

A dataset of nickel and cobalt based phosphides for the application of electrocatalytic oxygen evolution reaction in alkaline solution

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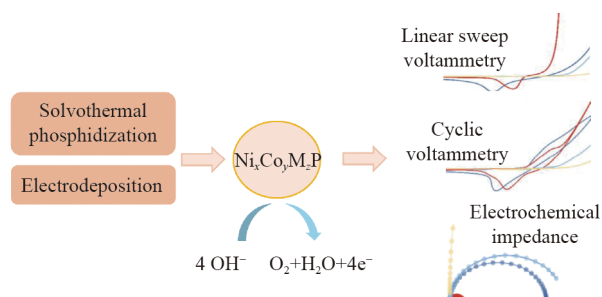
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Abstract: Hydrogen as the energy carrier is a promising solution to mitigate the environmental issues associated with the use of fossil fuels. Efficient and inexpensive electrocatalysts for oxygen evolution in alkaline media are crucial for advancing the widespread application of alkaline water electrolyzers for hydrogen generation. Transition metal phosphides are promising candidates as the (pre-)catalysts for electrocatalytic oxygen evolution reactions. This dataset compiles and compares the electrocatalytic oxygen evolution reaction activity of nickel- and cobalt-based phosphides. The metal phosphides reported were synthesized using solvothermal phosphidization or electrodeposition methods, and the oxygen evolution activities of these phosphides were evaluated using linear sweep voltammetry in 1 mol/L KOH. Besides, cyclic voltammetry and electrochemical impedance spectroscopy were performed on these metal phosphides. The total volume of this dataset is 14.5 MB, comprising 312 files. It serves as a valuable reference for the design of active metal phosphide-based materials for electrocatalysis.

Key words: nickel phosphide; cobalt phosphide; oxygen evolution reaction; alkaline solution



Hydrogen is among the most promising energy carriers to address the potential energy crisis and reduce environmental pollution caused by the utilization of fossil fuels. Producing hydrogen *via* water electrolysis can utilize the intermittent electricity generated from wind, solar, tidal, or other renewable energy sources. In contrast to the hydrogen evolution reaction that happens at the cathode of water electrolyzers, the oxygen evolution reaction (OER) requires consecutive transfer of four electrons, coupled with proton transfer, leading to sluggish kinetics. Therefore, active electrocatalysts are required to accelerate the kinetics of OER^[1-2].

Transition metal phosphides (TMPs) exhibit high electrical conductivity and abundant electrocatalytic active sites, making them ideal (pre-)electrocatalysts for OER^[3].

When used to electrocatalyze OER in alkaline media, the surface of metal phosphides undergoes restructuring to form metal oxides and oxyhydroxides, which are the actual active species for OER. The *in situ* formed metal phosphide core and oxide/oxyhydroxide shell offer abundant active sites, and introduce electronic interaction to achieve high OER activities^[4].

The synthesis of metal phosphides often relies on high temperature calcination using NaH₂PO₂ as the phosphorus source. Under elevated temperature (> 623 K), excessive phosphine gas is generated to react with the precursors. This high temperature calcination synthesis method is undesirable, as the phosphine gas is toxic, and mixed phases of the metal phosphides are frequently formed. To address these limitations, our group developed a low-temperature solvothermal

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phosphidization method, where metal-organic framework (MOF) precursors are reacted with white phosphorus to generate metal phosphides^[2–4]. The key advantages of this solvothermal phosphidization method are that metal phosphide nanoparticles can be synthesized at a lower temperature (< 473 K), and that the morphology of MOF precursors is preserved in metal phosphides. Furthermore, the structural features of the generated metal phosphide nanostructures can be readily tuned by altering the reactant ratio, solvent, ligand of the MOF, reaction temperature, etc. In addition, we have developed an alternative room-temperature electrodeposition method for preparing amorphous multi-metallic transition metal phosphides^[5].

This dataset reports the experimental electrocatalytic

OER activity of a series of Ni and Co-based phosphides synthesized *via* solvothermal phosphidization or electrodeposition method, and can providing a reference to facilitate the future design of metal phosphide-based materials for electrocatalysis.

1 Main part

1.1 Data profile

Table 1 lists the detailed information of this dataset, including the title, authors, data generation time, data format etc.

