Supporting Information

Ce-doped CoS₂ pyrite with weakened O₂ adsorption suppresses catalyst leaching

and stabilizes electrocatalytic H₂ evolution

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Computational Details

A plane-wave basis set density functional theory (DFT) was carried out to evaluate the stability of OER catalysts using Vienna Ab-initio Simulation Package (VASP).¹⁻³ The Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) functional was used for the exchange-correlation potential.⁴⁻⁶ All calculations were performed with an energy cutoff of 400 eV and accounted for spin polarization. A $16 \times 16 \times 16$ Monkhorst–Pack k-point mesh was employed in the calculations of bulk properties. The lattice volume was fitted with the third-order Birch–Murnaghan isothermal equation of state.⁷⁻⁹ The resulted lattice parameter was 5.505 Å, similar with the result (5.506 Å) from the Materials Project.¹⁰

The unit cell with a (2×2) slab was applied to model the CoS₂(001). The slab contained three Co layers and six S layers, in which the bottom one Co layer and two S layers were fixed and other layers were all relaxed. A 15 Å vacuum space along z-axis was used to separate the slab images. The Ce-doped CoS₂ slab was built through replacing one of the lattice Co atoms on the 2nd Co layer by a Ce atom (Fig. S1). The DFT + U methodology was used to treat the exchange interaction of the strongly localized Ce 4f electrons with an effective $U_{eff} = 4.5$ eV.¹¹ A 3 × 3 × 1 Monkhorst–Pack k-point mesh was employed. All geometry structures were allowed to be fully relaxed with the forces converged to less than 0.02 eV/Å and were optimized with a convergence criterion of 10⁻⁵ eV in energy.

The adsorption energy of O₂, E_{ad}, was defined as:

 $E_{ad}(O_2) = E(O_2 + slab) - E(slab) - E(O_2)$

 $E_{ad}(O_2)$ represented the adsorption energy of molecular O_2 . $E(O_2+slab)$ was the energy of slab model with an O_2 on surface. E(slab) and $E(O_2)$ were the energy of slab and O_2 , respectively.

The binding energy of S atom or O atom, E_{bind} was defined as:

 $E_{\text{bind}}(S) = E(\text{slab}) - E(\text{slab-S}_v) - E(S)$

 $E_{\text{bind}}(O) = E(O + \text{slab}) - E(\text{slab}) - E(O)$

 $E(\text{slab-S}_v)$ was the energy of slabs with a S vacancy and E(S) was the energy of a S atom. E(O+slab) were the energy of slab model with a O atom bonded on surface. E(O) was the energy of O atom.

Bader charge analysis was carried out by the code developed by Henkelman' group.¹²⁻¹⁴ The differential charge density plot was defined as that the electron density of the relaxed Ce-doped CoS_2 minus the electron density of a similar slab model with the Ce atom replaced by Co atom.

Experimental Section

Synthesis of Ce-Co₃O₄/Ti plate: Typically, the bare Ti plate (2 cm × 1 cm) were pre-cleaned by sonication in 5% HCl, acetone, ethanol and deionized (DI) water for 10 min consecutively. Specifically, 1 mmol mixture of $Ce(NO_3)_3 \cdot 6H_2O$ and $CoCl_2 \cdot 6H_2O$ with the desired molar ratio "x" (where x=[Ce³⁺]/([Ce³⁺]+[Co²⁺]), and x = 0, 0.1, 0.15 and 0.2, respectively) were added to a 15 mL of aqueous solution containing 5 mmol urea to obtain a transparent solution. Afterwards, the clean Ti plate was immersed into the reaction solution and then treated in a Teflon vessel (20 mL) at 120 °C for 8 h. After cooling down to room temperature, the Ti plate was rinsed by water/ethanol alternatively, dried at 60 °C, and subsequently annealed at 300 °C for 2 h in air to obtain Ce-Co₃O₄/Ti precursor. Co₃O₄/Ti precursor was also prepared *via* the same approach in the absence of Ce source.

