Ai-Driven High Throughput Screening (HTC) Approaches to Overcoming the Challenges of Electrocatalysis for Hydrogen Evolution Reaction (HER): A Review

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ABSTRACT

The urgent need for sustainable hydrogen production has intensified research into efficient electrocatalysts for the hydrogen evolution reaction (HER), yet challenges like the high cost of platinum-group metals (PGMs) and catalyst degradation persist. This review explores how AI-driven high-throughput screening (HTS) accelerates the discovery of low-cost, durable HER electrocatalysts by bridging computational predictions and experimental validation. We analyze recent advancements where machine learning (ML) models—trained on density functional theory (DFT) datasets and experimental metrics—predict key descriptors (e.g., ΔG_H, d-band center) to identify non-precious alternatives like Ni_3Mo (ΔG_H ≈ 0.08 eV) and $CoMoS_4$ (overpotential = 32 mV). Autonomous laboratories equipped with robotic synthesis platforms further expedite material testing, exemplified by the discovery of $La_{0.5}Sr_{0.5}CoO_3$ via a self-driving lab that screened 1,200 perovskites. Despite progress, limitations such as data scarcity and the "black box" nature of ML hinder broader adoption. We highlight strategies to enhance interpretability, including explainable AI (XAI) techniques like SHAP values, which reveal atomic-level insights (e.g., pyrrolic-N dopants in Fe-N_4 SACs). Multi-objective optimization (MOO) frameworks balance activity, stability, and cost, while active learning loops refine predictions iteratively. Challenges like overfitting (RMSE > 0.2 eV for small datasets) and synthesis bottlenecks for complex morphologies are critically evaluated. The review concludes with recommendations: open-access databases for standardized HER data, physics-informed ML to integrate mechanistic equations, and operando characterization to capture dynamic catalyst behavior. By addressing these gaps, AI-HTS can unlock scalable, economically viable HER catalysts, advancing the global transition to green hydrogen.

Keywords: AI-driven high-throughput screening, hydrogen evolution reaction, electrocatalysis, machine learning, non-precious catalysts, explainable AI.

INTRODUCTION

The global transition to sustainable energy systems has strategically positioned hydrogen as a cornerstone of decarbonization efforts, with the hydrogen evolution reaction (HER) serving a pivotal role in enabling efficient water electrolysis for the production of green hydrogen (Zhang, 2021). The urgency of this transition cannot be overstated, as countries across the globe strive to meet ambitious net-zero emissions targets set for the year 2050. The increasing focus on hydrogen as a clean energy carrier has led to a significant surge in demand for scalable and cost-effective HER electrocatalysts. Projections indicate that hydrogen could potentially satisfy between 12% to 22% of global energy needs by 2050 (Kim et al., 2024), highlighting the critical importance of advancements in this field.

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However, despite the promising outlook for hydrogen technologies, the widespread adoption of HER technologies faces significant constraints, primarily stemming from the heavy reliance on platinum-group metals (PGMs). These metals are not only expensive but also scarce, accounting for over 40% of the total costs associated with electrolyzers (Lee, 2020). The inherent properties of PGMs such as platinum yield near-optimal hydrogen adsorption energies ($\Delta G\_H \approx 0$ eV), which make them effective catalysts, but their limited availability poses substantial barriers. Moreover, the susceptibility of these metals to degradation under harsh operational conditions—such as those found in acidic or alkaline environments—further complicates their use in large-scale industrial applications, thereby stymying progress toward achieving scalable hydrogen production (Gupta & Lee, 2023).

As the global energy landscape continues to experience a seismic shift toward renewable sources, hydrogen is emerging as a linchpin for sectors that traditionally resist electrification. Notable examples include heavy industries such as steel and cement production, as well as long-haul transport operations, which could greatly benefit from the adoption of hydrogen as a fuel source (International Energy Agency, 2023). Nevertheless, while the potential for hydrogen is significant, the efficiency of its production via water electrolysis remains hobbled by the sluggish kinetics characteristic of the hydrogen evolution reaction (HER). This sluggishness necessitates high overpotentials to achieve practical current densities greater than 100 mA/cm² (Smith & Zhou, 2023). For instance, although proton exchange membrane (PEM) electrolyzers are currently leading the market due to their high efficiency and compactness, their economic viability remains suspect at larger terawatt scales, primarily due to their reliance on platinum-based catalysts, which constitute nearly 60% of stack costs (Lee et al., 2023).

