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How AI guided the development of green hydrogen production: in the case of solid oxide electrolysis cell?

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Abstract

The development of efficient and stable hydrogen production technologies is crucial for global clean energy transition. Solid oxide electrolysis cells (SOECs) have emerged as a promising technology for green hydrogen production due to their high efficiency, low-cost catalysts, and excellent adaptability to renewable energy sources. However, significant challenges remain in materials design, interface engineering, and system integration. This perspective reviews recent advances in artificial intelligence (AI)-guided SOEC development, focusing on machine learning approaches for design of key materials. Furthermore, we highlight how AI technologies can address the key challenges in both single-cell performances and system-level integration with renewable energy sources. Looking forward, we outline strategic directions for advancing AI-driven SOEC development toward commercial implementation, which may offer valuable insights and experiences within the field of energy conversion and storage.

Keywords: Hydrogen energy, solid oxide electrolysis cell, anode material, machine learning

MAIN TEXT

In the context of global climate change, clean energy transition has become a core development task for countries worldwide. The use of fossil fuels has led to massive greenhouse gas emissions, exacerbating global warming and environmental degradation[1-3]. Hydrogen energy, with its high energy density and zero-emission characteristics, particularly green hydrogen produced through water electrolysis using renewable energy sources (such as wind and solar power), has garnered significant attention[4,5]. However, the supply of renewable energy exhibits significant intermittency and instability. For instance, solar power generation heavily depends on sunlight conditions, with power generation capacity dramatically decreasing or even completely stopping during cloudy days, rainy weather, or at night when there is insufficient light. This intermittency poses severe challenges to the stable operation of water electrolysis hydrogen production equipment, necessitating the development of highly adaptable hydrogen production technologies[6,7].

The development of hydrogen production techniques for water electrolysis has gone through an evolutionary process from alkaline water electrolyzers (AWE), proton exchange membrane electrolyzers (PEMEC) to solid oxide electrolysis cell (SOEC)[7,8]. AWE, as the earliest technology to be industrialized, has the advantages of mature technology and relatively low cost. However, AWE has several key limitations: firstly, it requires the use of precious metal catalysts, such as Pt, to reduce the overpotential of the electrode reaction, which significantly increases the system cost; secondly, the low operating current density (typically between 0.2-0.4 $A{\cdot}cm^{-2}$) limits the hydrogen production efficiency; most importantly, it has a slow startup and shut-down process with poor dynamic response, making it difficult to adapt to the fluctuating characteristics of renewable energy sources[9,10]. PEMEC has achieved a significant improvement in performance by utilizing proton exchange membranes as the electrolyte. The technology operates below 100 °C with high proton conductivity and chemical stability, rapid startup, excellent dynamic response performance, and current densities up to 1-2 $A{\cdot}cm^{-2}$. However, the catalysts of PEMEC are expensive (use of Pt and Ir) and extremely sensitive to impurities, requiring stringent gas purification[11,12].

SOEC operating at 400-1,000 °C has high energy conversion efficiency (more than 80%) due to the faster electrochemical reaction kinetics and lower overpotential under high temperatures. Besides, SOEC can operate at current densities of 2-5 $A{\cdot}cm^{-2}$ or even higher with low-cost oxides as catalysts, which are abundant in resources[4,13-15]. Importantly, it can maintain stable operation under a wide range of power fluctuation conditions, showing excellent adaptability. Lastly, it can be system-integrated with high-temperature processes, such as industrial waste heat recovery, carbon capture, and so on, to further improve energy utilization efficiency. These advantages make SOEC a key technology for solving the problem of efficient utilization of renewable energy.

