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EMERGING STRATEGIES IN PHASE-TUNED PEROVSKITE MATERIALS FOR EFFICIENT HYDROGEN EVOLUTION: A MACHINE LEARNING PERSPECTIVE

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ABSTRACT

Phase-tuned perovskite materials have emerged as promising candidates for hydrogen production due to their excellent optoelectronic properties, flexible compositions, and structures. Phase engineering strategies, including strain induction, doping, and temperature-driven phase transformations, has significantly enhanced the tuning of bandgaps, charge transport, and catalytic activity. This review synthesizes current strategies for enhancing hydrogen evolution reactions (HER) efficiency in both oxide and halide perovskite systems through phase manipulation. The integration of machine learning (ML) into research accelerates the discovery of efficient HER catalysts by predicting optimal phase configurations, identifying novel compositions, and streamlining experimental efforts. Specifically, ML enhances phase tuning by analyzing vast compositional spaces, uncovering structure-property relationships, and guiding the design of phase-engineered perovskites with improved hydrogen evolution efficiency. Particular attention is directed towards AI-assisted studies on materials such as $La_{1-x}Sr_xFeO_3$ and $BaTiO_3$, which demonstrate strong correlations between phase configuration and HER performance. This review uniquely bridges the gap between phase engineering and data-driven approaches, highlighting how ML augments rational design by reducing trial-and-error experimentation. This work also outlines key challenges, including phase stability, model interpretability, and data limitations while proposing future directions for the development of robust, scalable perovskite-based photocatalysts. The insights presented serve as a foundation for advancing clean and efficient hydrogen production technologies.

Keywords: Artificial intelligence, Machine learning, Perovskites, Phase engineering, HER

INTRODUCTION

The increasing demand for renewable energy has driven attention towards hydrogen production via photocatalytic water splitting. Perovskite oxides and halides, characterized by their structural versatility and tunable electronic properties, hold significant promise for this application. It has been proven that strategies such as strain engineering, doping can substantially alter the photocatalytic performance of perovskite oxides, resulting to enhanced hydrogen evolution reaction (HER) efficiencies (Xiao *et al*., 2025). Furthermore, the leveraging of machine learning (ML) techniques has made easy the screening, optimization, and rational design of perovskite materials, as a result accelerating the discovery of efficient photocatalysts (Jacobs *et al*., 2023).

Phase engineering is the deliberate manipulation of a material's crystal structure, it has been identified as a unique strategy for tailoring the electronic and optical properties of perovskite materials to enhance photocatalytic performance of perovskite based materials. By inducing phase transitions, the band gaps and charge carrier dynamics can be modulate, thereby improving light absorption and charge separation efficiency (Jianjian *et al*., 2023). For instance, Bi-doped LaFeO3 shows a phase-driven improvement in photocatalytic activity of over 30% compared to its undoped form (Cao et al., 2024). These phase changes also affect octahedral tilting and metal-oxygen bond angles, which are crucial in facilitating better light absorption and longer carrier lifetimes. To accelerate this design process, machine learning (ML) has become increasingly valuable. ML algorithms, including random forest regressors and neural networks, are used to predict bandgaps, phase stability, formation energy, and HER activity based on structural and compositional features. Trained on data from high-throughput DFT simulations and experimental databases, these models can screen thousands of compositions within hours, drastically reducing the cost and time of discovery compared to conventional trial-and-error methods (Jacobs et al., 2023; Deng et al., 2025). Notably, ML-guided screening has identified previously overlooked perovskites with predicted HER efficiencies above 85% theoretical solar-to-hydrogen (STH) conversion benchmarks.

Despite these advances, several challenges persist. Stability under operational conditions, data quality variability, and the interpretability of ML models remain obstacles to implementation. Furthermore, vague classifications such as AI-assisted often overlook distinctions between supervised learning, deep learning, and model-experiment integration strategies. As the field evolves, addressing these limitations is crucial to fully unlocking the synergy between phase-tuned materials and ML-driven design. Additionally, the integration of AI and quantum computing holds promise for further accelerating the discovery and optimization of efficient photocatalysts (Wayo *et al*., 2024).

This review seek to synthesize recent advances in phase engineering of perovskite materials for HER, with a particular focus on the integration of ML approaches. We examine how these strategies intersect, provide examples of successful applications and propose future directions for data-driven materials discovery. By articulating current trends, key challenges, and emerging opportunities, this review intends to contribute a comprehensive roadmap for the rational design of perovskite-based photocatalysts for hydrogen production.

