

A dataset for electrocatalytic hydrogen evolution reaction performance of non-noble transition metal phosphides

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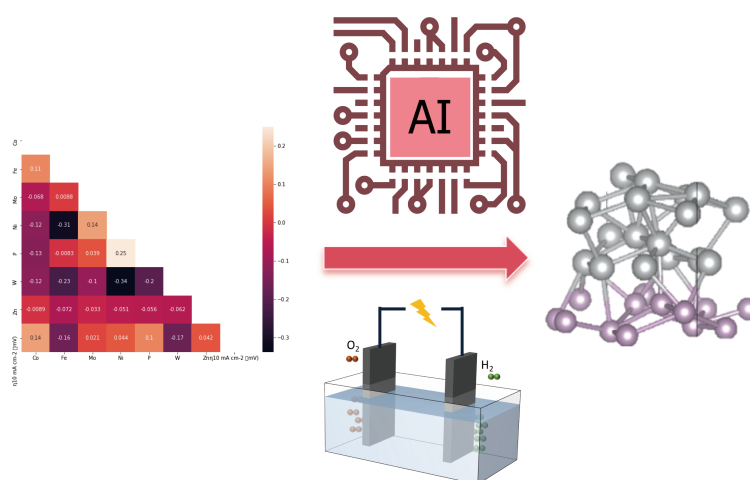
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Abstract: This dataset compiles the HER performance data of 203 non-noble transition metal phosphide (TMP) catalysts, covering detailed information on catalyst preparation (e.g., phosphating temperature, precursor, synthesis method), chemical composition (mass fractions of elements such as Ni, Co, Fe, P, Mo, W and Zn), and testing conditions (e.g., electrolyte type and concentration, electrode substrate). The key parameters for catalytic performance include the overpotential at 10 mA/cm² (η_{10}) and the Tafel slope. This dataset has been rigorously extracted, cleaned, and

standardized to ensure a high degree of structure and machine readability. This provides a reliable data foundation for data-driven methods, such as machine learning and statistical modeling, enabling rapid screening and design of high-performance HER catalysts, supporting performance prediction, in-depth structure-activity analysis and the rational development of novel catalysts.

Key words: water electrolysis for hydrogen evolution; transition metal phosphides; dataset; catalyst; machine learning



Hydrogen energy, recognized for its high energy density and zero-carbon emissions, which is widely regarded as a key clean energy source for achieving global energy transition and carbon-neutrality goals^[1–2]. Among various hydrogen-production technologies, water electrolysis for hydrogen evolution reaction (HER) can directly convert renewable electricity into chemical energy, offering high-purity hydrogen with a pollution-free process, thereby representing an ideal route for green hydrogen production^[3–4]. However, the high energy consumption caused by slow reaction kinetics hinders its large-scale commercial application. The solution to this problem relies

on high-performance electrocatalysts. Although noble-metal catalysts such as platinum (Pt) remain the performance benchmark, their extreme scarcity and high cost limit their widespread application. Therefore, developing non-noble metal-based catalysts that combine high activity, high stability, and low cost has become a challenge and research focus for promoting the large-scale application of HER^[5].

Among the many non-noble metal-based catalysts that have been developed, transition metal phosphides (TMPs) have become highly promising catalysts for the HER in recent years^[6–7]. During HER process, these catalysts can induce unique electronic restructuring, generating electron-

