Electronic Supplementary Material (ESI) for Nanoscale.

Partial sulfur vacancy created by carbon-nitrogen deposition of MoS_2 for high-performance overall electrocatalytic water splitting

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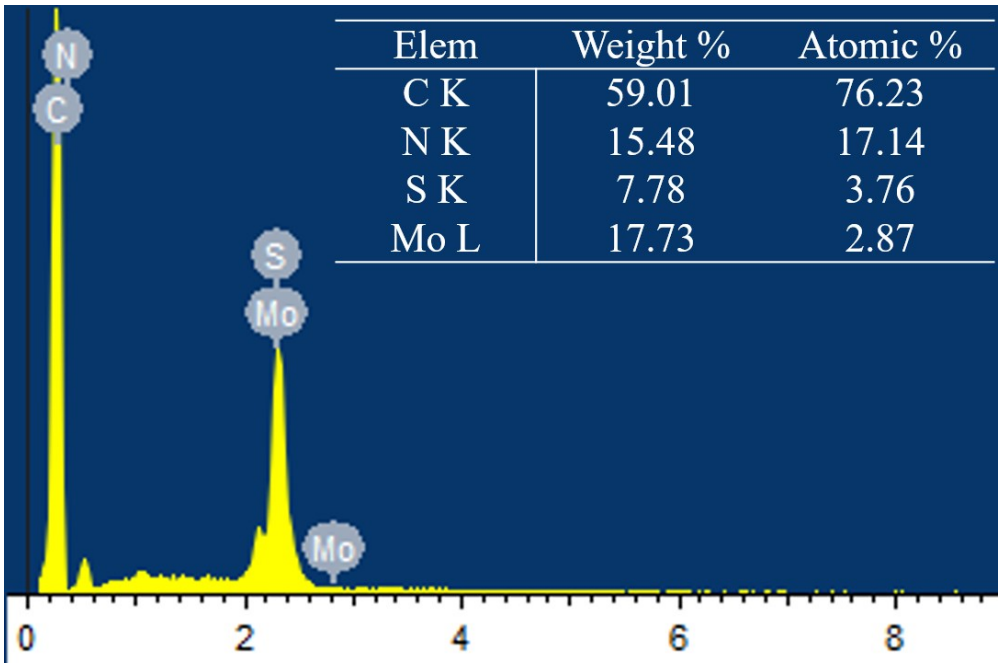

Elem	Weight %	Atomic %
C K	59.01	76.23
N K	15.48	17.14
S K	7.78	3.76
Mo L	17.73	2.87

Fig. S1. The EDX spectral analysis of the C-N-MoS_2/CC-700 material.

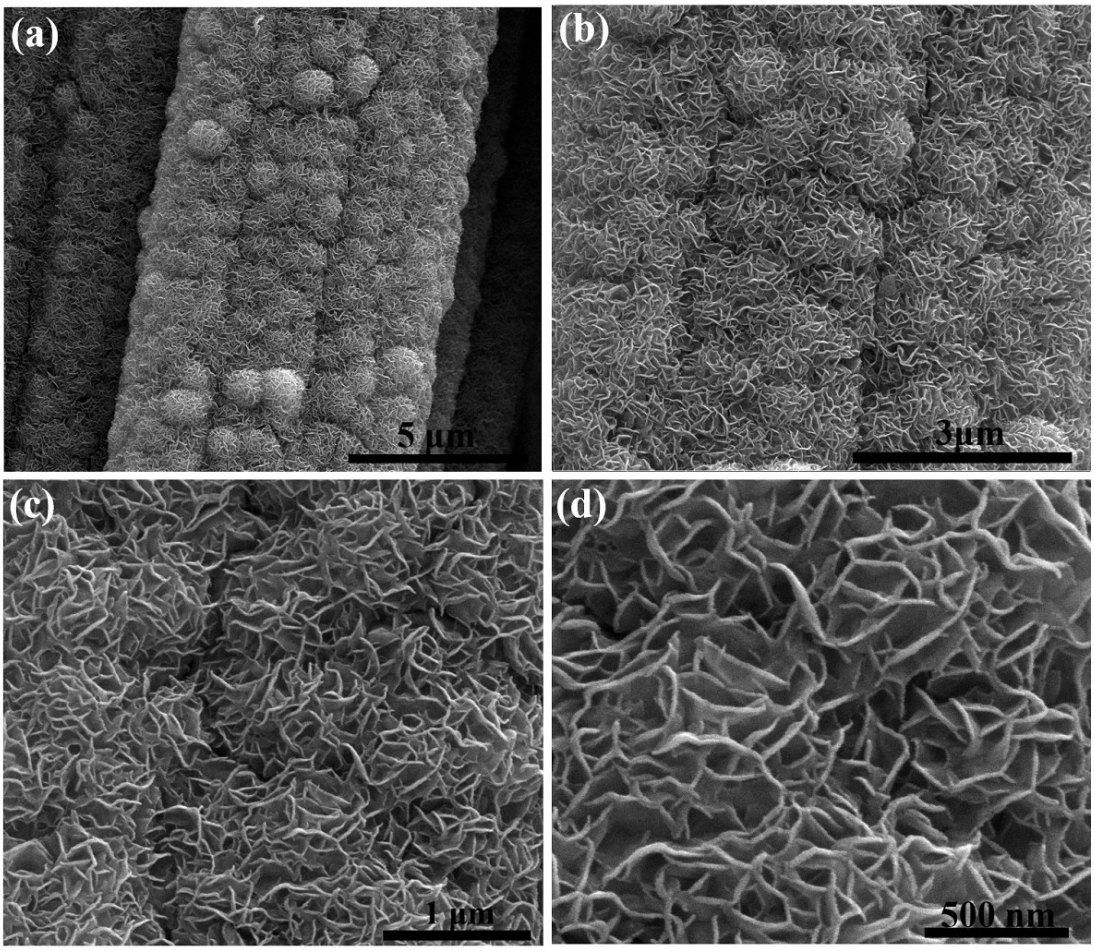

Fig. S2. The SEM image of the pure MoS_2/CC.

