Supporting Information

Defect engineering of Ni_3S_2 nanosheets with highly active (110) facets towards efficient electrochemical biomass valorization

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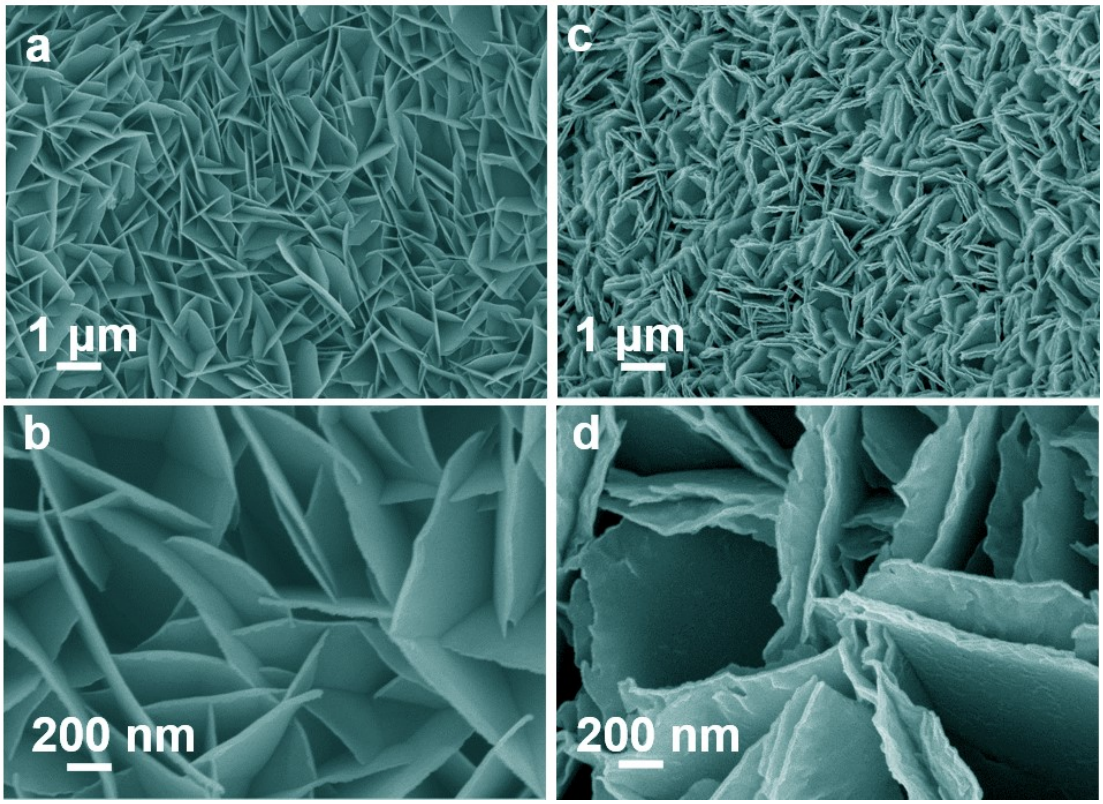

Figure S1. SEM images of (a,b) Ni_3S_2-3h and (c,d) Ni_3S_2-8h.

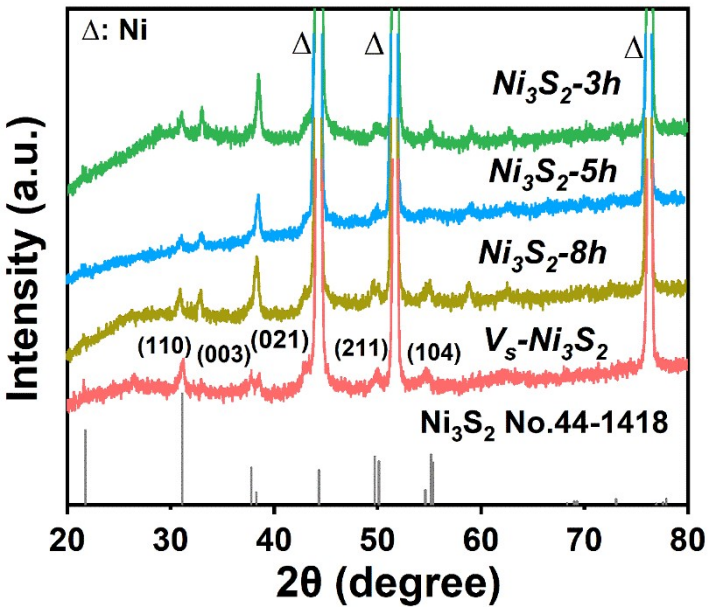

Figure S2. XRD patterns of different samples.