MATERIALS AND METHODS

Review Methodology

This review was conducted to synthesize recent advances at the intersection of phase engineering, perovskite photocatalysts and ML applications for hydrogen evolution. To ensure comprehensive and relevancy, literature was sourced from major scientific databases including Scopus,

Web of Science, ScienceDirect and IEE Xplore. Search terms used includes: Perovskite and phase engineering, photocatalytic hydrogen production, machine learning and perovskite, HER and AI and ML-assisted photocatalysis. A total of 70 articles were initially screened, from which 37 studies were selected for full-text analysis based on their methodological rigor, novelty and relevance to the review themes.

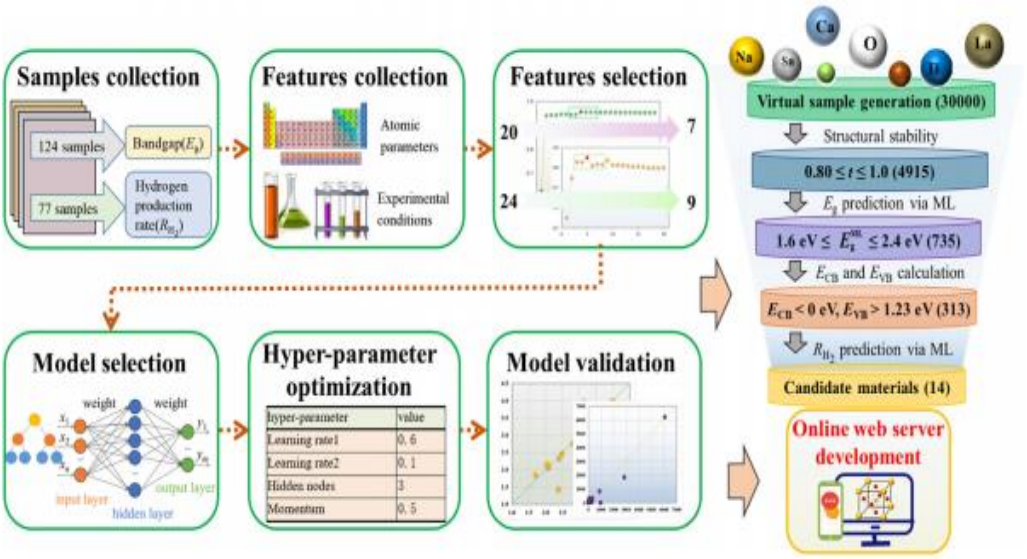

Figure 1: The flowchart of materials ML by Tao *et al*. (2021)

Table 1: Comparison Table of ML Models, Perovskite Types and HER Outcome

Work/Year	ML Model	Input Features	Perovskite System	Predicted Outcome	HER Performance/ Accuracy
Deng *et al*., (2025)	Random Forest (RF)	Bandgap, electronegativity, ionic radius	ABO_3 oxides ($LaFeO_3$, $SrTiO_3$)	HER activity, band alignment	~89%
Hung *et al*., (2025)	Convolutional Neural Network (CNN)	XRD pattern images	Mixed oxide perovskites	Phase classification and HER phase prediction	Accuracy ~93%
Luhan *et al*., (2024)	Neural Network (ANN)	Atomic radii, coordination number, formation energy	$BiFeO_3$, $BaTiO_3$ variants	Stability and HER potential	MAE ~0.12ev, 30% phase driven HER improvement
Jacobs *et al*., (2023)	Support Vector Machine	Structural descriptors + DFT data	Halide perovskites	Phase classification and HER phase prediction	Accuracy ~93% identified active mixed-phase $BiFeO_3$
Yang *et al*., (2021)	Active Learning (AL) with RF	Incremental DFT dataset	$La_{1-x}Sr_xFeO_3$	Optimal doping level for best HER performance	Reduced screening time by ~80%; accurate up to 95%
Zhou *et al*. (2018)	Unsupervised PCA + Clustering	DFT band structure vectors	ABO_3 perovskites	Grouped HER-efficient structures by geometry	Identified 5 new HER-relevant structural Motifs

Fundamentals of Perovskite Materials for Hydrogen Evolution

Perovskite materials have sparked intense attention over the years in the field of renewable energy conversion due to their unique structural versatility and excellent optoelectronic properties. The generic formula for perovskites is ABX_3, where A is a large cation (e.g., Cs^+, MA^+, or La^{3+}), while B is a smaller cation (e.g., Ti^{4+}, Fe^{3+}), and X typically denotes an anion such as oxygen or a halide. This structure allows for extensive chemical substitutions, enabling the precise control over electronic and structural properties for specific functionalities such as the hydrogen evolution reaction (HER) (Doggali *et al*., 2015).