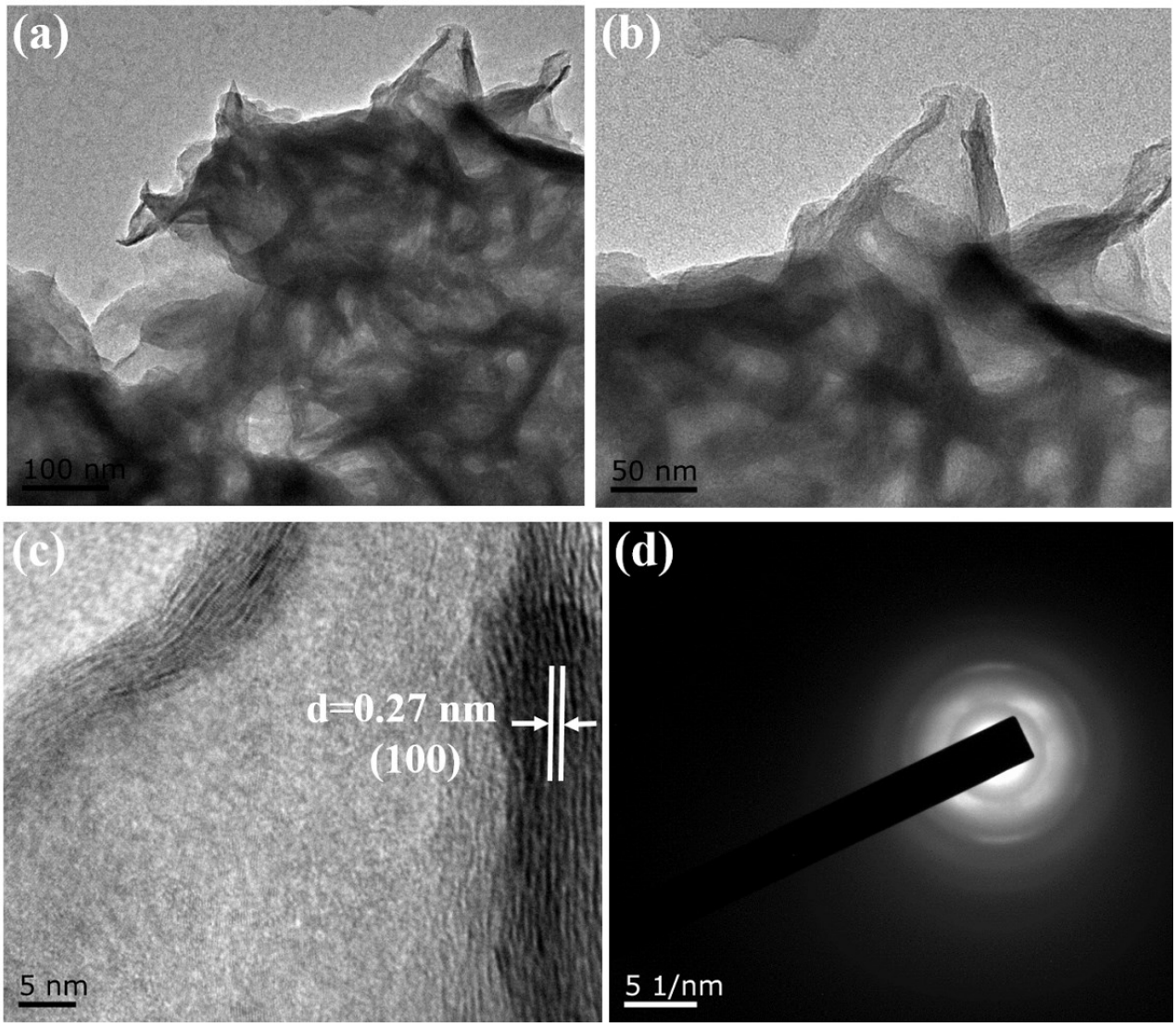

Fig. S3. (a) and (b) TEM image, (c) HRTEM image and (d) electron diffraction of the pure MoS_2/CC.

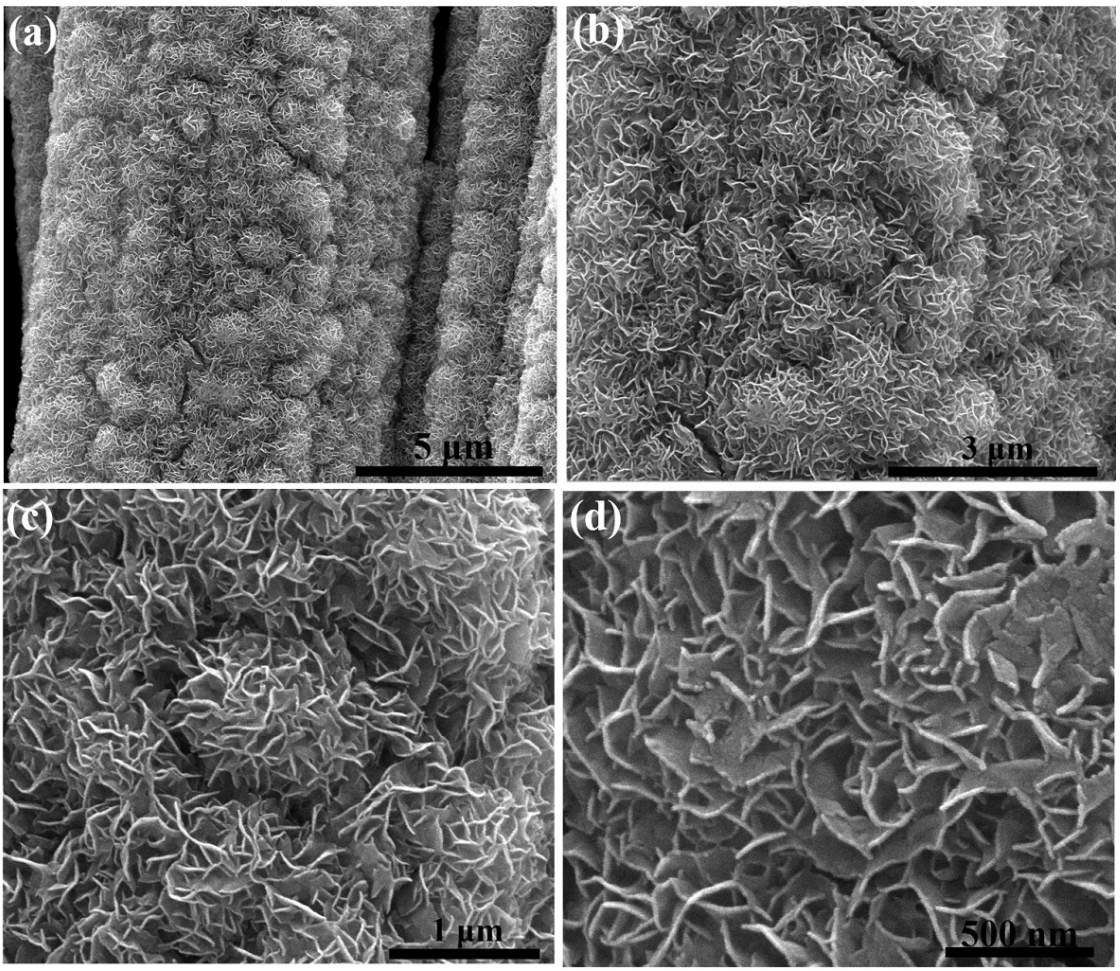

Fig. S4. The SEM image of the C-N-MoS_2/CC-550.

