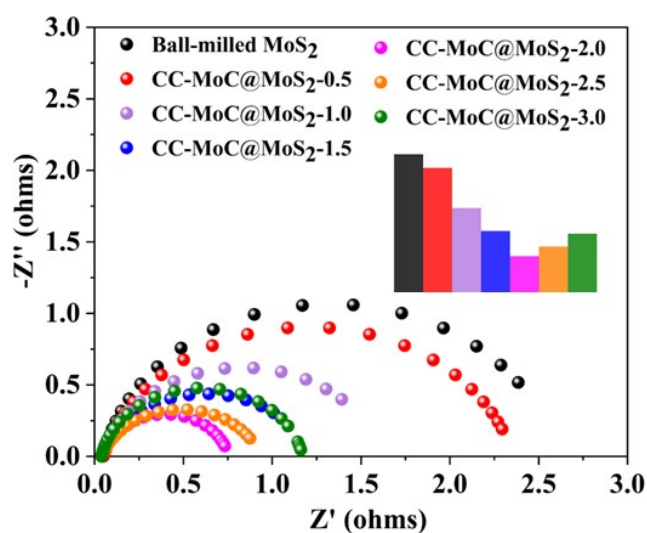


Fig. S12 The Nyquist plots of BM-MoS₂, CC-MoC@MoS₂-0.5, CC-MoC@MoS₂-1.0, CC-MoC@MoS₂-1.5, CC-MoC@MoS₂-2.0, CC-MoC@MoS₂-2.5 and CC-MoC@MoS₂-3.0.

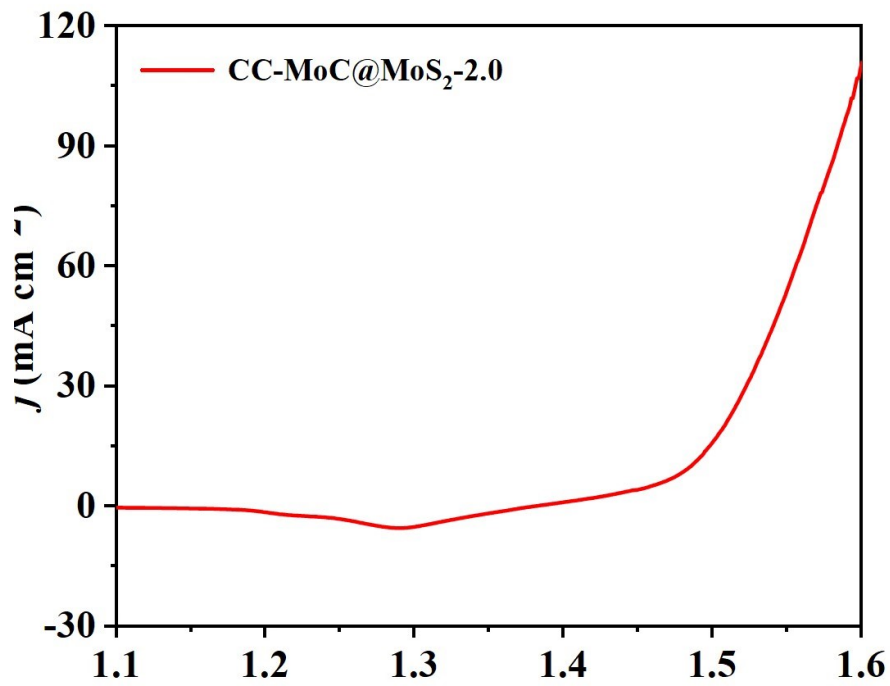


Fig. S13 LSV curve of CC-MoC@MoS₂-2.0 after a continuous CV of 5000 cycles.

Table S3: The η_{10} , Tafel slope, C_{dl} and R_{ct} values for OER of BM-MoS₂ and CC-MoC@MoS₂-X catalysts.