Table 1 Specifications of the Dataset

Data title (V0.1)	Electrocatalytic oxygen evolution activity database of nickel and cobalt-based phosphides
Author's name	LU Xinyu, WANG He, WANG Chao
Corresponding author's name	WANG Chao
Data content description	This database contains the experimental oxygen evolution reaction (OER) results for a series of Ni and Co-based phosphides in alkaline electrolyte (1 mol/L KOH). These metal phosphides were synthesized <i>via</i> the solvothermal phosphidization method or the electrodeposition method. The OER activity was evaluated by linear sweep voltammetry (LSV) at scan rates lower than 5 mV/s, using a standard three-electrode setup with a saturated calomel electrode (SCE) as the reference electrode, a graphite rod as the counter electrode, and 1 mol/L KOH as the electrolyte at room temperature. Additionally, the cyclic voltammetry and impedance spectroscopy data for part of the Ni and Co-based phosphides are included, obtained under identical experimental conditions
Data generation time	2020-2025
Data volume	15.2 MB
Data format	.csv, .bin, .txt, .opj
Data source location	https://doi.org/10.57760/sciencedb.32783
Citation format of data	LU Xinyu, WANG He, WANG Chao. Electrocatalytic oxygen evolution activity databased of nickel and cobalt-based phosphides[J]. J Fuel Chem Technol, 2026, 54, 20250386. LU Xinyu, WANG He, WANG Chao . Electrocatalytic oxygen evolution activity databased of nickel and cobalt-based phosphides[DS/OL]. V1. Science Data Bank, 2025. https://doi.org/10.57760/sciencedb.32783 . DOI:10.57760/sciencedb.32783.

1.2 Data value

The dataset presents here is generated from a systematic study of the Ni and Co-based phosphides towards the electrocatalytic OER in alkaline media. The phosphides were synthesized using low-temperature solvothermal method or an electrodeposition method. The data serve as the benchmark for the OER activity of metal phosphide-type materials (Table 2), with the corresponding compositions detailed in Table 3. In Table 2, key parameters in evaluating the OER performance of electrocatalysts are given, including overpotential at 10 mA/cm² (η_{10}), Tafel slope, number of electrochemically active atoms, double layer capacitance (C_{dl}), and charge transfer resistance (R_{ct}). The η_{10} is a widely accepted parameter in the area of OER. A lower η_{10} indicates superior OER activity. Tafel slope and R_{ct} values are related to the OER kinetics. Generally, lower Tafel slope values and R_{ct} values indicate the more favorable kinetics and thus higher catalytic OER activity. Besides, the mechanism of OER can

be inferred from the Tafel slope values. The number of electrochemically active atoms and C_{dl} are related to the number of active sites of the catalysts. Furthermore, users can use the data to compare the OER activity of metal phosphides that are synthesized with variations in methods, surface structures, metal doping, crystallinity and other properties. The format of these data includes .bin (original data file generated using CHI software), .opj (Origin project file), .txt (text file), and .csv (spreadsheet file), which can be easily plotted to compare with the user's experimental results. Through activity comparison and key electrochemical parameter analyses, reasons for the inferior or superior OER activity can be inferred to aid the rational design of more efficient metal phosphide-based electrocatalysts for alkaline OER reaction.

1.3 Data generation method or process

The data were generated using a CHI 660E potentiostat, with the corresponding software developed by the company.

The original data was stored as .bin format. To generate the data, metal phosphide nanostructures were synthesized using the solvothermal phosphidization or electrodeposition method described later. For the samples synthesized using the solvothermal phosphidization method, the working electrode was prepared by drop-casting of an ink that

contains the metal phosphide samples. The substrate used was a piece of cleaned nickel foam or carbon paper. Inks were prepared by dispersing certain amounts of powdery sample in water or water/ethanol mixed solvent, with 1% Nafion ionomer added as the binder.