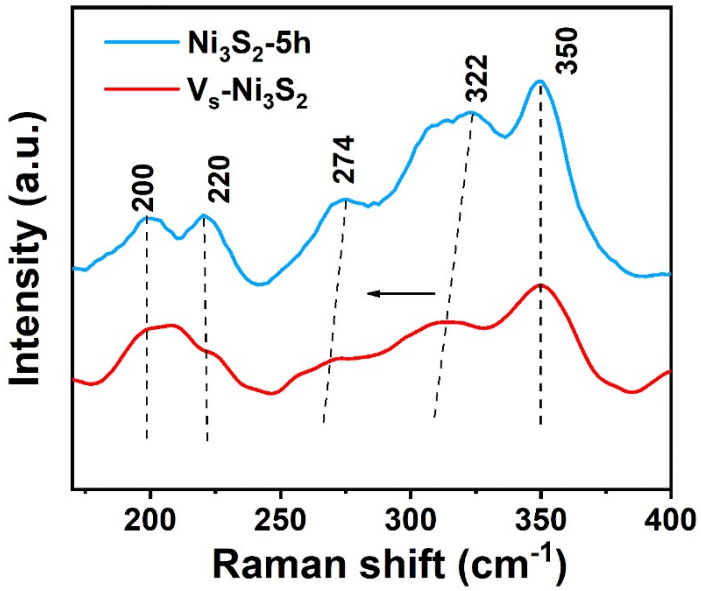

Figure S3. Raman spectra of Ni_3S_2-5h and V_s-Ni_3S_2.

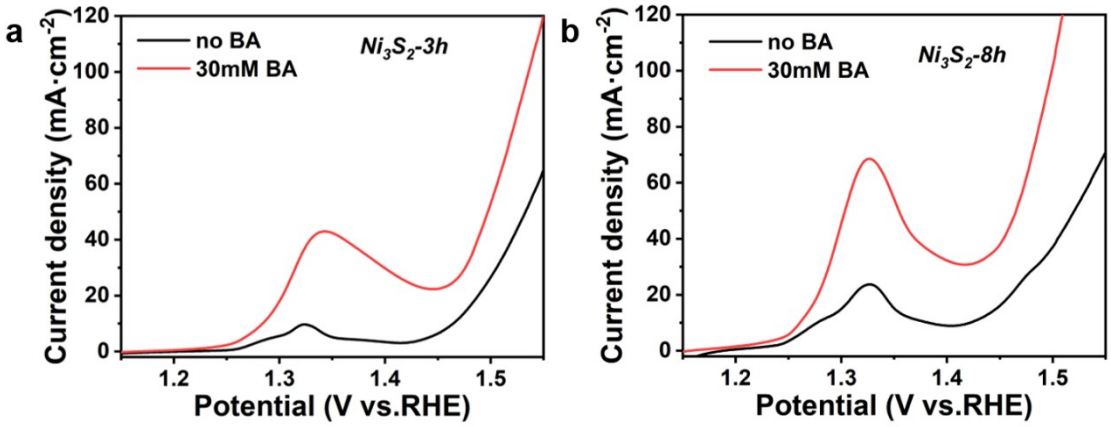

Figure S4. LSV curves with and without 30 mM BA using (a) Ni_3S_2-3h and (b) Ni_3S_2-8h catalysts.