Catalysts	η_{10} (mV)	Tafel slope (mV dec ⁻¹)	C_{dl} (mF cm ⁻²)	R_{ct} (Ω)
Ball-milled MoS ₂	285	112.12	2.98	2.553
CC-MoC@MoS ₂ -0.5	268	110.08	3.06	2.309
CC-MoC@MoS ₂ -1.0	262	91.22	3.25	1.586
CC-MoC@MoS ₂ -1.5	260	86.31	3.25	1.176
CC-MoC@MoS ₂ -2.0	248	47.09	4.02	0.716
CC-MoC@MoS ₂ -2.5	275	60.48	3.74	0.898
CC-MoC@MoS ₂ -3.0	257	79.56	3.08	1.131

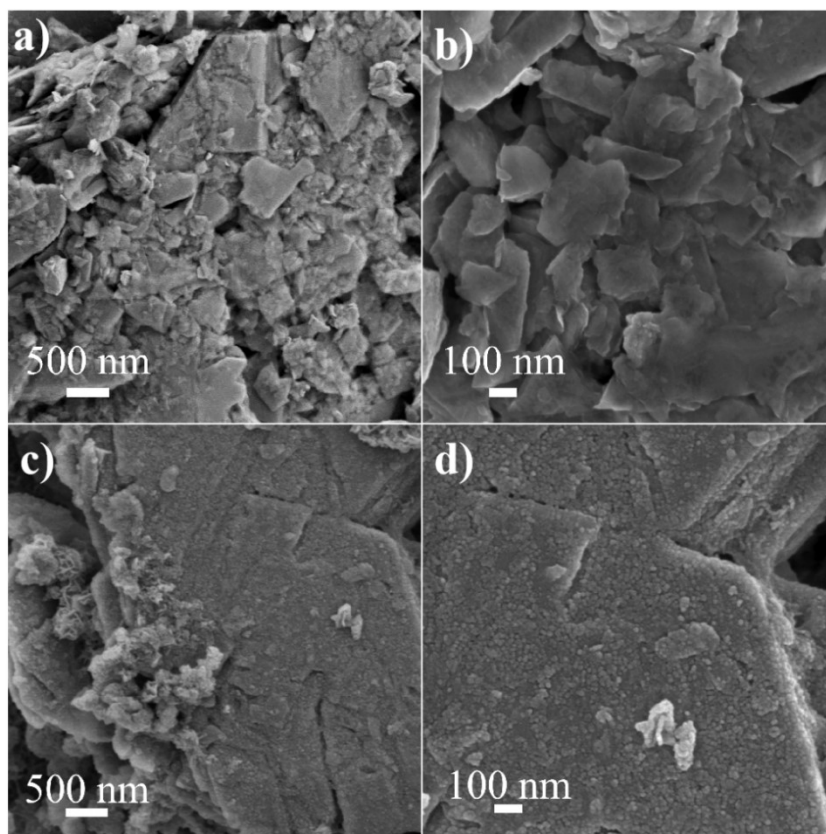


Fig. S14 SEM images of CC-MoC@MoS₂-2.0 (a, b) before and (c, d) after stability test.

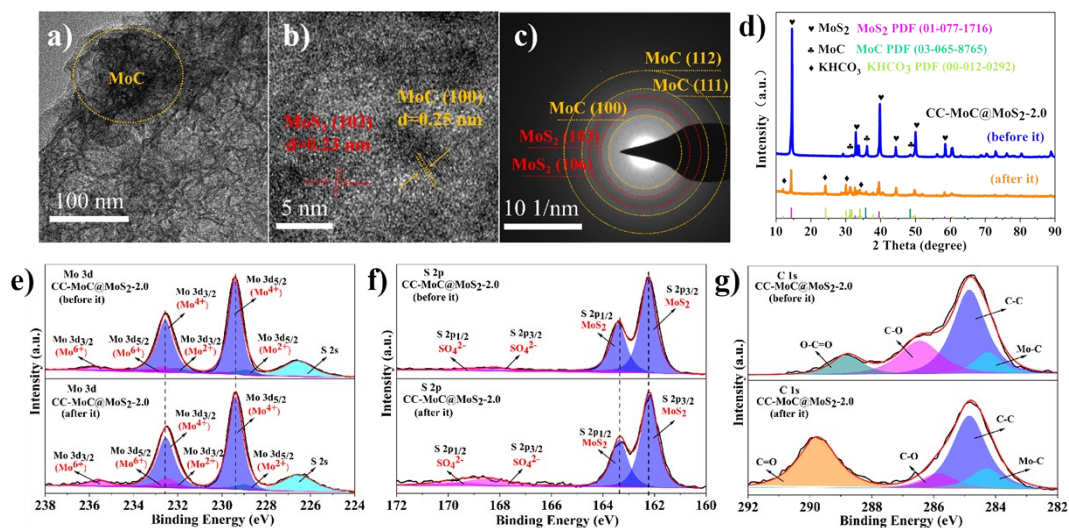


Fig. S15 (a, b) TEM images and (c) SAED pattern of CC-MoC@MoS₂-2.0 after stability test. (d) XRD patterns and XPS spectra of (e) Mo 3d, (f) S 2p, (g) C 1s of CC-MoC@MoS₂-2.0 before and after stability test.