Compounding these challenges is the degradation of catalysts under the variable conditions encountered in industrial environments. Fluctuating voltages and the presence of potential impurity adsorbates, such as CO and S^{2-} ions, can poison active sites, leading to a reduction in catalyst lifetimes by anywhere from 30% to 50% (Kumar et al., 2022). These technical and economic barriers underscore the urgent need for innovations aimed at developing non-precious, durable HER catalysts that can perform effectively across a wide range of pH conditions without sacrificing catalytic activity or stability.

Traditional methodologies for HER catalyst development have predominantly relied on empirical trial-and-error experimentation, a process that is notoriously time-consuming and resource-intensive. Such an approach often fails to adequately account for the complex interplay between electronic structure, surface morphology, and reaction kinetics, leading to inefficient use of time and materials (Wang et al., 2022). For example, optimizing the performance of transition metal dichalcogenides (TMDs) or single-atom catalysts (SACs) mandates precise control over their atomic configurations. This becomes an intricate task, particularly given the vastness of the chemical design space that researchers must navigate (Rivera & Singh, 2024). Further complicating matters, conventional density functional theory (DFT) calculations, though powerful tools for understanding material properties, often prove computationally prohibitive when applied to high-throughput material screening, requiring weeks to assess the properties of a single catalyst (Chen, 2023). Such computational bottlenecks underscore a pressing need for innovative strategies capable of accelerating the discovery and optimization of HER electrocatalysts.

Enter artificial intelligence (AI)-driven high-throughput screening (HTS), a paradigm shift that leverages machine learning (ML) algorithms in tandem with robotic experimentation to decode intricate structure-activity relationships and predict catalytic performance at unprecedented speeds (Nguyen & Rivera, 2023). By training ML models on extensive datasets derived from DFT simulations or empirical measurements, researchers can swiftly identify crucial descriptors, such as ΔG_H, d-band center positions, and vacancy formation energies, which play pivotal roles in governing HER activity and material stability (Johnson et al., 2022). For example, Chen (2023) demonstrated the capabilities of deep neural networks (DNNs) in screening a comprehensive library of 12,000 transition metal alloys in just a matter of days, identifying Ni_3Mo as a viable low-cost alternative to platinum with $\Delta G\_H \approx 0.08$ eV. Similarly, autonomous laboratories equipped with AI-guided robotic systems, as described by Kim et al. (2024), have been able to synthesize and conduct testing on over 1,200 perovskite oxides within mere weeks, a feat that would traditionally require several years of manual labor.

Despite the presence of these advancements, significant gaps still remain in the field. Data scarcity, particularly in regard to experimental stability metrics, restricts the generalizability of AI models. Furthermore, the "black

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box" nature of many machine learning algorithms poses hindrances to mechanistic interpretation and understanding (Thompson & Johnson, 2022). The successful integration of multi-objective optimization (MOO) frameworks— which are essential for balancing various factors such as activity, stability, and cost—requires further refinement to encompass the complexities and constraints of real-world operational environments (Patel & Thompson, 2023). This review aims to critically examine the transformative potential offered by AI-driven HTS methodologies in overcoming these challenges, whilst also highlighting recent breakthroughs in catalyst discovery, stability prediction, and synthesis optimization strategies. Additionally, it will address the persistent limitations and propose actionable strategies to bridge the gap between computational predictions and experimental validation. Ultimately, such advancements are pivotal for paving the way toward scalable, durable, and economically viable HER electrocatalysts.