Table 2 Electrochemical parameters of the nickel and cobalt-based phosphides in 1 mol/L KOH

Label	Crystalline phase	η_{10} /mV	Tafel slope /(mV·dec ⁻¹)	Electrochemical active atoms /(mol·cm ⁻²)	C_{dl} /(mF·cm ⁻²)	R_{ct} /Ω
NiP-1	Ni ₂ P	310	42	6.48×10^{-7}	—	—
NiP-2	Ni ₂ P	263	40	4.84×10^{-7}	—	—
NiP-3	Ni ₂ P	243	30	3.73×10^{-7}	—	0.85
NiP-4	Ni ₂ P	270	43	2.84×10^{-7}	—	—
NiP-5	Ni ₂ P	350	97	8.70×10^{-7}	—	2.16
NiP-6	Ni ₂ P	300	86	1.29×10^{-6}	—	1.39
NiP-7	amorphous	317	108	9.90×10^{-7}	—	0.89
NiP-8	Ni ₂ P	300	145	1.65×10^{-3}	2.22	4.99
NiP-9	Ni ₂ P	283	92	3.48×10^{-4}	2.01	3.16
NiP-10	Ni ₂ P	240	57	2.1×10^{-4}	2.14	2.69
NiP-11	Ni ₂ P	270	63	1.4×10^{-4}	1.90	2.82
NiP-12	Ni ₂ P	215	31	—	60.34	0.33
NiP-13	Ni ₂ P	310	67	—	80.72	2.08
NiP-14	NiCoP	248	49	4.1×10^{-7}	6.6	1.21
NiP-15	Ni ₂ P	293	99	1.8×10^{-7}	2.1	1.71
NiP-16	NiCoP	302	77	8.3×10^{-8}	4.6	1.39
NiP-17	Ni ₂ P	335	138	6.45×10^{-4}	—	3.50
NiP-18	Ni ₂ P	399	151	2.01×10^{-4}	—	10.60
NiP-19	Ni ₂ P	502	200	1.02×10^{-4}	—	25.90
NiP-20	amorphous	230	63	—	2.7	0.56
NiP-21	amorphous	312	168	—	9.8	3.20
NiP-22	amorphous	317	120	—	85.2	—
NiP-23	amorphous	277	64	—	183.6	—
NiP-24	amorphous	320	73	—	220.1	—
NiP-25	amorphous	350	102	—	332.9	—
NiP-26	amorphous	382	122	—	142.2	—
CoP-1	Co ₂ P	275	115	—	5.3	1.26
CoP-2	Co ₂ P	232	92	—	3.2	0.19
CoP-3	Co ₂ P	248	83	—	4.8	1.14
CoP-4	Co ₂ P	262	87	—	5.1	1.30
CoP-5	Co ₂ P	270	112	—	3.8	0.28
CoP-6	Co ₂ P	292	128	—	3.7	0.33
CoP-7	amorphous	301	142	—	4.6	0.30
CoP-8	amorphous	363	135	—	354.9	—
CoP-9	Co ₂ P	300	119	1.76×10^{-3}	21.44	2.31
CoP-10	Co ₂ P	240	53	1.59×10^{-3}	9.07	0.62
CoP-11	Co ₂ P	340	85	3.9×10^{-7}	4.8	5.09

