

Supporting information

Interfacial Engineering of an Advanced NiV-LDH@MoS₂ Heterostructure Electrocatalyst for Efficient Alkaline Hydrogen Evolution

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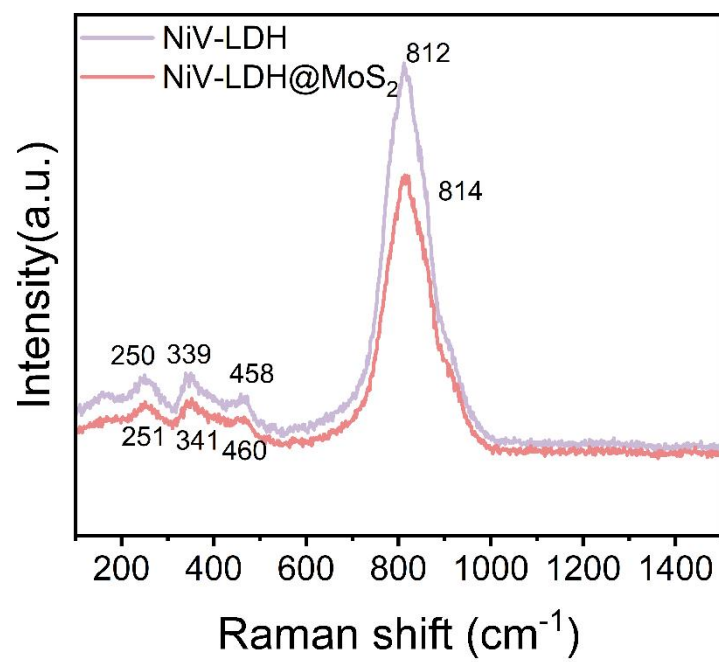


Figure S1. Raman spectra of NiV-LDH and NiV-LDH@MoS₂ under 532 nm excitation.

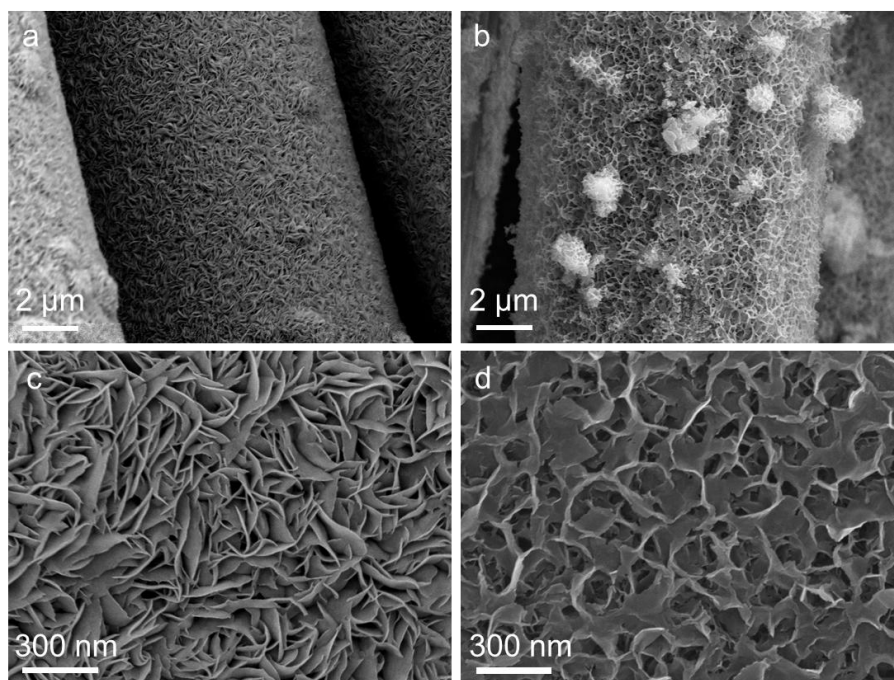


Figure S2. SEM images of (a, c) MoS₂ and (b, d) NiV-LDH.