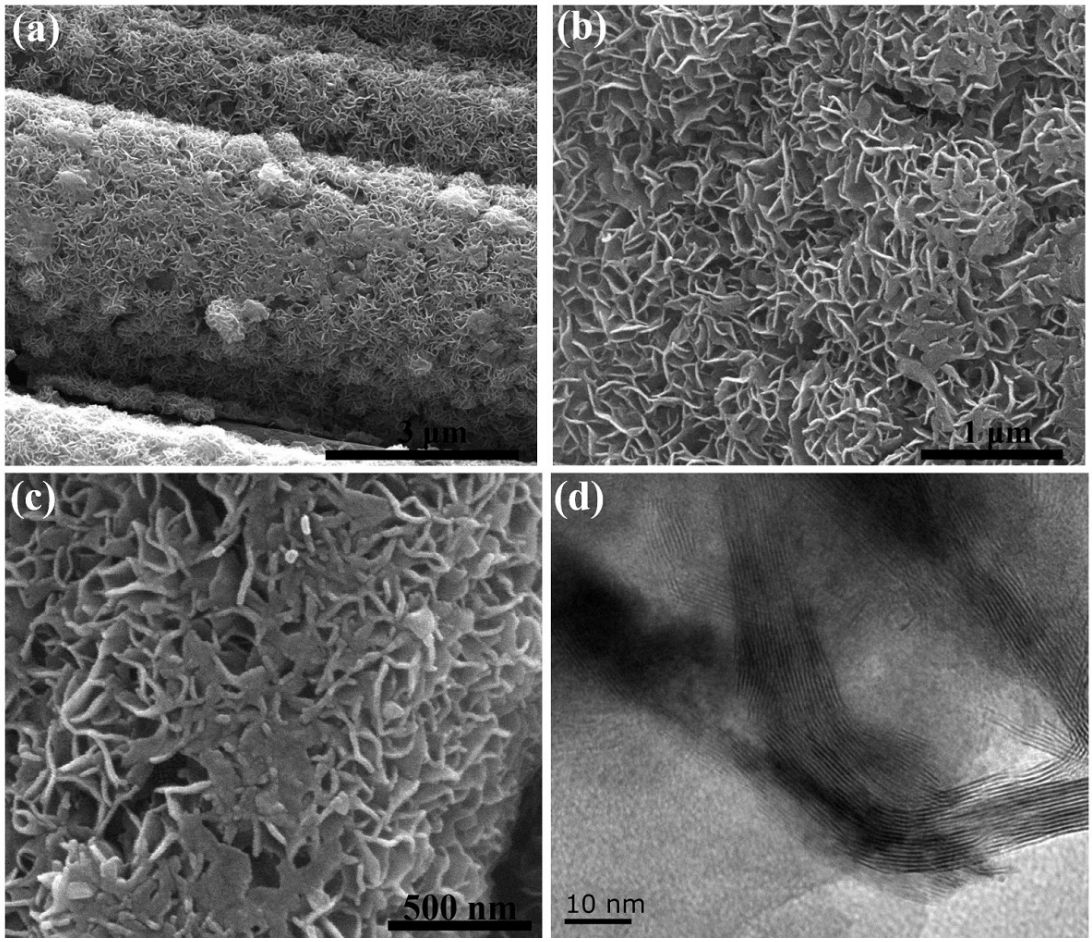

Fig. S5. The SEM image of the C-N-MoS_2/CC-600.

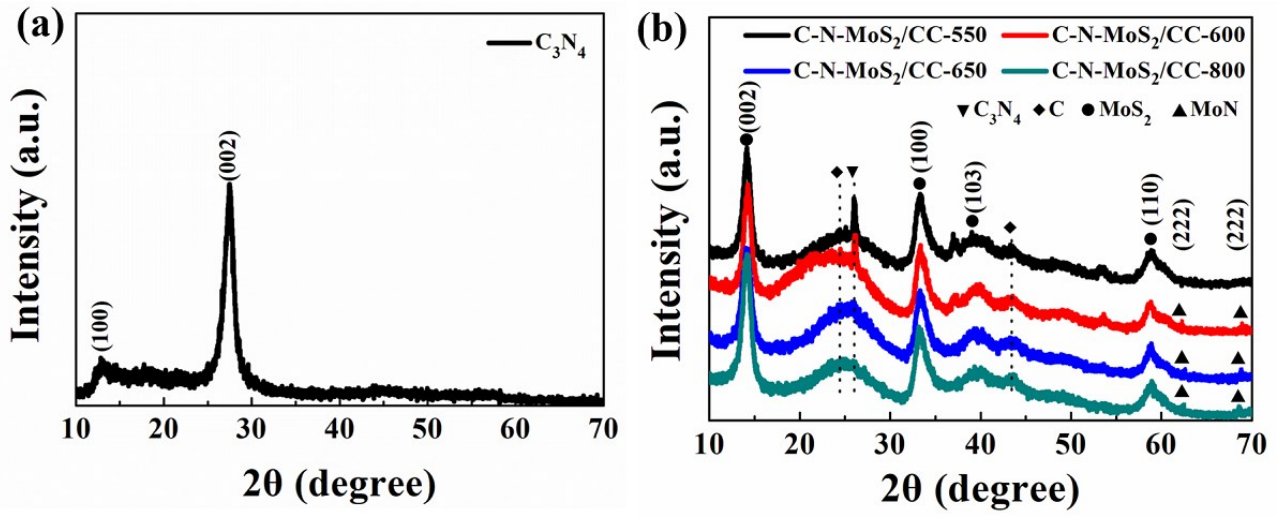

Fig. S6. The XRD patterns of the as-prepared catalyst: (a) C_3N_4, (b) C-N-MoS_2/CC-550, C-N-MoS_2/CC-600, C-N-MoS_2/CC-650 and C-N-MoS_2/CC-800.

