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Perspective

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Research and prospects of electrochemical technology and educational innovation in water pollution treatment

Qisheng Huang[1], Lei Huang[1], Zhenxing Wang[2], Haiyang Liao[1], Jia Yan[1], Huan Li[3], Yufang Guo[1], Hongguo Zhang[1]

[1]School of Environmental Science and Engineering, Guangzhou University, Guangzhou 510006, Guangdong, China.
[2]South China Institute of Environmental Sciences, Ministry of Ecology and Environment, Guangzhou 510655, Guangdong, China.
[3]Hunan Key Laboratory of Carbon Neutrality and Intelligent Energy, School of Resources & Environment, Hunan University of Technology and Business, Changsha 410205, Hunan, China.

Correspondence to: Dr. Lei Huang, Dr. Hongguo Zhang, School of Environmental Science and Engineering, Guangzhou University, No. 230 Outer Ring West Road, Panyu District, Guangzhou 510006, Guangdong Province, China. E-mail: znhuanglei@foxmail.com; hgzhang@gzhu.edu.cn; Dr. Huan Li, Hunan Key Laboratory of Carbon Neutrality and Intelligent Energy, School of Resources & Environment, Hunan University of Technology and Business, No. 569 Yuelu Avenue, Yuelu District, Changsha 410205, Hunan, China. E-mail: 2849@hutb.edu.cn

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Abstract
Electrochemical wastewater treatment technologies, such as electrodeposition, electroflocculation, and electrocatalytic electrosorption, are effective and environmentally friendly but have challenges in large-scale applications due to low efficiency, poor stability, and high electrode material costs. Density functional theory (DFT) and artificial intelligence (AI) offer strong support for the design of new electrode materials. These technologies enable efficient material screening and deeply investigate electrochemical mechanisms. However, current models struggle to simulate complex reactions, causing a gap between theory and practice. While new materials exhibit good performance in the lab, their long-term stability and high cost limit industrial use. Future efforts should focus on improving electrode material stability and efficiency, using DFT for more accurate predictions and AI for faster material discovery and optimization. Additionally, integrating educational innovation research in electrochemical techniques into these efforts will help train skilled professional students and encourage them to develop cutting-

edge thinking. Reducing material costs and enhancing reaction efficiency are also key to achieving industrial-scale applications.

Keywords: Electrochemical technology, electrocatalysis, machine learning, education

PERSPECTIVE

Electrochemical technology is one of the most widely used technologies today, particularly in water purification for both pre-treatment and advanced treatment processes. It can effectively remove various pollutants, such as heavy metal ions, microplastics, and so on[1,2]. The main techniques include electrodeposition, electroflocculation, electrocatalysis, and electrosorption[3-5]. The physicochemical nature of solvent molecules provides a natural reaction medium and a source of active species for removing pollutants. Under an electric field, water molecules can be effectively activated, enhancing interactions between various ions, contaminants, and electrode materials. Electrochemical reactions driven by the electric field facilitate the *in situ* generation of strong oxidants, reducing substances, flocculants, and precipitates on the electrode surface, enabling efficient contaminant recovery or removal[6]. Supplementary Table 1 presents the application fields of several electrochemical technologies, including data on costs, current development stages, and future solutions. It can be seen that the biggest challenges to their commercialization are the high cost of electrode materials and the low overall efficiency.

A number of electrode materials have been developed to enhance the efficiency and application of electrochemical technologies. For example, Zhang *et al.* developed a conjugated two-dimensional covalent organic framework (COF) catalyst by anchoring single platinum (Pt) atoms [Figure 1A][7]. The unique Pt-N_2 coordination modifies the electronic structure of the Pt active site, optimizing its binding energy to the hydrogen intermediate (H^*). Furthermore, the asymmetric coordination in the COF structure precisely modulates the electronic environment around the Pt-N_2 site atoms, thus improving the overall catalytic performance. Mansoor *et al.* introduced the MXene material ($Ti_3C_2T_x$) into the electrosorption system [Figure 1B], leveraging its high electrical conductivity, two-dimensional layered structure, and abundant surface functional groups to achieve efficient ammonia nitrogen removal and recovery[8]. Continued research into new electrode materials is expected to drive down costs while improving performance. Likewise, advances in synthesis technologies will further enhance efficiency and cost-effectiveness. Additionally, novel electrode materials will be discovered for various applications. In recent years, computational techniques such as density functional theory (DFT) calculations and molecular dynamics (MD) simulations have been integrated into electrochemical research, enabling a deeper understanding of electrode material mechanisms[9]. For example, Li *et al.* modulated the electronic structure and adsorption properties of Cu-N_4 sites by introducing main-group metal functional groups such as -COONa[10]. DFT calculations showed that -COONa coordination optimized intermediate adsorption energy, lowered reaction overpotential, and enhanced charge transfer and bonding strength at the active sites [Figure 1C]. However, the high computational cost of these techniques limits their large-scale application. Additionally, model construction in these techniques is highly system-specific, requiring extensive recalculations for new systems, which poses a challenge for the large-scale development of novel electrode materials.