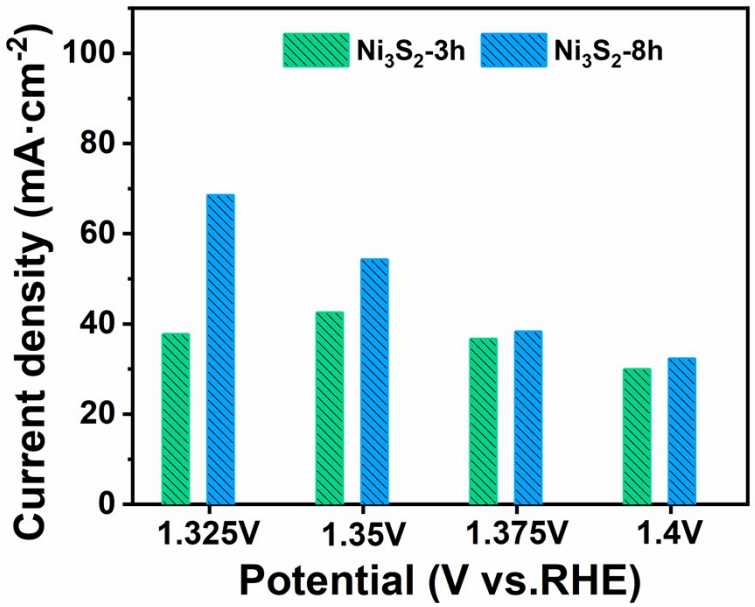

Figure S5. Comparison of current density at varied potentials over Ni_3S_2-3h and Ni_3S_2-8h in 30 mM BA.

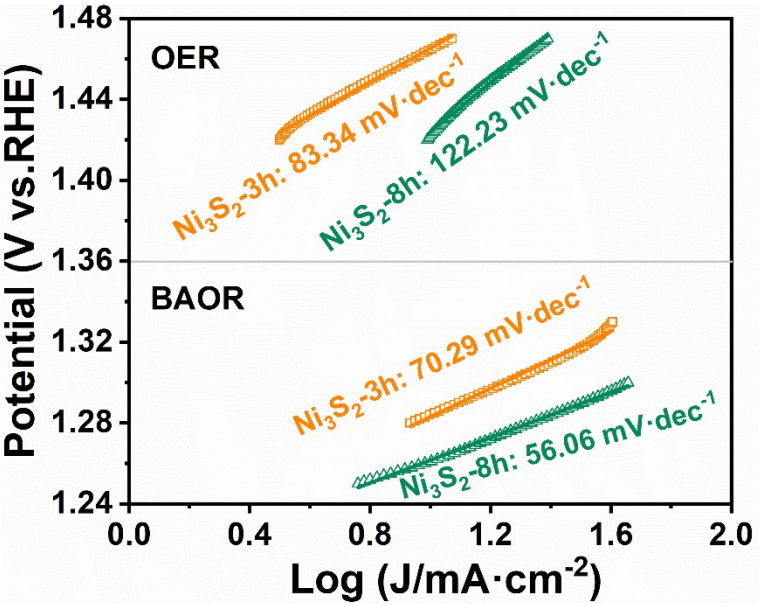

Figure S6. Comparison of current density at varied potentials over Ni_3S_2-3h and Ni_3S_2-8h in 30 mM BA.