Table 3 Elemental composition of nickel and cobalt-based phosphides by ICP-AES

Label	Mass content/%				Atomic content/%			
	Ni	Fe	Co	P	Ni	Fe	Co	P
NiP-1	28.8	—	—	71.2	17.8	—	—	82.2
NiP-2	19.2	0.7	—	80.2	11.3	0.4	—	88.3
NiP-3	16.2	5.8	—	78.0	9.6	3.6	—	86.8
NiP-4	15.0	7.7	—	77.3	9.0	4.8	—	86.3
NiP-5	71.3	—	—	28.8	57.0	—	—	43.0
NiP-6	50.0	—	—	50.0	34.8	—	—	65.2
NiP-7	32.1	—	—	67.9	20.2	—	—	79.8
NiP-8	79.3	—	—	20.7	67.2	—	—	32.8
NiP-9	46.4	13.3	—	40.0	16.99	5.0	—	27.2
NiP-10	72.0	13.8	—	14.2	63.8	12.7	—	23.5
NiP-11	60.4	23.4	—	16.2	52.6	21.1	—	26.3
NiP-12	68.2	13.5	—	18.3	58.6	11.99	—	29.44
NiP-13	36.6	—	—	63.4	23.6	—	—	76.4
NiP-14	25.3	12.2	25.7	36.7	19.2	9.6	19.2	52.1
NiP-15	43.5	20.1	—	36.4	32.9	15.7	—	51.4
NiP-16	27.5	23.6	—	48.9	19.1	17	—	63.8
NiP-17	56.3	—	—	43.7	40.8	—	—	59.2
NiP-18	33.4	—	—	66.6	21.2	—	—	78.8
NiP-19	23.6	—	—	76.4	14.2	—	—	85.8
NiP-20	47.9	33.5	—	18.6	40.8	29.6	—	29.6
NiP-21	83.7	—	—	16.3	73.3	—	—	26.7
NiP-22	14.8	—	13.9	71.3	9.1	—	8.4	82.4
NiP-23	15.0	—	13.5	71.5	9.3	—	8.2	82.6
NiP-24	15.2	—	13.6	71.2	9.4	—	8.3	82.3
NiP-25	15.3	—	13.2	71.5	9.4	—	8.0	82.5
NiP-26	15.5	—	12.0	72.3	9.5	—	7.3	83.2
CoP-1	—	—	75.0	25.0	—	—	61.2	38.8
CoP-2	—	27.7	41.6	30.7	—	22.6	32.2	45.2
CoP-3	—	18.9	56.6	24.5	—	16.1	46.0	37.9
CoP-4	—	4.2	75.3	20.5	—	3.7	63.4	32.9
CoP-5	—	—	53.4	46.6	—	—	37.6	62.4
CoP-6	—	—	73.6	26.4	—	—	59.4	40.6
CoP-7	—	—	74.0	26.0	—	—	59.9	40.1
CoP-8	—	—	22.2	77.8	—	—	13.0	87.0
CoP-9	—	—	81.0	19.0	—	—	69.2	30.8
CoP-10	—	11.2	81.2	7.6	—	10.9	75.5	13.6
CoP-11	—	5.1	55.4	39.5	—	3.9	40.8	55.3

After sonication for 20 min, appropriate amounts of inks were dropped onto the substrate surface to cover 1 cm² geometric area, to achieve the loading of the metal phosphide on the electrode surface at about 1 mg/cm². For the samples synthesized using the electrodeposition method, no ink was required to prepare the working electrode, as the electrodeposition method was used to generate a thin layer of metal phosphides at the substrate surface with good adhesion. The loading for the electrodeposited film is higher, typically at around 2 mg/cm². The OER activity was measured, and cyclic voltammogram (CV) and electrochemical impedance spectroscopy were performed

using the three electrode setup. Approximately 1 cm² geometric surface area of the working electrode was immersed in the 1 mol/L KOH electrolyte. The counter electrode was a cleaned graphite rod, and the reference electrode was a saturated calomel electrode (SCE). The electrochemical measurements were carried out at room temperature. The CV was scanned for 20 cycles in the potential region of 0–0.6 V vs. SCE to activate the working electrode till a stable CV was acquired. Then anodic or cathodic linear sweep voltammetry (LSV) was applied at 1, 2 or 5 mV/s covering the OER region. The overpotential of OER at a certain current density was acquired following the

Equation (1),

$$\eta = E_{\text{RHE}} - 1.229 \quad (1)$$

where E_{RHE} is the acquire potential in the reversible hydrogen scale and 1.229 V is the standard redox potential for OER. The Tafel slope value (b) is acquired by plotting the LSV curve in the OER region following Equation (2),

$$\eta = b \log j + a \quad (2)$$

where a is a constant, and j is the current density. To acquire the number of electrochemically active sites (n), CV at 50 mV/s is acquired covering the redox of $\text{Ni}^{2+/3+}$ peaks or $\text{Co}^{2+/3+}$ peaks. The total charge (Q) for the reduction peak is integrated. Following Equation (3), n can be acquired.

$$n = Q / zF \quad (3)$$

where F is the Faraday constant, and z is the number of electrons transferred in the redox processes (assumed to be 1). In some cases where the redox peaks are unable to be identified, the C_{dl} was used to estimate the number of surface active sites. CVs in the non-Faradaic region were collected at different scan rates. By plotting the difference between anodic current and cathodic current against the scan rate, the slope yields the C_{dl} value. The electrochemical impedance data were acquired at the applied potential corresponding to the η at 10 mA/cm², with the alternating potential amplitude at 10 mV and the frequency range in 10⁵–0.01 Hz. The solution resistance ranged from 0.5 to 1 Ω , and the LSV data were iR -corrected using the solution resistance value for each sample. The R_{ct} value is acquired from the impedance data.

