Supporting Information

Boosting hydrogen production from alkaline water splitting via electrochemical reconstructing active surface of transition metal sulfide electrocatalysts

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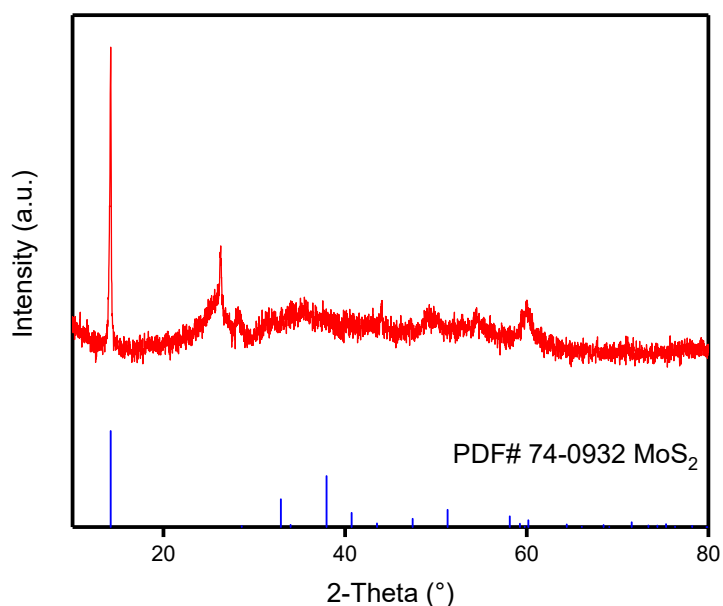
E-mail address: zhiguo@mail.sic.ac.cn (Zhiguo Yi)

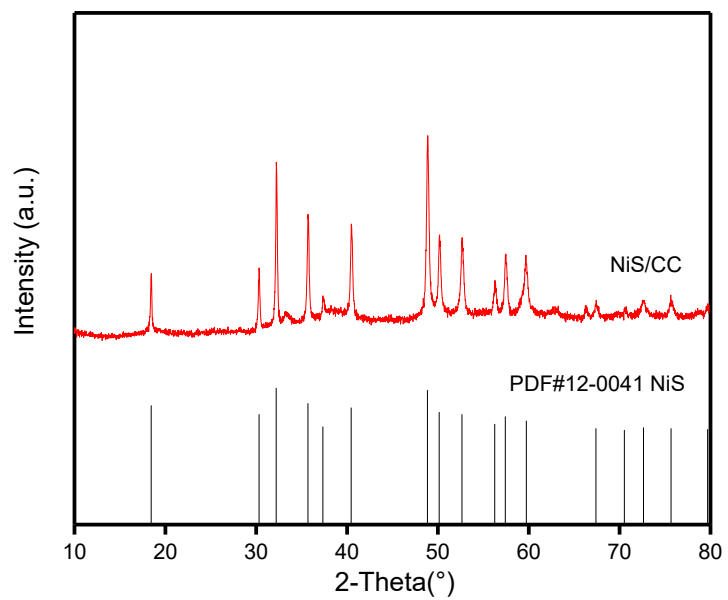Fig. S1 XRD pattern of the NMS (increased MoS_2 mass by 2 times)
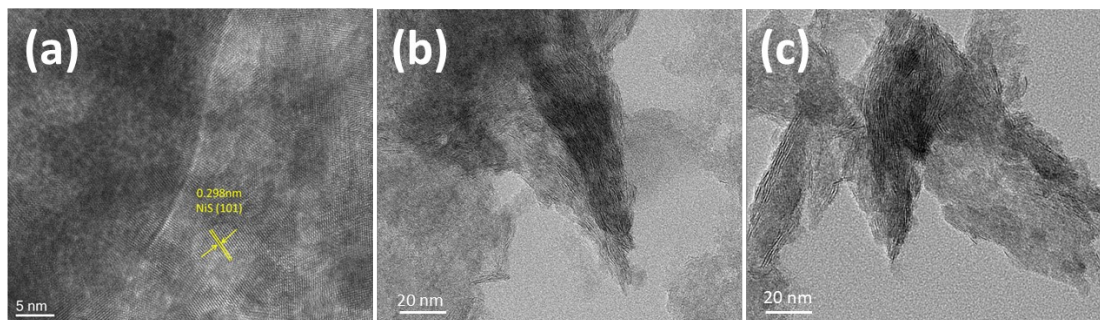
Fig. S2 XRD pattern of the NiS/CC