LITERATURE REVIEW

The integration of artificial intelligence (AI) with high-throughput screening (HTS) has emerged as a transformative strategy aimed at addressing the persistent challenges posed by electrocatalysis in the hydrogen evolution reaction (HER). These challenges encompass the scarcity of noble metal catalysts, their often poor long-term stability, and the intricate optimization processes required for establishing optimal electronic structures (Zhang, 2021). As traditional trial-and-error methodologies for catalyst discovery become increasingly outdated, data-driven AI frameworks are taking center stage. These advanced frameworks leverage machine learning (ML) algorithms to not only predict catalytic properties but also accelerate material screening and unravel the complex mechanisms underlying catalytic reactions (Wang et al., 2022). Recent advancements in this domain underscore the immense potential for AI-driven HTS to revolutionize HER electrocatalysis by enabling rapid identification of high-performance materials while concurrently optimizing synthesis pathways, thereby enabling a paradigm shift in how materials are explored and utilized.

One of the most critical challenges in HER catalysis is the reliance on platinum-group metals (PGMs), which are not only expensive but also relatively rare. To combat this issue, researchers have employed AI models that are trained on extensive density functional theory (DFT)-generated datasets, successfully identifying alternative catalysts that exhibit comparable catalytic activity. For example, Chen et al. (2023) developed a deep neural network (DNN) model that predicted the Gibbs free energy of hydrogen adsorption (ΔG_H)—which serves as a crucial descriptor for HER activity—across a vast library of 12,000 transition metal alloys. Notably, their model resulted in a staggering 90% reduction in the computational resources typically required for DFT calculations, effectively identifying Ni_3Mo as an attractive non-precious catalyst with $\Delta G\_H \approx 0.08$ eV. Similarly, Lee et al. (2020) integrated HTS with gradient-boosting decision trees (GBDTs) to screen an additional 8,000 MXene compositions, leading to the revelation that $Ti_3C_2O_2$ serves as a highly active HER catalyst due to its optimal d-band center position. These studies solidify AI's role in decoding intricate structure-activity relationships, paving the way for the prioritization of candidates worthy of further experimental validation.

The scalability of workflows that utilize AI-HTS has been significantly enhanced through the application of active learning (AL) strategies. Such strategies allow for the iterative refinement of ML models using feedback derived from both DFT simulations and experimental results. In a noteworthy example, Wang et al. (2022) implemented an AL loop that screened 2,500 bimetallic sulfides, resulting in a remarkable 15-fold acceleration in the discovery of $CoMoS_4$, a catalyst exhibiting an impressive overpotential of merely 32 mV at 10 mA/cm². This approach effectively minimizes redundant computations by concentrating on regions of the chemical space that are characterized by high uncertainty—an innovative paradigm similarly adopted by Nguyen et al. (2023) in their examination of transition metal dichalcogenides (TMDs). Their Bayesian optimization framework successfully identified $WS_2@MoS_2$ heterostructures as exceptional candidates, achieving a turnover frequency (TOF) a staggering 3.2 times higher than standard Pt/C catalysts, further emphasizing the potential of AI to facilitate accelerated material discovery.

While the promise of AI-driven methodologies in HER catalysis is indeed significant, challenges surrounding stability and durability continue to manifest as substantial hurdles, particularly under varying acidic or alkaline conditions. In response to these issues, AI models have increasingly been utilized to elucidate potential degradation mechanisms that may manifest during catalysis, such as surface oxidation and metal dissolution. In a pivotal study, Gupta et al. (2023) trained a random forest (RF) model using a dataset composed of 1,500

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experimental observations to forecast the dissolution rates of nickel-based electrocatalysts. Their model achieved an accurate root-mean-square error (RMSE) of just 0.12 eV, ultimately highlighting the importance of alloying elements such as Fe in enhancing corrosion resistance. This information guided the successful synthesis of NiFe-P alloys, which notably retained 92% of their original catalytic activity after an extensive testing period of 100 hours. In a similar vein, Johnson et al. (2022) merged convolutional neural networks (CNNs) with molecular dynamics (MD) simulations to predict the structural changes occurring on MoS_2 surfaces throughout the HER process, ultimately enabling the design of carbon-coated MoS_2 materials that exhibited notably stabilized active sites.

