Achieving highly efficient electrocatalytic hydrogen evolution with Co-doped MoS_2 nanosheets

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Supplementary Figures

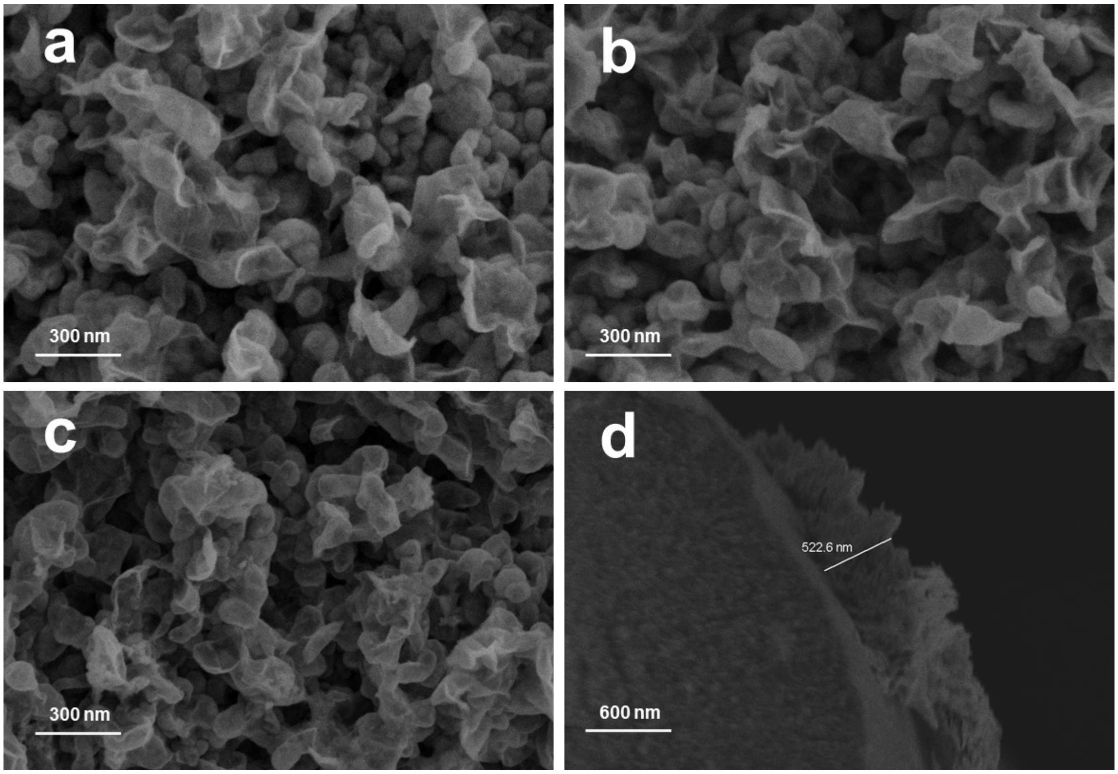

Figure S1. SEM images of samples (a) Co-1T-MoS_2, (b) Co-1T-MoS_2-2, (c) Co-1T-MoS_2-3, and (d) Cross-sectional view of the Co-1T-MoS_2-3.