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rich P sites and electron-deficient metal sites, thereby synergistically optimizing the hydrogen adsorption free energy and improving intrinsic activity^[8–9]. Furthermore, TMPs exhibit metallic-like conductivity, excellent mechanical strength, and corrosion resistance in acidic, alkaline, and even neutral electrolytes. Through strategies such as elemental doping (such as Fe, Co, Mo)^[10–12], structural engineering (including the construction of porous, hollow, or core-shell structures)^[13], and interface engineering (e.g., the construction of heterojunctions)^[14–15], researchers have developed a series of TMP-based catalysts with catalytic performance approaching that of commercial Pt/C. For instance, Zheng et al.^[16] used an *in situ* hydrothermal method to grow Ni₂P nanocrystals on black phosphorus (BP) nanosheets, constructing a Ni₂P/BP heterojunction. This resulted the formation of built-in electric field from BP to Ni₂P can promote interfacial charge transfer and optimize the *d*-band center of Ni active sites, leading to markedly improved HER activity in alkaline electrolyte. The catalyst requires only 85 mV overpotential at a current density of 10 mA/cm² and can operate stably for 125 h, showing promising application prospects. Furthermore, the synergistic strategy of rare earth doping and carbon coating provides a new approach to improve the overall performance of TMPs. For example, Su et al.^[17] constructed cerium-doped and carbon-coated NiCoP nanorod arrays on nickel foam (Ce-NiCoP@C/NF). The as-introduced Ce species can not only induce lattice distortion and enhance structural stability of NiCoP, but also significantly promote strong bonding between the carbon layer and the phosphide surface, effectively preventing carbon detachment. This catalyst achieved an HER overpotential of only 37 mV at 10 mA/cm² in alkaline medium and required a cell voltage of merely 1.51 V for overall water splitting, outperforming the commercial RuO₂||Pt/C system. However, TMP-based catalysts still face challenges such as limited numbers of active sites,

insufficient long-term operational stability, and difficulty in predicting the optimal stoichiometry, which require more systematic and in-depth research into their structure-activity relationship.

To address these challenges and accelerate the rational design of TMP catalysts, data-driven machine-learning (ML) techniques have shown unprecedented potential^[18–19]. ML can learn and uncover complex hidden patterns from massive, multi-dimensional experimental data, establishing accurate mapping models from material features (for example, elemental composition, synthesis parameters, and morphology) to target properties (including overpotential and Tafel slope), thereby enabling effective performance prediction and high-throughput screening of new materials^[20–21]. However, the accuracy and generalizability of ML models strongly depend on high-quality, standardized, and large-scale datasets. Currently, experimental data in this field are scattered across various publications, with inconsistent formats and testing standards, which hinders the effective application of ML in the HER. Therefore, this work aims to construct a standardized dataset for the HER performance of transition-metal phosphides in water electrolysis, as shown in Figure 1. This dataset systematically integrates catalyst preparation information, multi-element composition, testing conditions, and key catalytic parameters, aiming to establish a reliable data benchmark for this field. This provides a solid data foundation for subsequent ML-assisted catalyst design, in-depth structure-activity relationship analysis, and rapid discovery of new materials. Unlike traditional research papers that use datasets for ML training, this data paper focuses primarily on describing and validating the dataset, elucidating its generation, composition, and inherent limitations. Thus, this dataset helps promote data sharing, which provides valuable data resources for understanding the design and development strategies of water electrolysis catalysts.

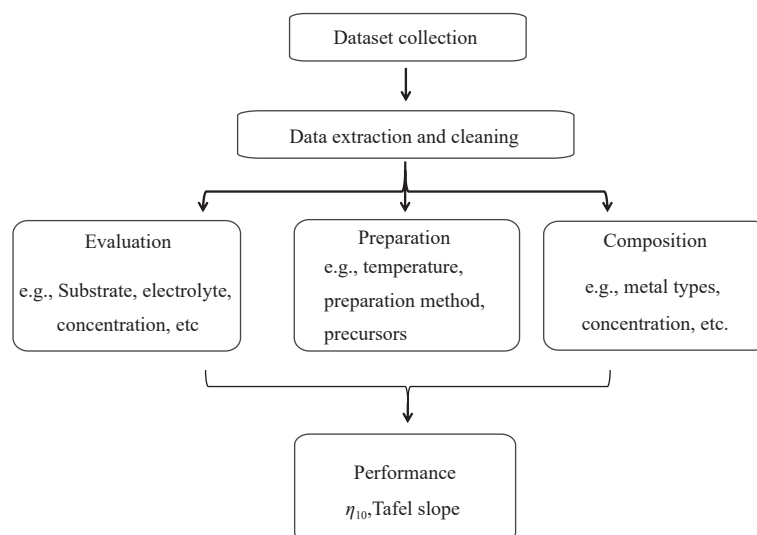


Fig. 1 The workflow for data collection in this work, and the key catalytic performance parameters are the overpotential at 10 mA/cm² (η_{10}) and the Tafel slope