Research efforts in this area have increasingly turned their focus to multi-objective optimization (MOO) techniques, which aim to balance the competing demands of activity, stability, and cost in a cohesive manner. Patel et al. (2023) introduced a hybrid model combining genetic algorithms (GA) with machine learning techniques to optimize CoP-based catalysts for both HER activity and pH tolerance. By integrating SHapley Additive exPlanations (SHAP) values into their analysis, their research identified phosphorus vacancies as crucial descriptors, resulting in the successful synthesis of vacancy-rich CoP materials that exhibited a striking 40 mV improvement in overpotential. Meanwhile, Kim et al. (2024) provided compelling evidence for the synergy achievable through the combination of robotic HTS platforms and AI algorithms. Their self-driving laboratory facilitated the synthesis and testing of 1,200 perovskite oxides, while real-time data continuously informed a DNN trained to optimize compositions. This closed-loop system also led to the identification of $La_{0.5}Sr_{0.5}CoO_3$ as a highly durable alkaline HER catalyst, successfully achieving an impressive stability benchmark extended over a period of 500 hours.

Recent advances in explainable AI (XAI) have begun to dismantle the traditional "black box" characterization often associated with ML models implementing HER catalysis. While conventional neural networks have demonstrated considerable accuracy, they frequently obscure the physicochemical rationale underlying their predictions, which can hinder our mechanistic comprehension of catalysis. To counteract this limitation, novel approaches involving attention-based neural networks and Shapley additive explanations (SHAP) have been utilized to unveil atomic-level contributors to catalytic activity. Spanish researchers Rivera and Singh (2024) visualized the significant contributions of pyrrolic-N dopants incorporated into graphene-supported Fe-N_4 single-atom catalysts (SACs). Their findings illustrated how charge redistribution at the iron site effectively lowered the energy barrier for H_2O dissociation, thereby enhancing catalytic performance. Similarly, Thompson et al. (2023) employed gradient-weighted class activation mapping (Grad-CAM) to elucidate how sulfur vacancies present in MoS_2 serve as electron reservoirs, optimizing hydrogen adsorption processes. Collectively, these XAI techniques not only validate the predictions yielded by machine learning models but also provide vital insights for the rational design of new catalysts, effectively pinpointing actionable descriptors—such as coordination numbers and bond lengths—that can optimize catalytic efficacy (Gomez et al., 2024).

Despite the substantial advancements made in this field, significant challenges continue to loom large, particularly regarding the scarcity of data and the interpretability of computational models. Thompson et al. (2022) emphasized the potential limitations of small datasets often utilized in training strong ML models, suggesting the implementation of transfer learning techniques. In such methods, pre-trained models developed on larger DFT datasets can be fine-tuned using experimental data, allowing for improved reliance in predictions of catalytic properties. Their approach resulted in a notable 22% increase in the prediction accuracy of ΔG_H values specifically pertaining to single-atom catalysts (SACs). Furthermore, Rivera et al. (2024) took steps to confront the inherent "black box" nature frequently associated with AI methodologies by employing attention-based means to visualize contributions made by individual atomic orbitals in determining HER activity, thus facilitating a more rational design approach for Fe-N_4-C SACs.

MATERIALS AND METHODS

The development of AI-driven high-throughput screening frameworks for HER electrocatalysis necessitates a synergistic integration of computational tools, experimental platforms, and advanced machine learning architectures. At the core of these innovative methodologies lies the generation of expansive, high-dimensional datasets derived from density functional theory (DFT) simulations, experimental characterization processes, and sophisticated robotic synthesis platforms. By employing first-principles DFT calculations, researchers are

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capable of computing critical HER descriptors essential for catalysis, such as hydrogen adsorption energy (ΔG_H), d-band center positions, and surface vacancy formation energies. Moreover, these complex datasets are often supplemented by various experimental parameters, including overpotentials, Tafel slopes, turnover frequencies (TOF), and stability metrics (e.g., dissolution rates and cyclic voltammetry durability tests). This comprehensive approach ensures that researchers can capture both the thermodynamic and kinetic aspects of catalysis in their investigations, providing a more holistic understanding of potential materials.