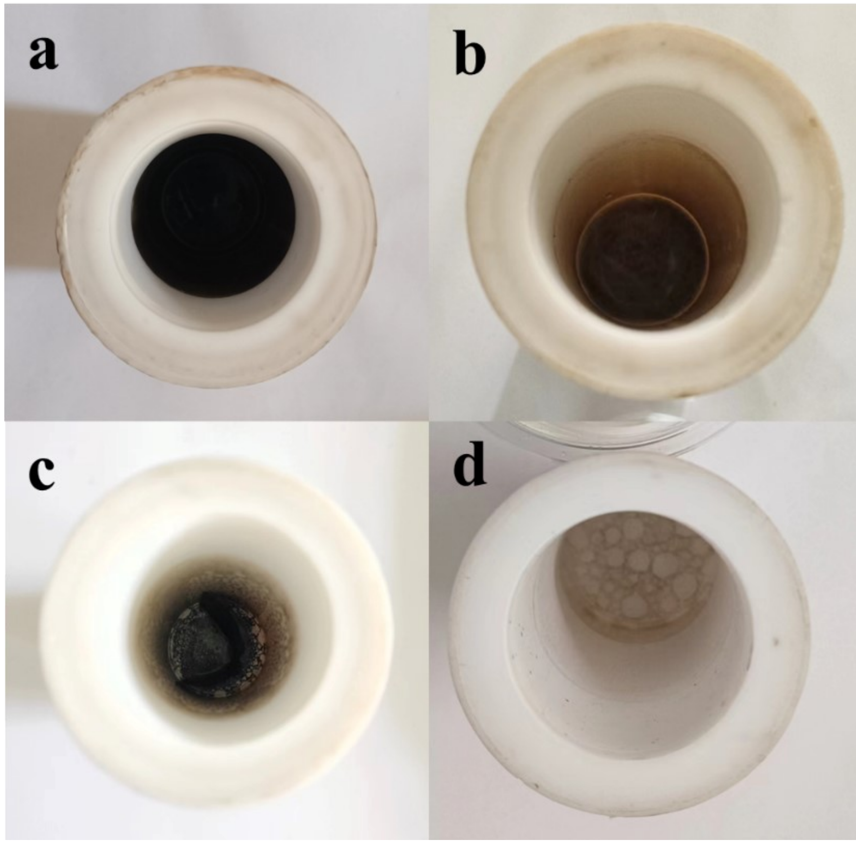

Figure S2. Internal state of the reaction autoclave of (a) Co-MoS_2, (b) Co-1T-MoS_2, (c) Co-1T-MoS_2-2, and (d) Co-1T-MoS_2-3.