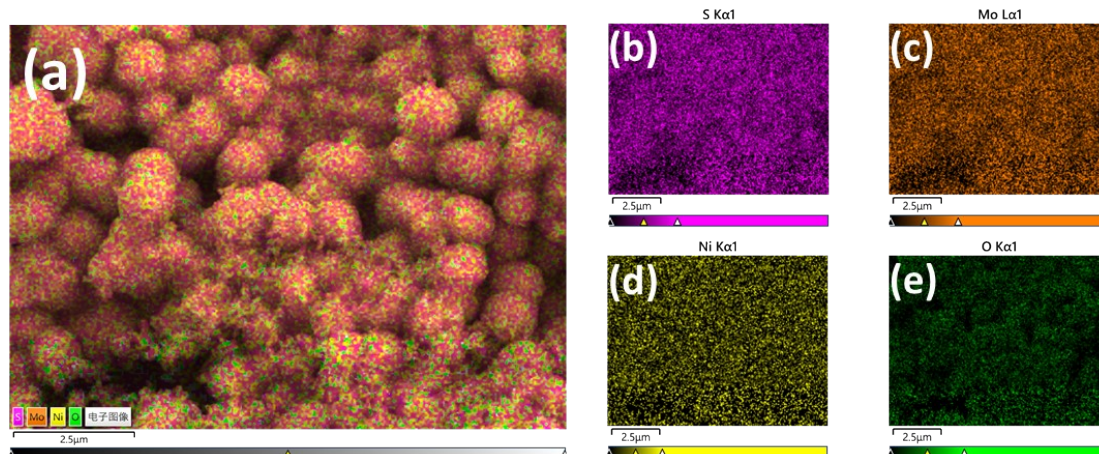Fig. S3 TEM images of NMS (a) and 40s-NMSO (b-c)

Fig. S4 SEM image of NMS (a) and its corresponding elemental mapping images for S (b), Mo (c), Ni (d) and O (e), respectively.
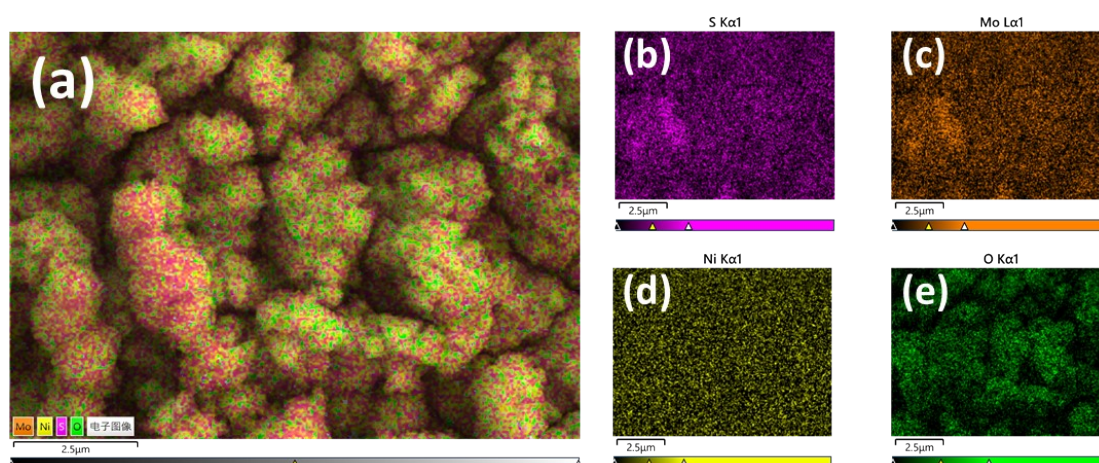