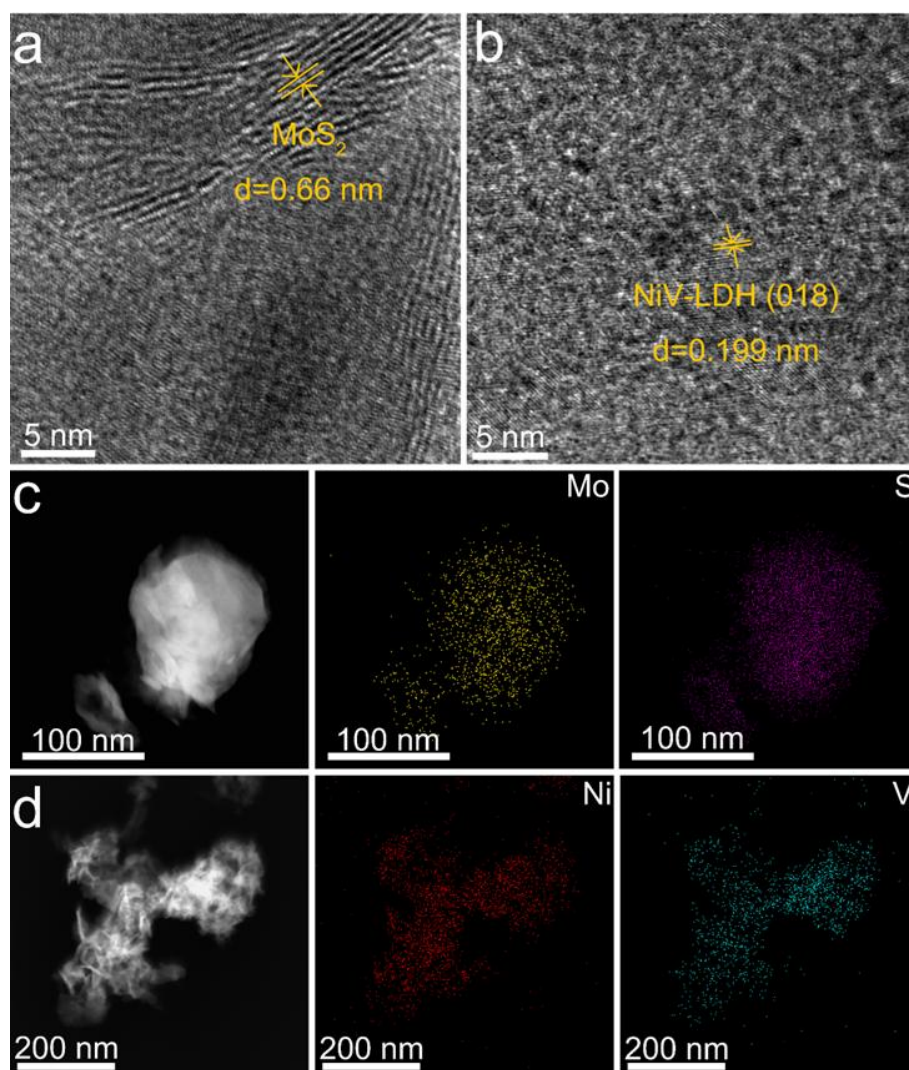


Figure S3. HRTEM images of (a)MoS₂ and (b) NiV-LDH. HAADF-STEM images and EDS elemental mapping images of (c)MoS₂ and (d) NiV-LDH.

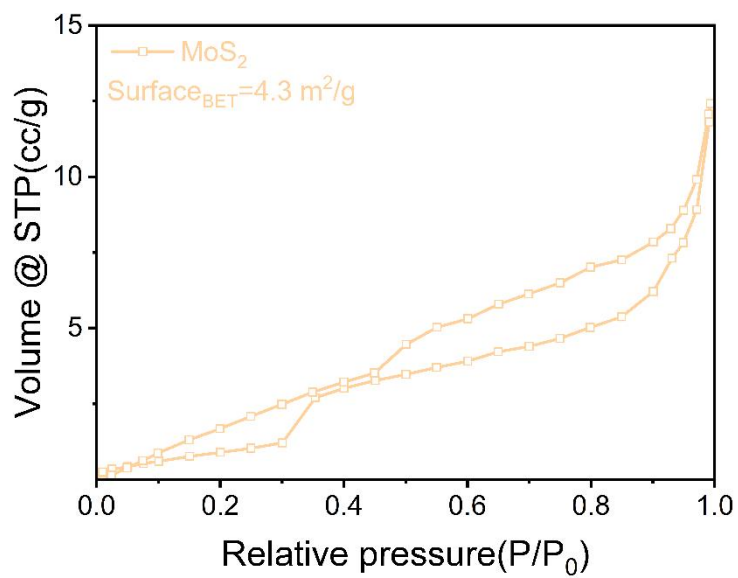


Figure S4. N₂ adsorption-desorption isotherm of MoS₂.

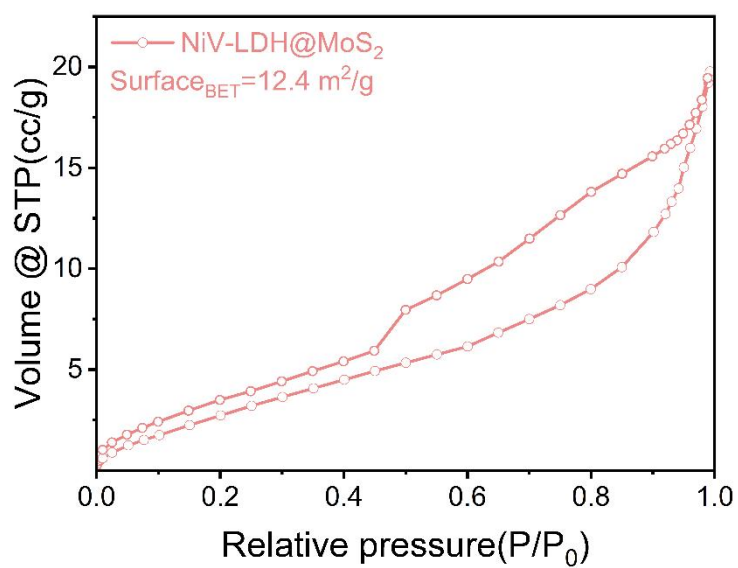


Figure S5. N₂ adsorption-desorption isotherm of NiV-LDH@MoS₂.