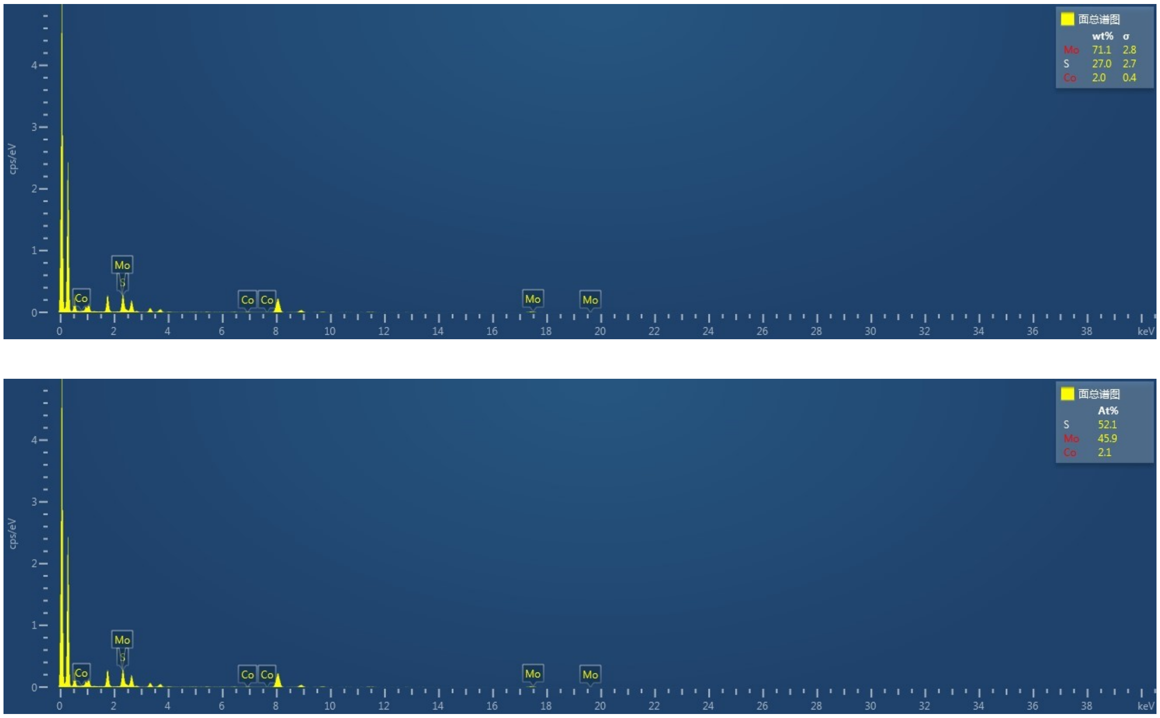

Figure S3.TEM-DES results

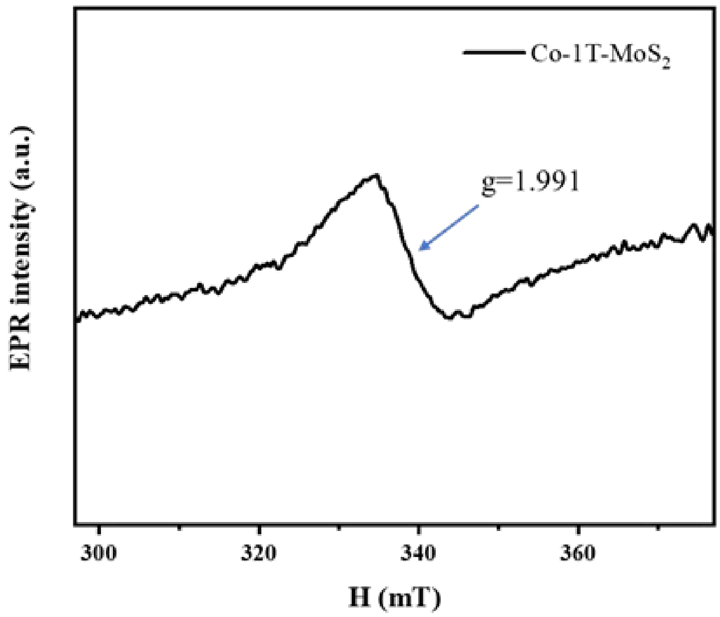

Figure S4. Electron paramagnetic resonance (EPR) spectra

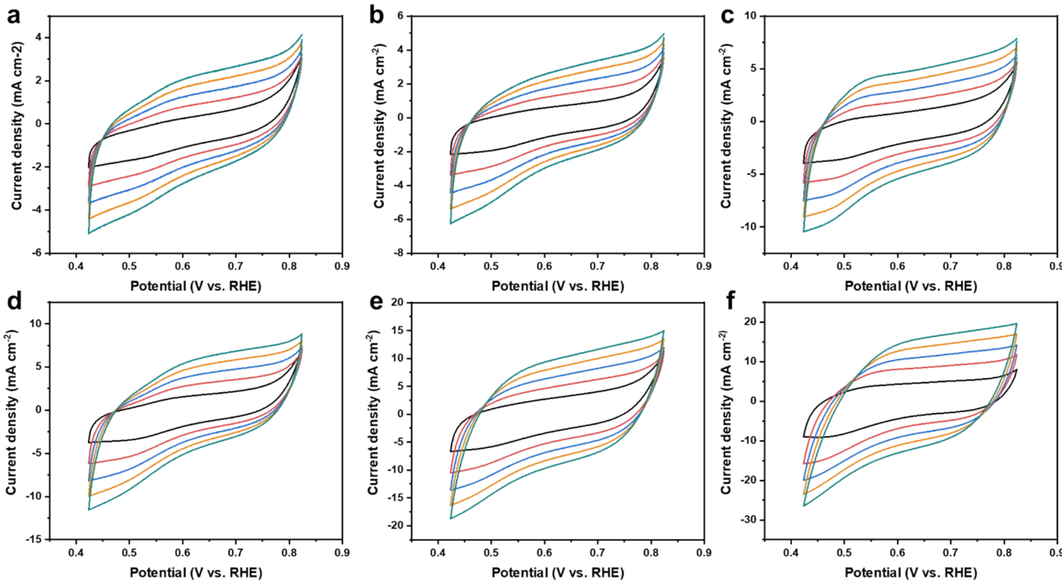

Figure S5. Cyclic voltammetry (CV) plots at different scan rates (20, 40, 60, 80 and 100 mV s^{-1}) of (a) MoS_2-blank, (b) Co-MoS_2, (c) 1T-MoS_2, (d) Co-1T-MoS_2, (e) Co-1T-MoS_2-2, and (f) Co-1T-MoS_2-3 used to calculate the double layer capacitance (C_{dl}).