Fig. S5 SEM image of 40s-NMSO (a) and its corresponding elemental mapping images for S (b), Mo (c), Ni (d) and O (e), respectively.
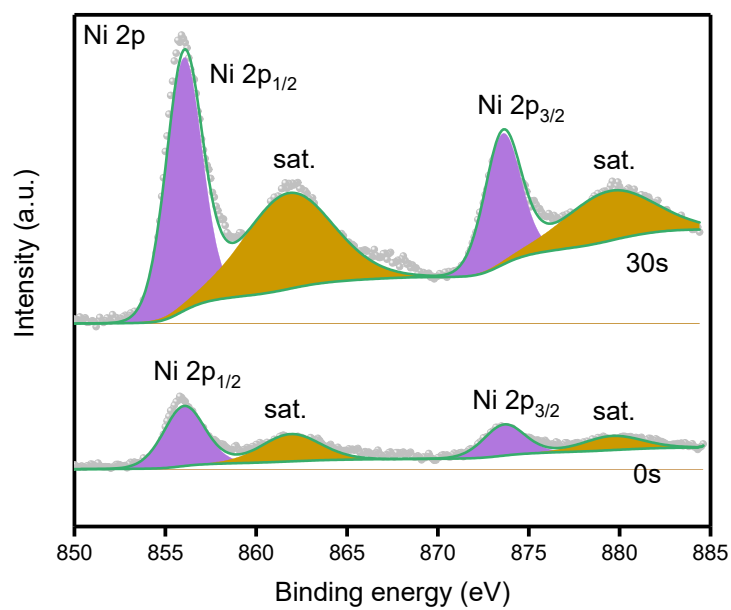
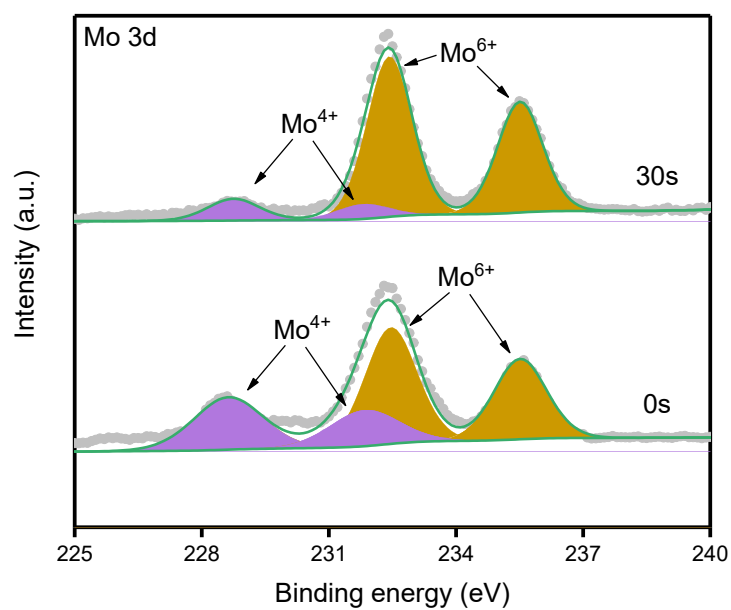Fig. S6 XPS spectra of Ni2p for the 30s-NMSO (upper) and NMS (bottom) samples