The crystallinity of the metal phosphides was acquired using a Rigaku Smartlab 9 kW Diffraction System using a Cu $K\alpha$ source ($\lambda = 0.15406$ nm). The composition of the metal phosphides was determined using the inductively coupled plasma-atomic emission spectroscopy (ICP-AES) with an iCAP 7400 analyzer. The measurement conditions are as follows: forward power 1350 W, plasma gas flow rate 12.0 L/min, nebulizer gas flow rate 1.0 L/min, auxiliary gas flow rate 1.0 L/min, sample uptake speed 50 r/min with white/orange Tygon tubing. A concentric nebulizer was used with a cyclonic spray chamber. ICP-AES analysis was performed without an internal standard. Each value was measured three times, and the results are reported in the form of mass ratio and atomic ratio in Table 3.

1.4 Data sample description

The data provided in this database include LSV, CV, and electrochemical impedance data. For NiP-1 to NiP-19, CoP-1 to CoP-7 and CoP-9 to CoP-11, the samples were synthesized using the solvothermal phosphidization method^[1–4,6–9]. These samples are powdery with nanostructures. The general procedure of this solvothermal phosphidization method is as follows: MOF (0.2 g) was dispersed in 30 mL *N,N*-dimethylformamide (DMF). Then 0.15 g white phosphorus (P_4) was added, and the suspension

was transferred into a 50 mL Teflon-lined stainless-steel autoclave. The autoclave was heated at 160 °C for 14 h, and the black precipitates were collected, washed with water, ethanol, and benzene, and dried. All these samples were synthesized following this typical procedure with slight modification as detailed below. NiP-1 to NiP-4 were prepared with NiFe-BTC (trimesic acid) MOF, where different amounts of Ni and Fe exist in the MOF. NiP-6, NiP-7 and NiP-8 were prepared by reacting 0.1 g Ni-BTC MOF with 0.025, 0.065 and 0.105 g P_4 , respectively. NiP-9 to NiP-11 were heterostructures of $\text{Ni}_2\text{P}/\text{FeOOH}$, where Ni_2P was formed using the solvothermal phosphidization method using 0.1 g Ni-BTC MOF and 0.065 g P_4 . Then, 0.02 g Ni_2P was dispersed in 20 mL of water and ethanol with 0.17, 1.33 and 6.67 mg/mL $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ for 4 h at room temperature to form NiP-9, NiP-10 and NiP-11, respectively. NiP-12 and NiP-13 were synthesized using NiFe-BTC-MOF and Ni-BTC MOF with 0.6 mmol P_4 at 180 °C for 12 h. NiP-14, NiP-15 and NiP-16 were synthesized using 0.3 g FeCoNi-BPDC (biphenyl-4,4'-dicarboxylic acid)-MOF, NiFe-BPDC-MOF, and NiCo-BPDC-MOF, respectively, and 0.27 g P_4 . NiP-17, NiP-18 and NiP-19 were synthesized using 0.1 g Ni-BDC (1,4-dicarboxybenzene), Ni-BPDC and Ni-NDC (2,6-naphthalenedicarboxylic acid) MOF, respectively, with 0.065 g P_4 . CoP-1 to CoP-4 were synthesized using CoFe-BTC-MOF with different Co to Fe ratios, with 0.09 g P_4 in DMF/ethylene glycol ($v:v = 1$) solvent at 170 °C for 16 h. CoP-5, CoP-6 and CoP-7 were synthesized using Co-BTC-MOF with 0.09 g P_4 in DMF/ethanol, DMF and DMF/glycerol ($v:v = 1$) solvents, respectively, at 170 °C for 16 h. CoP-9 and CoP-10 were prepared using 0.085 g Co-BTC MOF and CoFe-BTC MOF, respectively, at 170 °C for 14 h. CoP-11 was prepared using 0.3 g CoFe-MOF with 0.27 g P_4 at 160 °C for 16 h.