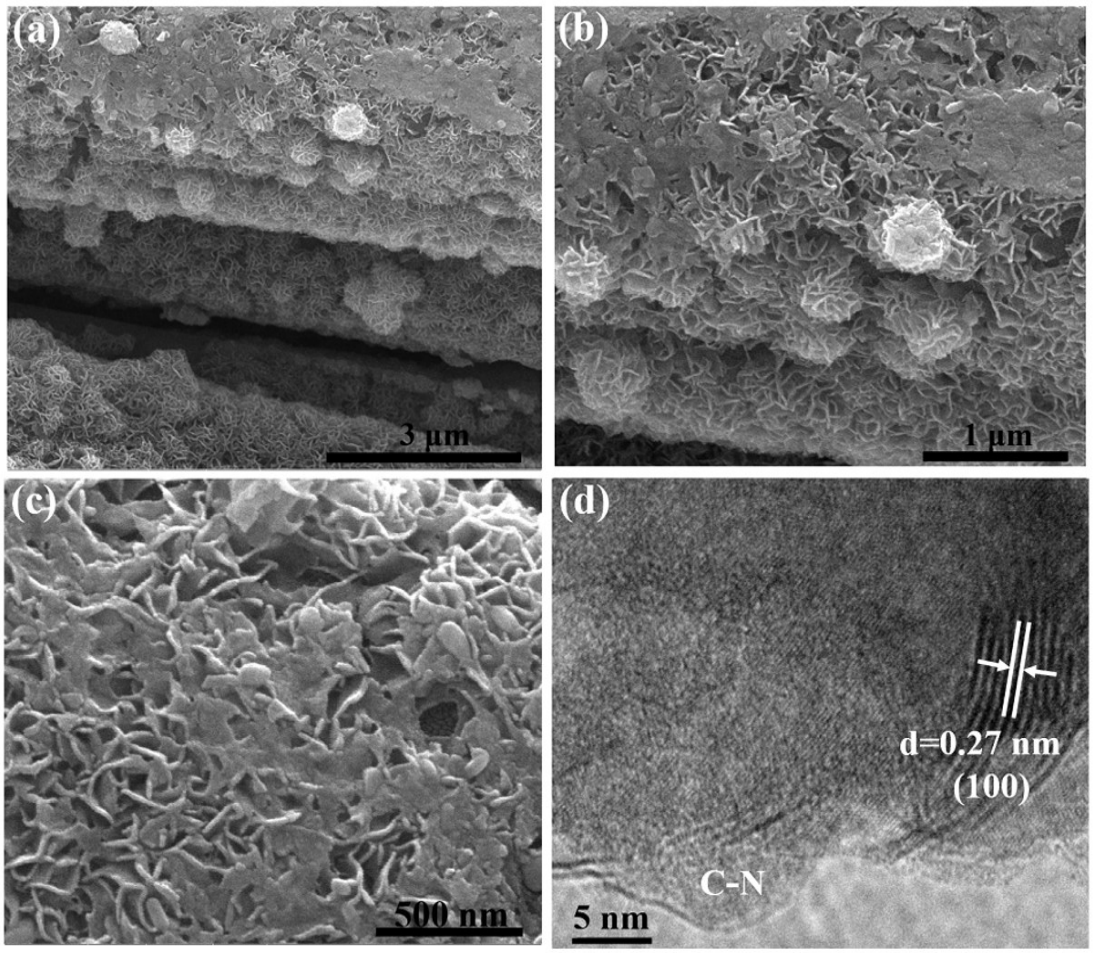

Fig. S7. (a), (b) and (c) The SEM image of the C-N-MoS_2/CC-650, (d) The TEM image of the C-N-MoS_2/CC-650.

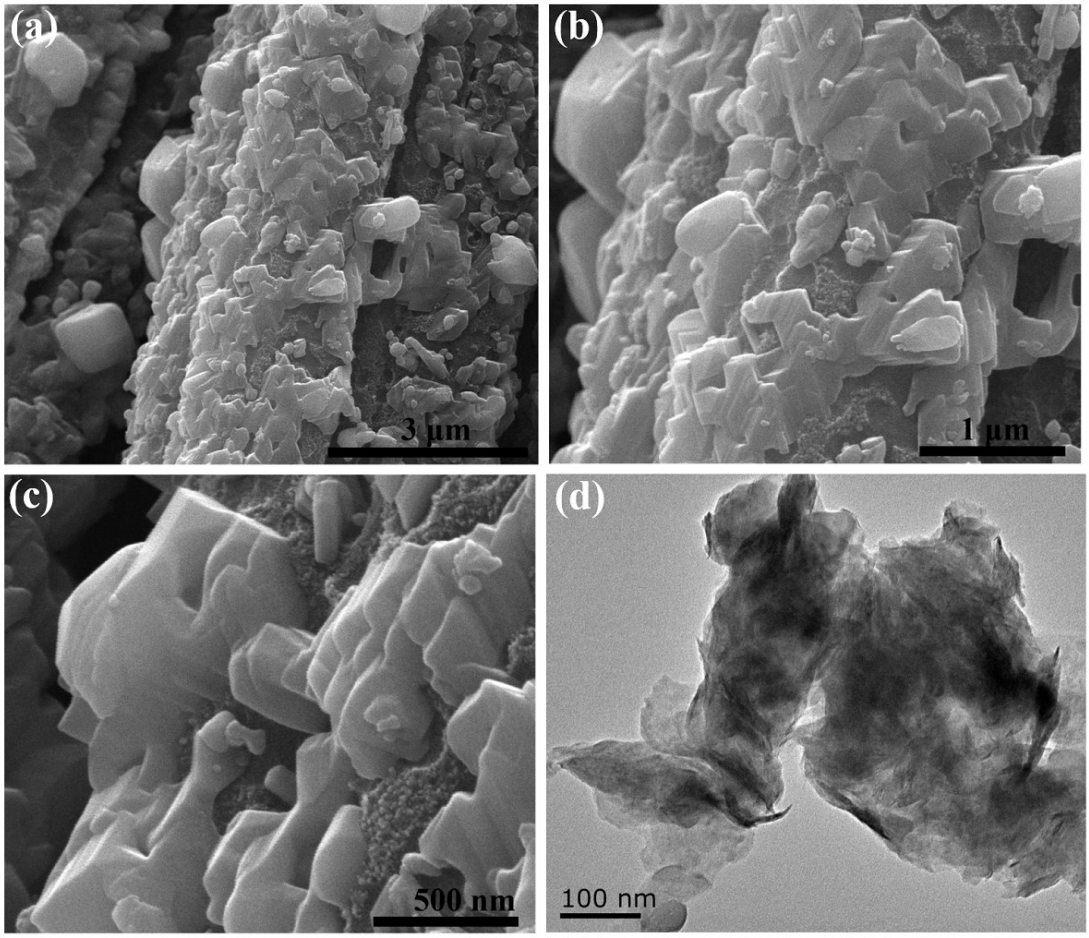

Fig. S8. (a), (b) and (c) The SEM image of the C-N-MoS_2/CC-800, (d) The TEM image of the C-N-MoS_2/CC-800.

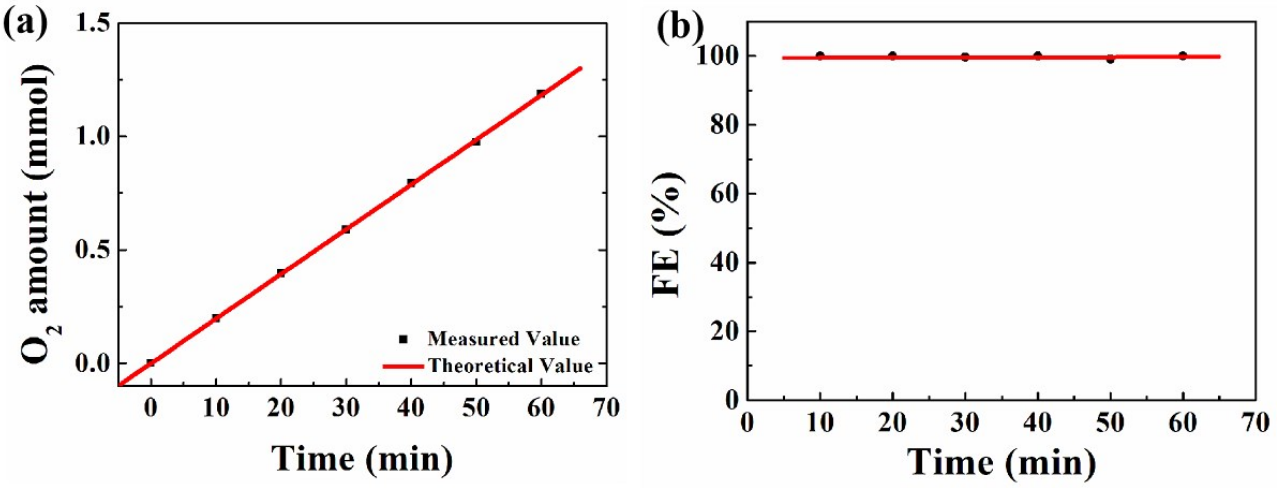

Fig. S9. (a) The O_2 amount of C-N-MoS_2/CC-700 generated at a current density of 10 mA cm^{-2} and (b) corresponding Faraday efficiency.