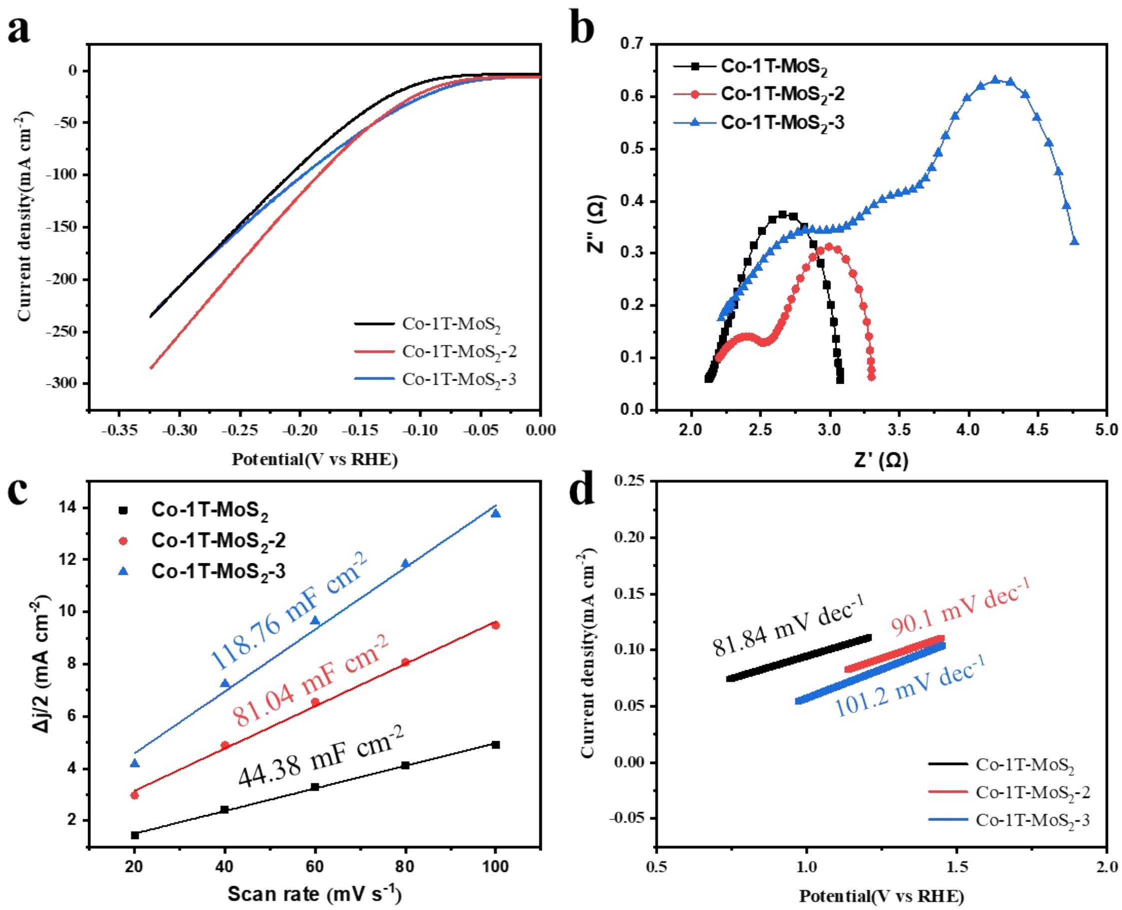

Figure S6. Electrochemical HER performance of Co-1T-MoS$_2$, Co-1T-MoS$_2$-2, and Co-1T-MoS$_2$-3. (a) Polarization curves at the range from -0.9 V to -1.25 V vs Hg/HgO by using a scan rate of 5 mV s^{-1} with 90% iR compensation. (b) Nyquist plots of electrochemical impedance spectra. (c) Linear regression of current densities at different scan rates for the calculation of C_{dl}. (d) Corresponding Tafel charts.

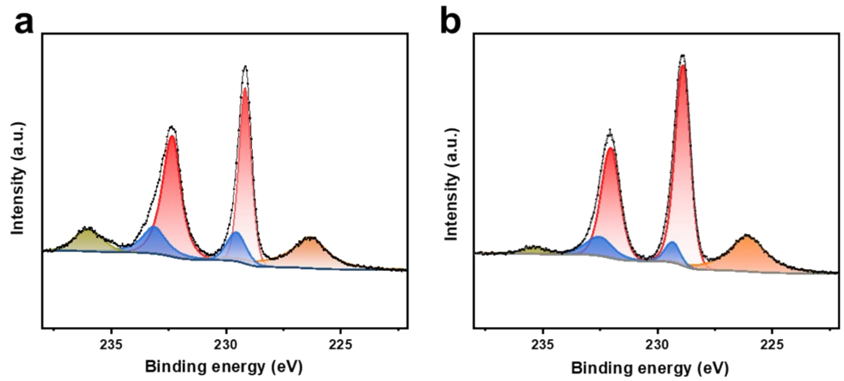

Figure S7. High-resolution XPS Mo 3d spectra after the durability test. (a) Co-1T-MoS_2-2, and (b) 1T-MoS_2.

