Constructing S-deficient nickel sulfide/N-doped carbon interface for improved water splitting activity
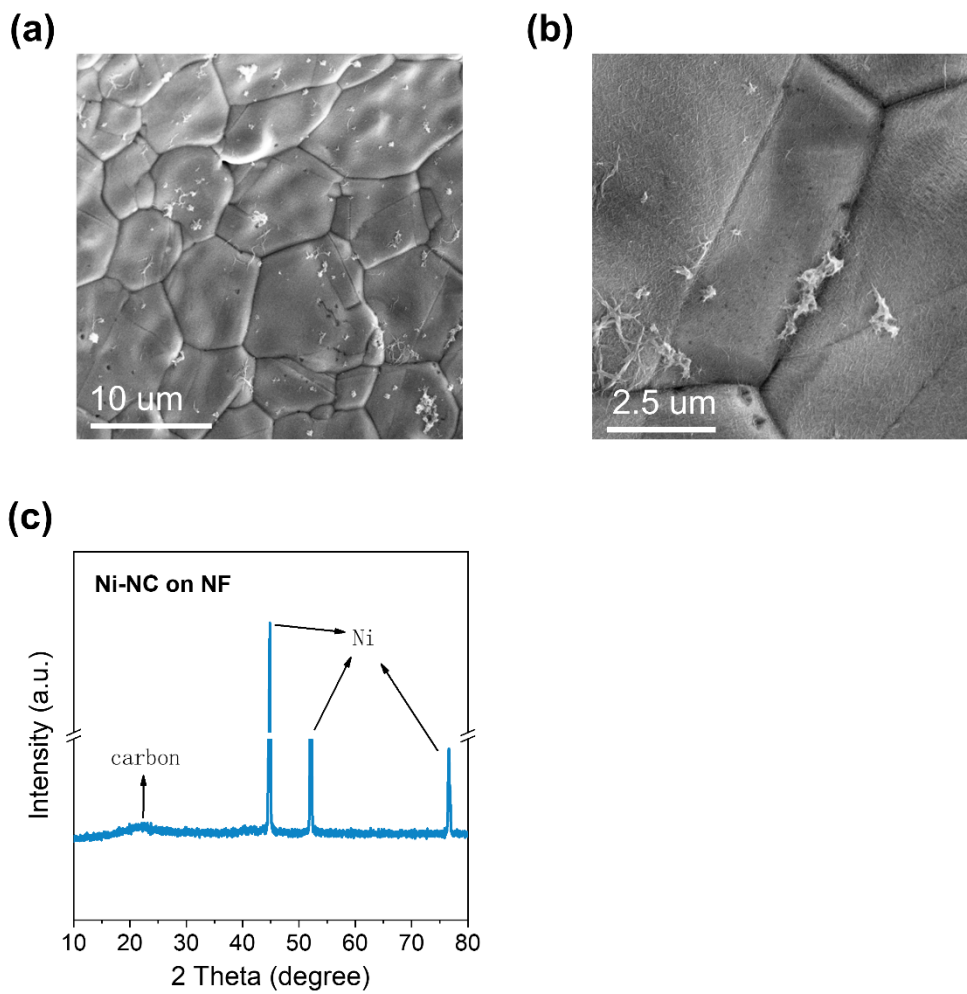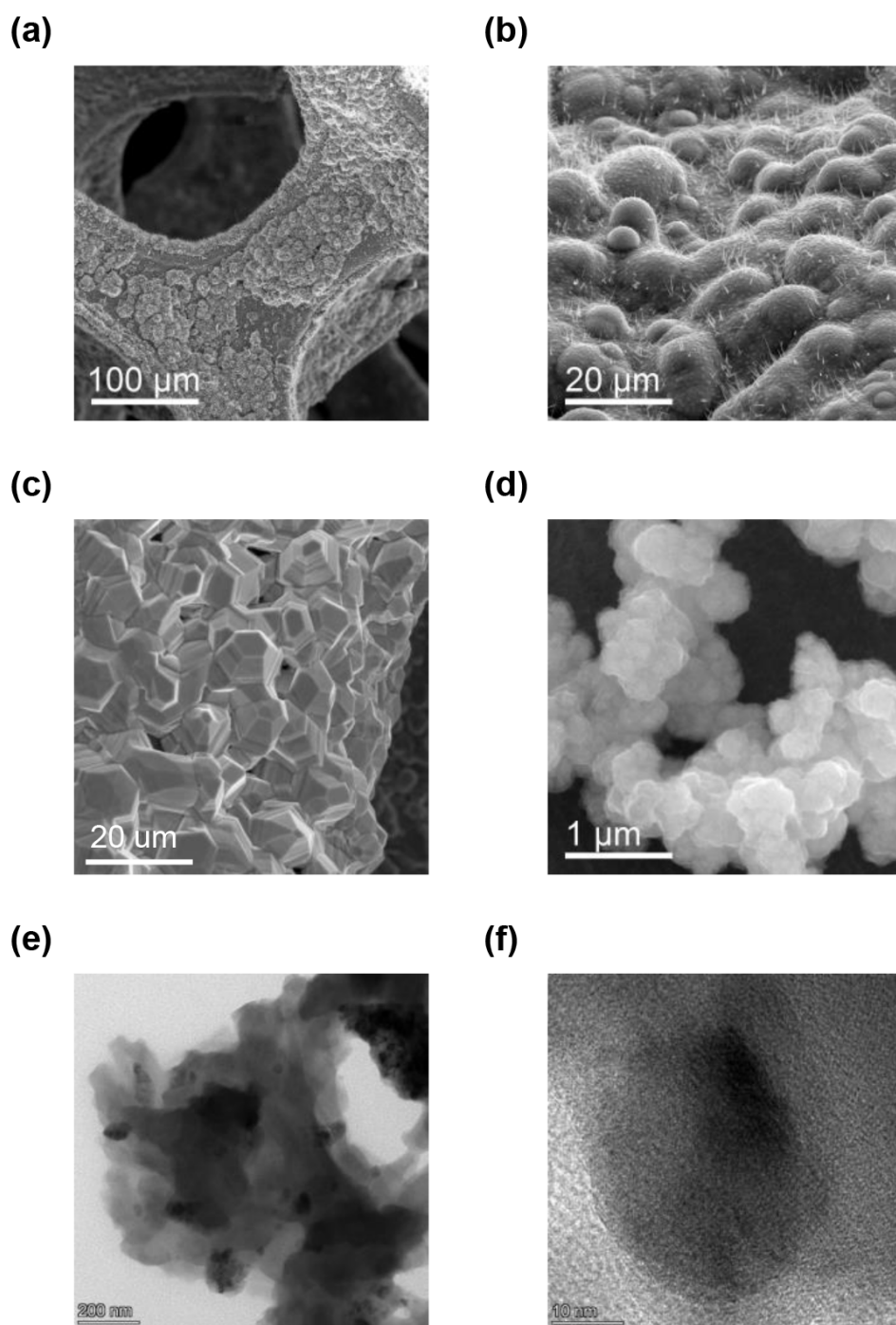
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