Despite the significant advantages of SOEC technology, it still faces many challenges on the way to commercialization. Firstly, the design of key materials, including anodes, cathodes and electrolytes, is the main bottleneck restricting the performances of SOEC, whose stability, catalytic activity, and ionic conductivity at high temperatures and high current densities still need to be further improved. As for anode materials, $Sm_{0.5}Sr_{0.5}CoO_{3-\delta}$ (SSC)[16,17], $(LaSr)CoO_{3-\delta}$ (LSC)[18], $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF)[19], and $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF)[20] are the widely used anodes for SOECs. As for the electrolyte, perovskite oxides $BaZr_{1-x-y}Ce_xM_yO_3$ (BZCM, M = Y, Yb, *etc.*) and yttria-stabilised zirconia (YSZ) are the most widely used electrolytes for SOEC[21-24]. Besides, oxides with $A_{n+1}B_nO_{3n+1}$ Ruddlesden-Popper structure, $A_2B_2O_5$ Brownmillerite structure, $ReMO_4$ structure, $A_2B_2O_7$ structure and $A_{10-x}B_6O_{26\pm\delta}$ apatite-type structure are also sometimes reported[25]. Ni-based cermets are used as typical anode materials, such as Ni-YSZ and Ni-BZCM cermets[26]. In addition, much effort still needs to be injected into the interfacial design of SOEC. Furthermore, the operating efficiency of SOEC is affected by various factors including temperature,

pressure, current density, *etc*. The problem of how to optimize these parameters under fluctuating renewable energy conditions is also an urgent issue[27]. If the solution to the above issues relies on traditional material development processes, there are often problems such as long material development cycles and high costs. The rapid development of artificial intelligence (AI) technology has provided new ideas and approaches to address these challenges. AI has demonstrated powerful capabilities in data processing, model building and optimization, and is able to effectively analyze and mine the complex relationships between material properties and structure. Through algorithms such as machine learning (ML) and deep learning, researchers can quickly screen potential high-performance materials and optimize their design[28-34].

Currently, some advances have been achieved, such as design of key materials and prediction of stability, relating to ML in SOEC[35-37]. As for the electrolyte, Hyodo *et al.* developed a gradient-augmented regression ML model to study the hydration structure-property relationship for perovskite oxides[38]. Gradient boosted regressor (GBR) model was trained by considering 80 descriptors based on the chemical compositions of perovskite oxides. After training, hydration structure-property maps were constructed, serving as a powerful tool to screen candidate materials from a vast number of compounds, thereby significantly accelerating the discovery process of proton-conducting oxides. Surprisingly, a new and outstanding material, $SrSn_{0.8}Sc_{0.2}O_{3-\delta}$, processing the proton conductivity of 1.4×10^{-3} S·cm^{-1} at 380 °C, was identified from 8,613 hypothetical perovskite oxides [Figure 1A]. This research provides a new avenue for the discovery of novel proton-conducting electrolytes for SOEC. Recently, Luo *et al.* reported that $BaSn_xCe_{0.8-x}Yb_{0.2}O_{3-\delta}$ (BSCYb) exhibits higher proton conductivity (0.02 S·cm^{-1}) and chemical stability (1,000 h), which is screened from 932 oxide candidate materials by calculating parameters such as oxygen vacancy formation energy, hydration energy [Figure 1B], and adsorption energies of H_2O and CO_2 [Figure 1C][39]. The current density of SOEC with BSCYb is 2.62 A·cm^{-2} at 600 °C and 1.3 V, ranking top among the reported cells[40].

Compared to the electrolytes, anodes of SOEC have received more attention[11,35-37]. In 2022, Wang *et al.* developed accurate and interpretable ML models with random forest and boosting (XGBoost) algorithms, *etc.*, to predict the hydrated proton concentration of oxides for the fast-screening promising anodes [Figure 2A-C], which is the first time to screen anode with the assistance of AI[36,41]. Initially, a database consisting of 792 samples was established, where 29 features, including temperature, water pressure, *etc.*, were designated as input variables, and the hydrated proton concentrations served as the target variable. After the model was trained, $(La,Ca)(Co,Ni)O_3$ family oxides were screened as the promising anodes of SOECs from thousands of perovskite oxides [Figure 2D]. For instance, the current density of the cell with a $LaCo_{0.9}Ni_{0.1}O_3$ anode achieved 1.44 A·cm^{-2} at 1.3 V and 650 °C[41]. After that, Zhai *et al.* introduced the ionic Lewis acid strength (ISA) - defined as the ability of ionic Lewis acids to accept electron pairs - as an effective physical descriptor of artificial neural networks (ANNs) model to design high oxygen reduction reaction (ORR) activity of perovskite oxides[11]. The screened oxide $Sr_{0.9}Cs_{0.1}Co_{0.9}Nb_{0.1}O_3$ (SCCN) shows small area-specific resistance (ASR) - the resistance encountered when current passes through a unit area of electrode material - (0.0101 Ω·cm^{-2}) and good stability (800 h) [Figure 3A and B]. In 2024, Li *et al.* predicted the oxygen vacancy concentration of Co-based and Fe-based perovskite oxides in a wide temperature range for the design of oxygen electrodes [Figure 3C][42]. They revealed that the predicted oxygen vacancy concentration is consistent well with ORR activity [Figure 3D and E]. This work provides a ML-guided route for developing oxygen electrocatalysts suitable for operation at different temperatures[42].