Fig. S7 XPS spectra of Mo3d for the 30s-NMSO (upper) and NMS (bottom) samples
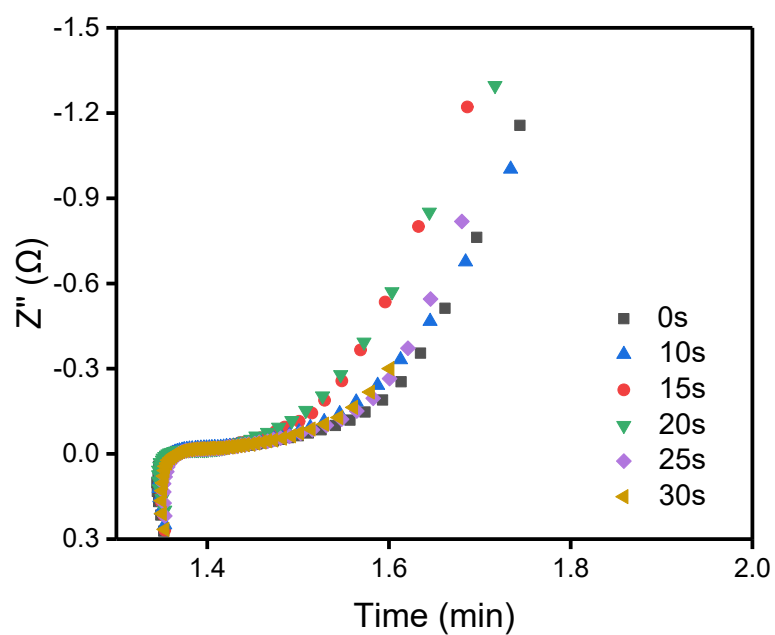
Fig. S8 Electrochemical impedance spectroscopy (EIS) of NMSO series catalysts in the frequency range from 100 kHz to 10 mHz
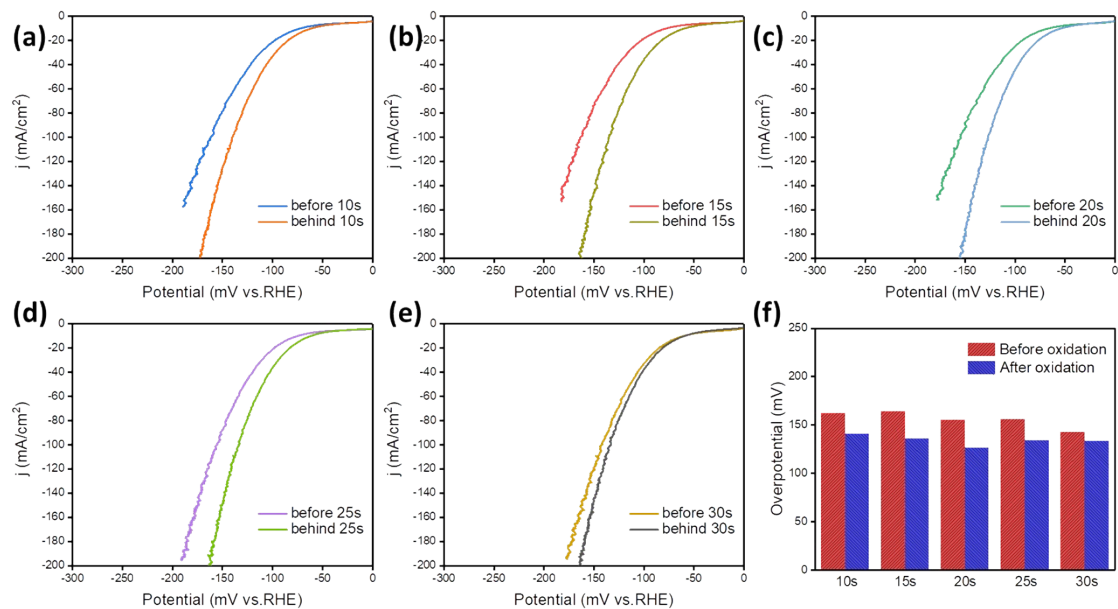

Fig. S9 (a-e) The LSV test diagram of each component catalyst before and after anodic oxidation. (f) The overpotential(η_{100}) comparison diagram of each component catalyst before and after anodic oxidation treatment
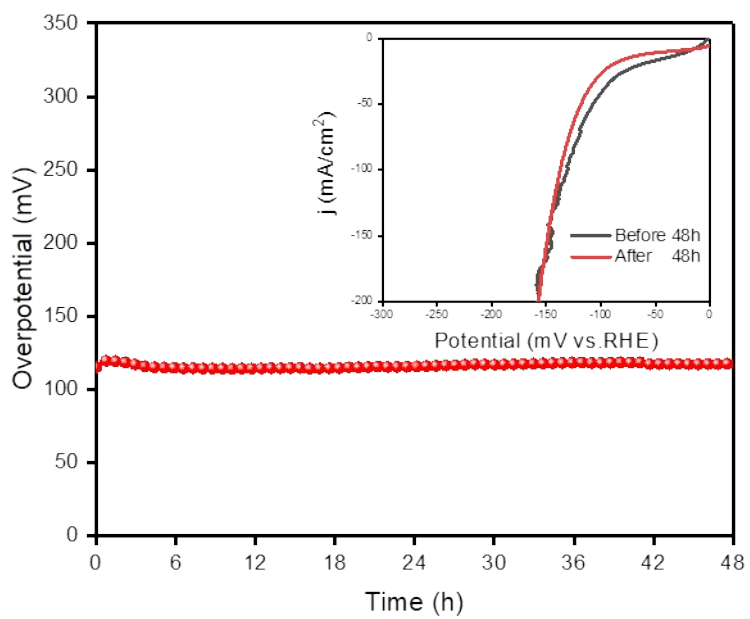
Fig. S10 Potential test figure of 20s-NMSO at constant current density of 100mA/cm^2. Inset shows ???
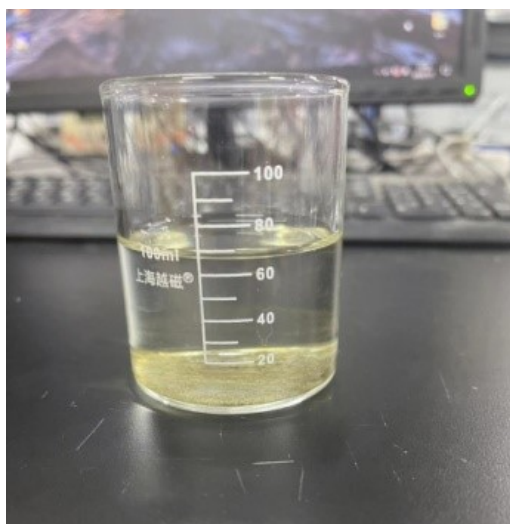