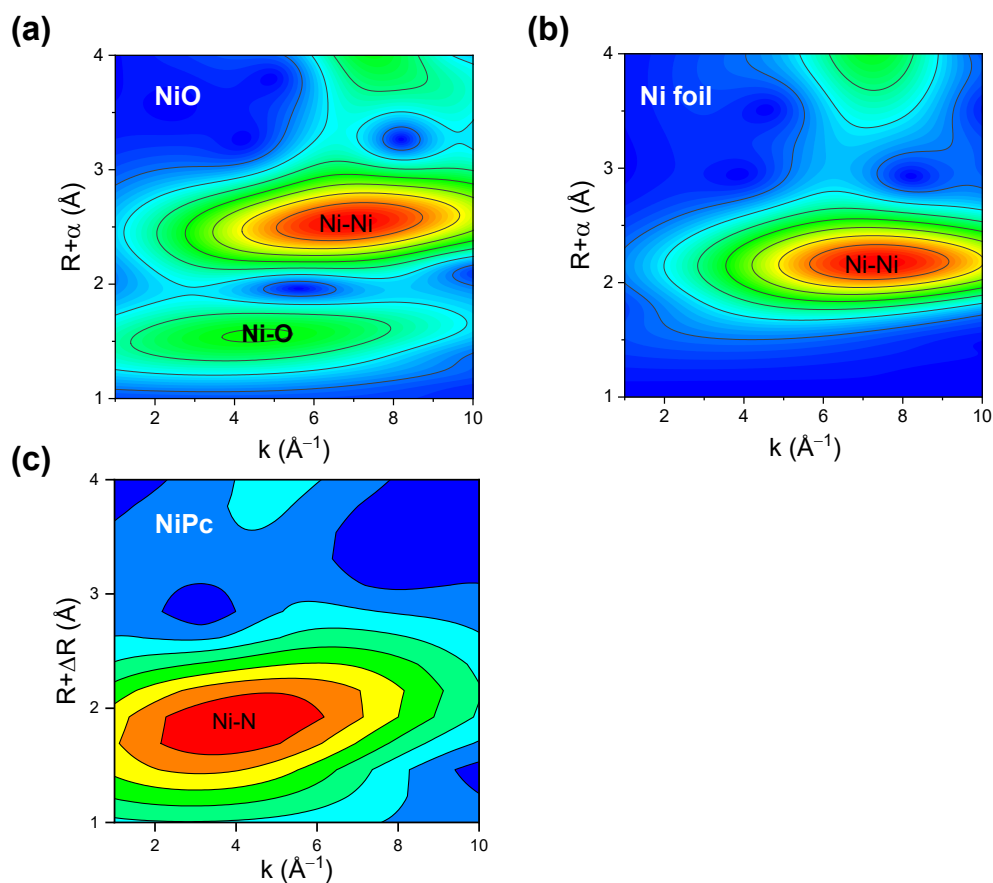
Figure S1. (a & b) SEM image and (c) XRD curve of precursive formamide-derived Ni-NC on nickel foam (NF)
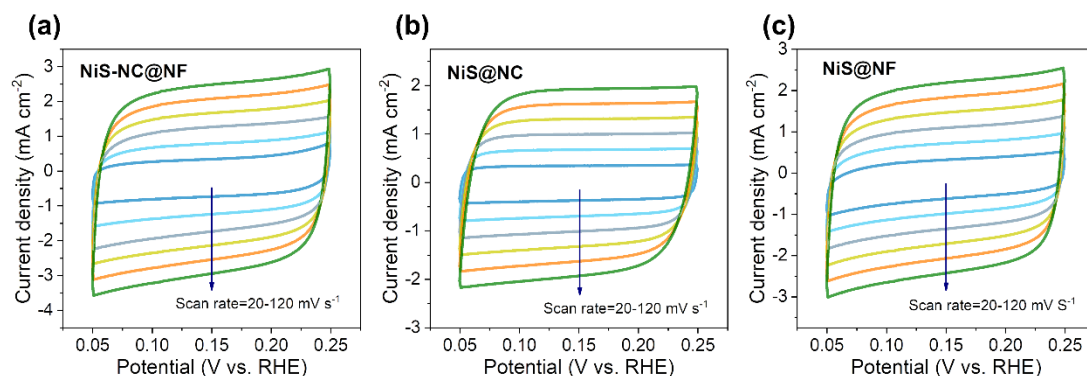
Figure S2. (a) SEM image and (b) enlarged