Despite the significant progress in AI-guided SOEC research and development, AI technology still needs to play a more active role in solving practical problems in terms of improving single-cell performance and suitability for renewable energy sources. The bottlenecks we are currently facing and the corresponding solutions can be approached from the following two levels: At the single-cell level, firstly, key material

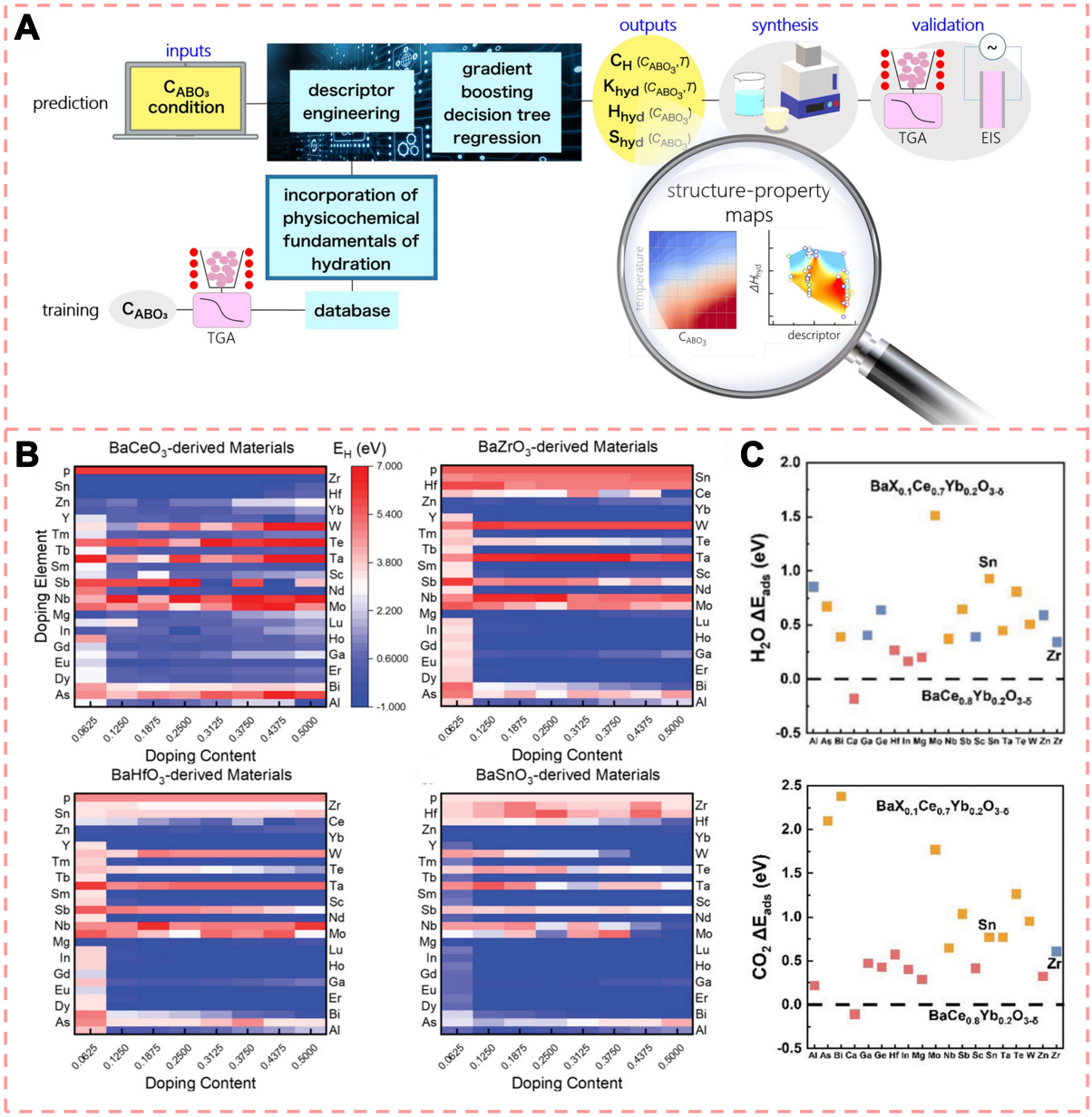

Figure 1. (A) Schematic workflow for the construction and discovery of proton conducting oxides using data-driven structure-property diagrams. This figure is quoted with permission from Hyodo *et al.*[38]; (B) High-throughput calculation results of hydration energy for $BaCeO_3$-derived, $BaZrO_3$-derived, $BaHfO_3$-derived, and $BaSnO_3$-derived oxides; (C) H_2O and CO_2 adsorption energies at 0 K. This figure is quoted with permission from Luo *et al.*[39].

performances, including insufficient catalytic activity, long-term stability to be improved, low electrolyte ionic conductivity, component compatibility issues, *etc.*, should be improved. Secondly, interface engineering challenges are manifested in poor component suitability and complex interfacial reaction mechanisms. Thirdly, material degradation mechanisms have not been fully elucidated, especially at high current density, affecting long-term system reliability.