1 Dataset description and discussion

1.1 Data value

The basic information of this dataset is described in Table 1. The core value of this dataset lies in providing a structured benchmark for the study of non-noble transition metal phosphide (TMP) electrocatalysts in HER. Through the integration of TMP catalysts, the dataset offers insights into revealing macroscopic performance trends and structure-activity relationships. The violin plots of overpotential and Tafel slope (Figure 2(a), (b)) visually illustrate the overall performance levels of existing TMP catalysts. The results show that the overpotential (η_{10}) is densely distributed in the range of 50–200 mV, while the Tafel slope is concentrated between 50–100 mV/dec, which provides a clear reference for evaluating the competitiveness of newly developed

catalysts. As shown in Figure 2(c), the relationship between overpotential and Tafel slope further demonstrates a certain positive correlation. Some of these TMP catalysts exhibit both low overpotential and low Tafel slope, representing a direction for high-performance optimization, which indicates the potential of TMP catalysts to replace noble metal Pt-based catalysts for HER. Furthermore, it can be clearly seen from Figure 2(c) that the pH environment of the electrolyte has a significant impact on the catalyst performance, which is relatively low in acidic electrolytes.

From the preparation parameters and composition information in the dataset, the violin plot of phosphidation temperature (Figure 3(a)) clearly shows that the phosphidation temperatures in the dataset are mainly concentrated between 200–400 °C, providing foundational data for the key process parameters in TMP catalyst preparation.

Table 1 Dataset basic information of electrocatalytic hydrogen evolution reaction performance of non-noble transition metal phosphides

Data title	A dataset for electrocatalytic hydrogen evolution reaction performance of non-noble transition metal phosphides
Author's name	ZHU Teng, WANG huanhuan, LI Yuming
Corresponding author's name	LI Yuming
Data content description	This dataset comprises 203 HER performance data points for TMP catalysts, covering various active metal elements (Co, Fe, Mo, Ni, W, Zn) and their combinations. Each data point includes a total of 20 feature fields grouped into three main categories: (1) synthesis information (including catalyst name, metal-component preparation method, phosphidation method, phosphidation temperature, phosphorus precursor); (2) composition information (including mass fractions of P, Ni, Co, Fe, Mo, W, Zn); and (3) performance testing information (including substrate electrode used, electrolyte type, electrolyte concentration). The output variables are the overpotential (mV) at 10 mA/cm ² and the Tafel slope (mV/dec).
Data generation time	2017–2025
Data volume	203 entries/83 KB
Data format	.xlsx
Data source location	https://doi.org/10.57760/sciencedb.j00124.00327
Citation format of data	ZHU Teng, WANG huanhuan, LI Yuming. A dataset for electrocatalytic hydrogen evolutionreaction performance of non-noble transition metalphosphides[J]. J. Fuel Chem Technol, 2026, 54(7): 20250390. ZHU Teng, WANG huanhuan, LI Yuming. A dataset for electrocatalytic hydrogen evolutionreaction performance of non-noble transition metalphosphides[DS/OL]. Science Data Bank, 2026, https://doi.org/10.57760/sciencedb.j00124.00327 . DOI:10.57760/sciencedb.j00124.00327.