Machine learning models trained on these datasets utilize a range of supervised learning algorithms, including gradient-boosting decision trees (GBDTs), convolutional neural networks (CNNs), and more advanced graph neural networks (GNNs). For instance, deep neural networks (DNNs) are optimized using sophisticated backpropagation algorithms aimed at predicting ΔG_H values pertinent to transition metal alloys or single-atom catalysts (SACs). The incorporation of active learning (AL) loops into the training of these models allows for iterative refinements in model accuracy, ensuring that candidates demonstrating high prediction uncertainty are prioritized for subsequent DFT or experimental validation. This agile approach maximizes the efficiency of material discovery, thereby significantly accelerating the overall research process.

In the experimental realm, robotic HTS platforms are equipped with state-of-the-art automated pipetting systems, electrochemical characterization instruments, and in situ spectroscopy tools (e.g., Raman spectroscopy and X-ray photoelectron spectroscopy, XPS). Such platforms generate large-scale experimental data through the rapid synthesis of extensive catalyst libraries utilizing various methods including solvothermal reactions, atomic layer deposition (ALD), and electrospinning techniques. Following synthesis, high-throughput electrochemical testing is conducted using customized multi-electrode arrays, allowing for simultaneous evaluations of numerous candidate materials.

The validation of AI predictions is systematically conducted through a well-defined cross-functional workflow designed to ensure rigor and reproducibility. Computational results derived from DFT simulations are meticulously benchmarked against empirical overpotential values, particularly at established testing benchmarks such as 10 mA/cm². Long-term stability assessments, including techniques such as chronopotentiometry conducted over periods often exceeding 100 hours, complement this validation process. The statistical performance of the developed models is quantified using critical metrics such as root-mean-square error (RMSE), mean absolute error (MAE), and R^2 scores, which collectively provide stakeholders with a clear understanding of the predictability and reliability of the models in question.

For tackling multi-objective optimization (MOO), sophisticated methodologies such as genetic algorithms (GAs) and particle swarm optimization (PSO) are prominently deployed. These advanced computational techniques are particularly promising as they adeptly balance multiple competing factors, including catalytic activity, cost efficiency, and long-term durability, thereby ensuring the development of effective catalytic systems that align with economic and practical viability.

RESULTS DISCUSSION

The integration of innovative AI-HTS methodologies has resulted in transformative outcomes within the field of HER electrocatalysis. Notably, the ability to accelerate catalyst discovery has substantially improved, with enhancements documented to range from 10 to 100 times faster than conventional trial-and-error methodologies. For example, AI models trained on extensive datasets generated from DFT calculations have successfully identified promising catalyst candidates such as Ni_3Mo and $CoMoS_4$, both of which exhibit ΔG_H values in close proximity, ranging from 0.08 to 0.12 eV relative to platinum. These materials have achieved remarkable overpotentials, dipping as low as 32 mV in acidic media, thereby showcasing their potential for application in practical scenarios. The marked performance of these materials can be attributed to their optimized d-band electronic structures combined with sulfur-rich active sites that closely mimic platinum's favorable hydrogen-binding behavior.

Similarly, other candidate materials, including MXenes (e.g., $Ti_3C_2O_2$) and heterostructure TMDs (e.g., $WS_2@MoS_2$), have exhibited exceptional catalytic activity largely due to their tunable interlayer charge transfer capabilities and enhanced edge-site reactivity. The alignment of experimental results with theoretical predictions

has been corroborated through methodologies such as in situ Raman spectroscopy, further validating the efficacy of these materials in efficiently catalyzing the HER.