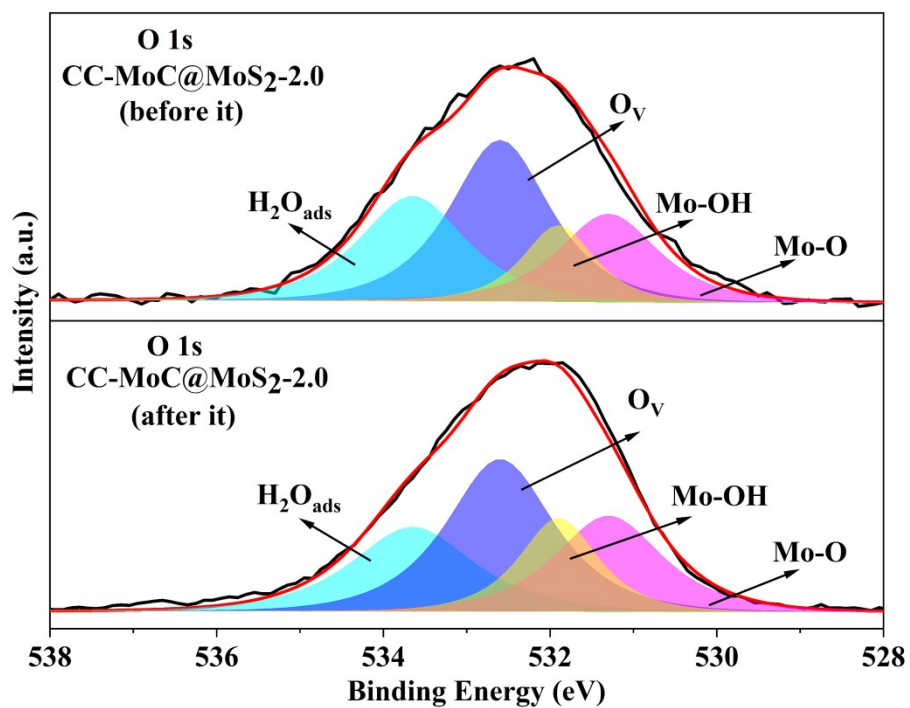


Fig. S16 High-resolution XPS spectra of O 1s of CC-MoC@MoS₂-2.0 before and after stability test.

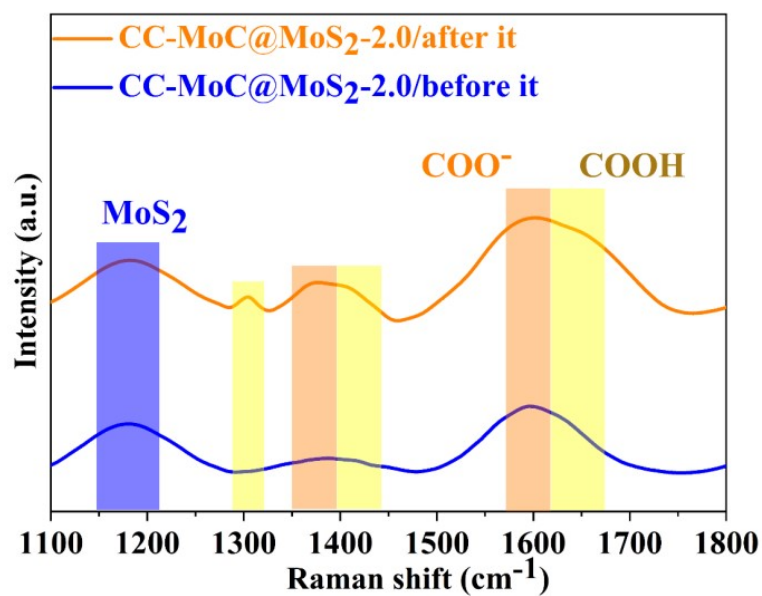


Fig. S17 Raman spectra of CC-MoC@MoS₂-2.0 before and after stability test.