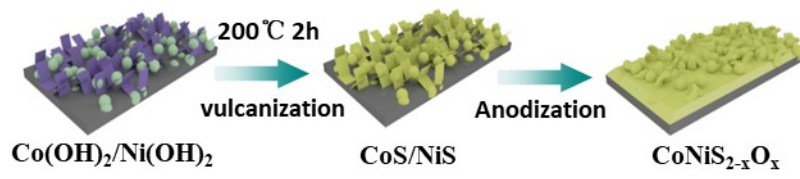Fig. S11 KOH solution after the anodic oxidation treatment
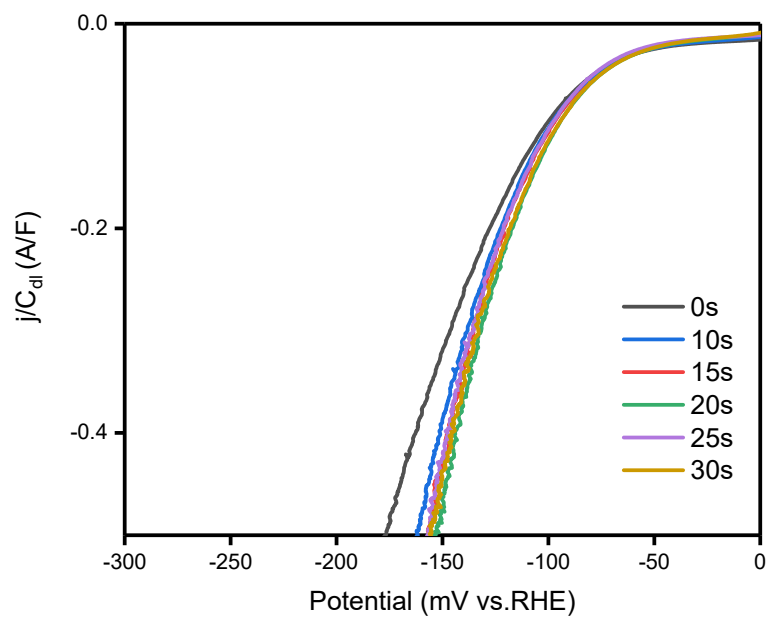
Fig. S12 Preparation procedure of NCSO