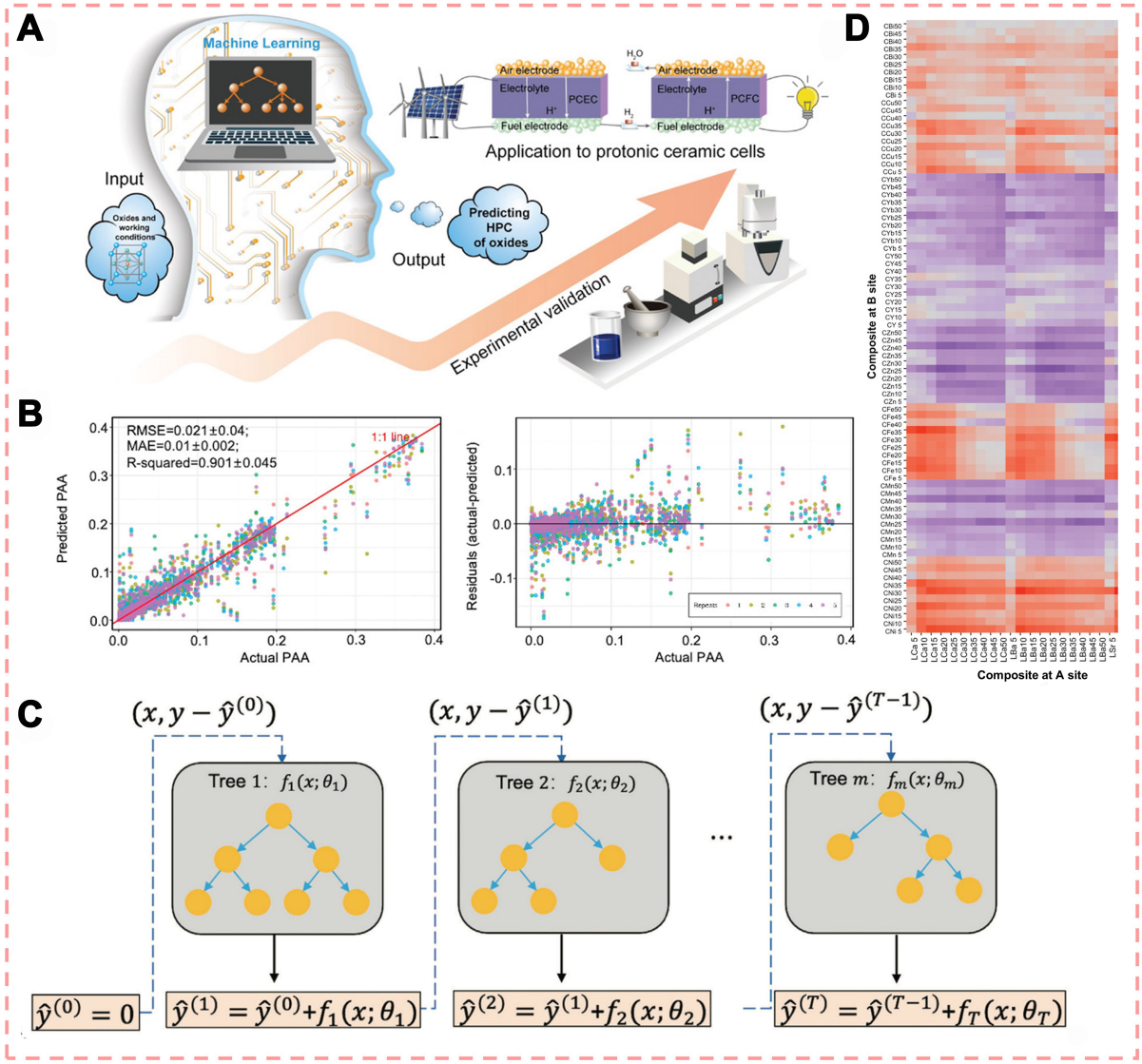

Figure 2. (A) Schematic diagram of the research process of screening anode of SOEC using ML models; (B) Comparison of actual and predicted values by the model, and the residuals of each predicted value by comparing with the actual values in XGBoost model; (C) General schematic diagram of the gradient boosting decision tree algorithm; (D) Part of the predicted hydrated proton concentration results. SOEC: Solid oxide electrolysis cell; ML: machine learning.

To address these challenges, AI-driven solutions breakthrough in three main directions: (1) Materials design optimization through deep data analysis and ML algorithms, mining existing material databases, and identifying key factors for performances, including ionic/electronic conductivity, thermal expansion co-efficiency, catalytic activity, porosity, *etc.*, predicting these performances of new material combinations, and guiding the optimization of material compositions and structures; (2) ML can be used to modify the interfaces in the cell. For instance, enhancing the compatibility and chemical reactivity between the electrolyte and anode, identifying optimal compositions, thicknesses, and preparation conditions for functional layers in between the electrolyte and anode, which plays a crucial role in reducing interfacial resistance, improving charge transfer, and enhancing overall cell performance; (3) Degradation mechanism analysis: analyze microstructure evolution, simulate electrochemical reaction process, predict material behavior under different working conditions, establish theoretical guidance framework, and promote