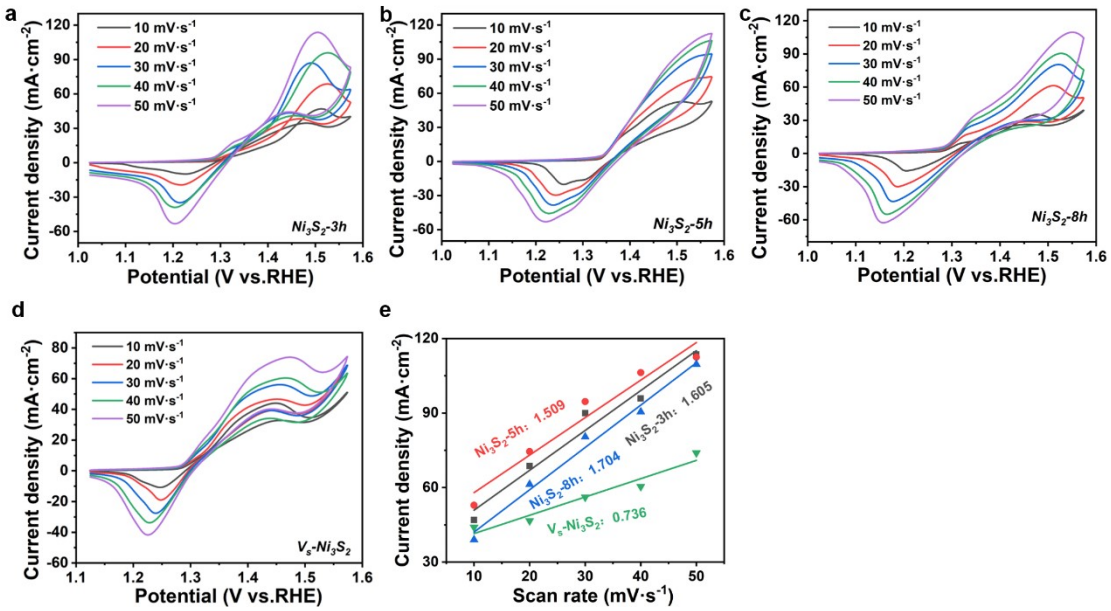

Figure S7. CV curves of (a) Ni_3S_2-3h, (b) Ni_3S_2-5h, (c) Ni_3S_2-8h and (d) V_s-Ni_3S_2. (e) The relationship between oxidation peak current in CV curves and scan rates.

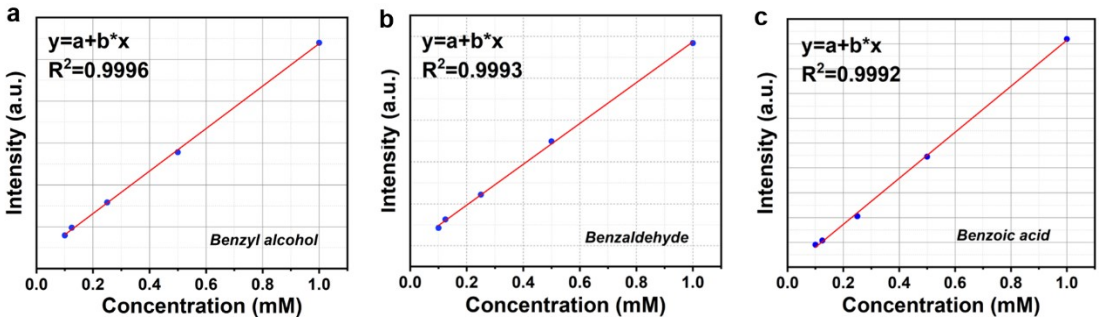

Figure S8. The standard curves of (a) benzyl alcohol, (b) benzaldehyde and (c) benzoic acid.

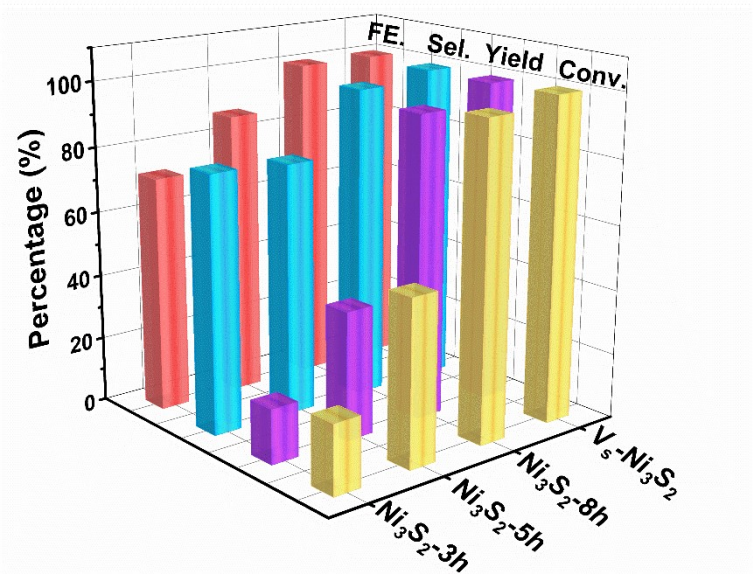

Figure S9. BAOR conversion, yield, selectivity and FE over different electrocatalysts at 1.35 V vs RHE.