For NiP-20 to NiP-26 and CoP-8, the samples were synthesized *via* electrodeposition from aqueous electrolytes containing metal ions and sodium hypophosphite^[5,10]. Samples are thin film at the surface of conductive substrates. The general procedure for electrodeposition is as follows. A three-electrode setup was used with a conductive substrate nickel foam or carbon cloth (1 cm²) as the working electrode. The counter electrode was a cleaned graphite rod, and the reference electrode was SCE. The CV method was used to deposit the metal phosphide layers. For NiP-20 and NiP-21, the electrolytes consisted of 0.025 mol/L $\text{Ni}(\text{NO}_3)_2 + 0.025$ mol/L $\text{Fe}(\text{NO}_3)_3 + 0.25$ mol/L NaH_2PO_2 and 0.025 mol/L $\text{Ni}(\text{NO}_3)_2 + 0.25$ mol/L NaH_2PO_2 , respectively. CV scan of -0.3 – (-1) vs. SCE was applied at 5 mV/s for 8 cycles. For NiP-22 to NiP-26, the electrolyte was 0.04 mol/L $\text{Ni}(\text{NO}_3)_2 + 0.01$ mol/L $\text{Co}(\text{NO}_3)_2 + 0.25$ mol/L $\text{CH}_3\text{COONa} + 0.25$ mol/L NaH_2PO_2 . CV scans of -0.3 – (-1) vs. SCE were applied at 5 mV/s for 5, 10, 15, 20 and 25 cycles over NiP-22, NiP-23, NiP-24, NiP-25 and NiP-26, respectively.

Analysis of these data reveals several correlations. For nickel phosphides with the Ni_2P crystalline phase (NiP-5 to

NiP-7), moderate crystallinity exhibits the optimum OER activity. Incorporation of Fe increases the OER activity, and the optimum extent of Fe incorporation lies in 30%–40% (NiP-1 to NiP-4, NiP-12 to NiP-13, CoP-1 to CoP-4 and CoP-9 and CoP-10). Deviation from this optimal Fe content, either higher or lower, compromises OER activity by affecting the OER kinetics, as observed by the increased Tafel slope and R_{ct} values. Forming $Ni_2P/Fe(O)OH$ heterointerface can enhance the OER activity (NiP-8 to NiP-11), with an optimum thickness of the surface $Fe(O)OH$ layer, reflected by the atomic percentage of Fe (NiP-10). Compared to samples from solvothermal phosphidation, metal phosphides prepared *via* electrodeposition usually exhibits higher C_{dl} values, which probably due to more uniform electrode surface coverage and higher specific surface area.

1.5 Data quality

To ensure the reliability and repeatability of sample preparation, all these samples were synthesized at least three times, and the electrochemical measurements were performed using different batches of samples. The reported results represent the average activity performance of these phosphides. In the three electrode tests, the pH value of the electrolyte was measured using a pH value meter, and the reference electrode potential was calibrated against a new SCE before and after each test. The overpotential values and R_{ct} are reported as the average from more than three independent tests.

1.6 Data usage methods and suggestions

It is recommended that when using these data, users should first identify the synthesis method before making a fair comparison, as the surface states of powder-based and electrodeposited working electrode differ significantly. Typically, metal phosphides synthesized *via* the solvothermal phosphidization method exhibit a higher surface phosphorus content. Furthermore, when comparing with OER activity data generated from other sources, attention should be paid to the key variables including the synthetic method, test temperature, electrolyte, active material loading, and the composition. The data provided in the .bin file are directly generated without any post-treatment. Some data is provided in the .opj file, where the potential is adjusted to the RHE scale, and where iR -compensation is applied. For convenience and optimal comparability, data in the .opj file are preferably recommended.

2 Conclusion

A database of the OER activity of Ni and Co-based metal phosphides is constructed based on experimental results.

The dataset encompasses phosphides synthesized *via* solvothermal phosphidization and electrodeposition methods. It provides key electrocatalytic parameters, and enables the analysis of the influence of metal doping, solvothermal condition (solvent and precursors), and crystallinity on the OER activity. This dataset can serve as a benchmark for evaluating Ni and Co-based phosphide materials for alkaline OER, and provides a foundation for designing more active metal phosphide-based electrocatalysts through comparative analysis. The metal phosphides reported in this dataset can be potentially applied as electrocatalytic materials for other critical reactions, including hydrogen evolution, alcohol oxidation, and carbon dioxide reduction reactions, which are vital for energy conversion devices such as fuel cells, electrolyzers, and metal-air batteries. In addition, these nanostructured metal phosphides can be applied as the electrode materials in lithium or sodium ion batteries, and as protective anticorrosion coating on metal surface protection.