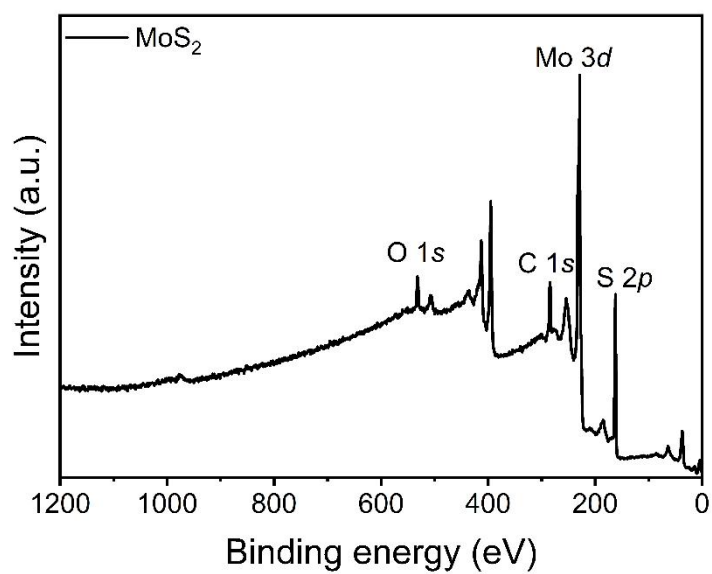


Figure S6. XPS survey spectrum of MoS₂.

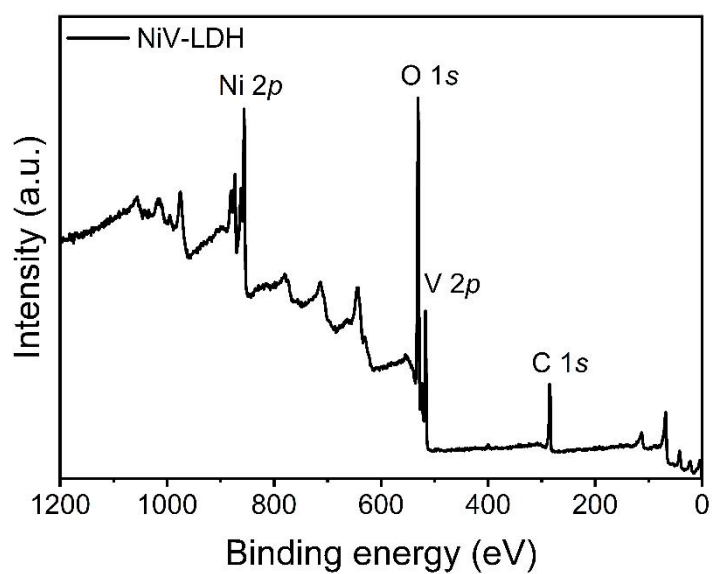


Figure S7. XPS survey spectrum of NiV-LDH.

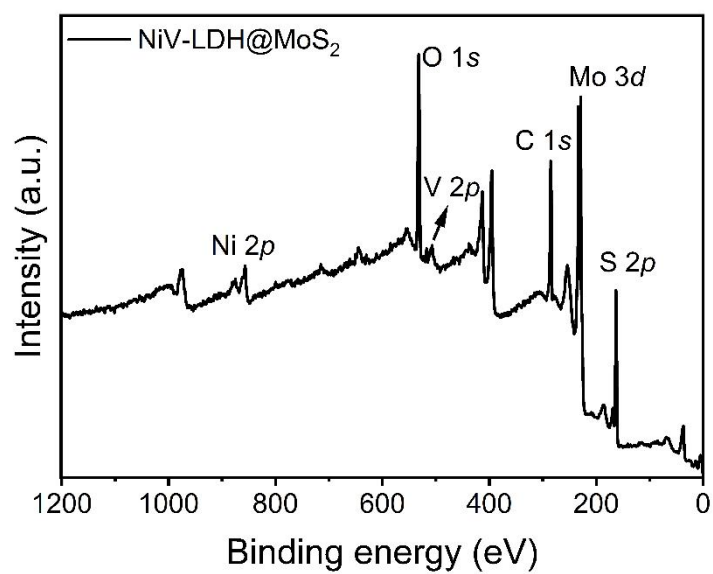


Figure S8. XPS survey spectrum of NiV-LDH@MoS₂.

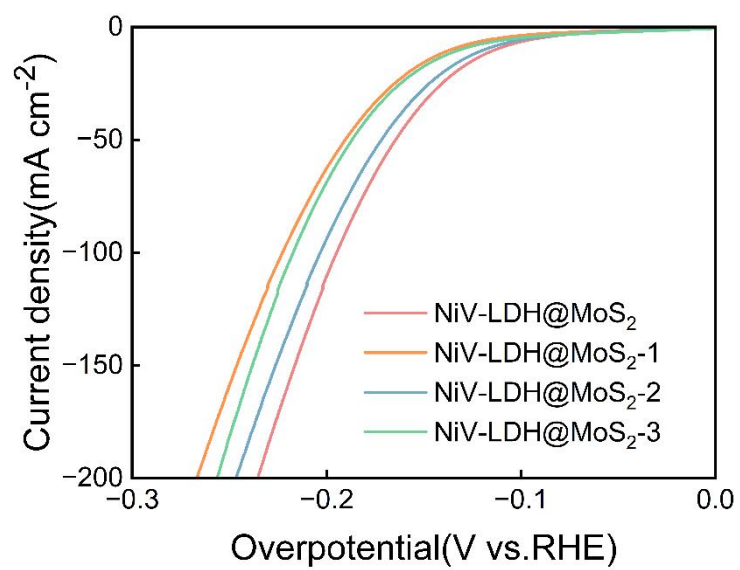


Figure S9. HER polarization curves of NiV-LDH@MoS₂-1, NiV-LDH@MoS₂-2, and NiV-LDH@MoS₂-3