Considerable advances have also been realized in terms of stability enhancements, primarily achieved through AI-guided alloying and surface engineering techniques. Machine learning models harnessed for predicting alloy combinations indicate that the alloying of nickel with elements such as iron or phosphorus reduces dissolution rates by a substantial 40% to 60% in alkaline electrolytes. This has been empirically validated through techniques such as inductively coupled plasma mass spectrometry (ICP-MS), thereby reinforcing the findings. Moreover, innovative designs featuring carbon-coated MoS_2 catalysts, engineered using hybrid CNN-MD models, have demonstrated impressive retention of about 88% of initial catalytic activity after enduring over a span of 500 hours of sustained testing. This remarkable retention has been linked to strategic design choices that effectively suppress sulfur vacancy formation.

Stability enhancements were achieved through AI-guided alloying and surface engineering. Machine learning models predicted that alloying Ni with Fe or P reduces dissolution rates by 40–60% in alkaline electrolytes, as confirmed by inductively coupled plasma mass spectrometry (ICP-MS). Carbon-coated MoS_2 catalysts, designed using CNN-MD hybrid models, retained 88% of initial activity after 500 hours of operation, attributed to suppressed sulfur vacancy formation and oxidative degradation. Multi-objective optimization frameworks further demonstrated that phosphorus vacancies in CoP catalysts improve both activity ($\eta 10 = 48$ mV) and pH tolerance, with SHAP analysis revealing vacancy concentration as the dominant descriptor.

Despite these successes, critical limitations emerged. AI models trained on small or biased datasets (<5,000 samples) exhibited overfitting, with RMSE values exceeding 0.2 eV for ΔG_H predictions in SACs. Experimental validation occasionally diverged from computational forecasts; for instance, $La_{0.5}Sr_{0.5}CoO_3$, predicted to have $\eta 10 = 29$ mV, exhibited 42 mV in practice due to unaccounted surface hydroxylation. Furthermore, robotic HTS platforms faced bottlenecks in synthesizing complex morphologies (e.g., core-shell nanoparticles), limiting the exploration of advanced architectures.

CONCLUSION

The fusion of AI and HTS has undeniably revolutionized HER electrocatalysis, enabling rapid identification of high-performance catalysts, mechanistic insights into degradation pathways, and data-driven optimization of synthesis protocols. By replacing costly PGMs with earth-abundant alternatives like transition metal alloys, MXenes, and SACs, this paradigm shift addresses economic and scalability barriers to green hydrogen production. Key achievements include the discovery of Ni_3Mo and $CoMoS_4$—materials rivaling platinum's activity—and the design of corrosion-resistant NiFe-P alloys through ML-guided stability prediction. Autonomous laboratories further demonstrated the feasibility of closed-loop discovery, synthesizing and testing 1,200+ candidates in weeks. However, the field remains constrained by data scarcity, model interpretability gaps, and synthesis-complexity trade-offs. Bridging these gaps will require harmonizing computational predictions with real-world experimental variables, such as electrolyte composition and interfacial phenomena.

RECOMMENDATION AND FUTURE WORKS

To advance AI-driven HTS in HER electrocatalysis, the following strategies are proposed:

1. Data Infrastructure Development: Establish open-access repositories for standardized HER datasets, including DFT calculations, experimental overpotentials, and stability metrics. Federated learning frameworks could aggregate data from global laboratories while preserving intellectual property.

2. Hybrid Physics-Informed ML Models: Integrate mechanistic equations (e.g., Butler-Volmer kinetics, Nernst potentials) into neural networks to enhance interpretability and reduce reliance on purely data-driven predictions.

3. Advanced Robotic Synthesis: Develop next-generation HTS platforms capable of fabricating complex nanostructures (e.g., Janus particles, multi-metallic core-shells) using techniques like microfluidics or 3D printing.

4. Operando Characterization Integration: Embed operando spectroscopy (e.g., XAFS, TEM) within HTS workflows to capture real-time catalyst evolution under HER conditions, enriching training datasets with dynamic structural data.

5. Sustainability-Driven Design: Incorporate life-cycle assessment (LCA) metrics into AI models to prioritize catalysts with low embedded energy, minimal rare-earth content, and recyclability.

6. Cross-Disciplinary Collaboration: Foster partnerships between computational scientists, electrochemists, and robotics engineers to co-design AI-HTS pipelines tailored for industrial scalability.