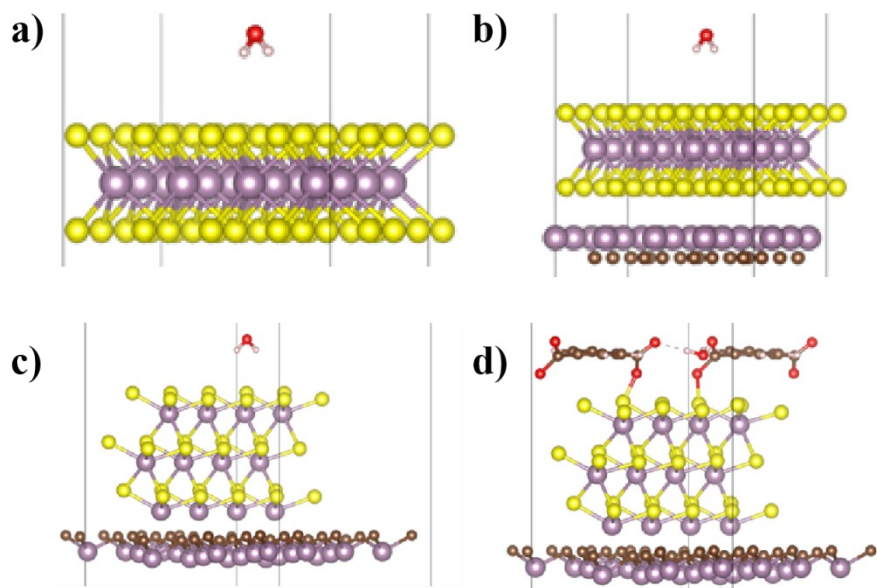


Fig. S18 Water adsorption models of (a) MoS₂, (b) MoC@MoS₂-I, (c) MoC@MoS₂-II and (d) CC-MoC@MoS₂-

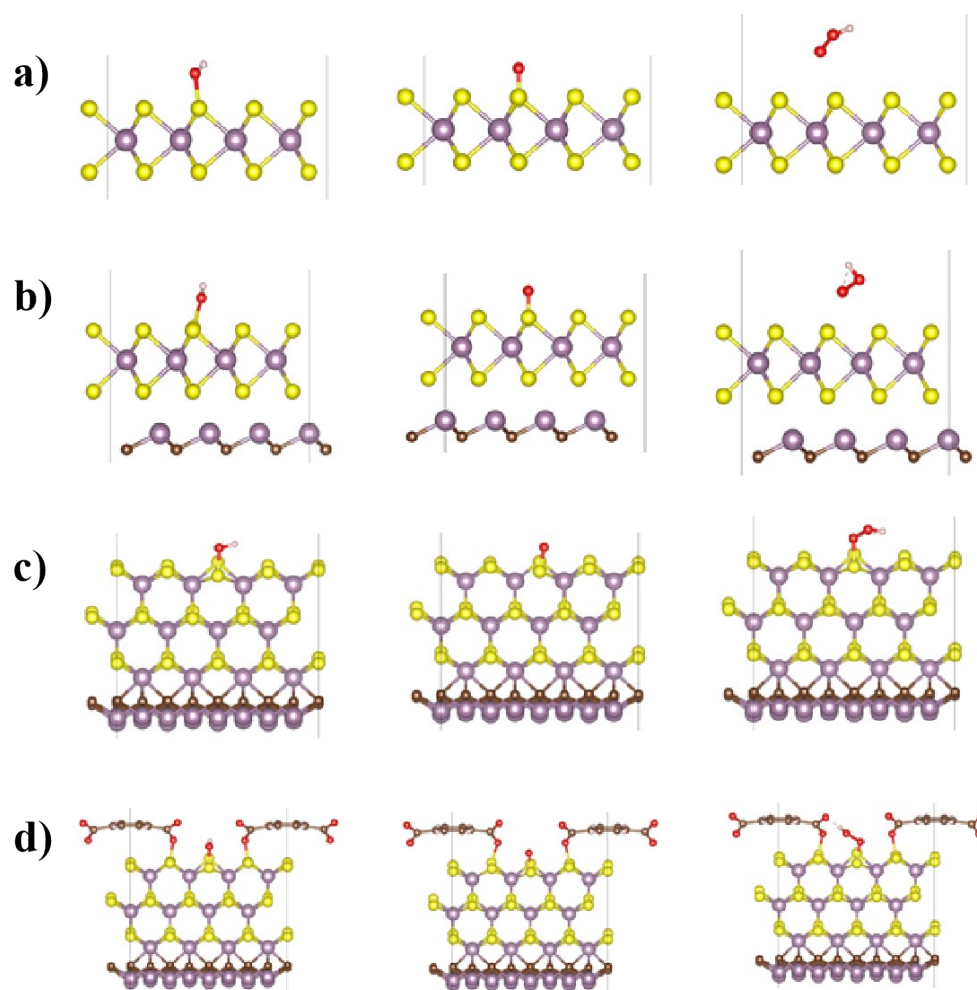


Fig. S19 Theoretical structural models of clean surfaces and *OH, *O, *OOH intermediates adsorbed on the surfaces of a) MoS₂, b) MoC@MoS₂-I, c) MoC@MoS₂-II and d) CC-MoC@MoS₂.