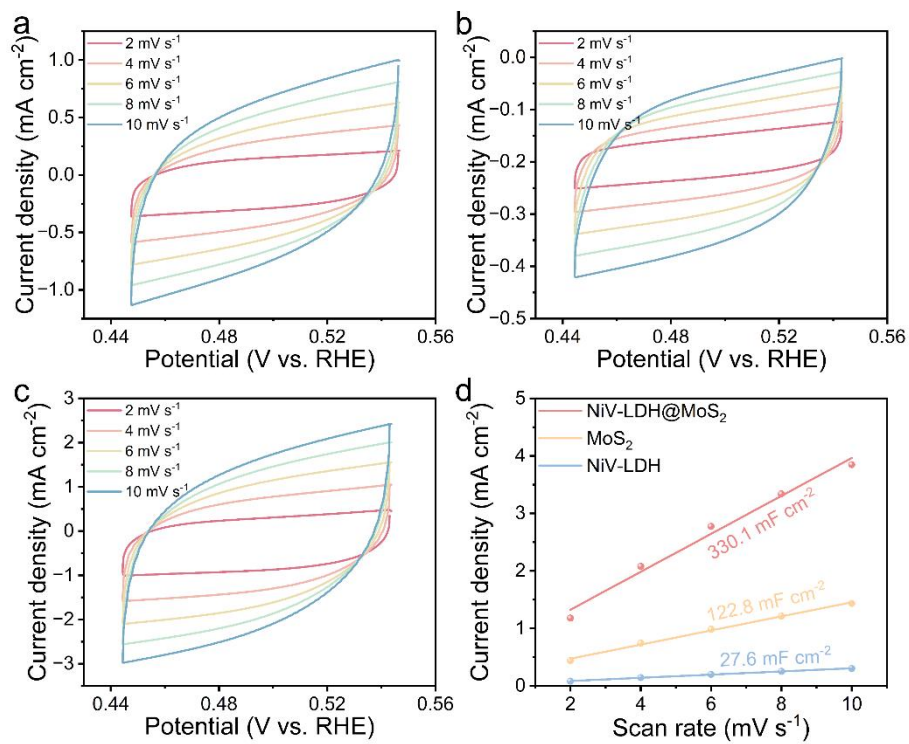


Figure S10. CV curves of (a) MoS_2 , (b) NiV-LDH , and (c) NiV-LDH@MoS_2 at the scan rates of 2,

4, 6, 8 and 10 mV s^{-1} . (d) The corresponding current variation as a function of scan rate.

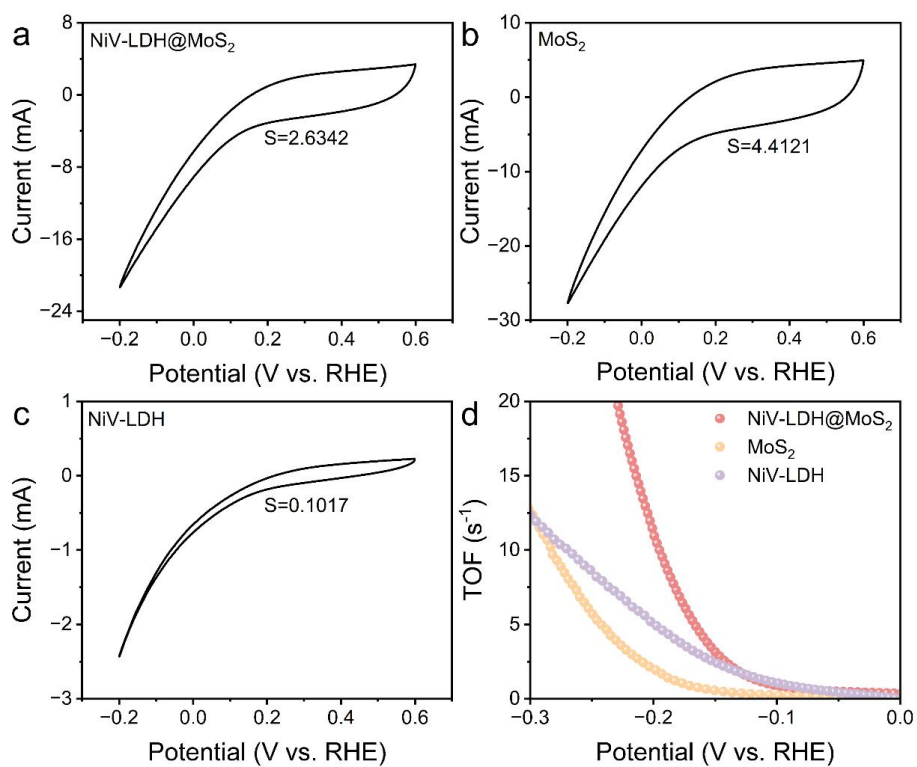


Figure S11. Electrochemical comparison in 1.0 M PBS: Cyclic voltammetry (CV) curves (a-c) and turnover frequency (TOF) plots (d) for NiV-LDH@MoS₂, MoS₂, and NiV-LDH recorded at a scan rate of 50 mV s⁻¹.