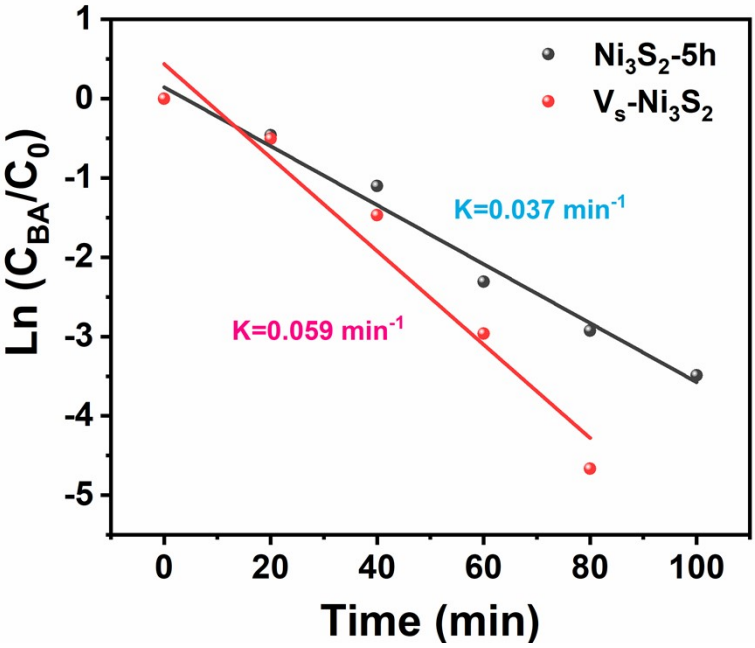

Figure S10 First-order kinetic models of the BA oxidation catalyzed by Ni_3S_2-5h and V_s-Ni_3S_2 catalysts.

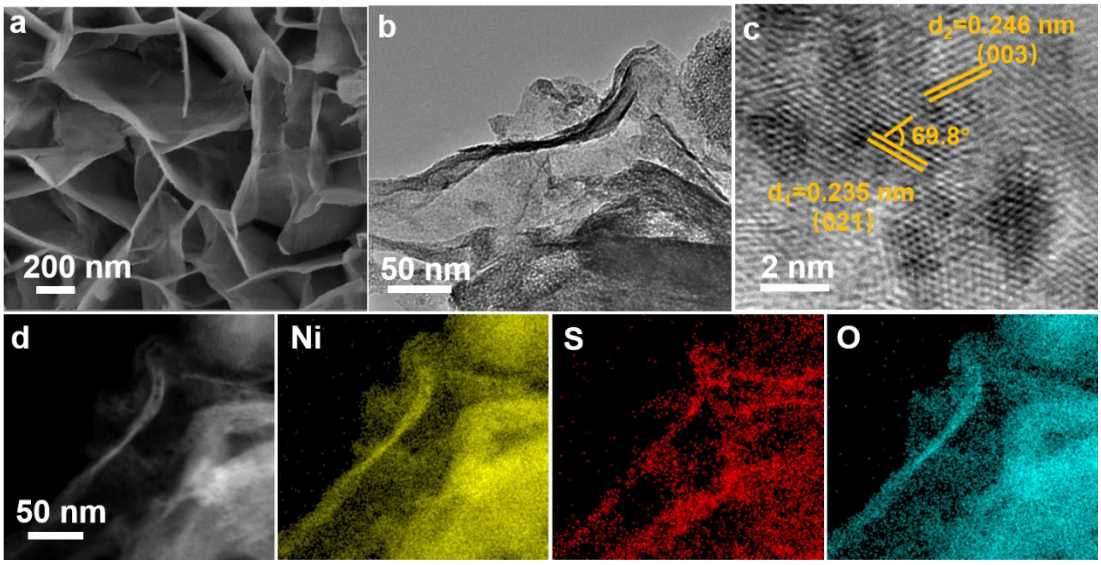

Figure S11. (a) SEM, (b) TEM, (c) HRTEM images and (d) mapping result of V_s-Ni_3S_2 catalyst after BA oxidation.