*Synthesis of Ce-CoS*₂/*Ti electrode:* The Ce-CoS₂/Ti electrode was obtained through a sulfidization process. Briefly, Ce-Co₃O₄/Ti was placed in the center of a quartz tube along with a quartz boat loading 2 g of sulfur situated at the upstream. Raising temperature to 300 °C at a ramping rate of 8 °C/min, the sulfidization happened at 300 °C for 2 h under the protection of Ar (100 sccm). As a comparison, the CoS₂/Ti electrode was fabricated from Co₃O₄/Ti through the same sulfidization process.

Preparation of Pt/C@Ti and IrO₂/C@Ti benchmark electrodes: The catalyst inks of the commercial 10 wt.% Pt/C and 20 wt.% IrO₂/C catalysts were prepared by dispersing 10 mg of two catalysts in 1 mL of the mixed solvent containing water, ethanol, and 5% Nafion with a volumetric ratio of 768 : 200 : 32. Then, the catalytic electrodes were prepared by drop-casting of the catalyst inks on the Ti plates to reach a catalyst loading of ≈ 2.1 mg cm⁻². The asprepared electrodes were dried at room temperature naturally.

Characterizations: Powder X-ray diffraction (XRD) data were acquired on a Shimadzu X-ray diffractometer with Cu K α radiation. Scanning electron microscopy (SEM) measurements were carried out on a Hitachi SU8010 scanning electron microscope at an accelerating voltage of 20 kV. Transmission electron microscopy (TEM) and energy-dispersive X-ray (EDX) measurements were performed on a JEOL 2100F TEM with an accelerating voltage of 200 kV. The X-ray photoelectron spectroscopy (XPS) measurements were performed on a Thermo Electron Model with Al K α as the excitation source. Raman spectra were obtained by a Horiba LabRAM HR800 with laser excitation wavelength at 532 nm. Inductively-coupled plasma mass spectrometry (ICP-MS) was performed on an Agilent ICPMS 7500CE. All samples for ICP-MS were pre-treated by aqua-regia to obtain clear solutions before measurements.

Electrochemical measurements: A CHI 660D workstation (CH Instruments, Inc., Shanghai) was employed to perform various electrochemical tests. HER and oxygen evolution reaction (OER) activity of the various electrodes were investigated in a three-electrode system, where the fabricated electrodes, saturated calomel electrode (SCE) and graphite rod as the working electrode, reference electrode and counter electrode, respectively. Linear sweep voltammetry (LSV) curves for various electrodes with a scan rate of 5 mV/s were recorded to evaluate their catalytic activities. The chronoamperometric and chronopotentiometric tests were utilized to evaluate the catalytic stability of various electrodes. All measurements were performed in 1.0 M KOH. The potentials reported herein are relative to the reversible hydrogen electrode (RHE). The calibration was performed in the high purity hydrogen saturated electrolyte with a Pt foil as the working electrode.¹⁵ Cyclic voltammetry (CV) was performed at a scan rate of 1 mV/s, and the average of the two potentials at which the current crossed zero was

taken to be the thermodynamic potential for the hydrogen electrode reaction. The CV result was shown in Fig. S8. Before the electrochemical test, E(RHE) = E(SCE) + 1.072 V for 1.0 M KOH electrolyte. After durability test, E(RHE) = E(SCE) + 1.071 V for 1.0 M KOH electrolyte.

For overall water splitting, a two-electrode cell system was built by employing the $Ce-CoS_2(2)/Ti$ electrodes as both negative and positive electrodes in 1.0 M KOH. The catalytic durability of the two-electrode full cell system for overall water-splitting was tested in 1.0 M KOH electrolyte at an applied potential to reach an initial catalytic current density of 10 mA/cm².

Activity-Durability factor (ADF) calculations: ADF values quantitatively reflect the relation between activity and durability for a catalyst, which can be expressed as, $ADF = j_{ex} / j_{corr}$. Herein, j_{ex} and j_{corr} represent the exchange current density and corrosion current density of catalysts, respectively.