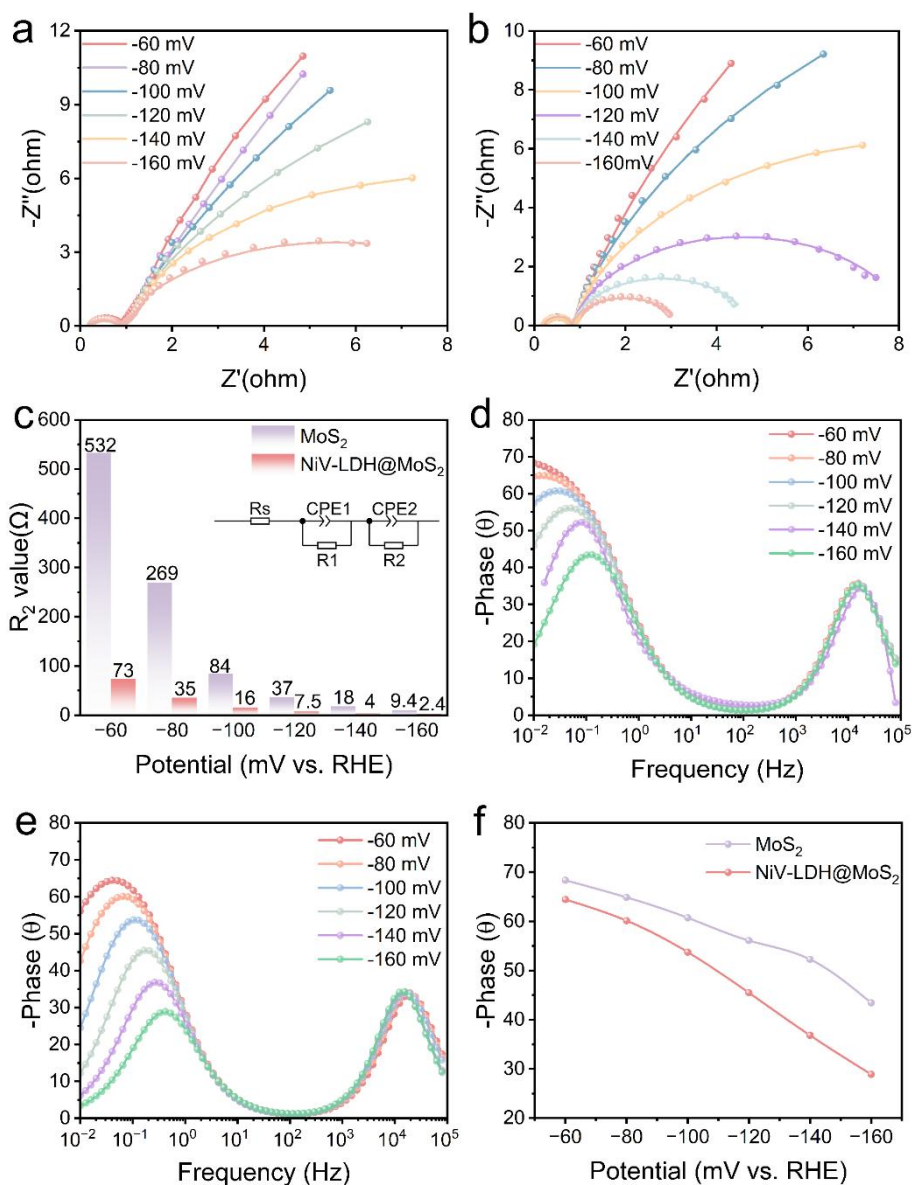


Figure S12. Nyquist plots of the electrocatalysts in 1 M KOH at various applied potentials of (a) MoS₂ and (b) NiV-LDH@MoS₂. (c) Comparison of R₂ values for MoS₂ and NiV-LDH@MoS₂ at different potentials; inset is the equivalent circuit for the simulation. Bode phase plots of (d) MoS₂ and (e) NiV-LDH@MoS₂. (f) Phase angle response of the electrocatalysts at various applied potentials.