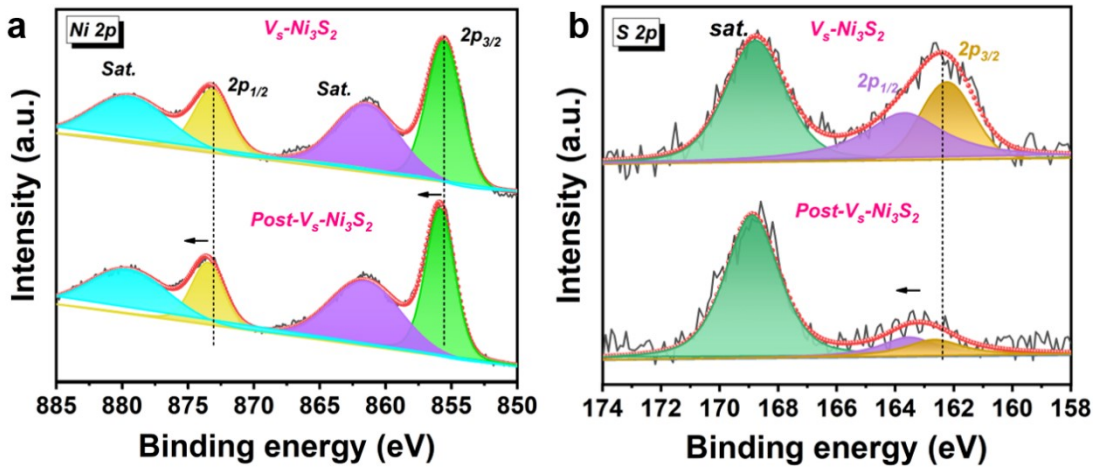

Figure S12. XPS spectra of (a) Ni 2p and (b) S 2p of V_s-Ni_3S_2 catalyst before and after BA electrolysis.

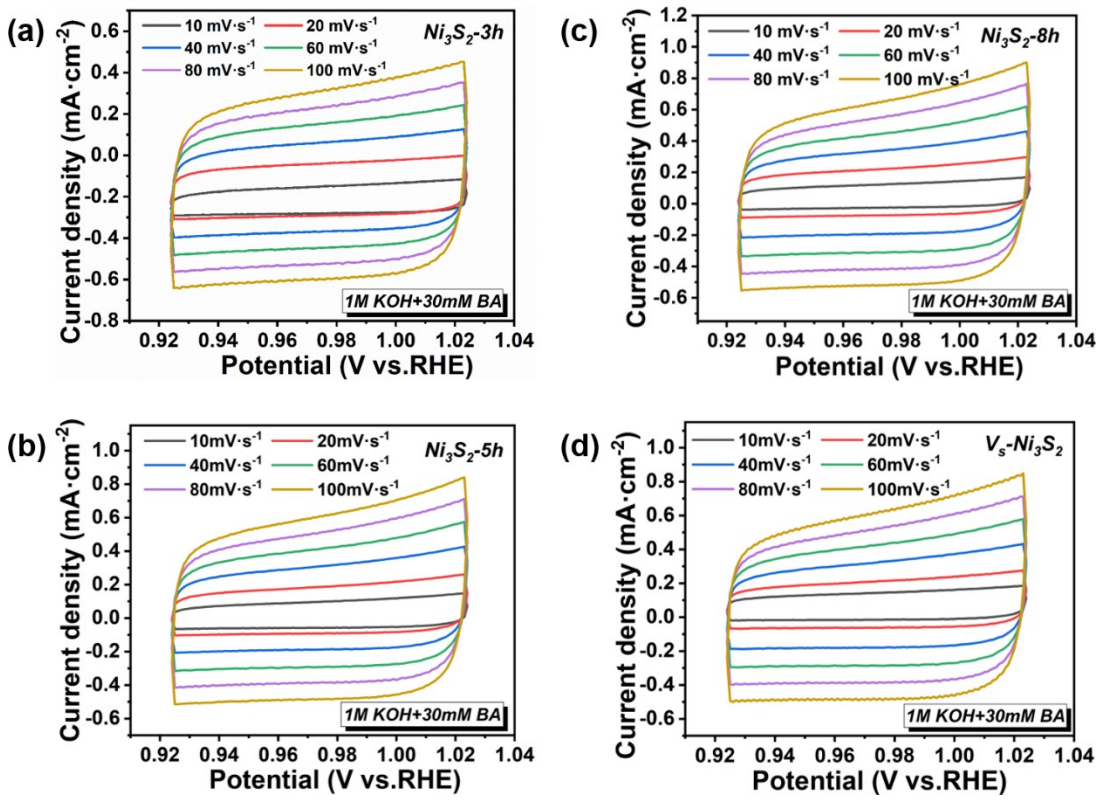

Figure S13. CV curves in non-Faradic region at varied scan rates for (a) Ni_3S_2-3h, (b) Ni_3S_2-5h, (c) Ni_3S_2-8h and (d) V_s-Ni_3S_2 catalysts in 1M KOH+30 mM BA.