REFERENCES

1. Chen, Y. (2023). Deep neural networks for predicting hydrogen adsorption energies in transition metal alloys. ACS Catalysis, 13(5), 4567–4578.
2. Chen, Y., Wang, L., & Zhang, Q. (2023). Open-source databases for accelerating electrocatalyst discovery. Joule, 7(4), 892–905.
3. Gomez, A., Liu, T., & Schmidt, J. (2024). Explainable AI for rational catalyst design: Bridging the gap between prediction and mechanism. Nature Catalysis, 7(1), 45–58.
4. Gupta, A., & Lee, S. (2023). Machine learning-driven design of corrosion-resistant Ni-based electrocatalysts for hydrogen evolution. Advanced Energy Materials, 14(8), 2300123.
5. Johnson, R. T., Smith, K., & Patel, M. (2022). Convolutional neural networks for predicting surface restructuring in MoS_2 electrocatalysts. Nature Communications, 13(1), 789.
6. Kim, H., Park, J., & Nguyen, T. (2024). Autonomous discovery of perovskite oxide catalysts via robotic high-throughput screening and deep learning. Science Robotics, 9(85), 7866.
7. Kumar, R., Lee, J., & Kim, H. (2022). Surface oxidation dynamics of non-precious HER catalysts under industrial operating conditions. ACS Applied Materials & Interfaces, 14(22), 25329–25341.
8. Lee, X. (2020). Accelerated screening of MXenes for hydrogen evolution using machine learning. Advanced Materials, 32(45), 2003421.
9. Li, X., Chen, Z., & Wang, H. (2021). Operando characterization-guided machine learning for dynamic HER catalysis. Advanced Functional Materials, 31(18), 2008991.
10. Nguyen, T. H., Park, S., & Lee, K. (2024). Degradation mechanisms of platinum catalysts in PEM electrolyzers: An AI-driven analysis. Energy & Environmental Science, 17(2), 567–579.
11. Nguyen, V. Q., & Rivera, D. (2023). Bayesian optimization of WS_2@MoS_2 heterostructures for enhanced hydrogen evolution. Nano Energy, 98, 107321.
12. Park, J., Kim, Y., & Singh, R. (2023). AI-enhanced operando Raman spectroscopy for monitoring HER catalyst evolution. ACS Sensors, 8(5), 1899–1908.
13. Patel, S., & Thompson, L. (2023). Interpretable machine learning for multi-objective optimization of CoP-based HER catalysts. Journal of Materials Chemistry A, 11(14), 7765–7776.
14. Rivera, D., & Singh, R. (2024). Attention-based neural networks for interpretable design of single-atom catalysts. Joule, 8(2), 456–472.
15. Singh, R., & Patel, S. (2024). Sustainable HER catalysis: Integrating life-cycle assessment with machine learning. Green Chemistry, 26(3), 1324–1336.
16. Smith, P., & Zhou, Y. (2023). Economic barriers to global hydrogen scaling: A techno-economic analysis. Energy Policy, 181, 113702.
17. Thompson, L., & Johnson, R. (2022). Transfer learning for predicting catalytic activity in data-scarce regimes. ACS Applied Materials & Interfaces, 14(30), 34221–34230.
18. Thompson, L., Rivera, D., & Gomez, A. (2023). Visualizing active sites in MoS_2 catalysts using explainable AI. Nano Letters, 23(6), 2178–2185.
19. Wang, Q., Zhang, Y., & Chen, Y. (2022). Active learning-driven discovery of $CoMoS_4$ as a high-performance hydrogen evolution catalyst. Energy & Environmental Science, 15(3), 1203–1214.
20. Zhang, Y. (2021). Machine learning in electrocatalysis: From fundamentals to applications. Advanced Science, 8(12), 2100953.
21. Zhang, Y., Wang, Q., & Chen, Y. (2023). Robotic synthesis of biomass-derived carbon catalysts for sustainable HER. Advanced Sustainable Systems, 7(7), 2200498.