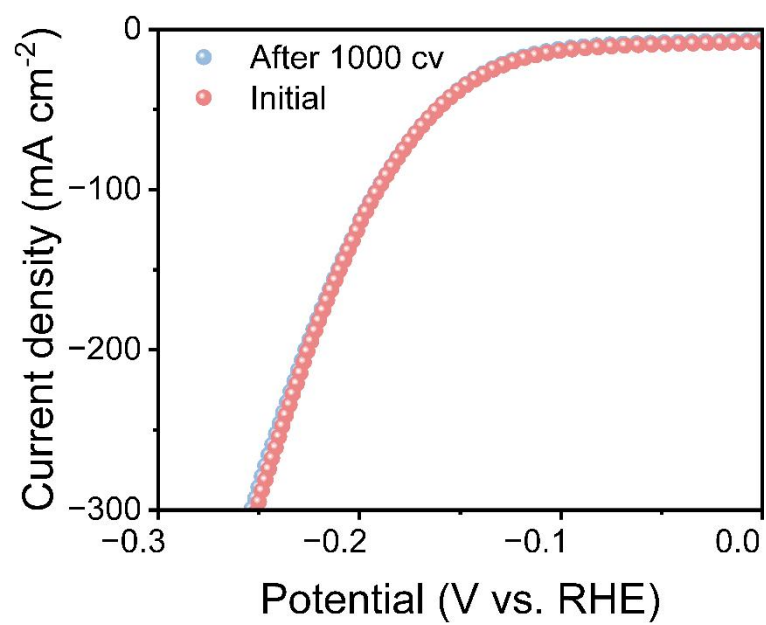


Figure S13. HER polarization curves of NiV-LDH@MoS₂ in 1 M KOH before and after 1,000 CV cycles.

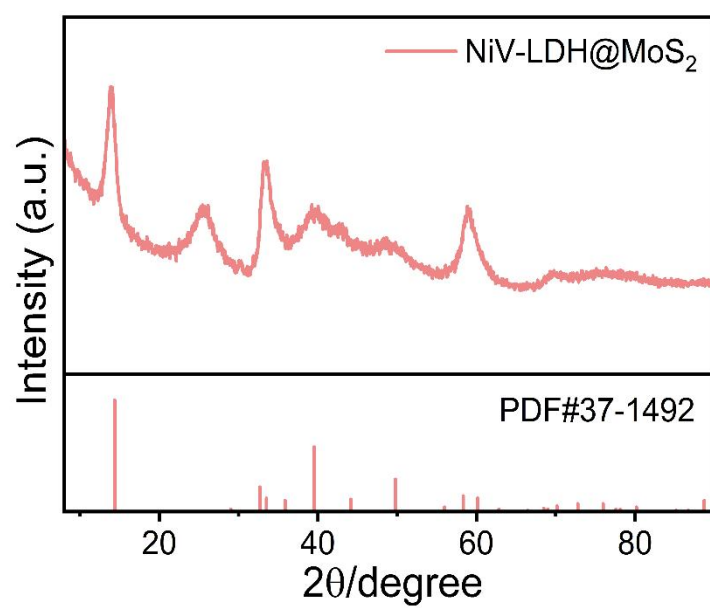


Figure S14. XRD pattern of NiV-LDH@MoS₂ after the stability test.

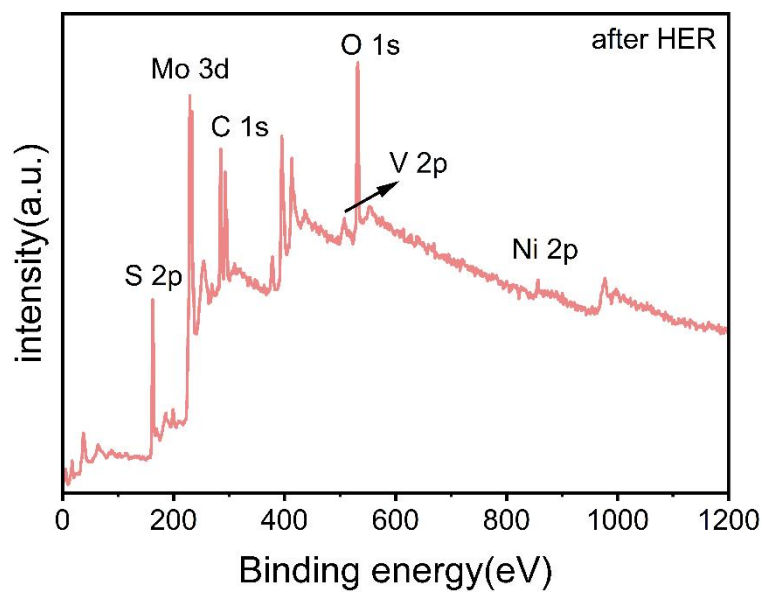


Figure S15. XPS survey spectra of NiV-LDH@MoS₂ after the stability test.