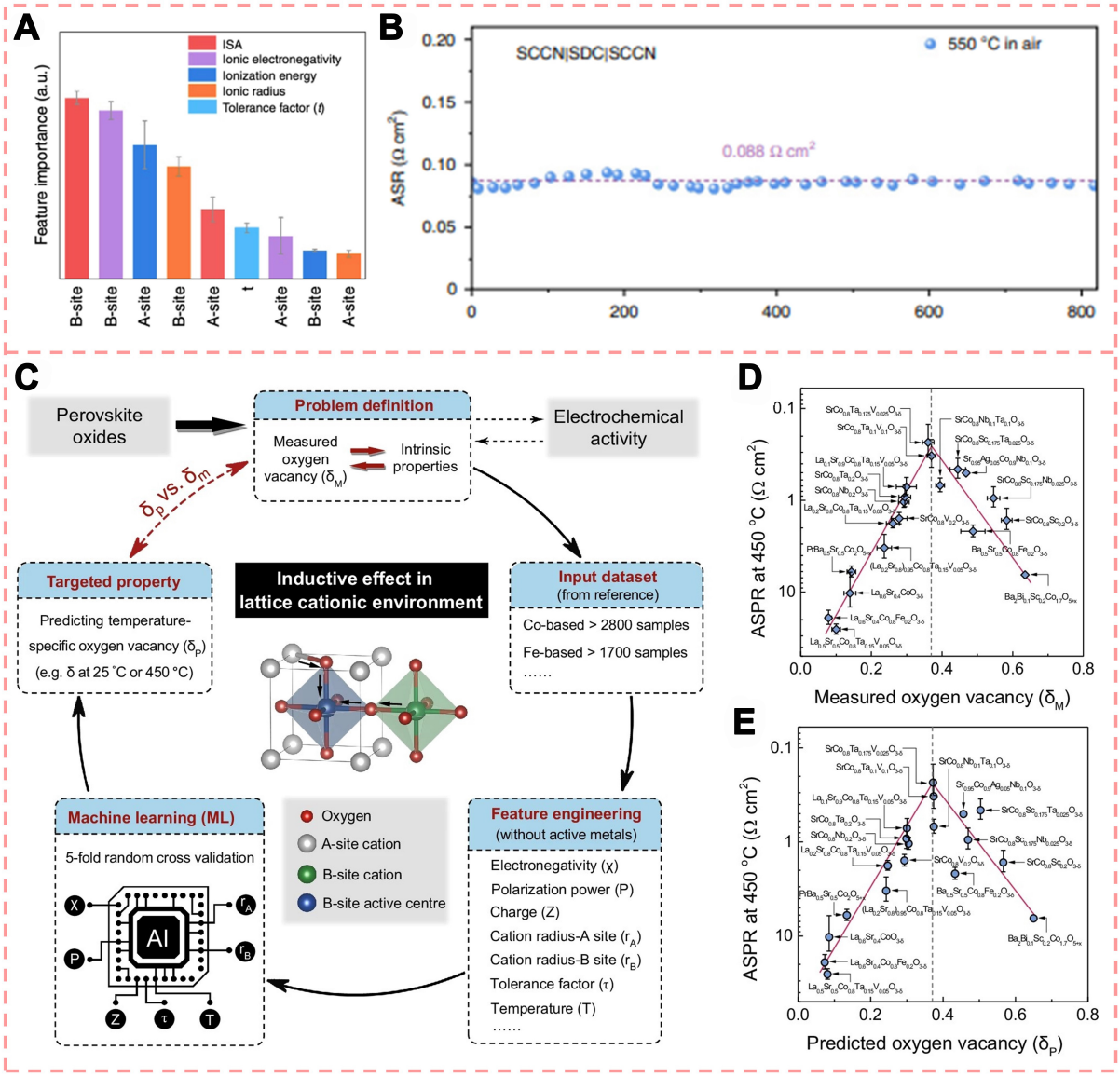

Figure 3. (A) Feature importance of the ionic descriptors based on the sensitivity analysis of the ANN model; (B) ASR values of $Sr_{0.9}Cs_{0.1}Co_{0.9}Nb_{0.1}O_3$ in a symmetrical cell measured for 800 h in air at 550 °C; (C) ML-assisted process for predicting oxygen vacancy concentrations; The ORR activity at 450 °C as a function of the (D) measured and (E) ML-predicted oxygen vacancy concentration. A-site and B-site: In cathode materials, ABO_3-type perovskite oxides, such as $LaCoO_3$, $LaCrO_3$, $LaNiO_3$, *etc.*, are commonly studied. For the doping of these oxides, the cell where the La element is located is generally referred to as the A-site, and the cell where Co/Cr/Ni is located is the B-site. ISA: Ionic Lewis acids are usually substances capable of accepting electron pairs. ASR: This refers to the resistance encountered when the current passes through a unit area of electrode material. Tolerance factor (t): A parameter used to measure the relationship between the size of different ionic radii and the stability of the crystal structure in a given crystal structure. Ionic electronegativity: A measure of an atom's ability to attract electrons when forming an ionic bond. It reflects the combined effect of an atom's electron affinity and ionization potential in a molecule or crystal. ANN: Artificial neural network; ASR: area-specific resistance; ML: machine learning; ORR: oxygen reduction reaction.

iterative innovation of key materials.

At the system level, adaptation between SOEC and renewable energy faces three core issues: power fluctuation adaptability (unstable output power, slow response speed, frequent start-stop affecting the life), thermal management (lack of precision in temperature control, thermal cycling stress, low efficiency), and

system control (complex synergistic, difficult to optimize the parameters, lagging failure warning). AI addresses these challenges by building systematic solutions: (1) constructing the prediction models to analyze weather, load, and other dynamic factors to accurately predict power generation and optimize operating parameters (temperature, current density, feed flow, *etc.*); (2) Developing intelligent control strategies to achieve synergistic operation of SOEC and renewable energy sources, including optimization of energy distribution, regulation of hydrogen production, and balancing of system efficiency; (3) Build power prediction and thermal field dynamic models to achieve power fluctuation smoothing and accurate temperature regulation. This multi-level, systematic AI-driven approach not only accelerates the development process of high-performance SOECs, but also provides a reliable guarantee for their stable operation under renewable energy conditions, which strongly promotes the large-scale application of green hydrogen energy. With the continuous innovation and deepened application of AI technology, SOEC technology will play an increasingly important role in the future energy transition.