Fig. S1 Structures of $CoS_2(001)$ and $Ce-CoS_2(001)$ surfaces. Top view of (a) $CoS_2(001)$ and (c) $Ce-CoS_2(001)$ surfaces. Side view of (b) $CoS_2(001)$ and (d) $Ce-CoS_2(001)$ surfaces.



Fig. S2 (a) Calculated binding energy of atomic oxygen on the adjacent Co sites of Ce for Ce-CoS₂ and the corresponding Co sites for CoS₂. (b) Calculated binding energy of atomic oxygen on the adjacent S sites of Ce for Ce-CoS₂ and the corresponding Co sites for CoS₂. Bader charge distributions for (c) CoS₂ and (d) Ce-CoS₂ surface. The significantly declined Bader charges of the Co and S sites neighbor to Ce clearly reflected the electron acceptance of such Co and S sites from the strong electron donor of Ce dopant. (e) Differential charge density analysis for Ce-CoS₂ multiple density of a similar slab model with the Ce atom replaced by Co atom. The Ce-CoS₂ model showed larger electron density of a simaller electron density in the green area compared to the CoS₂ model. The obvious electron cloud around Ce is mainly due to the intrinsically electrons to the adjacent Co and S sites, which neutralizes the partially positive charge of Co and increase the negative charge of S. The bond between O and Co can be regarded as a polar covalent bond, of which Co and O are partially positive and negative charged and constitute a dipole. Thus, the neutralization of the partially positive charge for Co and S are weakened dipole moment of Co-O and thus the force between dipoles will be smaller. Also, such electron-rich Co and S will lead to the stronger Pauli repulsion against O. Therefore, the corresponding Co-O and S-O interactions are weakened.



Fig. S3 Powder XRD patterns for the pure Co_3O_4 and various Ce-doped Co_3O_4 precursors.



Fig. S4 TEM and SEM images for the pure Co₃O₄ and various Ce-doped Co₃O₄ precursors.



Fig. S5 Raman spectra for the pure CoS₂ and various Ce-doped CoS₂ electrodes.



Fig. S6 TEM and SEM images for the pure CoS₂/Ti and various Ce-CoS₂/Ti electrodes.



Fig. S7 (a) The CV result of RHE calibration in 1.0 M KOH before durability test, E(RHE) = E(SCE) + 1.072 V. (b) The CV result of RHE calibration in 1.0 M KOH after durability test, E(RHE) = E(SCE) + 1.071 V.



Fig. S8 HER activities for various Ce-CoS₂ electrodes in 1.0 M KOH with IR-compensation.



Fig. S9 Exchange current density of CoS_2/Ti and $Ce-CoS_2(2)/Ti$ electrodes for HER.



Fig. S10 Nyquist plots for various catalytic electrodes in 1.0 M KOH electrolyte.



Fig. S11 (a) HER and (b) OER activities for various catalytic electrodes normalized to ECSA.



Fig. S12 The direct observation of electrolyte during long-term durability test for $Ce-CoS_2/Ti$ electrode. There is no obvious black precipitation (exfoliated catalyst) appearing in the bottom of the beaker during test, which reflects the remarkable mechanical stability of electrode.



Fig. S13 Comparison of the catalytic durability for CoS_2/Ti and $Ce-CoS_2(2)/Ti$ electrodes in normal or Ar-saturated 1.0 M KOH electrolyte.



Fig. S14 Faraday efficiency of CoS₂/Ti and Ce-CoS₂(2)/Ti electrodes for HER.



Fig. S15 High-resolution S 2p XPS spectra of fresh and spent CoS_2/Ti or $Ce-CoS_2(2)/Ti$ electrodes for HER operation.



Fig. S16 High-resolution Ce 3d XPS spectra of fresh and spent Ce-CoS₂(2)/Ti electrode for HER operation.