SEM view of NiS-NC on nickel foam (NF). SEM image of (c) NiS@NF and (d) NiS@NC. (e & f) TEM images of NiS@NC
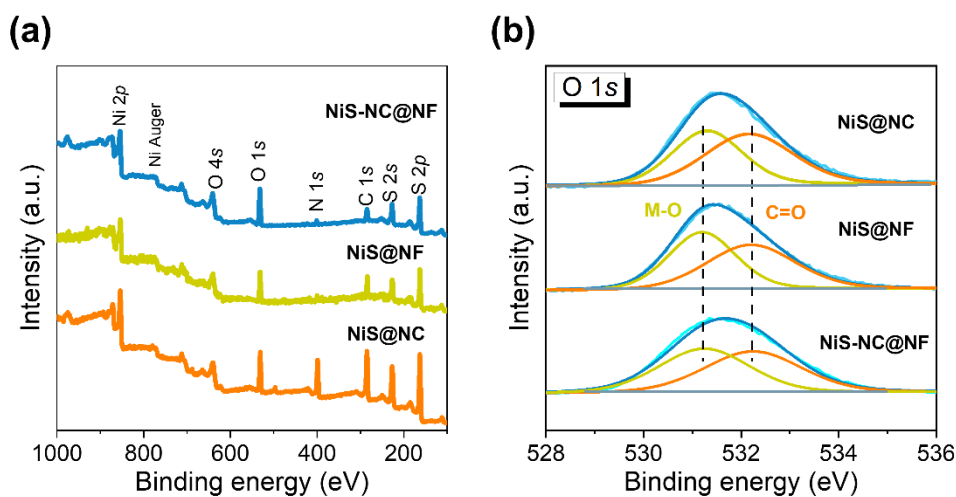
Figure S3. (a) XPS survey and (b) O 1*s* spectra of NiS-NC@NF and NiS@NC