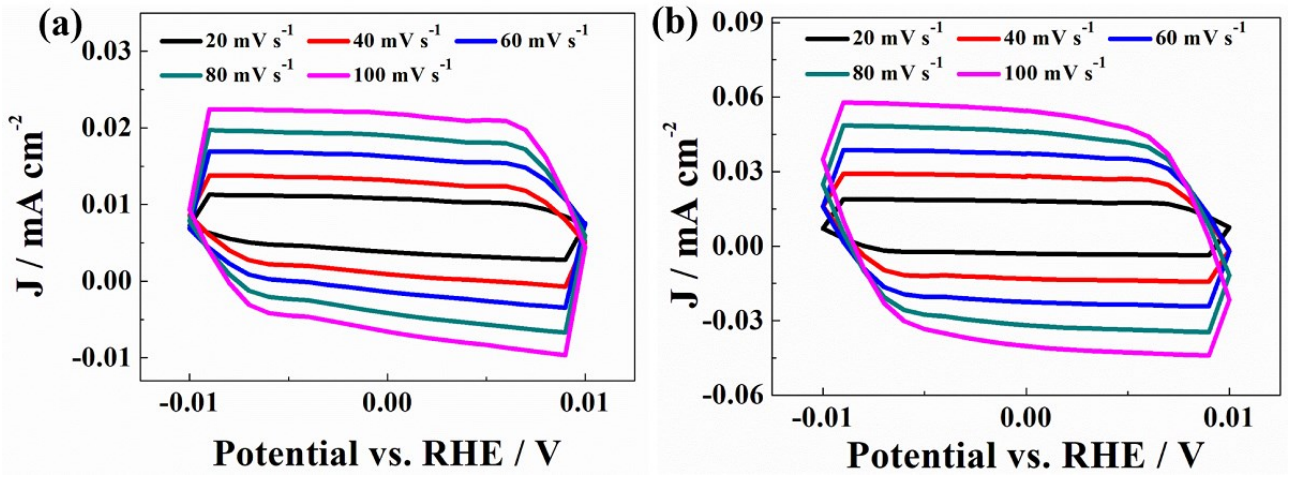

Fig. S10. CV curves at various scan rates in the potential range -0.01~0.01 V vs. RHE for (a) MoS_2/CC, (b) C-N-MoS_2/CC-700, respectively.

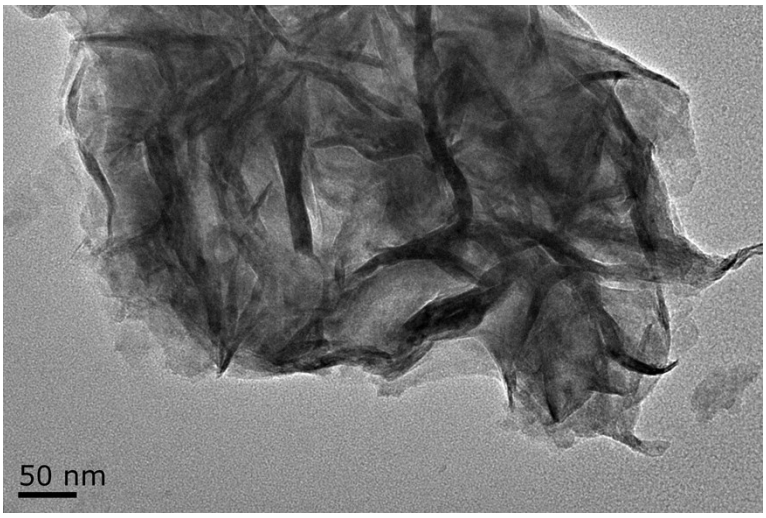

Fig. S11. The TEM image of the C-N-MoS_2/CC-700 after OER.