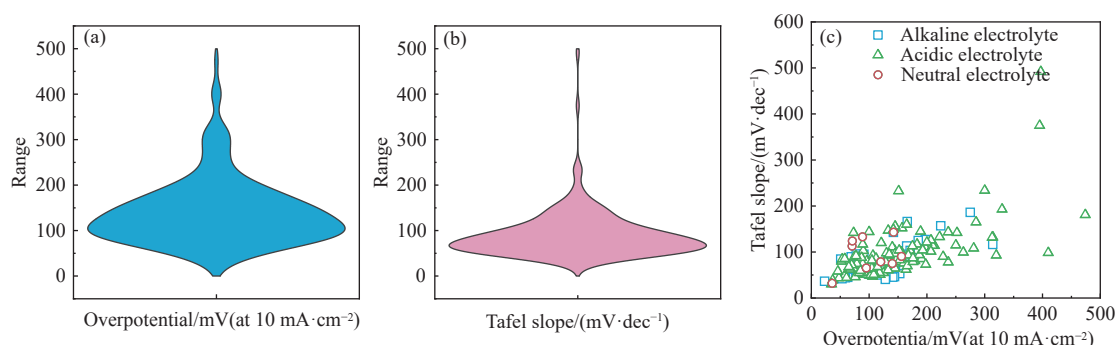


Fig. 2 (a) Violin plot of overpotential data measured at current density of 10 mA/cm²; (b) Violin plot of Tafel slope data; (c) The relationship between overpotential at current density of 10 mA/cm² and Tafel slope

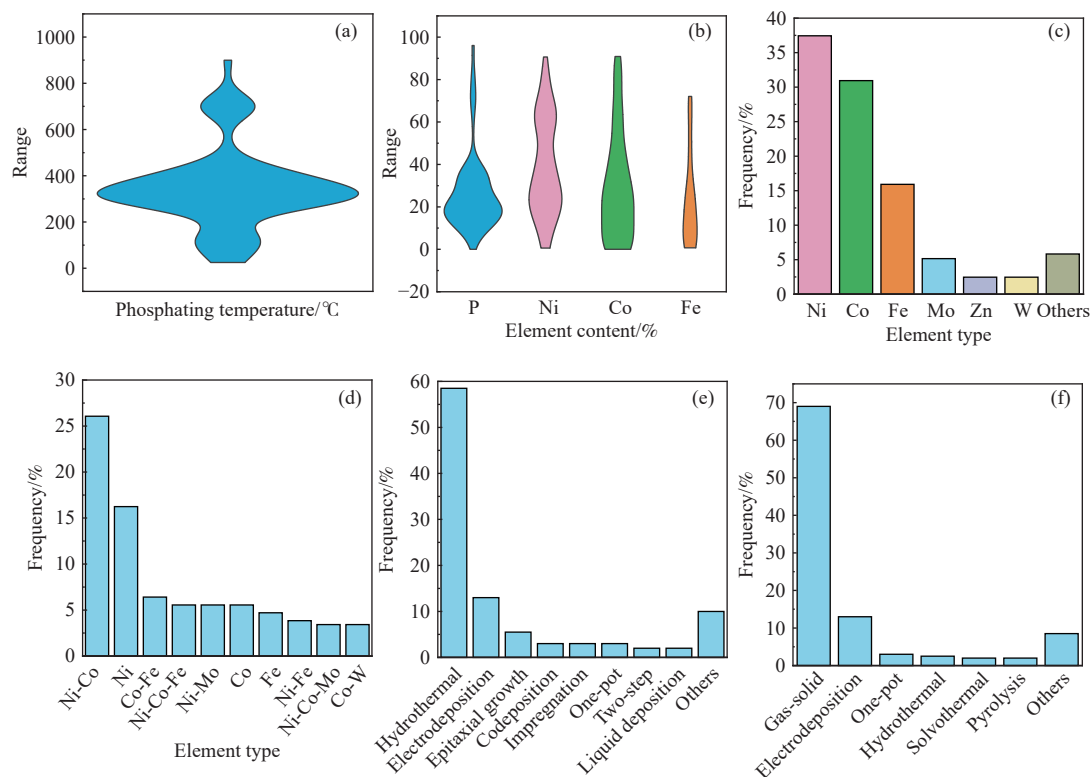


Fig. 3 (a) Violin plot of phosphidation temperature for catalyst preparation; (b) Violin plot of the weight content of selected catalyst elements; (c) Distribution of primary element types in catalyst composition; (d) Distribution of the top 10 most frequent multi-element composition types; (e) Statistics analysis of preparation methods for metal precursors; (f) Statistics analysis of phosphidation methods for catalysts