Fig. S13 LSV curves of NMSO series materials normalized by double layer capacitance
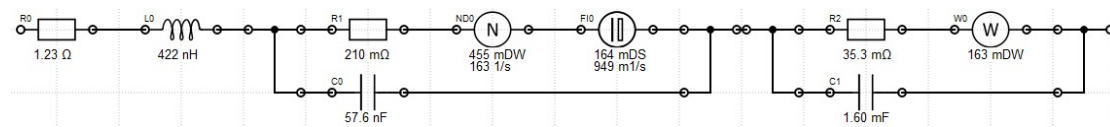
Fig. S14 Schematic diagram of circuit simulation for each component material.
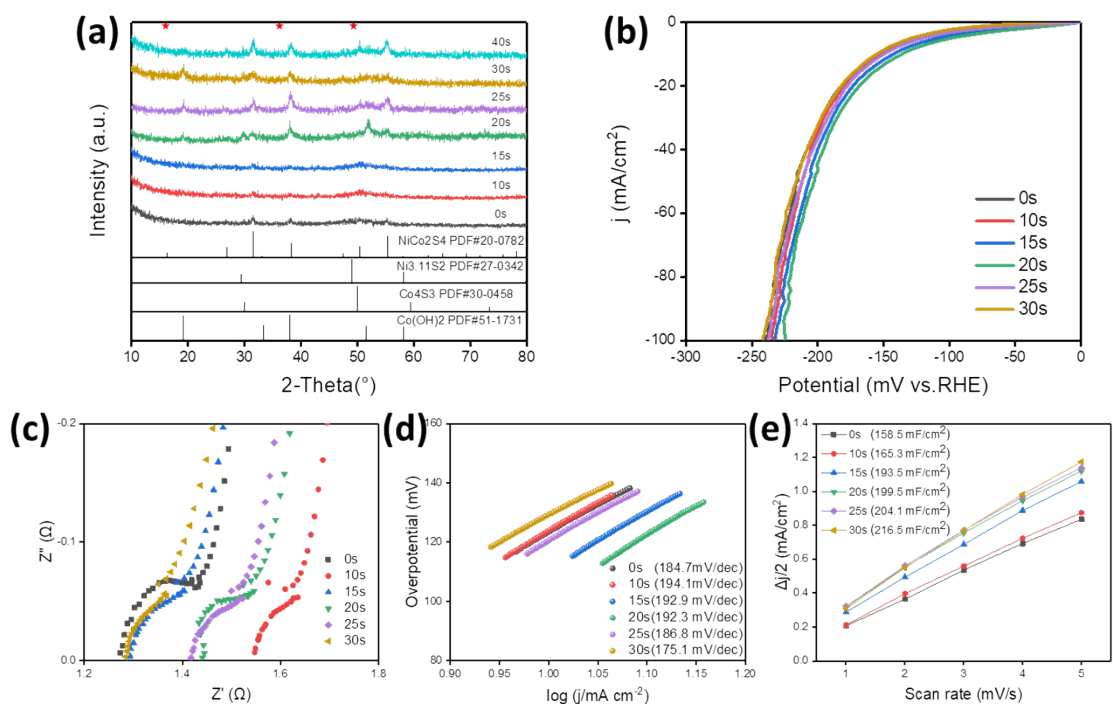
Fig. S15 (a) XRD patterns of NCSO after anodic treatment for different time.(b) HER polarization LSV curves of NCSO series at a scanning rate of 2 mV/s. (c) Electrochemical impedance spectroscopy (EIS) of NCSO series catalysts in the frequency range from 100 kHz to 10 mHz. (d) Tafel plots of NCSO series catalysts. (e) CV curves of NCSO series catalysts at the same abscissa at the scanning rates of 1,2,3,4 and 5 mV/s, the maximum difference in ordinates.

Fig. S16 The PDOS diagram of NiS with different contents of O doping: (a) O 100%; (b) O 66%; (c) O 33%; (d) O 0%.

Fig. S17 SEM images of : (a) NCS; (b) 20s-NCSO; (c)   30s-NCSO.