Table S4: The calculated E^* (eV), Gibbs free energy change $\Delta_r G$ (eV) and theoretical overpotential η (eV) values of the OER performance (calibration at 298.15 K, the unit of physical quantity is eV, U = 0 V).

System	E^*	$G_{\text{H}_2\text{O}}$	G_{H_2}	G_{O_2}	$\Delta_r G_1$	$\Delta_r G_2$	$\Delta_r G_3$	$\Delta_r G_4$	η
MoS ₂	-364.73				1.40	-	-	-	-
MoC@MoS ₂ -I	-661.31				1.11	-	-	-	-
MoC@MoS ₂ -II	-696.01	-14.22	-6.80	-9.92	-0.47	-0.26	1.03	-0.30	1.03
CC-MoC@MoS ₂ - 2.0	-809.10				-0.11	-0.53	0.94	-0.30	0.94

Table S5: The energies of proton generation and migration of different electrocatalysts calculated by CI-NEB method.

System	Reaction	$E_{\text{transition}}$ (eV)
MoC@MoS ₂ -II	Proton generation	0.47
CC-MoC@MoS ₂		0.42
MoC@MoS ₂ -II	Proton transfer	0.84
CC-MoC@MoS ₂		0.72

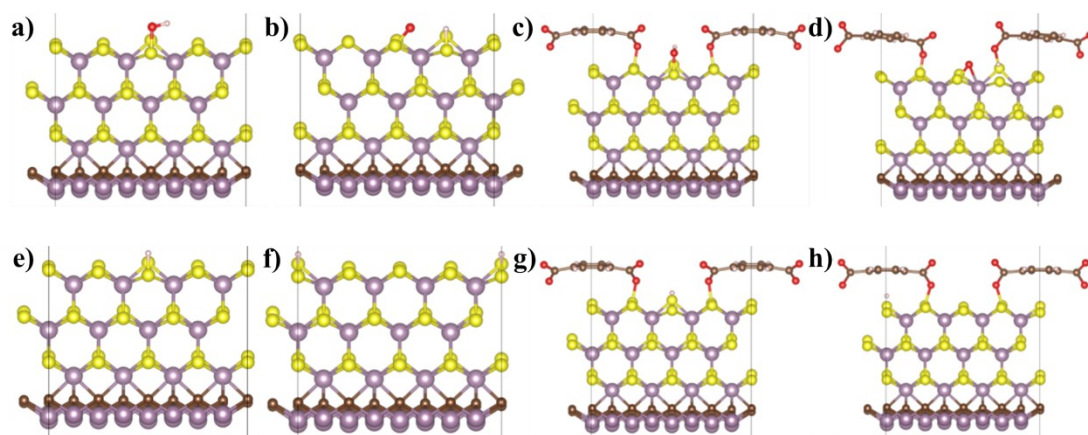


Fig. S20 Schematic illustration of the proposed proton transfer processes of MoC@MoS₂-II and CC-MoC@MoS₂-2.0. The initial and final proton generation states of MoC@MoS₂-II (a, b) and CC-MoC@MoS₂-2.0 (c, d). The initial and final states of proton migration of MoC@MoS₂-II (e, f) and CC-MoC@MoS₂-2.0 (g, h).