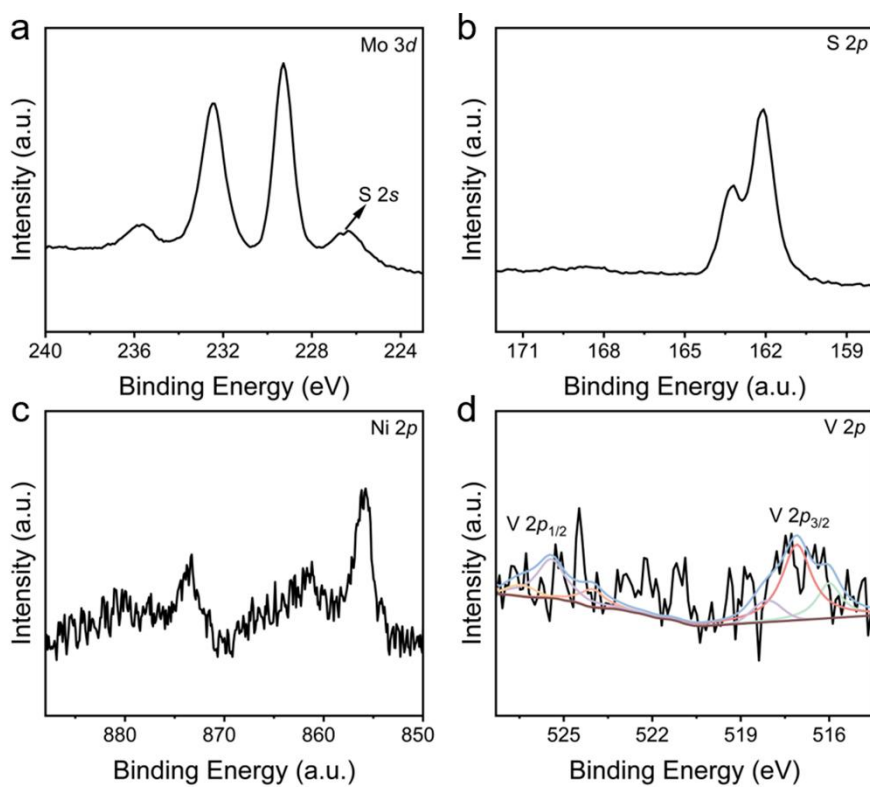


Figure S16. The (a) Mo 3d, (b) S 2p, (c) Ni 2p and (d) V 2p XPS spectra of NiV-LDH@MoS₂

after stability test.

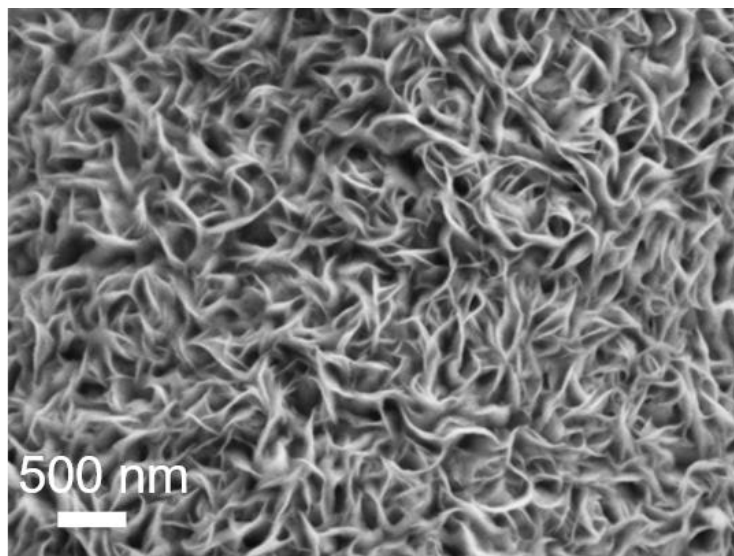


Figure S17. Post-stability test SEM image of NiV-LDH@MoS₂.

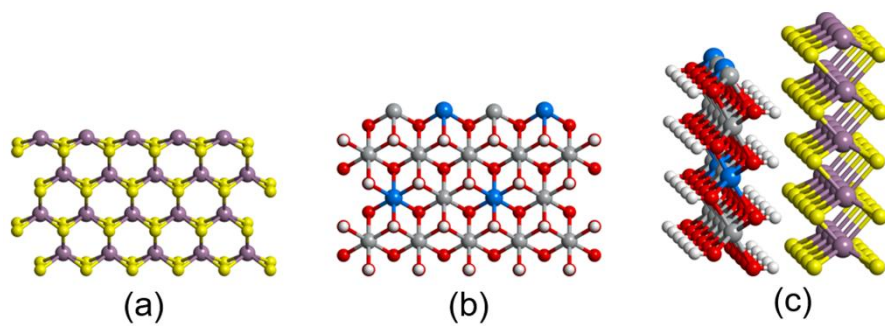


Figure S18. The established structural models of (a) MoS₂, (b) NiV-LDH, and (c) the NiV-LDH@MoS₂ heterostructure.

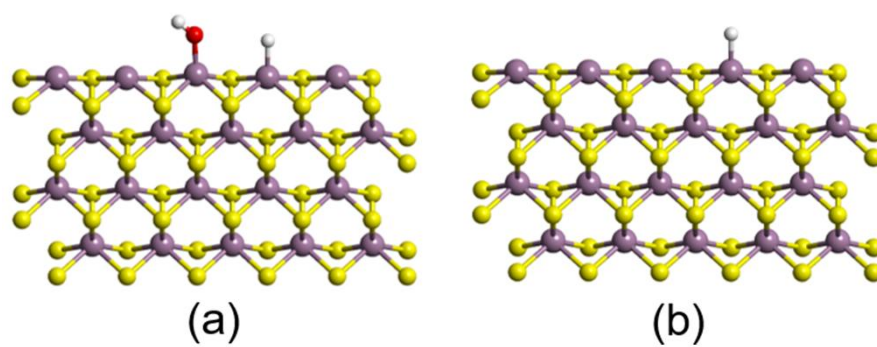


Figure S19. Structural Model: HER Intermediates on MoS_2 .