The introduction of artificial intelligence (AI) technology can effectively compensate for the shortcomings of traditional calculation methods. Models trained through machine learning can accurately predict electrode materials with better performance, often achieving a prediction accuracy exceeding 80%[11]. Although DFT techniques can also predict electrode materials to some extent, DFT may not be able to accurately capture all physical effects due to the limitation of the approximation of the exchange-correlation

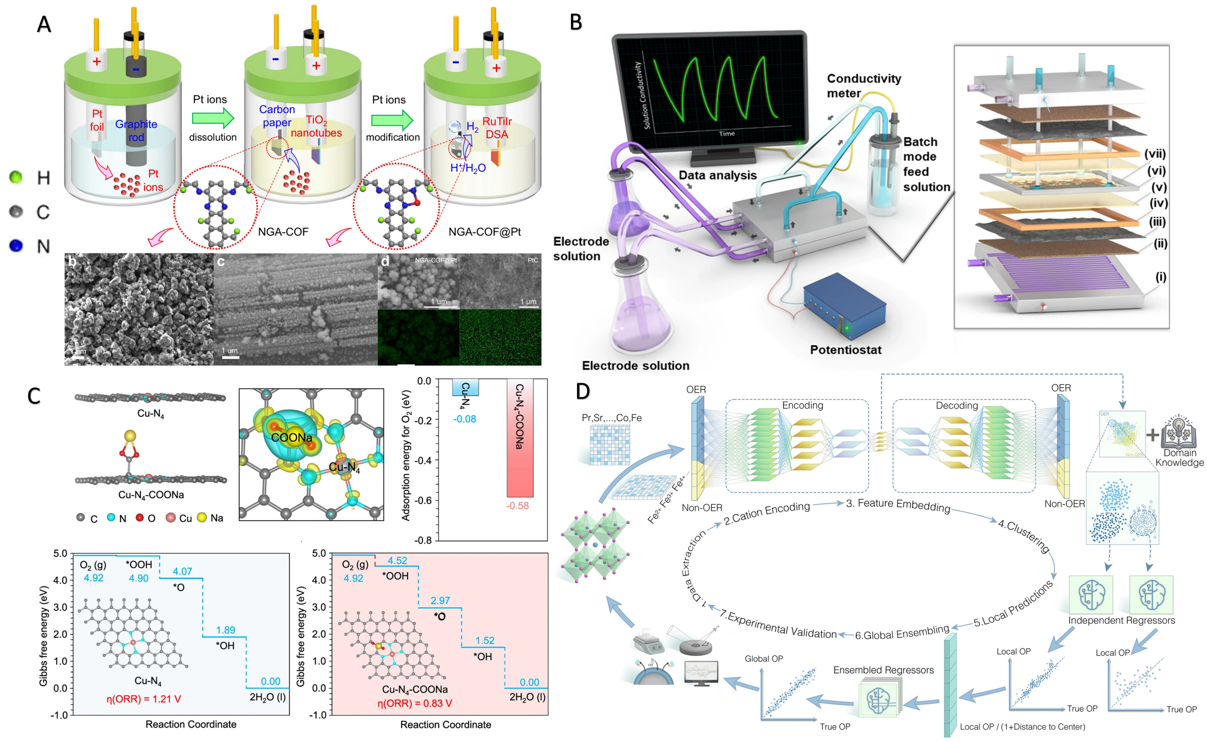

Figure 1. (A) Electrocatalyst synthesis and morphology characterization[7]; (B) Schematic illustration of capacitive deionization operation[8]; (C) DFT calculations for ORR catalysis[10]; (D) Transfer learning workflow to discover perovskite electrocatalysts for the oxygen evolution reaction[12]. ORR: Oxygen reduction reaction; DFT: density functional theory.

functional, especially when dealing with transition metal catalysts, interfacial effects, or electrochemical reactions under high temperature and pressure conditions. To solve this problem, Jiang *et al.* proposed a transfer learning paradigm [Figure 1D] by combining pre-trained models, integrated learning and active learning techniques[12]. Using this approach, they screened 16,050 new chalcogenide oxides, and identified two chalcogenide-structured electrode materials, $Pr_{0.1}S_{r0.9}Co_{0.5}Fe_{0.5}O_3$ (PSCF) and $Pr_{0.1}S_{r0.9}Co_{0.5}Fe_{0.5}Mn_{0.2}O_3$ (PSCFM) with better oxygen evolution reaction (OER) activity. Nowadays, advanced research has increasingly incorporated AI techniques (mostly machine learning) to predict material properties. These predictions are then experimentally verified, followed by further investigations into the mechanisms of the electrode materials using DFT and MD calculations. However, building machine learning models for electrode material prediction requires extensive data collection, often necessitating researchers to manually extract large volumes of relevant data from published literature. Despite the labor-intensive and repetitive nature of this process, no effective tools have yet emerged to automate it. More importantly, the availability of high-quality data points in published manuscripts is often limited, and the presence of non-reproducible data could misguide the model, significantly affecting the accuracy of subsequent predictions. As a result, extensive experimental validation becomes necessary. To address these challenges, new algorithms need to be developed to enhance the reliability and efficiency of predictive modeling in this field.