Fig. S17 High-resolution (a) Co 2p and (b) S 2p XPS spectra of fresh or spent CoS_2/Ti and $Ce-CoS_2(2)/Ti$ electrodes for long-term immersion in electrolyte.



Fig. S18 The direct observation of electrolyte during long-term durability test for CoS₂/Ti electrode.



Fig. S19 XRD patterns of the stored CoS_2 and $Ce-CoS_2(2)$ catalysts in ambient condition.



Fig. S20 EDX elemental mapping and line scan of a nanowire in spent Ce-CoS₂(2)/Ti electrode for HER operation.



Fig. S21 CV curves of (a) CoS_2/Ti and (b) Ce-CoS₂(2)/Ti electrodes with various scan rates in 1.0 M KOH. (c) C_{dl-OER} calculated from the CV curves.



Fig. S22 High-resolution (a) Co 2p, (b) S 2p and (c) Ce 3d XPS spectra of fresh and spent Ce-CoS₂(2)/Ti electrodes for OER operation. (d) Raman spectra of fresh and spent Ce-CoS₂(2)/Ti electrodes for OER operation. (e) EDX line scan and elemental mapping of a nanowire in spent Ce-CoS₂(2)/Ti electrode for OER operation. When the XPS profiles of Ce-CoS₂(2)/Ti before and after OER operation shown in Figure S22 are compared, it can be seen that the Co 2p core level XPS spectra of the spent Ce-CoS₂(2)/Ti (Figure S22a) presented the complete disappearance of the intensive peak at 778.3 eV, which are characteristic of the Co species in fresh Ce-CoS₂(2)/Ti, and a newborn characteristic XPS peak at 781.1 eV, which is similar to the Co species in cobalt oxides (CoO_x) composed by dominant Co^{3+} and few Co^{2+} . Meanwhile, the XPS spectra in S 2p region for spent Ce-CoS₂(2)/Ti (Figure S22b) also delivered the completely disappeared peaks at 162.5 eV and 163.6 eV (sulfur species in Ce-CoS₂) and sharply raised peak at \sim 168 eV (oxidized sulfur species). This finding suggested the species evolution of CoS_2 component in Ce-CoS₂ to the CoO_x species. Also, the XPS spectra in Ce 3d region showed a dramatical main peak shift from 883.0 eV for fresh catalysts to 886.5 eV for spent catalysts, which reveals the significantly raised valence state of Ce heteroatoms in Ce-CoS₂ and reflects their species evolution during OER (Figure S22c). Raman spectra (Figure S22d) further supports the species evolution of $Ce-CoS_2$, in which the Raman characteristic peaks of pyrite structures for spent Ce-CoS₂(2)/Ti completely vanished and five new peaks have emerged. Raman peaks at 471, 502, 551 and 601 cm⁻¹ reflected the formation of CoO_x composed by dominant CoOOH and few $Co(OH)_2$, while the peak located at 450 cm^{-1} corresponded to the vibration of Ce-O bond and thus demonstrated the formation of oxidized Ce species (CeO_x) under OER conditions. EDX mapping and line scan (Figure S22e) investigations for spent Ce-CoS₂(2)/Ti presented that the Co, Ce and S elements still showed the uniform distribution in the whole nanowire and the total content of S was sharply reduced, while the O element significantly concentrated on the surface of the nanowire. The aforesaid finding revealed that Ce-CoS₂ structures evolved into CoO_x/Ce -CoS₂ core-shell structures with surface CeO_x species $(CeO_x(a)CoO_x/Ce-CoS_2).$