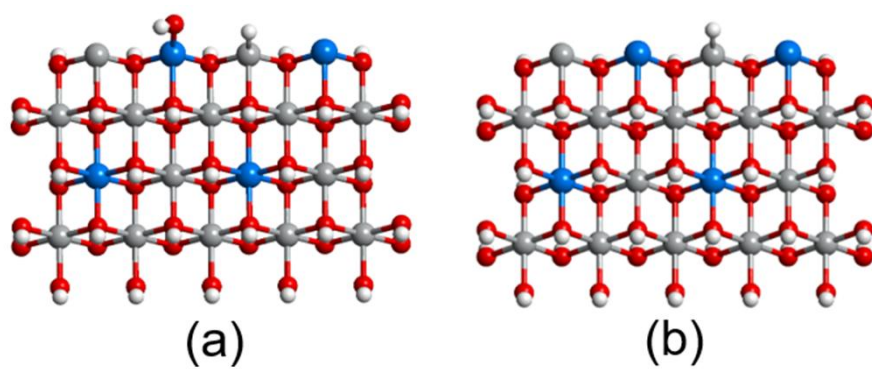


Figure S20. Structural Model: HER Intermediates on NiV-LDH.

Table S1 ICP-OES results of NiV-LDH@MoS₂ sample.

Catalyst	Ni (ppm)	V (ppm)	Mo (ppm)
NiV-LDH@MoS ₂	0.03	0.01	1.11

Table S2 EIS fitting parameters of equivalent circuits for MoS₂ in 1.0 M KOH

Potential(mV)	R _s	CPE ₁ -T	CPE ₁ -P	R ₁	CPE ₂ -T	CPE ₂ -P	R ₂
-60	0.2333	2.977E-5	1.013	0.6493	0.45535	0.79197	532
-80	0.2312	2.859E-5	1.014	0.6493	0.46008	0.78896	269
-100	0.2333	2.755E-5	1.014	0.6464	0.46458	0.7936	84
-120	0.2351	2.724E-5	1.015	0.6436	0.46659	0.79775	37
-140	0.2325	2.7633E-5	1.012	0.6449	0.46609	0.79937	18
-160	0.2462	2.276E-5	1.035	0.6273	0.46201	0.79938	9.4

Table S3 EIS fitting parameters of equivalent circuits for NiV-LDH@MoS₂ in 1.0 M KOH

Potential(mV)	R _s	CPE ₁ -T	CPE ₁ -P	R ₁	CPE ₂ -T	CPE ₂ -P	R ₂
-60	0.2371	2.198E-5	1.019	0.58031	0.38689	0.84179	73
-80	0.2334	2.337E-5	1.021	0.58359	0.38878	0.84671	35
-100	0.2319	2.562E-5	1.018	0.58462	0.38758	0.85295	16
-120	0.2463	2.251E-5	1.041	0.56902	0.38443	0.86006	7.5
-140	0.2446	2.188E-5	1.045	0.56593	0.38166	0.855	4
-160	0.2425	2.114E-5	1.051	0.56044	0.38025	0.83525	2.4

Table S4 Performance comparison of NiV-LDH@MoS₂ with other non-precious-metal HER catalysts in 1 M KOH electrolyte.

Catalyst	Overpotential (mV) (@ 10 mA·cm ⁻²)	Tafel slope (mV dec ⁻¹)	Reference
NiV-LDH@MoS ₂	103	76.9	This Work
MoS ₂ /Ni ₃ S ₂	110	88	[1]
FeNi@FeNi/NF	127	143.1	[2]
(Ni, Fe)S ₂ @MoS ₂	130	101.2	[3]
NiFe LDH-POM/NF	156	67	[4]
CoS ₂ @CoFe-LDH	162	91	[5]
Ni-Co-Fe LDH@NiNCs	174	65.5	[6]
Al ₄₀ CoFe ₃₀	178	62	[7]
MoS ₂ /NiCoS	189	75	[8]
N-NiMoO ₄ /NiS ₂	200	74.2	[9]
Mo-Ni ₃ S ₂ /NixPy	202	68.4	[10]
CoFe@NiFe-200/NF	240	88.88	[11]
MoS ₂ /NiS	244	97	[12]

Structures of NiV-LDH@MoS₂ and interface formation energy

The interface formation energy quantifies the thermodynamic stability of an interface between two materials (A and B) and is calculated as:

$$E(\text{formation}) = E(\text{NiV-LDH@MoS}_2) - E(\text{MoS}_2) - E(\text{NiV-LDH})$$

where $E(\text{NiV-LDH@MoS}_2)$ is the total energy of the relaxed interface system, $E(\text{MoS}_2)$, $E(\text{NiV-LDH})$ are the energies of MoS₂ and NiV-LDH, respectively. The calculated results are listed below:

Table S5 The calculated formation energy of NiV-LDH@MoS₂, unit: eV.

	$E(\text{NiV-LDH@MoS}_2)$	$E(\text{MoS}_2)$	$E(\text{NiV-LDH})$	$E(\text{formation})$
NiV-LDH@MoS ₂	-203.99451459	-90.79375300	-111.58688932	-1.61387227

Table S6 The calculated hydrogen adsorption energy on Ni and V sites of NiV-LDH@MoS₂, unit:

eV.

	E(surface+H)	E(surface)	E(H ₂)	$\Delta E(\text{ads})$	$\Delta G(\text{H}^*)$
Ni site	-739.06824917	-735.31652855	-6.77082607	-0.36630758	-0.12630758
V site	-738.74712146	-735.31652855	-6.77082607	-0.04517987	0.19482013

Reference

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