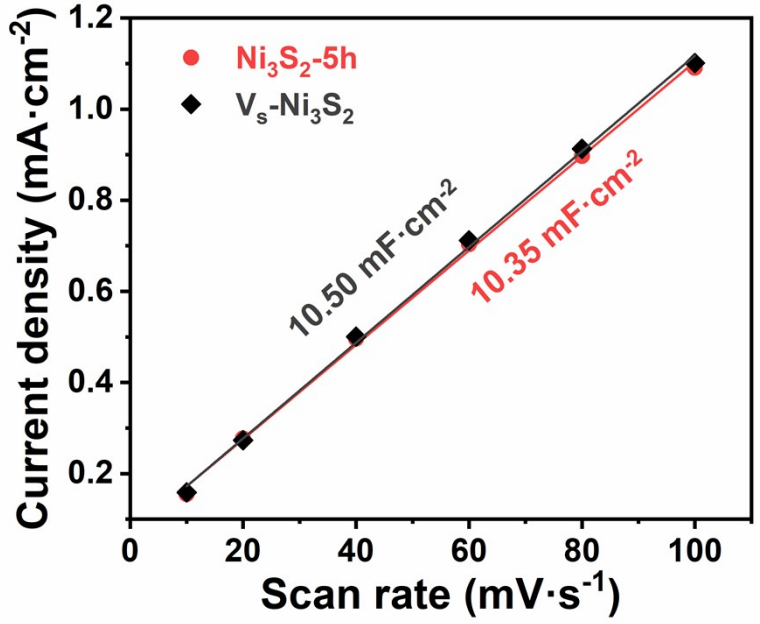

Figure S14. ECSA values of Ni_3S_2-5h and V_s-Ni_3S_2 catalysts.

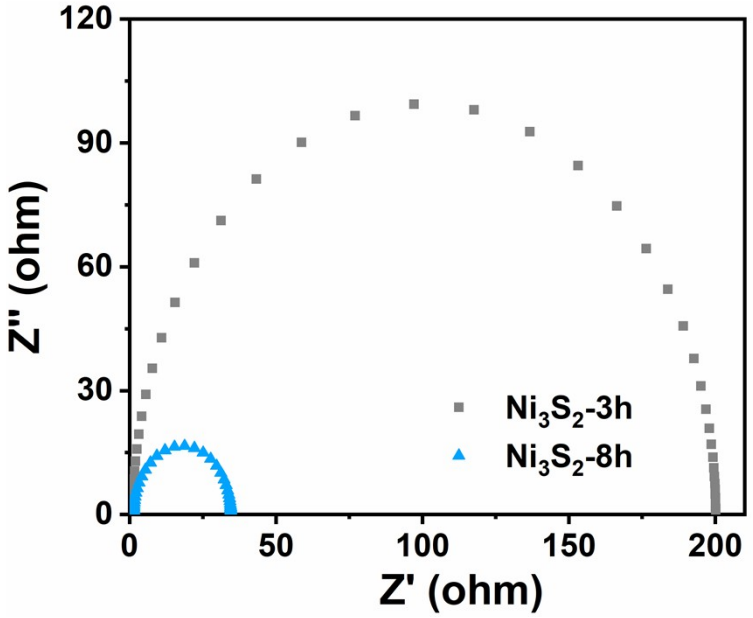

Figure S15. EIS of Ni_3S_2-3h and Ni_3S_2-8h catalysts.