Fig. S23 (a) Inferred mechanism for the improved OER performance of $Ce-CoS_2(2)/Ti$ electrode. **(b)** KOH concentration-dependent OER Tafel slope profiles for CoS_2/Ti and $Ce-CoS_2(2)/Ti$ electrodes. *KOH electrolyte concentration reflected the hydroxy concentration around catalysts. For sure, the richer hydroxy around catalysts is favorable to achieve higher OH* coverage on active sites during OER. Such raised OH* coverage could directly aim at the rate-determining step for the 6-coordinated Co sites in CoOOH species and thereby accelerate the overall OER kinetics, which was characterized by the declined Tafel slopes. By regulating KOH electrolyte concentration. Tafel slope values for CoS_2/Ti and Ce-CoS_2(2)/Ti both presented strongly negative dependency with KOH electrolyte concentration. That is to say, hydroxy adsorption kinetics was indeed crucial for overall kinetics of such pyrite-derived OER catalysts and highly depended on the concentration of ambient hydroxy. Interestingly, Ce-CoS_2(2)/Ti presented the smaller Tafel slopes compared to that of CoS_2/Ti in the same concentration of KOH electrolyte and the Tafel slope values for CoS_2(2)/Ti is the lower concentration of KOH, corresponding to the faster OER kinetics of Ce-CoS_2(2)/Ti is timulated by the hydroxy enrichment effects of CeO_x component. Notably, the Tafel slope value for CeS_2(2)/Ti in 0.001 M KOH was even smaller than that of CoS_2/Ti in 0.01 M KOH was particularly significant under the low OH* coverage and up to 10 times.*



Table 52. Calculated CC content in fresh COS'' if and various $CC-COS''$ if clothous

Catalytic electrodes	CoS ₂ /Ti	Ce-CoS ₂ (1)/Ti	Ce-CoS ₂ (2)/Ti	Ce-CoS ₂ (3)/Ti
Total mass of catalysts (mg)	~ 4.2	~ 4.2	~ 4.1	~ 4.3
Measured Co concentration (ppm)	19.4	19.9	17.9	17.7
Corresponding mass of Co in catalysts (mg)	1.94	1.99	1.79	1.77
Measured Ce concentration (ppm)	0	1.4	2.0	4.3
Corresponding mass of Ce in catalysts (mg)	0	0.14	0.20	0.43
Calculated mass of S in catalysts (mg)	2.26	2.07	2.11	2.10
Calculated Ce content (atom %)	0 %	1 %	1.47 %	3.12 %

Catalysts	η_{10} [mV]	Tafel slope [mV dec ⁻¹]	Stability [hour]	Reference
Ce-CoS ₂ (2)/Ti electrode	-82	59.4	250	This work
Ni _{0.33} Co _{0.67} S ₂ /Ti	-88	118	18	Ref. 16
Fe _{0.1} NiS ₂ /Ti	-200	108	10	Ref. 17
NiS ₂	-219	157	19	Ref. 18
V-NiS ₂	-110	90	20	Ref. 19
FeS ₂ /C/NF	-202	98	4	Ref. 20
$Ni_{0.7}Fe_{0.3}S_2$	-155	109	14	Ref. 21
<i>h</i> -NiS _x	-60	99	10	Ref. 22
Fe _{0.54} Co _{0.46} S _{0.92} /CNTs	-70	65	72	Ref. 23
Ni ₃ S ₂ /NF	-223	_	200	Ref. 24
Fe-Ni ₃ S ₂ /NF	-47	95	20	Ref. 25
N-doped Ni ₃ S ₂	-155	113	50	Ref. 26
NiCo ₂ S ₄ /NF	-210	58.9	50	Ref. 27
FeS_2/CoS_2	-78	44	80	Ref. 28
CoS_2/MoS_2	-97	70	10	Ref. 29
$Co(S_{0.71}Se_{0.29})_2$	-122	85.7	20	Ref. 30
CoPS	-107	88.3	100	Ref. 31
CoPS@NPS-C	-191	106	30	Ref. 32
$(Co_{1-x}Ni_x)(S_{1-y}P_y)_2$ /graphene	-117	85	50	Ref. 33
$Co_{0.9}S_{0.58}P_{0.42}$	-141	72	20	Ref. 34
$Ni_{0.90}Fe_{0.10}PS_3$	-72	73	50	Ref. 35

Table S3. Comparison of HER performance with state-of-the-art pyrite catalysts and other transition metal-based electrocatalysts working in 1.0 M KOH.

