Materials LAB

PERSPECTIVE

Materials Lab 2024, 3, 230021

Artificial intelligence in accelerating the development of air electrode materials for proton conducting solid oxide cells

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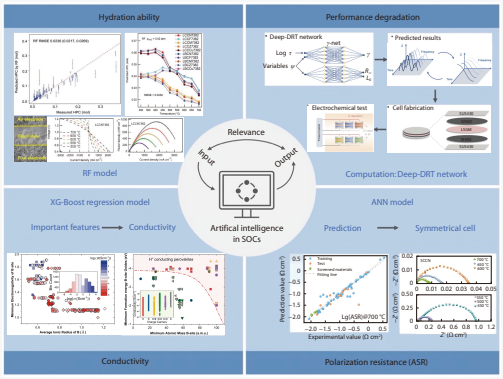
Proton conducting solid oxide cells (P-SOCs) operating at intermediate temperature, working in both fuel cell mode for power generation and electrolysis mode for hydrogen production, gain much attention due to their unique advantages. However, the lack of efficient air electrode is the main obstacle to get high-performance P-SOCs, moreover, developing such materials relies on the high-cost and time-waste traditional way. The application of artificial intelligence (AI) to the field of P-SOCs can solve the problems that the traditional way faced. In this perspective, we discussed the current reports relating to the development of air electrode materials of P-SOC by constructing machine learning models. Finally, the future directions of AI guiding the discovery of key materials and high-performance P-SOCs are proposed.



The exponential growth in consumption of limited fossil fuels not only leads to a serious energy crisis, but also causes many adverse environmental impacts in the past several decades. Consequently, renewable energy resources, such as wind, solar and tidal energy, are required to achieve the satisfaction of future energy demands. However, features of the intermittent nature and site dependency make these natural energies are not suitable for power supply core in large electricity grid, which requires storage or energy carriers. Hydrogen has been regarded as a clean fuel for many applications, such as, heating, electricity, and vehicles, and also can serves as an energy carrier because it is easily converted to liquid compounds by physical and chemical sorption process. Several types of electrochemical cells have been systematically investigated for hydrogen utilization and production, including proton exchange membrane cells (PEMCs),[1] proton-conducting solid oxide cells (P-SOCs),[2] and oxygen-ion conducting solid oxide cells (O-SOCs)[3] operated at low (< 300 °C), intermediate (400–700 °C) and high (> 700 °C) temperatures, respectively. PEMCs largely rely on high activity of platinum group metals (PGM) catalysts (like Pt, Ir and Ru) for electrode reactions, which increases the cost of system and limits their applications.[4] The commercialization of O-SOCs is hindered by delamination between cell components and significant degradation. P-SOCs are promising alternative to the O-SOCs because of some unique merits, such as, lower mobility activation energy for proton transfer, and ease of gas separation, which are expected to have better component compatibility, low cost, and high conversion/energy efficiencies at intermediate temperatures.[5-6]

The typical P-SOCs consist lamellar structure, including dense thin film electrolyte with composition of Ba(Zr, Ce, M)$O_{3-\delta}$ (M = Y, Yb, etc.) sandwiched by the porous air and fuel electrodes.[7] One of the major challenges for P-SOCs is the relatively high air electrode reaction resistance due to the sluggish kinetics for oxygen reduction and oxygen evolution reactions (ORR and OER) in fuel and electrolysis cell modes, respectively.[8-9] The basic requirements of air electrodes should include high specific area of active sites, sufficient electronic and ionic conductivity, chemically compatible with electrolyte and excellent hydrothermal stability. To date, significant efforts have been devoted to design air electrodes for P-SOCs, and the typical materials can be classified to ABO_3 perovskite, $AA'B_2O_{5+\delta}$ double-layered perovskite, Ruddlesden-popper phases with the general formula $A_{n+1}B_nO_{3n+1}$, layered ferrites (e.g., $Sr_2Fe_2O_5$) and layered swedenborgite (e.g., $YBaCo_4O_{7+\delta}$)

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Received 27 April 2023; Accepted 23 August 2023; Published online

DOI: 10.54227/mlab.20230021

from the crystal structure.[10-12] In addition to the material design of chemical composition, the microstructure and surface modification have been employed to promote the electrode reactions, such as, ultraporous air electrodes,[13] infiltration processes,[14] oxide layer deposition[15-16] and *in situ* exsolution.[17-18]

