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EDITORIAL

Breaking limits in electrocatalysis design

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Electrons can be considered the simplest form of reagent and can be efficiently supplied by directly applying a potential to a solid electrode or catalyst.[1] This highlights the critical importance of electrochemical catalysis in producing clean energy and valuable chemicals. It facilitates the transformation of fundamental scientific discoveries into practical technologies that underpin modern energy systems, including batteries, hydrogen fuel production, and carbon-neutral chemical manufacturing. The roots of this field trace back to Faraday's early work on electrolysis, and over time, scientists have developed detailed theories to explain how electrons move and drive reactions at material surfaces.

Thanks to these advances, electrocatalysis has become a powerful bridge between basic science and real-world energy solutions. It helps us design better catalysts and devices for a low-carbon future. However, electrocatalysis is also notoriously a "dirty" science. This is due to the inherent complexity of real-world experiments, where catalyst surfaces are rarely pristine and undergo continuous transformation during reactions. Surface inhomogeneity, such as steps, kinks, grain boundaries, and defect sites-combined with in situ phase transformations and reconstruction, means that two ostensibly identical electrodes can behave very differently. The presence of trace contaminants in electrolytes, including impurities at the parts-per-million level, as well as subtle fluctuations in pH or ionic strength, further complicates the reproducibility of experimental results.

From a theoretical perspective, the majority of models continue to assume idealized surfaces and simplified environmental conditions, which do not fully correspond to practical realities. For instance, even the simple hydrogen evolution reaction exhibits discrepancies between theoretical predictions and experimental observations when conducted on platinum electrodes, attributable to complex surface transformations occurring under operational conditions. To advance the understanding and enhancement of electrocatalysis, it is imperative that researchers realize and incorporate its inherent complexity.