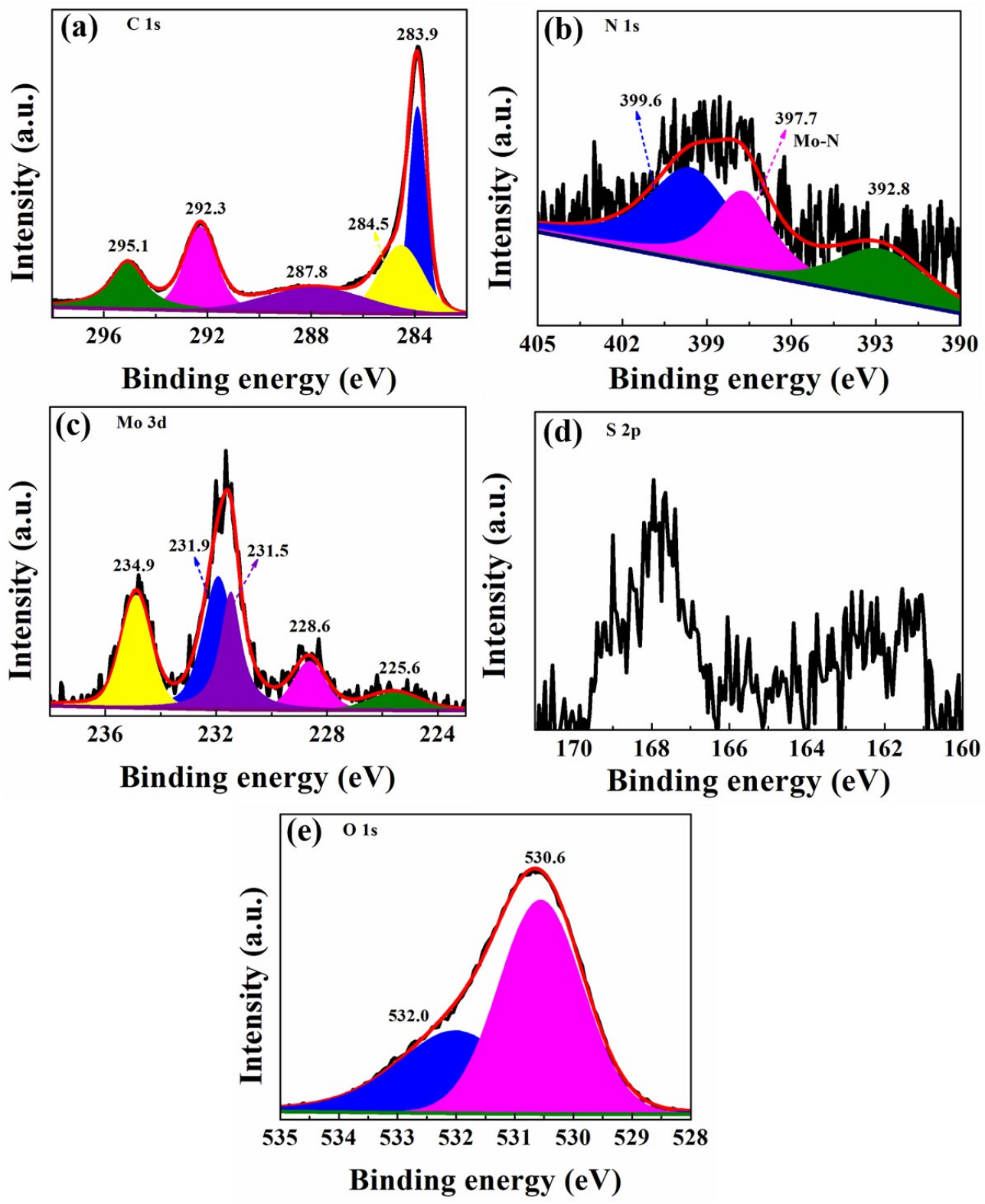

Fig. S12. The XPS spectra of the C-N-MoS_2/CC-700 after OER.

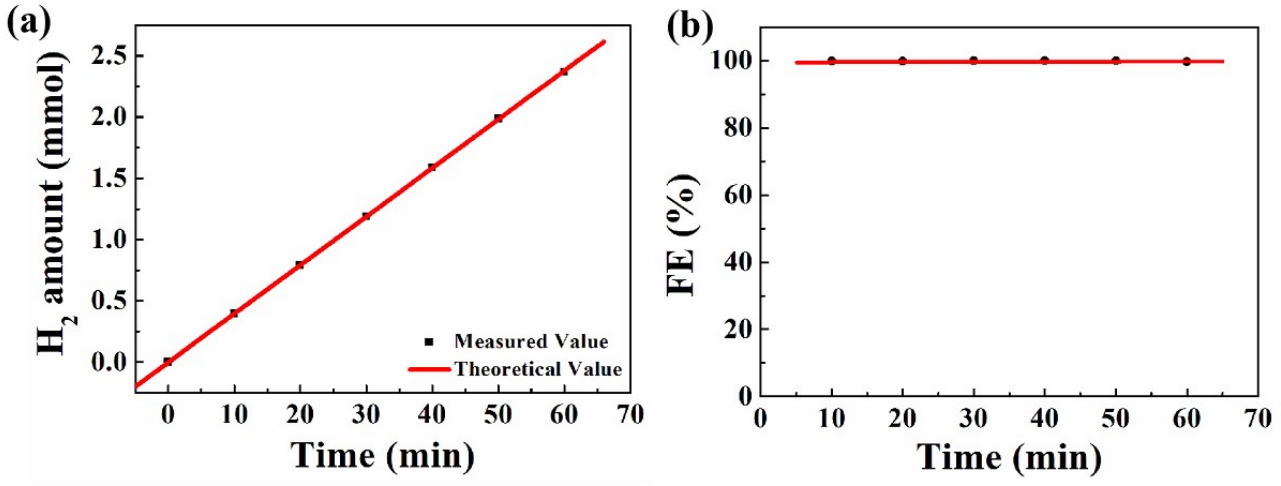

Fig. S13. (a) The H_2 amount of C-N-MoS_2/CC-700 generated at a current density of 10 mA cm^{-2} and (b) corresponding Faraday efficiency.

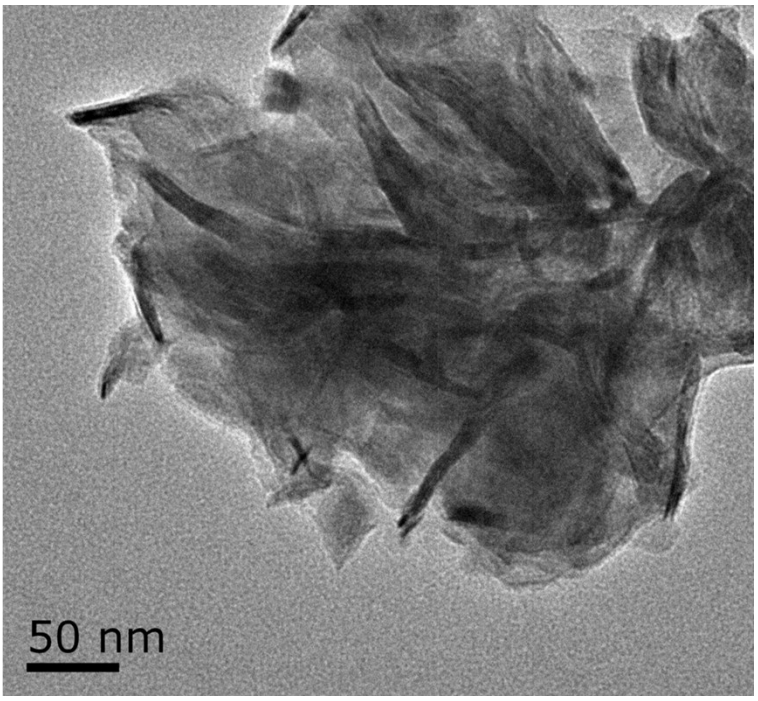

Fig. S14. The TEM image of the C-N-MoS_2/CC-700 after HER.