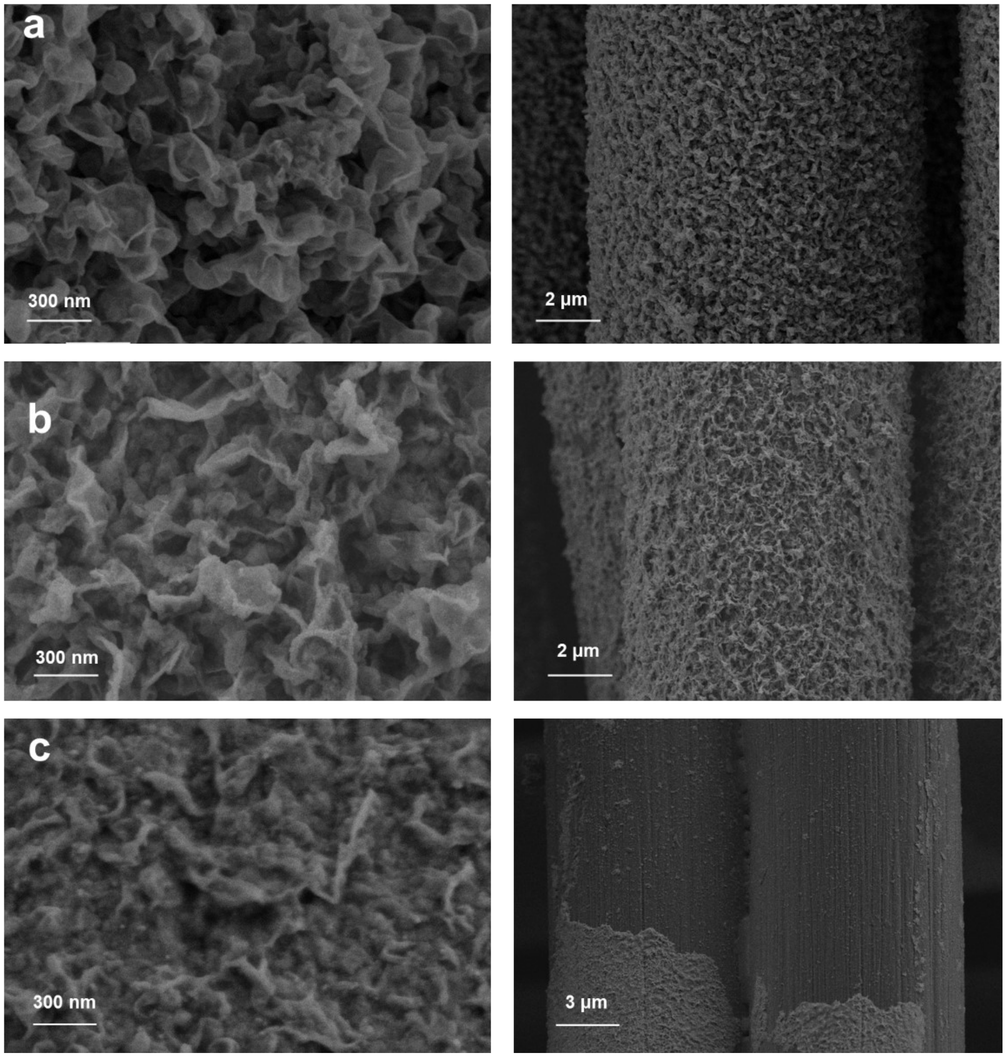

Figure S8. SEM images of samples after the durability test.(a) Co-1T-MoS_2-2, (b) 1T-MoS_2, and (c) Co-1T-MoS_2-210°C.