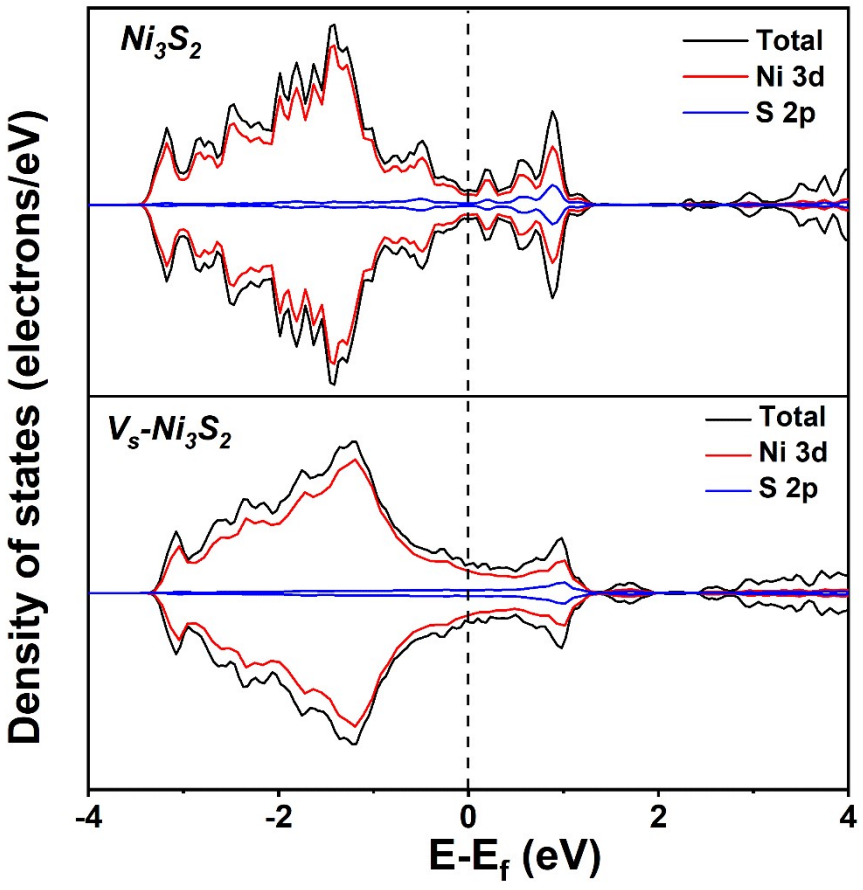

Figure S16. Projected density of states (PDOS) of Ni_3S_2 and V_s-Ni_3S_2.

Table S1. The electrocatalytic performances of the four catalysts in OER.

	η@50mA cm^{-2} (mV)	Tafel slope ($mV\ del^{-1}$)
Ni_3S_2-3h	303	83.34
Ni_3S_2-5h	259	105.03
Ni_3S_2-8h	291	122.23
V_s-Ni_3S_2	286	98.91

Table S2. The electrocatalytic performances of the four catalysts in BAOR.

	Peak current density ($mA\ cm^{-2}$)	Tafel slope ($mV\ del^{-1}$)	ECSA ($mF\ cm^{-2}$)	TOF@1.325 V (h^{-1})	R_s (Ω)	R_{ct} (Ω)
Ni_3S_2-3h	42.96	70.29	8.53	57.0	1.229	198.9
Ni_3S_2-5h	75.16	57.52	10.35	101.2	0.965	158.6
Ni_3S_2-8h	68.51	56.06	11.12	97.7	1.369	33.22
V_s-Ni_3S_2	93.92	48.15	10.50	295.4	0.894	1.396

Table S3. The electrocatalytic performances of the four catalysts in this study.

Catalyst	Potential (V vs. RHE)	Time (min)	Conv. (%)	Sel. (%)	Yield (%)	F.E. (%)
Ni_3S_2-3h	1.35V	100	21.21	79.07	16.77	72.23
Ni_3S_2-5h	1.35V	100	96.98	96.51	93.6	99.99
Ni_3S_2-8h	1.35V	100	50.79	77.67	39.45	87.35
V_s-Ni_3S_2	1.35V	100	100	99.34	99.34	99.99

Reaction condition: organic substrate concentration of 30 mM with 20 mL volume, 1M KOH, electrolytic potential of 1.35 V. The products were evaluated by HPLC analysis.

Table S4. The catalytic performance of BA electro-oxidation in literatures.

Catalyst	BA Concentration	Potential (V vs.RHE) or Current	Time (min)	Conv. (%)	Sel. (%)	F.E. (%)	Refs.
1.0 h-$Ni(OH)_2$	40 mM	20 mA	/	99.99	99.30	98.62	[1]
hp-Ni	10 mM	1.423 V	/	~99.99	/	98	[2]
Co_3O_4 NWs	50 mM	/	/	99	92	56.82	[3]
Mo–Ni	25 mM	1.35 V	/	/	/	/	[4]
A-Ni-Co-H/NF	100 mM	1.5 V	15	99	99	/	[5]
NiCu NTs	20 mM	1.424 V	120	100	98	90	[6]
$Co_{0.83}Ni_{0.17}$/AC	10 mM	1.425 V	-	100	99.4	96	[7]
V_s-Ni_3S_2	**30 mM**	**1.325 V**	**100**	**100**	**97.8**	**99.99**	**This work**

References

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