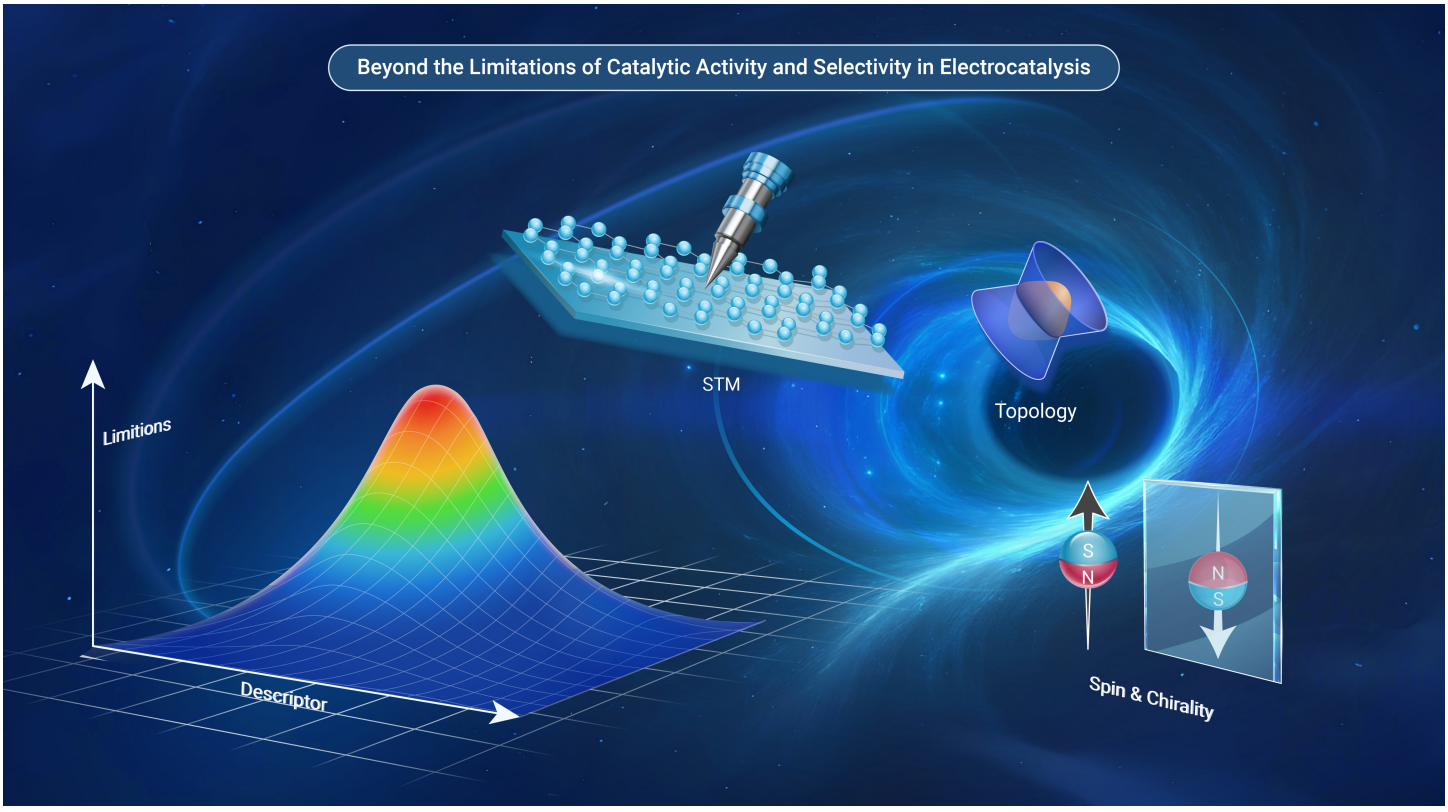

Figure 1. Electrocatalysis for clean energy and chemical synthesis: Challenges and opportunities.

Overly idealized theoretical models. Over the years, scientists have built theoretical models to explain and predict how electrocatalysts work. d-band theory successfully explains the trends of small molecules such as CO_2 and H_2 adsorption across metal and alloys,[2] while microkinetic models based on Nernst-Volmer kinetics offer a starting point for predicting current-potential relationships. These models simplify complex chemical reactions into more manageable mathematical relationships and have been instrumental in advancing the field, particularly in the early stage of catalyst design. However, a significant limitation of these theories is their reliance on idealized conditions, such as atomically flat, pristine crystal surfaces, and precisely controlled environments. Moreover, they decouple charge transfer from mass transport, despite the fact that real systems are affected by diffusion, migration, and surface coverage.

To move beyond simplified models, predictive electrocatalysis requires advanced, multi-scale theories that reflect the real interfacial complexity and dynamic behavior of catalytic systems. We propose that multi-scale simulations are necessary to capture structural and temporal changes at interfaces. In addition, ab initio molecular dynamics or hybrid methods are required to reflect solvation and ion interactions in performing site-specific energy calculations. Effective approaches such as constant-potential density functional theory (DFT) and explicit solvation models, which adjust the system's electron count to maintain a fixed electrode potential, enable accurate modeling

of potential-dependent adsorption energies, charge transfer, and electric double-layer effects. These methods also capture specific cation effects and interfacial structural changes that influence catalytic activity and selectivity, which are critical for understanding complex reactions such as CO_2 reduction.

Lagging experimental techniques. Although powerful tools like scanning tunneling microscopy and electrochemical X-ray photoelectron spectroscopy have greatly expanded our understanding of electrochemical surfaces, they still lag behind theoretical developments. This challenge arises from the inherent difficulty in investigating solid-liquid interfaces under realistic, operational conditions. Combining different techniques (like spectroscopy, microscopy, and electrochemical tests) in operando setups sounds promising, but often involves difficult compromises in controlling temperature, pressure, and voltage. These technical challenges continue to constrain our capacity to directly correlate atomic-scale phenomena at active sites with the overall catalytic performance observed.

The rapid development of in situ techniques, such as the integration of electrochemical systems with advanced microscopy, offers new opportunities to probe high spatial resolution, temporal resolution, and chemical specificity in electrocatalytic systems. Taking electrochemical CO_2 reduction on copper as an example, in situ Electrochemical-Transmission Electron Microscopy enables direct observation of the dynamic formation and dissolution of Cu_2O/Cu interfaces under varying potentials. This finding successfully explains the enhanced selectivity toward C_2 products such as ethylene. Atomic-scale imaging captures the migration and reconstruction of surface atoms, directly linking structural dynamics to catalytic activity. It is well known that many catalysts undergo significant surface structure reconstruction during electrochemical processes. With the advent of electrochemical-atomic force microscopy (EC-AFM), it is now possible to investigate crystal dissolution and redeposition in real time. For instance, in the case of platinum used for the oxygen reduction reaction (ORR), EC-AFM imaging has revealed real-time roughening and smoothing of Pt surfaces with nanometer-scale resolution, allowing identification of preferred dissolution sites under specific potential conditions. Nonetheless, a critical challenge persists: current analytical techniques are unable to simultaneously deliver the comprehensive spatial, temporal, and chemical resolution required under realistic operating conditions.