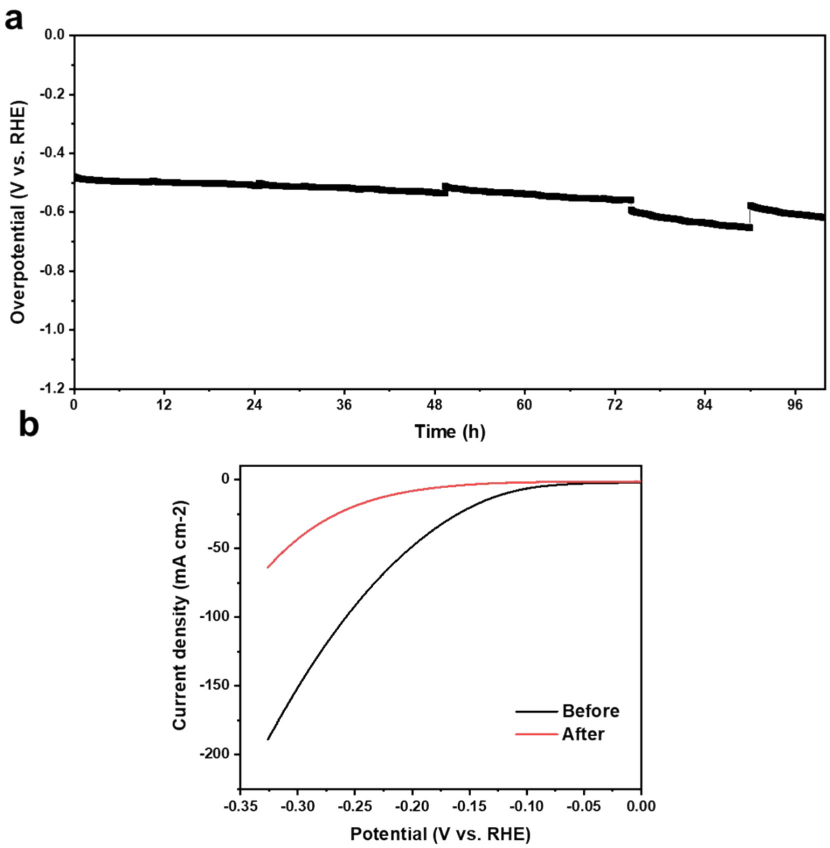

Figure S9. (a) Chronopotentiometry durability curve of Co-1T-MoS_2-210°C at 100 mA cm^{-2} for 100 h. (b) Polarization curves of Co-1T-MoS_2-210°C before and after stability tests.

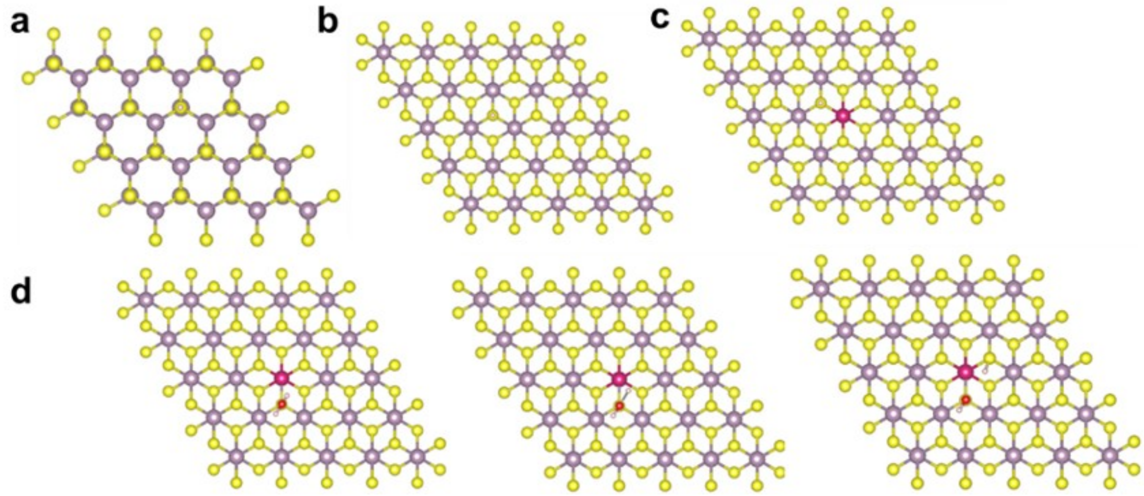

Figure S10. The optimized calculation models of H* adsorption on (a) 2H-MoS_2, (b) 1T-MoS_2, and (c) Co-1T-MoS_2 (d)The optimized calculation models of H_2O dissociation on Co-1T-MoS_2 (yellow atom is S atom, purple atom is Mo atom, pink atom is Co, red atom is O, and white atom is H).

Supplementary Table

Table S1. Comparison of HER performance of Co-1T-MoS_2 with other MoS_2-based electrocatalysts.