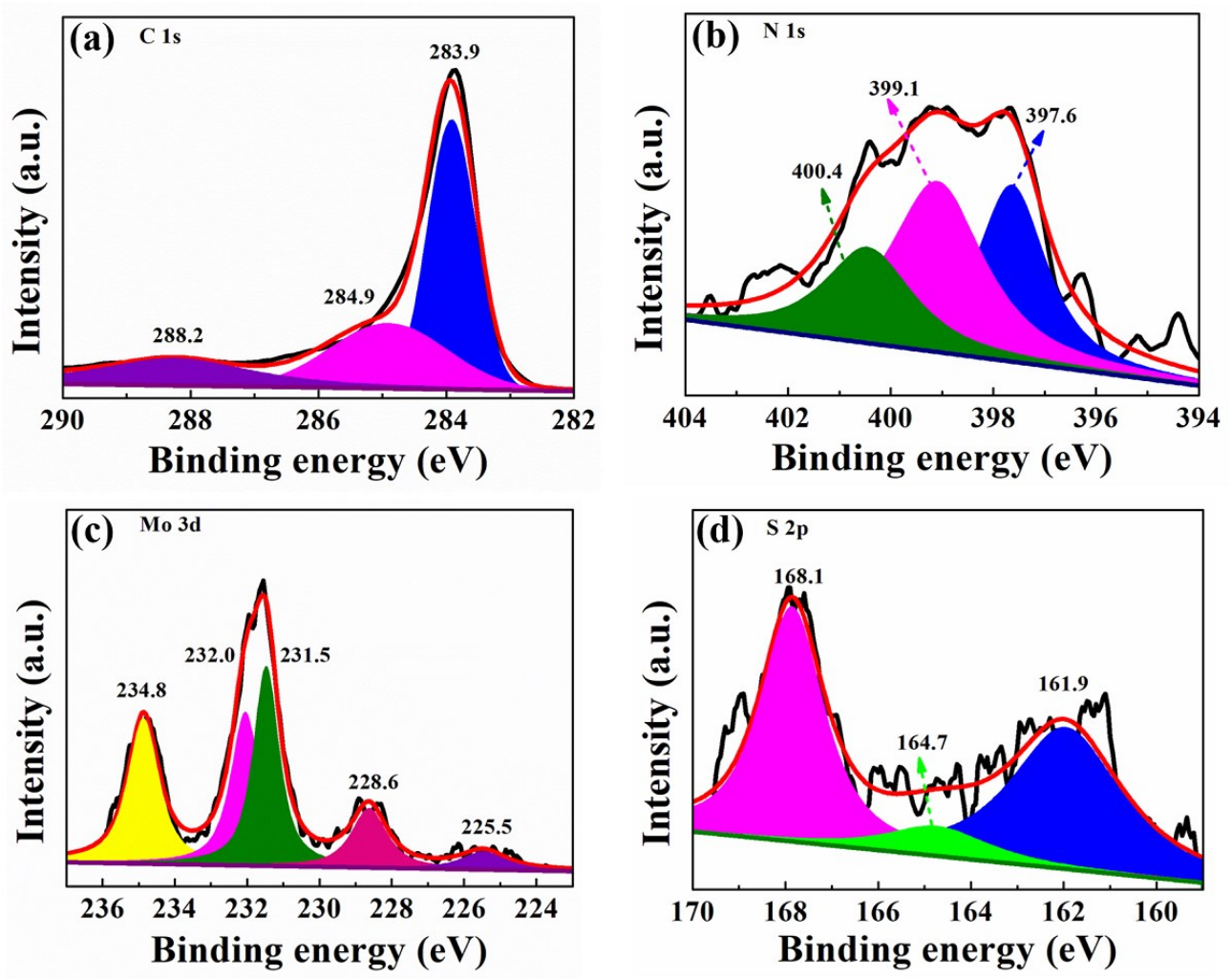

Fig. S15. The XPS spectra of the C-N-MoS_2/CC-700 after HER.

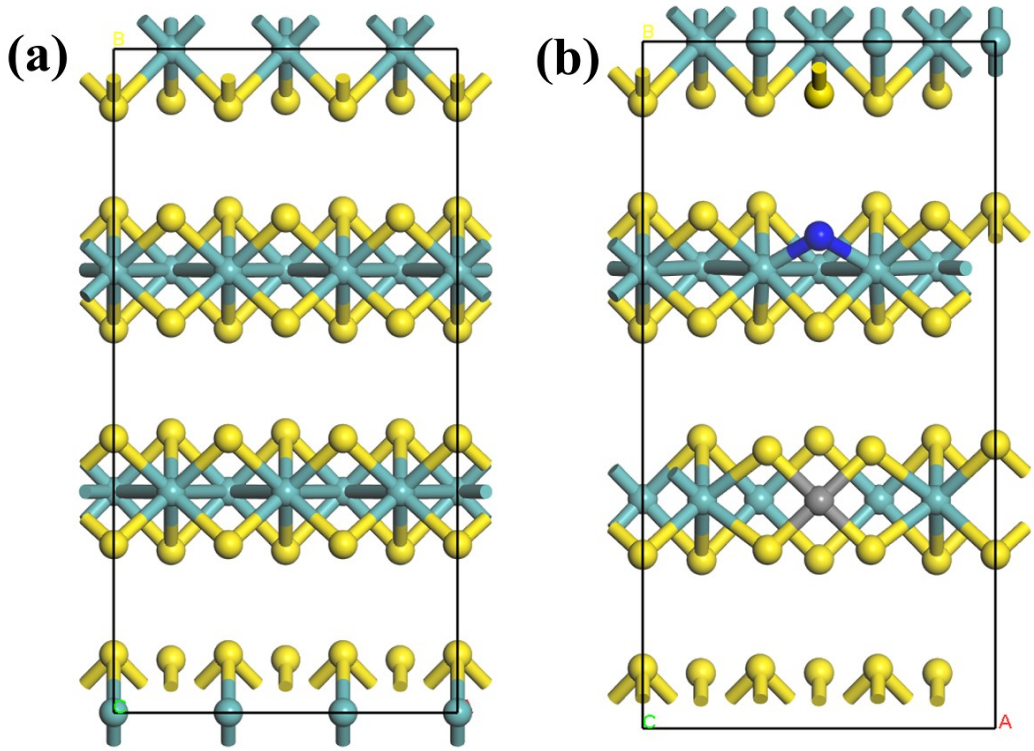

Fig. S16. The optimized atomic structure model for (a) MoS_2 and (b) C-N-MoS_2-700.

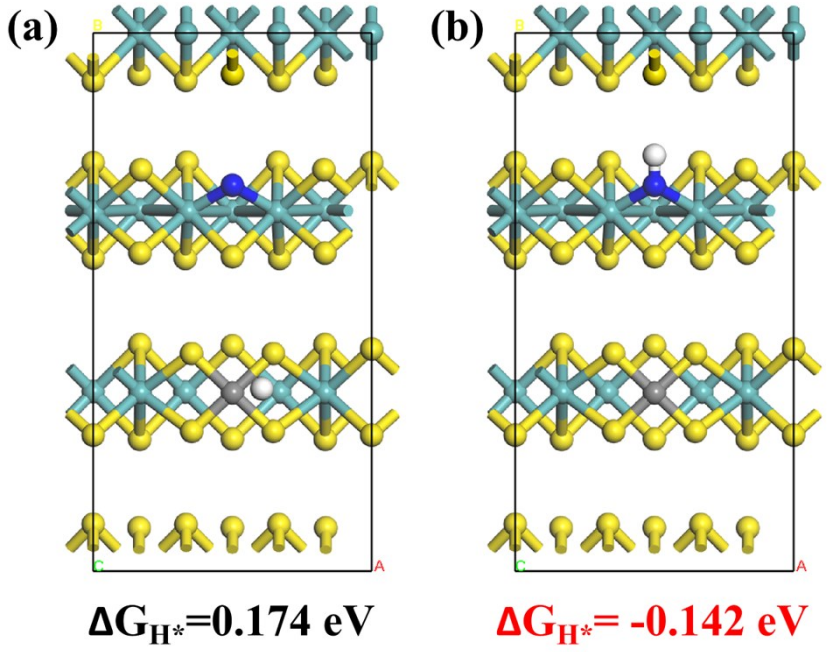

Fig. S17. The influence of different adsorption active sites.