Despite the promising potential of ML to advance SOECs, several significant issues must be addressed to fully realize its impact. One of the primary concerns is the inadequate standardization of data collection protocols[37]. Currently, there is a lack of unified standards for collecting, processing, and sharing data related to SOECs. These results are in inconsistent data quality and formats, making it difficult to integrate datasets from different sources and limiting the ability to train robust and generalizable ML models. The standardization of data collection protocols is essential to ensure that data is consistent, reliable, and interoperable across different research groups and platforms. Another critical issue is the lack of interpretability and low accuracy of AI models. Many existing AI models used in SOEC research are complex and often act as black boxes, making it challenging to understand how predictions are derived[8,11,39]. This lack of transparency hampers the trust and adoption of ML models by researchers and engineers. Moreover, the accuracy of these models often remains insufficient, with a lack of empirical support and specific examples to demonstrate their reliability and effectiveness. Detailed discussions and empirical studies are needed to validate the accuracy of ML models and provide specific examples of how they can be interpreted to guide practical applications. For instance, more research is required to show how AI models can be used to predict the long-term stability of SOEC or to optimize the composition of key materials with high precision.

Addressing these challenges requires a concerted effort to develop standardized data collection protocols and enhance the interpretability and accuracy of ML models. For instance, to clarify the degradation mechanism of SOEC, integrating *in-situ* analysis techniques, physically informed models, and high-quality databases is highly needed. *In-situ* analysis techniques, such as *in-situ* X-ray diffraction (XRD), electron microscopy, and spectroscopy, provide real-time data on the structural and chemical changes occurring in SOEC operation. This data can be used to train AI models, ensuring that they capture the dynamic behavior of oxides under actual operating conditions. These techniques also reveal the underlying mechanisms of degradation, such as phase transformation, microstructure evolution, and chemical degradation, which can be incorporated into ML models to improve their accuracy. Physically informed models integrate fundamental physical laws and principles related to SOEC degradation, such as the Nernst equation, Butler-Volmer equation, and heat transfer equations. This ensures that the models are grounded in the fundamental physics of the system. Multi-physics modeling approaches can account for the coupled effects of electrochemistry, thermodynamics, and mechanics in SOECs, providing a more comprehensive understanding of degradation mechanisms. High-quality databases are crucial for training reliable ML models. These databases should obey the standardizing data collection protocols, ensuring that the data is consistent and reliable, improving the quality of the training datasets. By overcoming these issues, AI can become a more powerful and reliable tool for advancing SOECs, ultimately contributing to the development

of more efficient and sustainable green hydrogen production technologies.

CONCLUSION

The integration of AI technologies with SOEC development represents a paradigm shift in accelerating green hydrogen production technologies. AI-driven approaches have demonstrated remarkable advances in key materials discovery and performance optimization, significantly reducing development cycles and costs. In the future, the continuous advancement of AI capabilities, coupled with expanding experimental datasets, will further enhance our ability to design high-performance, stable, and cost-effective SOEC single cells and systems. To fully realize the potential of AI in SOEC development, future efforts should focus on: (1) Establishing standardized protocols for data collection and sharing to build more comprehensive databases; (2) Developing more interpretable and accurate ML models that can better capture the complex relationships between materials properties and performance; (3) Integrating real-time AI-driven control systems for optimal operation under fluctuating renewable energy conditions. These developments will be crucial in establishing SOEC technology as a cornerstone of the global transition to sustainable energy systems.

DECLARATIONS

Authors' contributions

Conceptualization, resources, writing, and editing: Yuan, B.; Zhang, X.
Conceptualization, data curation, writing: Tang, C.
Conceptualization, supervision, and review: Ye, S.; Wang, N.

Availability of data and materials

Not applicable.

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Conflicts of interest

All authors declared that there are no conflicts of interest.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

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