In the early stage, P-SOCs are employed with the O^{2-}/e^{-} double conductors for the air electrodes, such as $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF), $Sm_{0.5}Sr_{0.5}CoO_{3-\delta}$ (SSC) and $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF), which are widely used in the O-SOCs. However, the proton-accessible electrode reactions areas are limited near the gas-electrode-electrolyte triple-phase boundary (TPB) in P-SOCs owning to the mismatch of primary ionic carries between air electrode and electrolyte materials (H^{+}), thus most of the peak power densities (PPD) and current densities in P-SOCs are below 0.5 W cm^{-2} and 0.5 A cm^{-2} at the temperatures lower than 600 °C.[19] In more recent year, $H^{+}/O^{2-}/e^{-}$ triple conductors with hydration ability have been extensively examined for the air electrodes in P-SOCs, as inspired by that triple conductors could spatially expand reaction zone from TPB to the whole surface of the air electrode.[9, 20] The application of triple conductors in P-SOCs significantly increased the performance, for instance, the triple conducting material, $PrBa_{0.5}Sr_{0.5}Co_{2-x}Fe_xO_{5+\delta}$ (PBSCF) was successfully applied as air electrode in P-SOCs with peak power density near 1.10 W cm^{-2} and current density of 1.92 A cm^{-2} at 600 °C (1.3 V).[15] However, the other triple conductor of $Ba_{0.95}La_{0.05}Fe_{0.8}Zn_{0.2}O_{3-\delta}$ (BLFZ) with high proton concentration of 0.1 mol $unit^{-1}$ at 250 °C,[21] was reported to perform a current density of 0.46 A cm^{-2} at 650 °C and 1.3 V.[22] These results indicate it does not mean that pure or high protonic conducting oxides are excellent air electrodes, the catalytical activity and electronic conductivity should be considered at the same time. Therefore, developing outstanding air electrodes with smaller reaction resistance is critical to improve the electrochemical performance of P-SOCs. As the operating condition of air electrode contains steam, especially in electrolysis mode, thus, the thermal stability and compatibility between components are the second challenge for P-SOCs, which is almost impossible to finished in a short time due to the abundancy in the material and components. In addition, the effective anode areas are very limited and large-scale P-SOCs with high performance should be designed and evaluated. But, the design of air electrode materials, long-term durability and large-scale cells rely on careful control of material composition, preparation methods, a lot of time for measurement, and so on. So, some new technologies need be discovered to promote the development of air electrode materials for P-SOCs.

Fortunately, with the rapidly developed artificial intelligence (AI) and the expansion of the materials database, AI is gradually applied to the materials science for discovering new materials or predicting some properties with high-efficiency, speediness, low-cost, etc. Machine learning (ML) techniques, focusing on a data-driven perspective, have accelerated the design for energy material exploration to next stage. Wang et al. summarized the latest developments in ML models of supervised learning (SL), transfer learning (TL) and unsupervised learning (UL) to understand the relationship between the required data scale of materials attributes and ML models. And gave perspective that SL models can shorten the material design cycle from the existing databases, while the combined use of TL and UL are applied as the amount of material attributes with inadequate labels sharply increases.[23] The rechargeable batteries with the application of ML from microscale and macroscale were reviewed by Chen et al. and a quantitative "structure-function" correlation can be established to predict ionic conductivity of solids as well as forecast battery lifespan, thus, provided an outlook on future combination of experiments, multi-scale simulations and ML.[24]

In the case of solid oxide cells, Zhang et al. introduced deep learning techniques to simultaneous fault diagnosis in oxygen-ion conducting solid oxide fuel cell (O-SOFC) systems. An innovative and intelligent diagnostic technique based on stacked sparse auto-encoders (SSAE) was applied to solve simultaneous fault problems and enable proper fault diagnosis in O-SOFC systems.[25] The structure-property correlation in oxygen-ion and proton conductors was summarized by Coduri et al. and the application of AI computational approach to accelerate the discovery of oxide-ion and proton conductors was also introduced.[26] However, the available examples in P-SOCs and O-SOCs of the application of AI to develop new materials are still scarce[27-32]. (Fig. 1). As for the air electrodes of P-SOCs, there are also few reports relating to the AI accelerating the materials design. Wang et al. reported the highly accurate and explainable machine learning model with random forest algorithm to screen the proton-conduction oxides for the air electrodes of P-SOCs. The high-efficiency $(La_{0.7}Ca_{0.3})(Co_{0.8}Ni_{0.2})O_3$ (LCCN7382) was selected from 3200 oxides by predicting the hydrated proton concentration, then it was tested for verifying the accuracy of the model, finally, the oxide as the air electrode of P-SOC operated in fuel cell and electrolysis modes with excellent electrochemical performances.[33] J. Hyodo et al. demonstrated the accelerated discovery of the proton-conducting oxides for P-SOCs using data-driven structure-property maps for hydration of 8613 oxides by machine learning (ML) model with gradient boosting regression. The model finds that $SrSn_{0.8}Sr_{0.2}O_3$, which was not previously recognized as the proton conductor, is a new promising proton-conducting oxide.[34]

Not only proton concentration, but also the electronic conductivity, catalyst ability for electrode reaction (resistances of symmetrical cells), activation energy and long-term durability of air electrodes materials can be taken as directional parameters for AI. However, the use of AI methods to predict P-SOC air electrode materials still encounters challenges. First, the key central theme of AI algorithms for material design is the need of vast database of experimental results for training and verification. In this respect, high quality data of P-SOCs should be set and some hand-crated descriptors based on structural properties need be considered. Second, the properties of air electrode materials are determined by multiple parameters and features, thus it is necessary to seek highly accurate, explainable, and better generalization capability models. Another challenge for AI methods is knowing how to detect and correct errors that may occur in the data.