Data availability statement

The data supporting the results in this study has been published in sciencedb database and can be obtained through DOI: [10.57760/sciencedb.32783].

Declaration of Competing Interest

The authors declare no conflict of interest.

References

- [1] XING Y, LIU S, LIU Y, et al. Construction of nickel phosphide/iron oxyhydroxide heterostructure nanoparticles for oxygen evolution[J]. Nano Energy, 2024, 123: 109402.
- [2] WANG C, CHAI L, LUO C, et al. Solvothermal preparation of nickel-iron phosphides hollow nanospheres derived from metal-organic frameworks for water oxidation reaction[J]. Appl Surf Sci, 2021, 540: 148336.
- [3] WANG C, CHAI L, CUI X, et al. Amorphous/crystalline heterostructured nickel phosphide nanospheres for electrocatalytic water and methanol oxidation reactions[J]. J Phys Chem C, 2021, 125(39): 21443–21452.
- [4] LIU S, CUI X, WANG Q, et al. Iron and oxygen codoped cobalt phosphide solvothermally prepared from a metal-organic framework for oxygen evolution[J]. J Phys Chem C, 2022, 126(36): 15205–15214.
- [5] WANG C, WU Y, ZHOU Z, et al. Electrodeposited amorphous nickel-iron phosphide and sulfide derived films for electrocatalytic oxygen evolution[J]. Int J Hydrog Energy, 2022, 47(97): 40849–40859.
- [6] GAO J, LIU S, LI Z, et al. Cobalt phosphide nanoparticles synthesized by solvothermal phosphidization of metal-organic frameworks for electrocatalytic oxygen evolution[J]. Int J Energy Res, 2023, 2023(1): 3893229.
- [7] TONG J, XING Y, XIAO X, et al. Iron-doped cobalt

- phosphide nanowires prepared via one-step solvothermal phosphidization of metal-organic frameworks for the oxygen evolution reactions[J]. Green Chem, 2024, 26(9): 5308–5325.
- [8] WANG Z, LIU S, DU J, et al. Iron-doped nickel phosphide hollow nanospheres synthesized by solvothermal phosphidization of layered double hydroxides for electrocatalytic oxygen evolution[J]. Green Chem, 2024, 26(13): 7779–7788.
- [9] LIU X, HU Z, XING P, et al. Construction of iron-doped nickel cobalt phosphide nanoparticles via solvothermal phosphidization and their application in alkaline oxygen evolution[J]. J Colloid Interface Sci, 2025, 677: 441–451.
- [10] CHAI L, LIU S, PEI S, et al. Electrodeposited amorphous cobalt-nickel-phosphide-derived films as catalysts for electrochemical overall water splitting[J]. Chem Eng J, 2021, 420: 129686.

镍基及钴基磷化物碱性电催化析氧反应数据集

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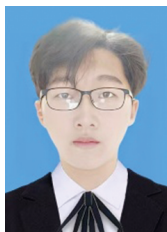
摘 要: 氢能作为能源载体是缓解化石燃料使用带来的环境问题的有前景的解决方案。开发高效且廉价的碱性析氧电催化剂对加速碱性水电解槽的广泛应用至关重要。过渡金属磷化物有望成为高活性且稳定的析氧催化剂。此数据集收集并比较了镍和钴基磷化物的电催化析氧反应活性。数据集中的金属磷化物样品由溶剂热磷化或电沉积技术合成, 并使用线性扫描伏安法在 1 mol/L KOH 中评估了这些磷化物的析氧活性。此外, 还对这些金属磷化物进行了循环伏安法和电化学阻抗谱分析。数据集大小为 14.5 MB, 包含 312 个文件。此数据集的数据能够为设计高性能金属磷化物电催化剂提供实验依据。

关键词: 磷化镍; 磷化钴; 析氧反应; 碱性

中图分类号: O646.51

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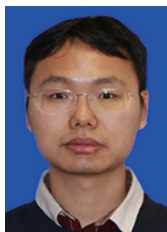
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