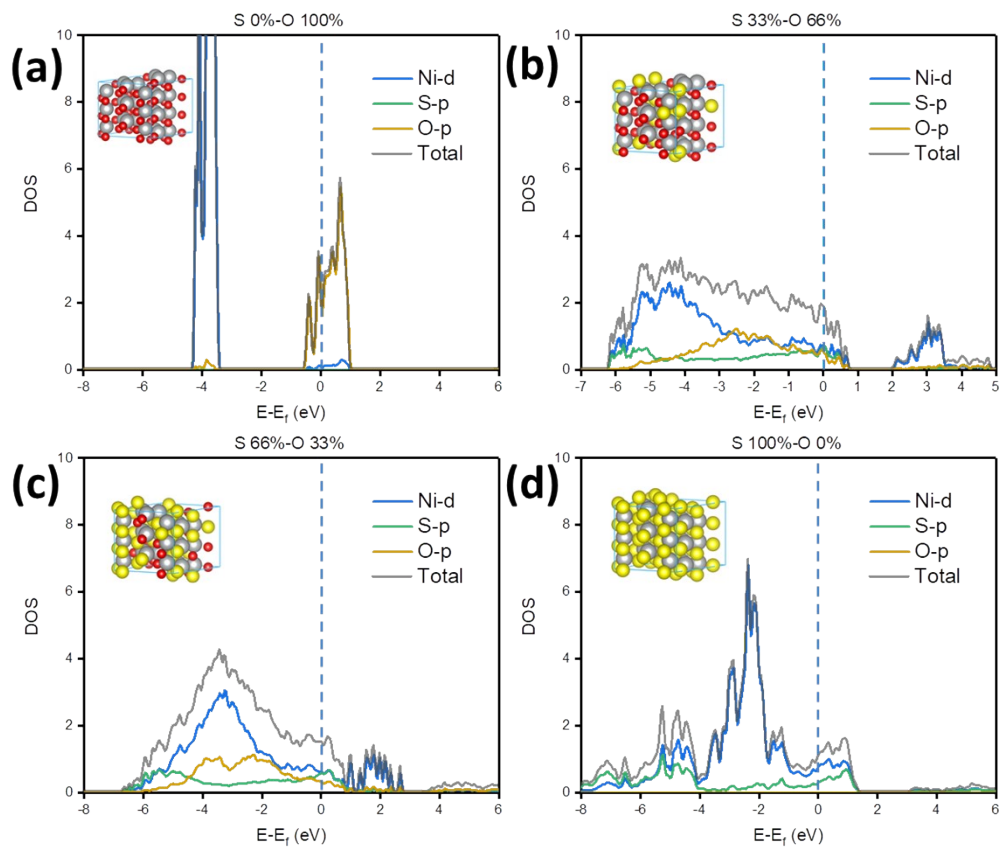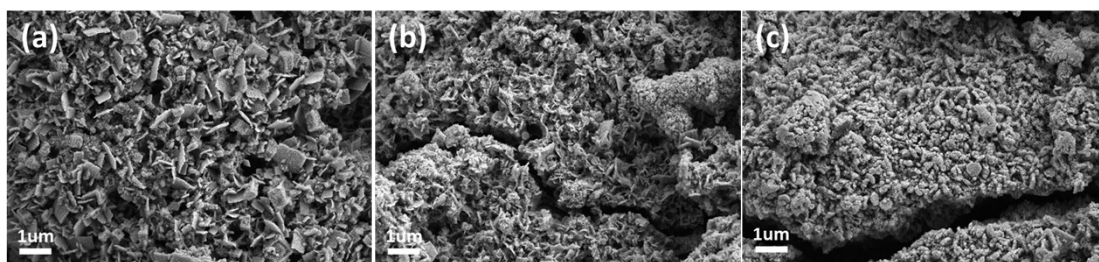Fig. S18 Three-dimensional in situ infrared absorption spectra of the initial time after anodic potential access

Fig. S19 Three-dimensional in situ infrared absorption spectra of the initial time after anodic potential access