Statistical analysis of element occurrence frequency further validates the importance of the dataset from another dimension. As shown in Figure 3(b)–(d), Ni, Co, Fe and P are the most frequently used elements in the dataset, reflecting the current consensus and preference for elements and their combinations in TMP catalysts. Synthetic method analysis (Figures 3(e), (f)) shows that for TMP catalysts, the preparation of metal precursors and phosphating methods are mainly based on hydrothermal synthesis, which highlights the importance of expanding the synthetic methods in this field. Combining this data-driven approach with feature importance and statistical analysis promises to guide experiments, optimizing research directions and element selection strategies. Furthermore, it can reduce the blind spots inherent in traditional trial-and-error methods.

1.2 Data generation method or process

This dataset was constructed following a rigorous data engineering workflow, comprising three key stages: data collection, extraction, and cleaning and standardization. All raw data were derived from publicly available, high-quality academic journals and underwent systematic literature review to ensure the authority and representativeness of the data sources. From each publication, three major categories of information were extracted, and those are synthesis information (including metal-precursor preparation method, phosphidation method, phosphidation temperature,

phosphorus precursor, and electrode substrate), composition information (element type, mass fraction, etc.), and catalytic evaluation information (electrolyte type and concentration). In the data processing phase, the extracted data were first standardized. For elemental composition data, a data-pivoting and grouping-summation approach was used to unify dispersed element contents into normalized mass fractions. Categorical variables such as synthesis methods and electrolyte types were converted into a machine-readable numerical format by one-hot encoding. Regarding catalytic performance, the overpotential at 10 mA/cm² (η_{10}) and the Tafel slope were adopted as the output variables, because η_{10} is explicitly reported in most publications and serves as a key indicator for cross-study comparison. Although the onset potential is also an important parameter for HER, it was not included as a catalytic performance indicator in this dataset due to inconsistencies in related literature and unclear definitions. This systematic data-processing workflow ensures internal consistency and machine readability of the dataset, which lays a solid foundation for subsequent data analysis and modeling.

1.3 Data sample description

This dataset is organized in a structured table format, where each row corresponds to an independent catalyst sample and each column represents a specific feature or catalytic performance. A typical data record includes the

following information, including the major elemental composition distribution of the catalyst, such as phosphorus content (~10%–40%), nickel content (~20%–60%), and cobalt content (~10%–40%); preparation conditions including phosphidation temperature (predominantly within 300–400 °C), phosphidation method (mainly gas-solid phase method), and electrode substrate (including carbon cloth, nickel foam, glassy carbon electrode, etc.); as well as electrochemical performance parameters such as overpotential (50–200 mV) and Tafel slope (40–100 mV/dec) at a current density of 10 mA/cm². As shown in Figure 3, the violin plot of the frequency distribution of element content and element combination types helps in understanding the data. The results of data analysis indicate that despite the diverse combinations of metal elements, several multi-component systems, such as Ni-Co, Co-Fe and Ni-Co-Fe, are currently the mainstream in TMP-based HER catalyst research. These statistical trends can not only reflect the differences in catalyst composition and preparation conditions, but also relate to the catalytic performance, thereby providing a visual analysis for understanding composition-performance relationships.

1.4 Data quality

To ensure the reliability and accuracy of the data, each data point is annotated with its original literature source, establishing a complete data-lineage record. During the data-extraction stage, strict selective standard was applied, and only samples that provided full preparation details, elemental composition, and key catalytic performance data were collected, while records with incomplete information were excluded.

To address potential discrepancies in test conditions across the literature, we implemented data standardization to maximize data comparability. For example, we used the overpotential at a current density of 10 mA/cm² as the core catalytic performance indicator, which represents different testing conditions in a uniform normalized manner. Regarding missing values, samples lacking critical features such as elemental content and/or overpotential value were removed, and this can ensure that all final data possess a high degree of information completeness. In addition, we conducted consistency tests such as correlation heatmap analysis to examine the intrinsic relationships between variables, thereby effectively identifying and handling potential outliers or contradictory data, and ensuring the overall quality and reliability of the dataset.