Ref No.	Catalyst	Electrolyte	η10 (mV)	1T-phase content (%)	Tafel slope (mV/dec)	R_{ct} (Ω)	Stability
This work	Co-1T-MoS_2-2	1M KOH	69	83	81.84	0.98	100 h @100 mA cm^{-2}
1	1T/2H–MoS_2@CC	1M KOH	135	88	84.5	-	100 h @100 mA
2	P-1T-MoS_2	0.5M H_2SO_4	153	82	43	16	1000 cycles
3	CoMoS-C	0.5M H_2SO_4	135	-	50	14.3	1000 cycles
4	Co-1T-MoS_2-bpe	1M KOH	118	80	83	-	10 h @100 mA
5	R-MoS_2	1M KOH	111	34	105	21.73	5000 cycles
6	Co-MoS_2-1.4	0.5M H_2SO_4	59	79.2	32	-	1000 cycles
7	1T-MoS_2 (SBH+DMF)	0.5M H_2SO_4	248	79.4	56	121	48 h @ 260 mV
8	1T-MoS_2	0.5M H_2SO_4	136	70	45	3.3	12 h @10 mV
9	$Co_xMo1_{-x}S_2$	0.5M H_2SO_4	357	-	120	-	10 h @ 3800 mV
10	Co-1T-MoS_2	0.5M H_2SO_4	84	-	47	53	-
11	CTAB/MoS_2	0.5M H_2SO_4	182	50	45.9	6.09	3000 cycles
12	MA-MoS_2	0.5M H_2SO_4	270	70	56	386	1000 cycles
13	1T/2H-MoS_2/NH_4^+	0.5M H_2SO_4	159	61.16	55.5	12.2	1000 cycles
14	Pt:Ru(1:4)-MoS_2	0.5M H_2SO_4	84	-	68.5	88.3	10h @10mAcm^{-2}
15	2Ru-MoS_2	0.5M H_2SO_4	70	-	110	-	10h @10mA
16	MoS_2/S(1:1)	0.5M H_2SO_4	151	55	38	1.39	1000 cycles
17	Cl-MoS_2	0.5M H_2SO_4	158	-	60.8	35.1	-
18	ZnSAs/1T-MoS_2	0.5M H_2SO_4	177	-	84.9	18.41	3000 cycles
19	$Ce_{0.1}$-MoS_2	0.5M H_2SO_4	113	-	57.36	9.34	10h @10mA
20	Ni-MoS_2	1M KOH	124	69	64	-	1000 cycles
21	Ni-MoS_2	1M KOH	98	-	60	-	2000 cycles

Table S2. Comparison of ICP test results for Co-MoS_2 and Co-1T-MoS_2

<table>
<tr><th>Sample</th><th>M_0 (g)</th><th>V_0(mL)</th><th>Test elements</th><th>C_0 (mg/L)</th><th>f</th><th>C_1(mg/L)</th><th>C_X(mg/kg)</th><th>W(%)</th><th>$n_{Co/Mo}$ (%)</th></tr>
<tr><td rowspan="3">Co-MoS_2</td><td>0.0101</td><td>25</td><td>Mo</td><td>3.819</td><td>1</td><td>3.819</td><td>9452.970</td><td>0.945</td><td rowspan="3">1.35</td></tr>
<tr><td>0.0101</td><td>25</td><td>S</td><td>2.302</td><td>1</td><td>2.302</td><td>5698.020</td><td>0.570</td></tr>
<tr><td>0.0101</td><td>25</td><td>Co</td><td>31.819 (ug/L)</td><td>1</td><td>31.819</td><td>78759.901 (ug/kg)</td><td>0.008</td></tr>
<tr><td rowspan="3">Co-1T-MoS_2</td><td>0.0123</td><td>25</td><td>Co</td><td>1.305</td><td>1</td><td>1.305</td><td>2652.439</td><td>0.265</td><td rowspan="3">7.8</td></tr>
<tr><td>0.0123</td><td>25</td><td>S</td><td>19.124</td><td>1</td><td>19.124</td><td>38869.919</td><td>3.887</td></tr>
<tr><td>0.0123</td><td>25</td><td>Mo</td><td>5.392</td><td>5</td><td>26.960</td><td>54796.748</td><td>5.480</td></tr>
</table>

m_0 (g): The quality of the sample taken when the sample is analyzed; V_0 (mL): After the sample is digested, the volume of the fixed volume; C_0 (mg/L): Test the elemental concentration of the solution; f: Dilution factor; C_1 (mg/L): Elemental concentration of the digestion solution/original sample solution; C_X (mg/kg) & W(%): Elemental content of the sample; C_X(ug/kg)=C_0*f*V_0*10^{-3}/m_0*10^{-3}=C_1*V_0/m_0; W(%)=C_X/10^{-9}*100%

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