In the field of photocatalytic hydrogen production, useful material parameters of perovskites include suitable bandgap energies (typically 1.5–2.5 eV), high carrier mobility, and band edge alignment with the redox potentials of water. For HER, the conduction band minimum (CBM) of the perovskite must lie above the hydrogen evolution potential (0 V vs. NHE), while the valence band maximum (VBM) should be below the oxygen evolution potential (+1.23 V vs. NHE) to facilitate overall water splitting (Shah *et al.,* 2017). Materials

such as $SrTiO_3$, $BiFeO_3$, and $LaFeO_3$ have demonstrated potential in satisfying these conditions under visible light.

However, despite these attractive properties, the practical integration of conventional perovskites is hampered in HER applications. These limitations include photocorrosion, poor chemical stability in aqueous environments, and charge carrier recombination. But, the structural phase of perovskites plays a crucial role in determining their photocatalytic performance, as phase changes can significantly alter material's band structure and surface reactivity (Temerov *et al*., 2022)

Addressing these limitations necessitates the incorporation of strategic material design approaches such as doping, compositional tuning, and more recently, phase engineering. These methods allow for precise control over lattice distortions, octahedral tilting, and electron distribution, ultimately inducing changes in both charge dynamics and catalytic activity (Feng *et al.,* 2025). Notably, recent studies have demonstrated that subtle changes in the perovskite crystal phase can significantly affects HER efficiency by facilitating better charge mobility and creating more active surface sites.

As research advances, the need for multiscale understanding and linking of atomic-scale features to macroscopic catalytic performance is becoming evident. Computational tools such as density functional theory (DFT), in combination with machine learning (ML) models, now play a important role in predicting and optimizing perovskite behavior under operational conditions (Nyangiwe *et al*., 2025). This has laid the foundation for a data-driven, rational design of high-efficiency perovskite materials for hydrogen evolution.

Phase Engineering Strategies in Perovskite Photocatalysts

Phase engineering has emerged as a noble strategy to enhance the photocatalytic performance of perovskite materials, particularly for hydrogen evolution reactions (HER). Perovskites can exist in multiple structural phases such as orthorhombic, cubic, rhombohedral, and tetragonal, depending on factors like temperature, ionic radius mismatch, and doping concentration. These phase variations strongly influence the material's electronic structure, charge transport properties, and surface reactivity (Dawa *et al*., 2024).

The tuning of phase stability and transitions has proven effective in optimizing the band edge positions and improving charge carrier separation efficiency. For instance, studies on $LaFeO_3$ have demonstrated that by tuning the doping level of Bi, Ce or Y at the A-site (La^{3+}), one can induce transitions between various crystallographic phases, resulting in enhanced light absorption and photocatalytic activity (Cao *et al*., 2024). In the same fashion, altering the B-site cation (e.g., Fe^{3+} replaced with Mn^{3+} or Ti^{4+}) can modify the metal–oxygen bond angle, thereby regulating the perovskite's phase and electronic conductivity.

One effective method of phase engineering is strain induction, which involves applying external or internal stress (via epitaxial growth or lattice mismatch) to distort the perovskite lattice. This strain effects can lead to change in electronic structure, shift in band edge, impact defect density, and improve charge mobility (Kahlaoui *et al*., 2020; Wang *et al*., 2025). For example, tensile strain in $SrTiO_3$ thin films has been shown to induce a transition to a pseudo-cubic phase with improved charge transport and HER efficiency.

Another strategy includes temperature- or pressure-driven phase transformations, which allow researchers to reversibly tune the crystal structure and correlate it with catalytic performance. Although such techniques are more challenging to implement in practical devices, they offer deep insight into the structure–property relationships that govern HER activity (Maciejewska *et al*., 2023; Jayakrishnan *et al.,* 2023; Toriqul *et al*., 2024).

Importantly, phase boundaries within mixed-phase perovskites can act as active sites or facilitate directional charge separation. For instance, $BiFeO_3$ with coexisting rhombohedral and tetragonal phases has shown superior hydrogen production under visible light compared to its single-phase counterparts (Chen *et al*., 2015; Baloni *et al*., 2022). This is attributed to the internal electric fields and enhanced carrier dynamics at the phase interfaces.

As a frontier approach, AI and machine learning techniques are now being integrated to predict favorable phase configurations for specific applications. Trained on high-throughput computational data, ML models can identify composition to desired phase property relationships more efficiently than conventional trial and error approach (Alghadeer *et al*., 2024; Badini and Pugliese. 2023). This enables the targeted design of phase-engineered perovskites with optimal band alignment and catalytic activity for hydrogen evolution.

AI and Machine Learning Approaches in Perovskite Photocatalysis

The integration of artificial intelligence (AI) and machine learning (ML) into materials science has rapidly transformed the discovery and optimization of photocatalysts for hydrogen evolution, particularly within complex systems such as perovskites. Traditional trial and error experimental methods and even first-principles calculations are often time demanding when exploring vast compositional and structural design spaces. AI-driven approaches offer high-throughput, cost-effective pathways to accelerate the identification of efficient perovskite-oxides materials with desirable photocatalytic properties (Hung *et al*., 2025; Luhan *et al*., 2024; Ali *et al*., 2020; Weng *et al*., 2020).