Anyway, considering that AI applied in P-SOCs brings many advances, we should pay more attention to this for accelerating the development of high-performance P-SOCs. In specific, on the one hand, the ML models with various algorithm, such

DOI: 10.54227/mlab.20230021

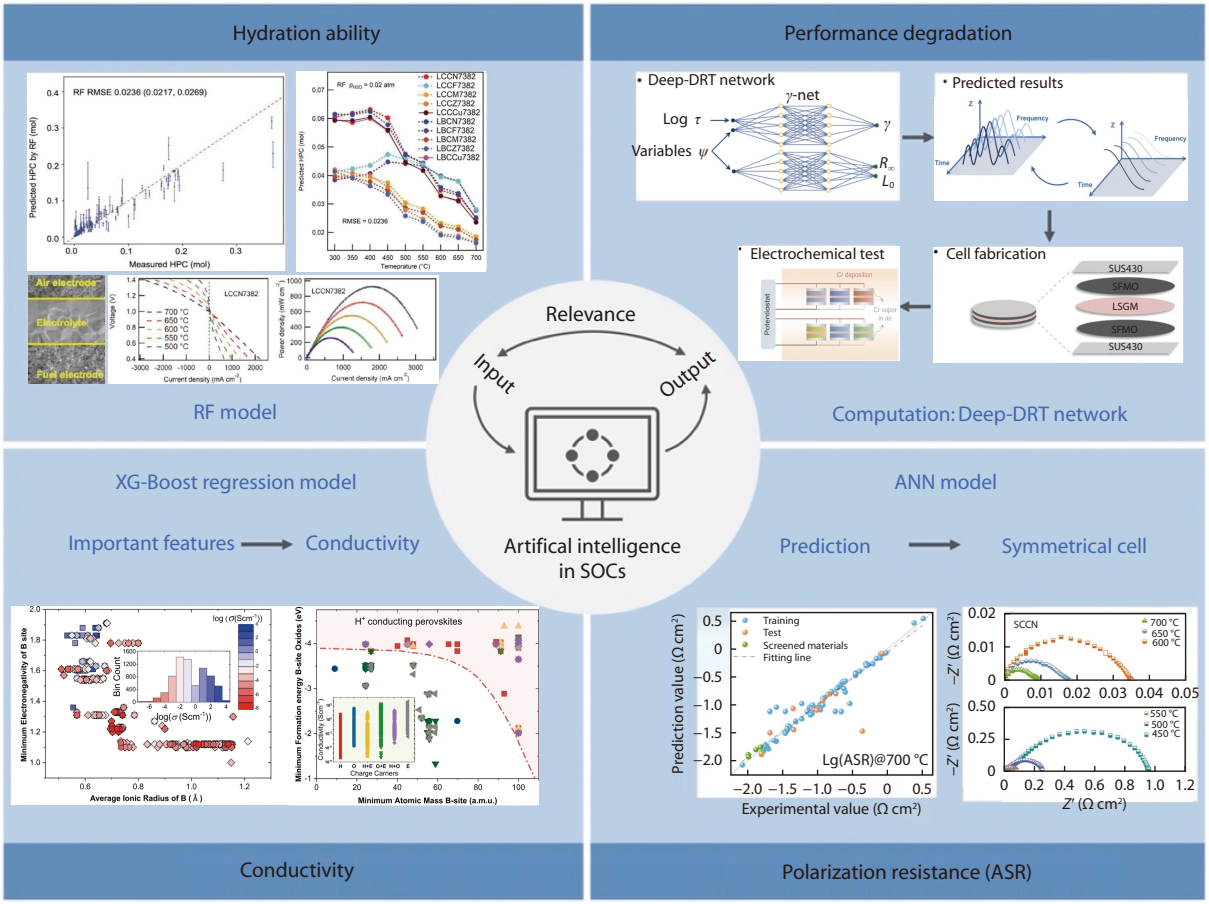

Fig. 1 Application of AI in P-SOCs and O-SOCs for predication of hydration ability, conductivity, polarization resistance and performance degradation.[27, 28, 33, 35] Copyright 2019, Nature; Copyright 2022, Royal Society of Chemistry; Copyright 2022, Wiley-VCH; Copyright 2021, Nature.

as support vector machine (SVM), artificial neural network (ANN), gradient boosting regression (GBR), can be constructed for the discovery of key materials in terms of electrolyte and air electrode for P-SOCs. On the other hand, the electrochemical performances can be predicted by building the accurate and explainable ML models. In short, AI technique should be introduced to the field of P-SOCs for the rapid development of this devices.

■ CONFLICTS OF INTEREST

The author declare no conflict of interest.

■ ACKNOWLEDGEMENTS

This work was supported by GuangDong Basic and Applied Basic Research Foundation (No. 2022A1515110612 and 2022A1515110470 (recipient: B.Y. Yuan and N.Wang), and Guangdong Engineering Technology Research Center for Hydrogen Energy and Fuel Cells.

■ AUTHOR CONTRIBUTIONS

This manuscript was drafted by C. Tang, F. Zheng, B. Yuan, Z. Huang and revised by L. Zhao, S. Ye and N. Wang. All authors have approved the final version of the manuscript.

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