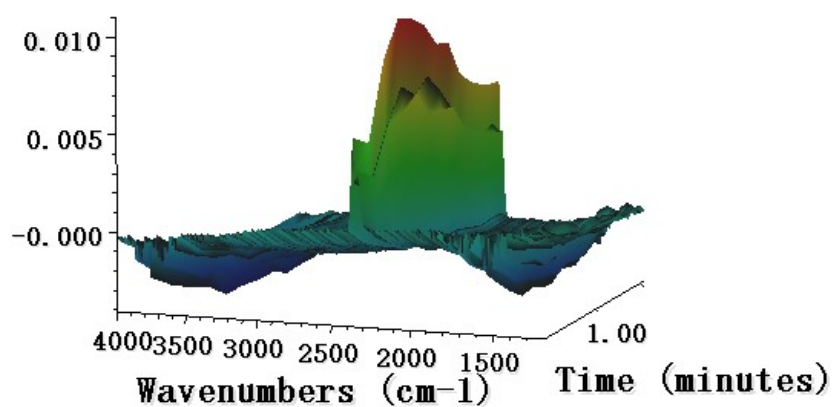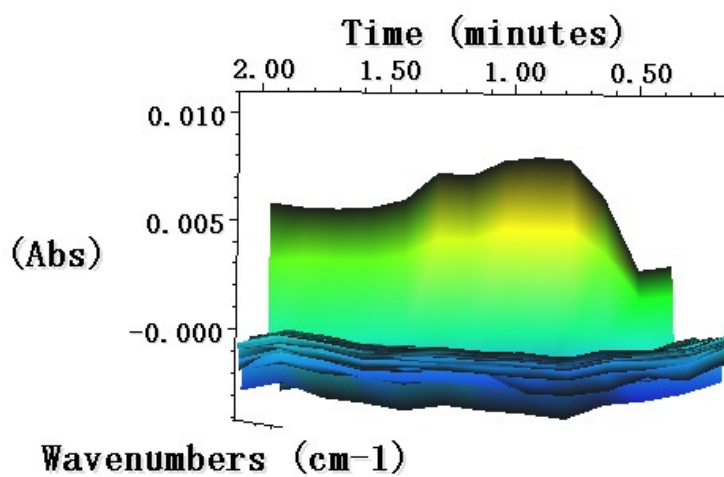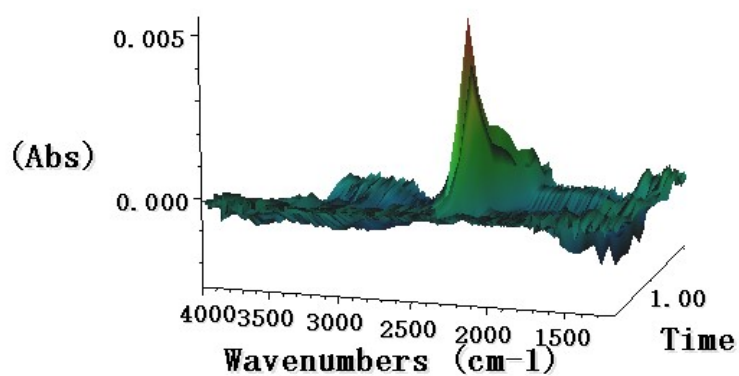Fig. S20 Three-dimensional in situ infrared absorption spectra at the second time after anodic potential access
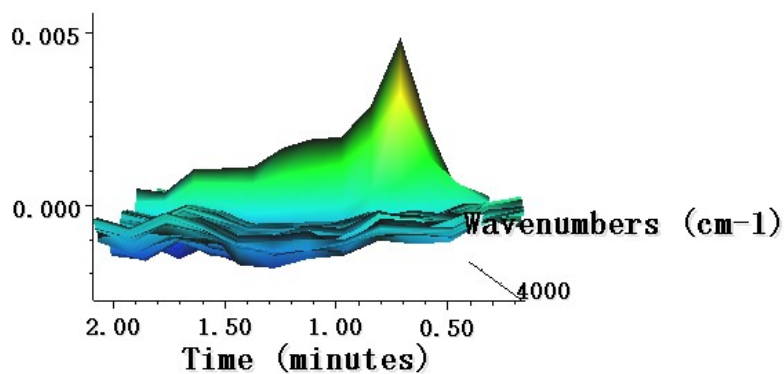

Fig. S21 Three-dimensional in situ infrared absorption spectra at the second time after anodic potential access

Tab. S1 The BET specific surface area of each component

Sample ID.	NMS	15s-NMSO	30s-NMSO
BET surface area (m^2/g)	11.430	30.201	52.059

Tab. S2 EDS quantitative test results of NMS

Element	Wt%	Wt% Sigma	Atomic percentage
O	24.08	0.31	50.58
S	18.50	0.29	19.38
Ni	44.73	0.47	25.60
Mo	12.69	0.67	4.44

Tab. S3 EDS quantitative test results of 15s-NMS

Element	Wt%	Wt% Sigma	Atomic percentage
O	23.70	0.29	49.68
S	18.22	0.27	19.06
Ni	49.44	0.47	28.24
Mo	8.64	0.65	3.02

Tab. S4 EDS quantitative test results of 30s-NMS

Element	Wt%	Wt% Sigma	Atomic percentage
O	28.13	0.31	55.36
S	15.28	0.25	15.00
Ni	53.16	0.48	28.51
Mo	3.43	0.64	1.13

Tab. S5 The quantitative results of each element of NMS calculated by XPS

Element	S	S2-	S6+	Mo4+	Mo6+	Ni2+
At%	9.52	18.89	34.81	7.79	13.16	15.83

Tab. S6 The quantitative results of each element of 30s-NMSO calculated by XPS

Element	S	S2-	S6+	Mo4+	Mo6+	Ni2+	O2-
At%	3.49	5.93	6.42	1.77	11.46	50.16	20.76

Tab. S7 R_{ct} obtained after fitting the EIS results of each component

Element	0s	10s	15s	20s	25s	30s
$R_{ct}(m\Omega)$	217	202	197	178	190	210