Therefore, colleges and universities must keep up with the times in electrochemical education. Many course contents have yet to be updated to reflect recent developments. For instance, there is limited coverage of electrosorption technology, new electrode materials, and advanced *in-situ* characterization techniques. As a result, many emerging research results have been detached from the production and research status quo described in traditional textbooks. In the era of AI, the introduction of new machine learning and deep learning models is driving the rapid development of electrochemical technology, necessitating corresponding changes in education. Integrating scientific research with teaching can bridge this gap, fostering a synergy that meets the growing demand for highly skilled professionals in modern society. Enhancing electrochemical education not only helps students grasp the latest research developments, but also cultivates their innovative thinking and problem-solving abilities, strengthening the connection between scientific research and practical applications in education.

OUTLOOK

To summarize the previous section, electrochemical technology holds a broad application prospect in the field of water pollution treatment. The future will be considered in the following multiple directions:

(1) Integration of AI: AI will play a crucial role in accelerating the design and development of materials for electrochemical technology. By leveraging AI algorithms such as machine learning and deep learning, large volumes of experimental data can be processed efficiently to predict optimal material combinations, significantly reducing the iterative cycles of traditional experiments and improving the efficiency of electrocatalyst development. However, as discussed above[13], some AI-predicted electrode materials may be challenging to synthesize due to complex or stringent conditions. To address this, the development and application of more efficient and practical algorithms are essential. Future research should focus on developing electrode materials that combine ease of synthesis with high performance.

(2) Electrocatalytic degradation of emerging pollutants: The degradation of novel pollutants through electrocatalytic technology is one of the important directions for the future advancement of electrochemical technology. Emerging pollutants (such as pharmaceutical residues, endocrine disruptors, antibiotics, *etc.*) pose serious environmental and health risks due to their complex chemical structures and poor biodegradability. With the continuous expansion of industrial production, the diversity and complexity of these pollutants are increasing, demanding higher-performance electrode materials for electrocatalytic applications. To meet this challenge, researchers should tailor electrode material development to specific application scenarios, ensuring precise targeting and optimization. The advancement of new electrocatalytic materials (e.g., single-atom catalysts, COFs, MXene, *etc.*), combined with in-depth research on reaction mechanisms, is expected to transform electrocatalysis into a green, efficient, and sustainable solution, providing strong technical support for the treatment of emerging pollutants and contributing to the comprehensive upgrading and innovation of environmental protection technology.

(3) Scaling up electrosorption technology and enhancing resource recovery: The large-scale development and resource recovery capabilities of electrosorption technology will be pivotal for its future progress. Electrosorption, an electric field-driven adsorption process, offers advantages such as high efficiency, low energy consumption, and strong selectivity. The key to its industrial application lies in the development of large-scale, modular equipment tailored for real-world deployment. Additionally, as the technology matures, its application in recovering valuable resources from wastewater (such as metal ions, salts, and organics) will further enhance its economic and environmental benefits. Efficient resource recovery not only minimizes waste but also significantly reduces wastewater treatment costs, supporting the dual goals of resource recycling and environmental protection. In the future, advancements in material science and engineering will unlock greater potential for electrosorption technology, particularly in the intelligent design of large-scale equipment, cost-effective resource recovery, and multi-scenario applications.

CONCLUSION

The future development of electrochemical technology is expected to follow a wide and diverse trend. It is believed that researchers will be able to study and understand the reaction mechanisms at microscopic interfaces in electrochemical processes by integrating advanced computational theories and AI techniques. Meanwhile, it points out the challenges in the industrialization process and highlights the important role of educational reform in training future technological innovators. Future research should further incorporate practical data to tackle economic and stability problems associated with large-scale applications of electrochemical wastewater treatment technologies. Additionally, educational reform is essential for fostering technological innovation and talent training. Emphasizing interdisciplinary education and the construction of teaching systems for emerging technologies will be key to advancing the industrialization process.

DECLARATIONS

Authors' contributions

Manuscript draft, drawing pictures, design: Huang, Q.
Guidance, framework proposed, funding acquisition: Huang, L.; Wang, Z.
English revision: Liao, H.
English summary: Yan, J.
Guidance, English summary: Li, H.
Data statistics, English summary: Guo, Y.
Guidance, editing review: Zhang, H.

Availability of data and materials

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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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