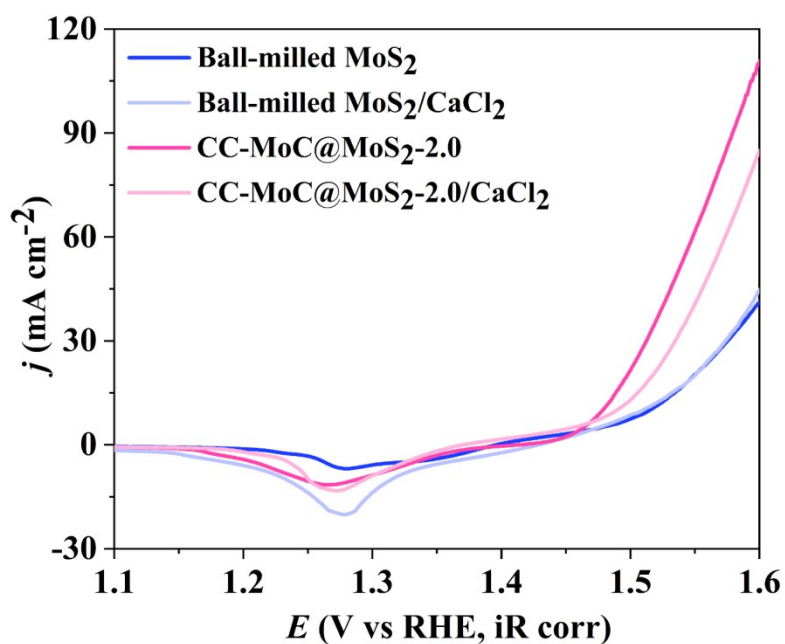


Fig. S21 LSV curves of BM-MoS₂ and CC-MoC@MoS₂-2.0 with and without CaCl₂ in the electrolyte.

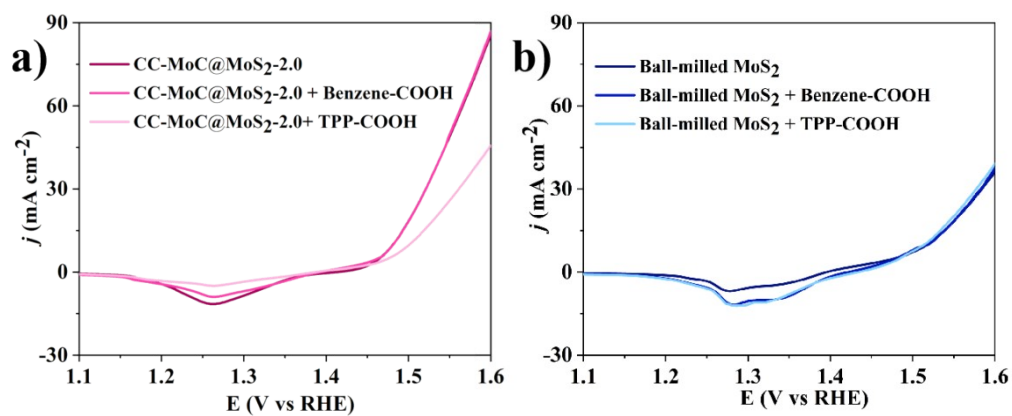


Fig. S22 LSV curves of (a) CC-MoC@MoS₂-2.0 and (b) BM-MoS₂ catalysts in 1 M KOH with the titration of 5 mM TPP-COOH or Benzene-COOH.

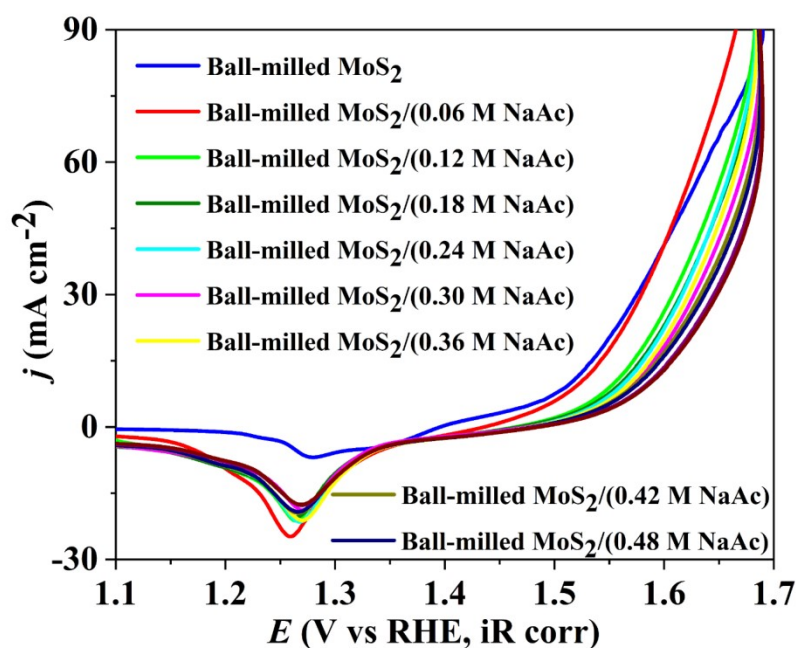


Fig. S23 LSV curves of BM-MoS₂ catalysts in 1 M KOH with NaAc solutions of different concentrations.

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