Some catalyst parameters, such as catalyst particle size, are important factors influencing the HER performance. However, the available data on these parameters are scattered and incomplete, resulting in low data quality. Therefore, these parameters have not been included in the current version of the dataset. It is recommended that future studies systematically report such information to facilitate more efficient and comprehensive machine-learning analysis.

1.5 Data usage methods and suggestion

This dataset supports a variety of application areas and analytical methods. For machine learning research (Figure 4), the dataset can be used for regression tasks (predicting overpotential or Tafel slope). Before modeling, researchers can refer to the feature importance histograms provided in this study (e.g., SHAP analysis results) to determine the priority of key features and perform appropriate feature engineering. Preliminary modeling results indicate that for the overpotential, the random forest (RF) model achieved an R^2 of 0.72 on the training set and 0.437 on the test set, while for the Tafel slope, the XGBoost model yielded an R^2 of 0.722 (training set) and 0.307 (test set). The corresponding root-mean-square errors (RMSE) were 0.0018 (training set) and 0.0037 (test set) for the RF-predicted overpotential and 0.125 (training set) and 0.126 (test set) for the XGBoost-predicted Tafel slope. Therefore, it is recommended that RF and XGBoost algorithms be used as the starting point for predictive modeling of this dataset.

For the field of catalysis, the dataset can be directly employed for in-depth statistical analysis. Scatter plots between elemental composition and catalytic performance (e.g., the influence of P or Ni content on overpotential) provide an intuitive way to explore univariate trends. Cluster analysis combined with violin plots of catalytic performance distributions enables rapid assessment of the potential HER activity of different active components. A particularly valuable approach is the integration of model-interpretability tools such as SHAP, which can quantitatively uncover key factors governing catalytic performance from trained machine-learning models. For instance, SHAP analysis clarifies intrinsic determinants of HER performance. It suggested that lower phosphorus content tends to lower the overpotential, which can be due to the modulation of electronic structure of metal sites with an optimal amount of phosphorus. Besides, the combination of low Ni and high Fe contents would lead to the increase of overpotential, highlighting the need for precise tuning of bimetallic synergy. Moreover, lower phosphidation temperatures favor the formation of highly active catalysts. For Tafel slope, higher phosphorus content would reduce its value, implying the improved reaction pathways and charge-transfer kinetics. These findings reveal the complexity of performance-governing factors. For example, the effects of phosphorus content on thermodynamic parameters (overpotential) and kinetic parameters (Tafel slope) differ, indicating a need to find the optimal balance point. These key features and mechanisms can serve as important descriptors for constructing catalyst performance prediction models, which helps in the rational design of high-performance catalysts. When developing novel catalysts, key focus should be placed on the preferred metal element combinations (e.g., Ni-Co and Co-Fe) and optimized phosphating temperature ranges revealed by the dataset.