Table S3.	Continued
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Catalysts	η_{10} [mV]	Tafel slope [mV dec ⁻¹]	Stability [hour]	Reference
Ce-CoS ₂ (2)/Ti electrode	-82	59.4	250	This work
Ni ₅ P ₄ pellet	-49	98	16	Ref. 36
MoP	_	48	20	Ref. 37
FeP nanorod array	-218	146	_	Ref. 38
CoP mesoporous nanorod	-54	51	32	Ref. 39
NiCoP/carbon nanofibers	-130	83	20	Ref. 40
Mo ₂ C/N-doped porous carbon	-45	46	20	Ref. 41
Ni ₃ C/CNTs	-132	49	50	Ref. 42
CoMoC	-118	44	24	Ref. 43
NiMoN	-109	95	36	Ref. 44
Ni ₃ FeN	-158	42	8	Ref. 45
Ni ₃ N _{1-x} /NF	-55	54	50	Ref. 46
Co ₂ B	-233	92.4	55	Ref. 47
MoB/g-C ₃ N ₄	-130	46	48	Ref. 48
Porous MoO ₂	-25	41	12	Ref. 49
Ni/NiO-Cr ₂ O ₃	-36	_	48	Ref. 50

Table S4 . Fitting parameter values of the EIS	data of the various	catalytic electrodes	tor HER.
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Electrodes	$R_s[\Omega]$	$R_1 [\Omega]$	<i>n</i> ₁	CPE ₁	^a C _{dl-HER} [mF]
CoS ₂ /Ti	2.67	45	0.85	0.026	16
Ce-CoS ₂ (1)/Ti	2.88	40	0.83	0.03	18
Ce-CoS ₂ (2)/Ti	2.77	21	0.81	0.051	31
Ce-CoS ₂ (3)/Ti	2.45	42	0.86	0.03	20

 $\frac{1}{a C_{dl-HER}} = [CPE_1/(R_s^{-1} + R_1^{-1})^{1-n}]^{(1/n)}$

Catalytic electrodes	"ECSA for HER [cm ²]	"ECSA for OER [cm ²]
CoS ₂ /Ti	400	820
$Ce-CoS_2(1)/Ti$	450	-
Ce-CoS ₂ (2)/Ti	775	1027.5
Ce-CoS ₂ (3)/Ti	500	-
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^a ECSA for HER = $C_{dl-HER}/0.040$ mF cm⁻² ^b ECSA for OER = $C_{dl-OER}/0.040$ mF cm⁻²

	Table S6. BE	T results for	the various	catalysts	loaded	on Ti
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Catalysts	Surface Area [m ² /g]	Pore Size [nm]
CoS_2	20	13
$Ce-CoS_2(1)$	33	17
$Ce-CoS_2(2)$	44	21
$Ce-CoS_2(3)$	35	16

Table S7. Calculation of the representative ADF values for CoS_2/Ti and $Ce-CoS_2(2)/Ti$.

Catalytic electrodes	$j_{\rm ex}$ [mA cm ⁻²]	$j_{\rm corr} [{ m mA}~{ m cm}^{-2}]$	Activity Dtability Factor
CoS ₂ /Ti	0.129	0.72	0.18
Ce-CoS ₂ (2)/Ti	0.29	0.05	5.8

Table S8. The content of each elements in spent $Ce-CoS_2(2)/Ti$ electrode under HER operation.