Figure S4. Wavelet transformed (WT) EXAFS of NiO, Ni foil, and NiPc references

Figure S5. CV curves of (a) NiS-NC@NF, (b) NiS@NC and (c) NiS@NF measured at different scan rates.
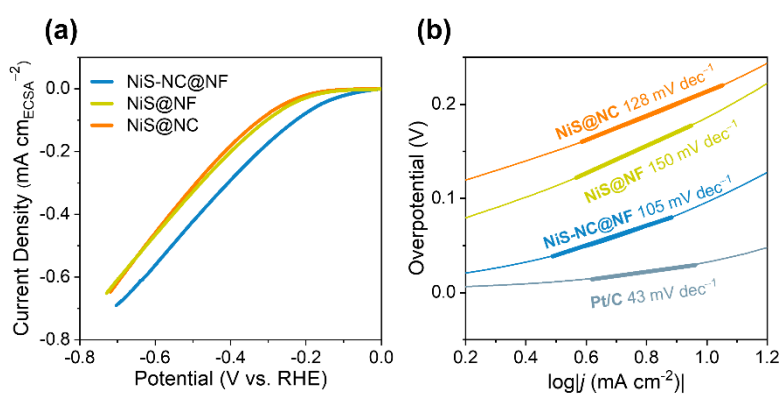
Figure S6. (a) HER polarization curves after normalized by ECSA and (b) Tafel plots of NiS-NC@NF and NiS@NC.
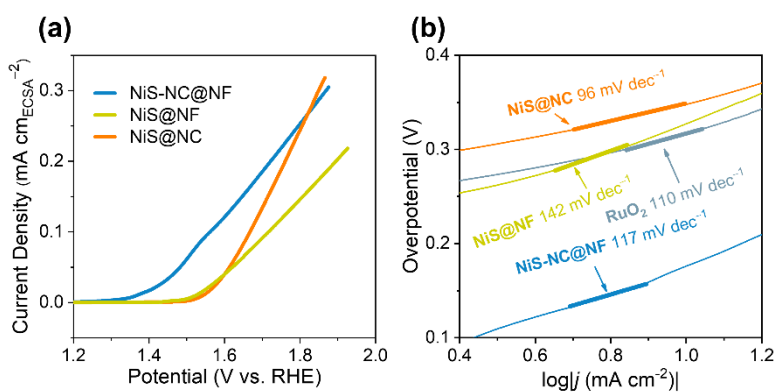
Figure S7. (a) OER polarization curves after normalized by ECSA and (b) Tafel plots of NiS-NC@NF and NiS@NC.
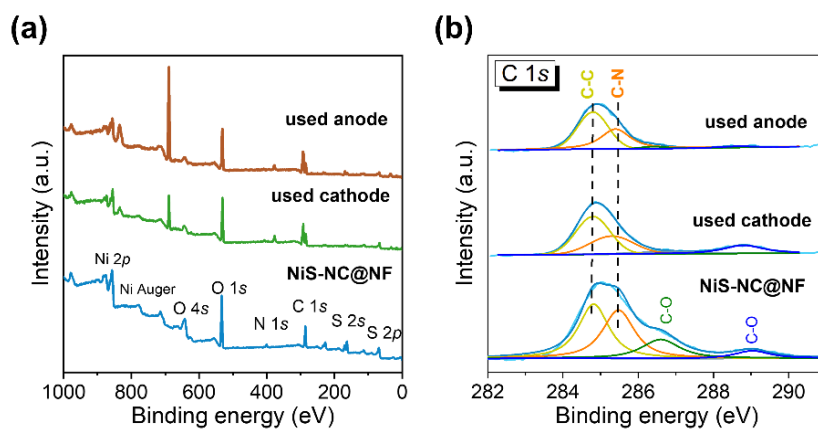
Figure S8. (a) XPS survey and (b) C 1*s* spectra of used NiS-NC@NF after long-term operation as anode and cathode for overall water splitting.

