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AI driven design of new materials for clean energy.

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ABSTRACT

Electrocatalytic clean energy production powered by renewable electricity is gaining increasing attention to address rapidly growing energy demands while advancing toward a more environmentally sustainable future. However, the practical implementation of such processes remains hindered by the sluggish kinetics of key electrochemical reactions, including the oxygen evolution reaction (OER) and C-N coupling. These reactions typically demand high energy input in the form of elevated operating potentials, as well as the use of expensive noble metals., thereby limiting the overall energy efficiency and scalability of the electrochemical systems.

To address these challenges, the development of efficient, stable and cost-efficient electrocatalysts is essential. First-principle simulations and artificial intelligence (AI) algorithms offer powerful tools to gain atomic-level insights into reaction mechanisms and to accelerate catalyst discovery. In this context, we firstly employ existing experimental findings and density functional theory (DFT) calculations to elucidate the electrocatalytic reaction mechanisms, identify rate-determining step and evaluate possible by-products. Building upon these insights, we establish several AI-assisted electrocatalyst designing frameworks, aimed at locating materials with high intrisic activity, selecitivity towards target product (e.g. H_2, O_2 and urea), operational stability, and minimal reliance on noble metals. The performance of the predicted materials is validated through both theoretical calculations and experimental studies, confirming the effectiveness and accuracy of the proposed design strategies. Furthermore, this design protocol is readily extendable to a broader range of electrocatalytic reactions, offering a scalable and generalizable approach for sustainable green chemical production. The AI-assisted methodology outlined here presents a new paradigm for the rational design of electrocatalysts, paving the way for efficient and economical process of clean energy production.

KEY WORDS

DFT calculation, artificial intelligence, clean energy

BIOGRAPHY

Yiran Jiao is currently a Ph.D. candidate at the School of Chemical Engineering, the University of Adelaide, under the supervision of Professor Yan Jiao. His research focuses on the rational design of

materials for clean energy production, with particular emphasis on the integration of first-principles simulations and artificial intelligence.