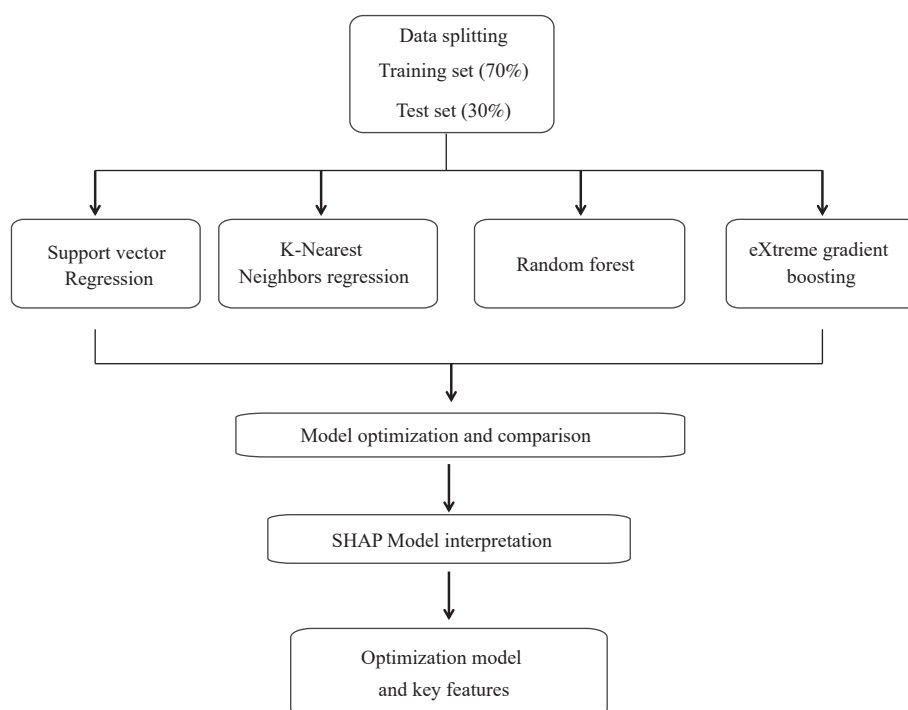


Fig. 4 Workflow for machine learning used in this study

Furthermore, the performance prediction model based on this dataset can be used for preliminary screening of candidate formulations before experiments. In addition, scatter plots can be used to compare predicted and actual values to evaluate the reliability of the model, which significantly improves research efficiency and reduces experimental costs and time.

In the field of HER, the onset potential is also an important performance parameter. However, due to inconsistent reporting or large variations in test conditions across the collected literature, this parameter was not included as a catalytic performance parameter in this dataset. Therefore, it is recommended that future studies uniformly report onset potential to facilitate more comprehensive analysis.

2 Conclusion

This study successfully constructed a dataset on the hydrogen evolution reaction (HER) performance over transition metal phosphides (TMPs) based catalysts. This dataset integrates preparation details, multi-element compositions, testing conditions, and key catalytic performance of catalysts reported in multiple published studies, forming a structured and standardized data resource. Through statistical analysis and visualization, this dataset reveals the macroscopic trends in the catalytic performance, elemental composition, and process selection of current TMP catalysts, providing a benchmark for catalyst evaluation and design. Furthermore, the effectiveness of the dataset in predicting catalytic performance was validated using multiple machine learning algorithms. Moreover, the application of SHAP model

interpretation quantitatively identified phosphorus content, nickel content, and phosphidation temperature as the most critical features influencing HER performance, offering clear directions for rational catalyst design.

This dataset provides the first systematic database of TMP-based catalysts in the HER field, demonstrating the significant potential of data-driven methods in accelerating the screening and development of high-performance catalysts. Through data sharing and model collaboration, this dataset is expected to promote the rapid advancement of green hydrogen production technologies.

Declaration of Competing Interest

The authors declare no conflict of interest.

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非贵金属基过渡金属磷化物电解水析氢性能数据集

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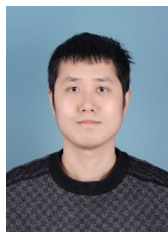
摘 要: 本数据集收集与整理了来自 203 种非贵金属基过渡金属磷化物(TMPs)催化剂的电解水析氢反应(HER)性能数据。数据涵盖了广泛的催化剂制备信息(如磷化温度、前驱体、制备方法)、化学元素组成信息(如 Ni、Co、Fe、P、Mo、W、Zn 等元素的质量分数)以及性能测试条件(如电解质类型与浓度、电极基底)。关键性能指标为在 10 mA/cm² 电流密度下的过电位(η_{10})和塔菲尔斜率。本数据集经过严格的提取、清洗与标准化处理, 具有高度的结构化和机器可读性, 为通过数据驱动方法(如机器学习、统计建模)快速筛选和设计高性能 HER 催化剂提供了坚实的数据基础, 可用于催化剂的性能预测、构效关系深度分析以及新催化剂的理性开发。

关键词: 电解水制氢; 过渡金属磷化物; 数据集; 催化剂; 机器学习

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