Table S1. XPS element contents of NiS@NC, NiS@NF and NiS-NC@NF

Sample	Ni	S	C	N	O
NiS@NF	11.70	30.70	39.25	-	18.35
NiS@NC	6.22	26.35	38.23	17.80	11.41
NiS-NC@NF	11.93	15.06	35.39	2.42	35.2
Used NiS-NC@NF cathode	12.6	4.98	29.13	4.83	48.46
Used NiS-NC@NF anode	13.68	8.29	25.97	2.52	49.54

Table S2. EXAFS fitting parameters at the Ni K-edge of samples (S_0^2=0.70, 0.77)

Sample	Shell	N^a	R (Å)^b	$\sigma^2 \times 10^3$ (Å^2)^c	ΔE_0 (eV)^d	R factor
Ni foil	Ni-Ni	12*	2.48±0.01	6.2±0.2	6.9±0.4	0.001
NiO	Ni-O	6.0±0.7	2.08±0.01	5.2±0.9	−1.4±1.6	0.004
	Ni-Ni	12.6±0.7	2.95±0.01	6.0±0.3	−3.0±0.6	
NiS	Ni-S	3.9±0.4	2.26±0.01	6.9±0.9	2.0±0.1	0.001
	Ni-Ni	1.8±0.4	2.52±0.01	5.5±1.3	1.1±2.9	
NiPc	Ni-N	3.6±0.3	1.89±0.01	2.7±0.7	1.33±1.1	0.0133
NiS-NC@NF	Ni-S	1.9±1.2	2.18±0.04	8.1±7.3	7.3±4.2	0.008
	Ni-Ni	2.1±1.6	2.46±0.03	5.9±4.1	6.9±0.9	

$^a N$: coordination numbers; $^b R$: bond distance; $^c \sigma^2$: Debye-Waller factors; $^d \Delta E_0$: the inner potential correction. R factor: goodness of fitting.

Table S3. HER EIS calculation parameters of of NiS@NC, NiS@NF and NiS-NC@NF obtained by fitting the Nyquist plots of Figure S8.

Sample	Rs (Ω)	Rct (Ω)	CPE-T (mF)	CPE-P (mF)
NiS@NF	2.09	6.61	0.11	0.74
NiS@NC	2.14	8.71	0.13	0.85
NiS-NC@NF	2.17	3.82	0.05	0.61

Table S4. OER EIS calculation parameters of of NiS@NC, NiS@NF and NiS-NC@NF obtained by fitting the Nyquist plots of Figure S8.

Sample	Rs (Ω)	Rct (Ω)	CPE-T (mF)	CPE-P (mF)
NiS@NF	1.29	11.01	0.08	0.68
NiS@NC	1.53	12.09	0.09	0.81
NiS-NC@NF	1.27	4.21	0.06	0.54