Machine learning models such as random forest, support vector machines, and neural networks have been employed to predict key descriptors like band gap, conduction band position, formation energy, and hydrogen adsorption energy based on compositional and structural features of perovskites (Zhou *et al*., 2018; Deng *et al*., 2025; Hung *et al*., 2025). These models are trained on datasets derived from either density functional theory (DFT) calculations or experimental repositories such as the Materials Project or NOMAD. Once trained, the models can screen thousands of perovskite compositions rapidly for stability and photocatalytic efficiency prediction rapidly.

In particular, AI has shown remarkable potential in guiding phase engineering through correlations between nature and type of dopant, lattice strain, phase and phase transitions (Abdullah *et al*., 2025). For instance, convolutional neural networks have been utilized to classify perovskite crystal phases based on XRD patterns and to predict phase transition pressures under different chemical environments. These capabilities enable researchers to virtually screen for phase-tuned perovskite compositions that can maximize hydrogen evolution efficiency.

Furthermore, unsupervised learning techniques such as principal component analysis (PCA) and clustering algorithms help in understanding the latent variables controlling HER activity across a broad materials landscape. These methods can group similar materials by performance and structural characteristics, unraveling hidden structure to property relationships (Chander and Vijaya, 2021; Tshitoyan *et al*., 2019).

Recent efforts have also focused on coupling ML with active learning frameworks where models are continuously refined through feedback from new experiments or simulations. This iterative process has led to the discovery of novel doped perovskites and heterostructures with enhanced light absorption and charge separation capabilities (yang *et al*., 2021). Moreover, generative models such as variational autoencoders and generative adversarial networks are being explored to design new hypothetical perovskite compositions for tailored application.

Also, explainable AI techniques are gaining attention in perovskite photocatalysis to ensure that predictions are interpretable and scientifically grounded. By quantifying feature importance and identifying causal relationships, researchers can better understand why a particular composition or phase yields high HER performance (Doshi-Velez & Kim, 2017). AI/ML approaches are not just tools for prediction but are becoming integral to the rational design of next-generation perovskite photocatalysts. When combined with first-principles methods and experimental validation, they pave the way for data-driven discovery and rapid advancement of sustainable hydrogen production technologies.

Challenges, Limitations, and Future Directions

Despite the tremendous potential of phase-tuned perovskites for hydrogen evolution, several critical challenges remain. The table below provides a summary of the challenges, along with their corresponding implications and proposed solutions

Table 2: Challenges, Implication and Proposed Solutions

Challenges	Implication	Proposed Solution
Lack of standardized ML datasets	Limits model generalization	Create shared benchmarking datasets for perovskite-HER research
Poor phase stability under HER conditions	Short catalyst lifetimes	Develop hybrid phase systems with protective oxide layers
Overfitting in ANN/CNN models	Misleading performance metrics	Apply dropout, cross-validation, and model explainability tools
Difficulty in doping control during synthesis	Limits reproducibility	Use ML to predict optimal synthesis condition (e.g temperature, pH, etc.)
Disconnect between ML and fabrication	Slows experimental translation	Encourage collaborative ML-materials labs: include fabrication data in training
Lack of environmental impact analysis	Risk of toxic byproducts or unstable materials	Prioritizing lifecycle assessment during ML-based material selection

CONCLUSION

This review has synthesized the current state of research on phase-tuned perovskite materials for efficient hydrogen evolution reactions (HER), highlighting the synergy between phase engineering and machine learning (ML). The key contributions of this paper include the identification of phase engineering strategies that enhance HER performance in perovskite materials, the discussion of ML's role in accelerating the discovery of efficient HER catalysts and optimizing phase-tuned perovskites and finally, the outline of challenges and opportunities in scaling up synthesis methods and integrating phase-engineered perovskites into practical devices

Future Research Directions

To advance the field, future research should prioritize better data curation, development of explainable ML techniques, and scale-up synthesis methods. High-quality, standardized datasets are essential for training ML models and predicting HER performance. Explainable ML can uncover underlying structure-property relationships, improving model interpretability. Cost-effective, high-throughput synthesis methods are crucial for scaling up phase-engineered perovskites.

Limitations of the Review

This review has several limitations, including a focus on theoretical and computational studies, limited discussion of experimental data, and a regional bias towards research conducted in specific geographic areas. Future reviews could benefit from a more comprehensive inclusion of experimental studies and a broader geographic scope.

By addressing these challenges and pursuing future research directions, we can accelerate the development of efficient, scalable, and sustainable HER systems based on phase-tuned perovskite materials.

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