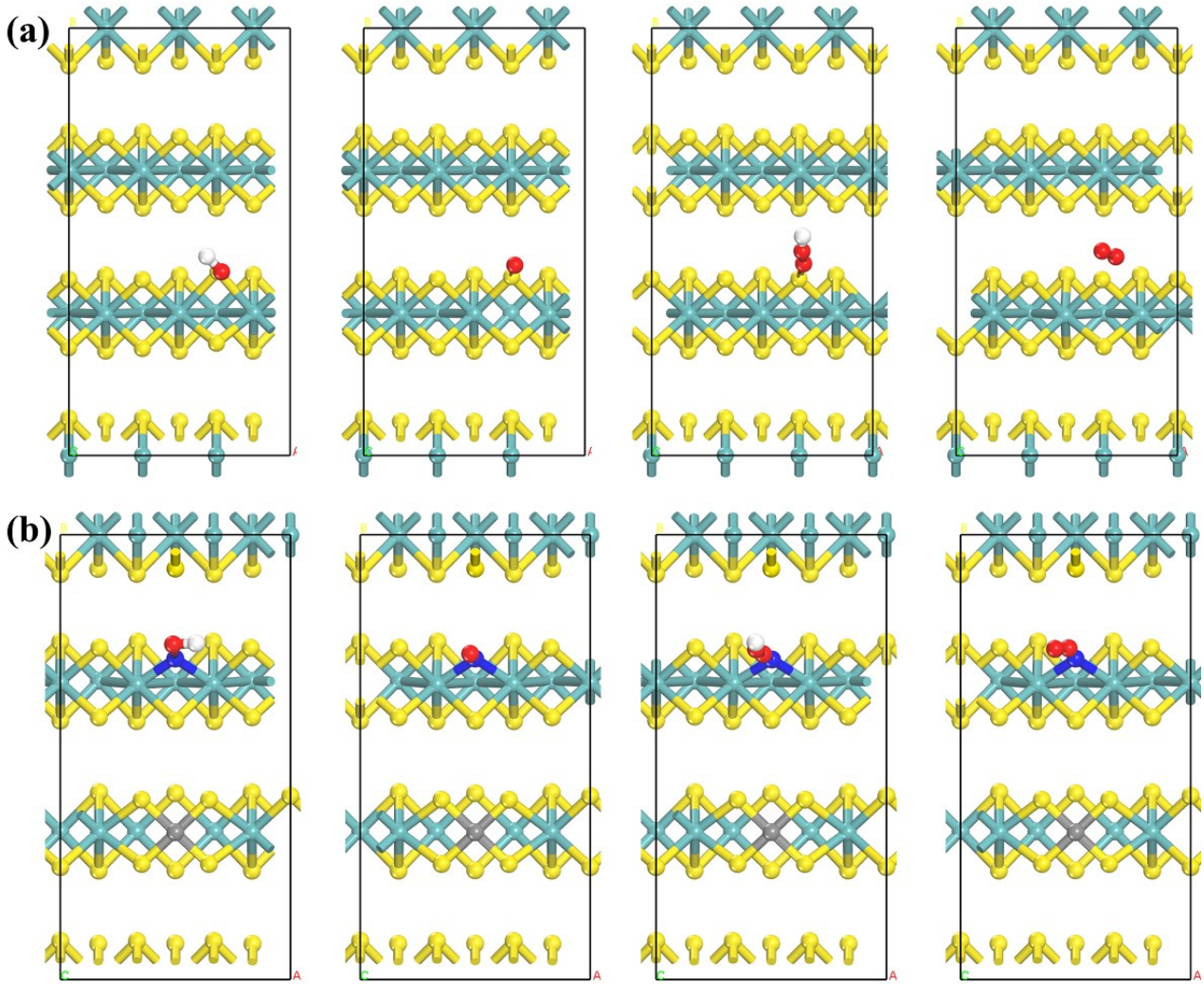

Fig. S18. The intermediates configuration of OER for (a) pure MoS_2 and (b) C-N-MoS_2-700.

Table S1 The atomic ratio of the prepared catalyst analyzed by XPS.

Sample	Atomic concentration (%)				Atomic ratio
	C	N	Mo	S	C/N
C-N-MoS_2/CC-550	53.77	38.67	3.14	4.42	1.4
C-N-MoS_2/CC-600	62.71	30.29	3.02	3.98	2.1
C-N-MoS_2/CC-650	67.32	25.80	2.99	3.89	2.6
C-N-MoS_2/CC-700	74.39	18.98	2.87	3.76	3.9
C-N-MoS_2/CC-800	77.14	16.17	2.90	3.79	4.8

Table S2 The comparison of OER performance with state-of-the-art electrocatalysts.

Materials	Supports	Electrolytes	$\eta_{J=10\ mA\ cm^{-2}}$ (mV)	References
CN-MoS_2/CC-700	CC	1 M KOH	230	This work
MoS_2/NiS	GC	1 M KOH	350	1
CoNC@MoS_2/CNF	GC	1 M KOH	325	2
$Co(OH)_2$@aMoS_{2+x}	-	1 M KOH	380	3
Co_9S_8@MoS_2/CNFs	-	1 M KOH	430	4
MoS_2-Ni_3S_2 HNRs	NF	1 M KOH	249	5

Table S3 TOF of the as-prepared catalysts at overpotential of 200, 250 and 300 mV corresponding to OER.

TOF s^{-1}(mV) / Samples	η=200	250	300
MoS_2/CC	0.00843	0.0120	0.0150
C-N-MoS_2/CC-550	0.0201	0.0294	0.0375
C-N-MoS_2/CC-600	0.0326	0.0494	0.0821
C-N-MoS_2/CC-650	0.0471	0.0657	0.1050
C-N-MoS_2/CC-700	0.0827	0.1260	0.1530
C-N-MoS_2/CC-800	0.0122	0.0150	0.0179

Table S4 The comparison of HER performance with state-of-the-art electrocatalysts.

Materials	Supports	Electrolytes	$\eta_{J=10\ mA\ cm^{-2}}$ (mV)	References
C-N-MoS_2/CC-700	CC	1 M KOH	90	This work
MoS_{2+x} nanoparticles	-	1M KOH	310	1
CoNC@MoS_2/CNF	CC	1M KOH	143	2
MoS_2/NiCoS	GC	1 M KOH	189	6
MoS_2/NiS	GC	1 M KOH	244	7
CoS_x@MoS_2	Ni foil	1 M KOH	146	8
MoS_2@CoO	CC	1 M KOH	325	9
NiS_2/MoS_2	GC	1 M KOH	204	10
OGNs@MoS_2-40	-	1M KOH	125	11

Table S5 TOF of the as-prepared catalysts at overpotential of 200, 250 and 300 mV corresponding to HER.

TOF s^{-1}(mV) / Samples	η=200	250	300
MoS_2/CC	0.00985	0.0190	0.0250
C-N-MoS_2/CC-550	0.0269	0.0334	0.0415
C-N-MoS_2/CC-600	0.0386	0.0586	0.0861
C-N-MoS_2/CC-650	0.0651	0.0889	0.1190
C-N-MoS_2/CC-700	0.1130	0.1470	0.1860
C-N-MoS_2/CC-800	0.0181	0.0223	0.0272

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