Catalytic electrodes	Fresh	Spent
Total mass of catalysts (mg)	~ 4.1	~ 4.0
Measured Co concentration (ppm)	17.9	17.2
Measured Ce concentration (ppm)	2.0	2.0
Measured Co content in catalysts (wt. %)	43.7 %	43.1 %
Measured Ce content in catalysts (wt. %)	4.9 %	5.0 %
Calculated S content in catalysts (wt. %)	51.4 %	51.9 %

Catalysts	η_{10} [mV]	Tafel slope [mV dec ⁻¹]	Stability [hour]	Reference
Ce-CoS ₂ (2)/Ti electrode	233	53.4	250	This work
Fe _{0.1-} NiS ₂ /Ti	200	73	15	Ref. 17
NiFeS ₂	262	56.4	10	Ref. 51
$CoS_{4.6}O_{0.6}$	290	67	10	Ref. 52
V-NiS ₂	290	45	20	Ref. 19
FeS ₂ /C/NF	240	-	5	Ref. 20
<i>h</i> -NiS _x	180	96	10	Ref. 22
Ni ₃ S ₂ /NF	260	_	200	Ref. 24
NiCo ₂ S ₄ /CC	260	40.1	50	Ref. 27
FeS_2/CoS_2	240	42	70	Ref. 28
CoS_2/MoS_2	272	45	10	Ref. 29
$Co(S_{0.22}Se_{0.78})_2$	283	65.6	20	Ref. 30
CoPS@NPS-C	326	98	30	Ref. 32
$(Co_{1-x}Ni_x)(S_{1-y}P_y)_2$ /graphene	285	105	100	Ref. 33
$Co_{0.9}S_{0.58}P_{0.42}$	266	48	20	Ref. 34
$Ni_{0.90}Fe_{0.10}PS_3$	_	69	50	Ref. 35
Ni ₂ P/Ni//NF	200	_	100	Ref. 53
$(Co_{0.52}Fe_{0.48})_2P$	270	30	_	Ref. 54
NiCoP/carbon nanofibers	268	83	20	Ref. 40
Ni ₃ FeN	280	46	8	Ref. 45
Co ₂ B	380	45	60	Ref. 47
Porous MoO ₂	260	54	12	Ref. 49
nNiFe LDH/NGF	310	45	3.4	Ref. 55
NiFeO _x	> 220	31.5	100	Ref. 56

Table S9. Comparison of OER performance with state-of-the-art transition-metal-based electrocatalysts working in 1.0 M KOH.

Catalysts	Cell voltage at 10 mA/cm ² [V] Stability [hour]		Reference
Ce-CoS ₂ (2)/Ti electrode	1.56	180	This work
V-NiS ₂	1.56	20	Ref. 19
$Ni_{0.7}Fe_{0.3}S_2$	1.625	14	Ref. 24
<i>h</i> -NiS _x	1.47	10	Ref. 22
Ni ₃ S ₂ /NF	1.76	150	Ref. 21
Fe-Ni ₃ S ₂ /NF	1.54	10	Ref. 25
NiCo ₂ S ₄ /NF	1.63	50	Ref. 27
FeS ₂ /CoS ₂	1.47	21	Ref. 28
CoS_2/MoS_2	1.6	10	Ref. 29
$Co(S_{0.71}Se_{0.29})_2$	1.63	20	Ref. 30
$(Co_{1-x}Ni_x)(S_{1-y}P_y)_2$ /graphene	1.65	50	Ref. 33
$Co_{0.9}S_{0.58}P_{0.42}$	1.59	30	Ref. 34
Ni ₂ P/Ni//NF	1.49	40	Ref. 53
NiCoP/carbon nanofibers	1.65	10	Ref. 40
$(Co_{0.52}Fe_{0.48})_2P$	1.53	50	Ref. 54
Co/CoP	1.54	12	Ref. 57
NiSe	1.63	20	Ref. 58
CoNiSe	1.62	10	Ref. 59
NiMo HNRs/Ti mesh	1.64	10	Ref. 60
Co ₂ B	1.81	60	Ref. 47
Porous MoO ₂	1.53	24	Ref. 49
NiFe LDH/NF	1.70	3	Ref. 61
NiFeO _x	1.51	100	Ref. 56

Table S10. Comparison of electrocatalytic overall water splitting performance of various transitionmetal-based catalysts in 1.0 M KOH.

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