While advanced characterization and theoretical modeling have significantly progressed, catalyst synthesis remains a major bottleneck in electrocatalysis research. A central challenge lies in the precise control of nanocatalyst atomic structures, including crystal facets, defect sites, and atomic composition. For instance, although Pt nanocrystals are widely used in fuel cell catalysis, synthesizing Pt nanoparticles with uniform size, shape, and facet orientation, such as well-defined {111} or {100} surfaces remain nontrivial. Even minor deviations in shape or facet exposure can lead to significantly different reaction pathways or stability profiles during operation. Furthermore, achieving atomic-level doping or alloying, such as in Pt-Ni or Pt-Co systems, is complicated by segregation effects or non-uniform distribution during high-temperature treatments. A similar problem lies in the controlled synthesis of MoS_2-based catalysts, with their edge sites are far more active than the inert basal plane. Additionally, scaling up these precise synthesis methods for practical applications also remains a significant challenge.

Breaking linear scaling relationships. In electrocatalysis, linear scaling relationships describe a trend: the binding strengths of important reaction intermediates (like *O and *OOH) often change together across different catalysts. This makes it easier to screen catalysts, for example, using volcano plots-but also creates a problem. If one try to improve the binding of one intermediate, it often worsens the binding of another. This trade-off sets a limit on how active a catalyst can be, especially for those reactions coupled with multi electrons such as ORR.

To get around this, scientists are exploring new material properties that can "break" this rigid link and allow more independent control over each step in a reaction. One promising approach uses topological materials.[3] These materials exhibit atypical electronic structures that induce distinct electron behavior at the surface, which can selectively modulate the adsorption of specific intermediates.

Another strategy leverages spin effects, which can be further modulated by external fields including magnetic and strain fields. In these materials, electrons with different spin orientations exhibit distinct interactions with reactive species. This leads to spin-dependent adsorption, where some reaction steps are stabilized more than others-again helping break the typical scaling pattern. Chiral materials, exhibiting a "handedness" in structure, can induce spin-polarized electron transfer at the crystal surface.[4] This approach can selectively stabilize spin-sensitive intermediates, such as triplet $*O_2$, without influencing other species. While more experiments and stronger theoretical support are needed to fully understand these quantum effects, these strategies already highlight the remarkable potential of quantum materials in reshaping catalyst design.

Unlocking AI's potential. One of the primary difficulties in catalysis research lies in understanding the complex relationship between atomic-scale features and macroscopic catalytic performance. Over the years, scientists have introduced many descriptors, such as coordination number, d-band center, adsorption energy, or more advanced ones like topological surface states, to help predict catalyst behavior. However, these descriptors often lack generality and struggle to describe the heterogeneous, dynamic conditions present at real catalytic interfaces.

In this context, artificial intelligence (AI) is opening new avenues. While DFT remains a powerful tool, it is computationally limited to small systems. AI-driven methods, such as machine learning force fields, graph neural networks, and symbolic regression, can now simulate systems containing millions of atoms, offering unprecedented insight into catalyst dynamics under realistic reaction conditions.[5] For instance, graph neural networks can elucidate how local atomic arrangements affect reactivity, while symbolic regression can identify meaningful equations that characterize structure-activity relationships.

To take advantage from AI support, the field needs a comprehensive catalyst database that brings together simulation data, experimental results, and AI predictions. To overcome these challenges, community-driven initiatives have emerged. The Open Catalyst Project provides large-scale, open-access DFT datasets optimized for machine learning, with standardized formats and consistent methodologies. Similarly, Catalysis-Hub.org aggregates reaction energetics data from across the literature, supporting open data exchange and reproducibility.

Toward a smarter, cleaner catalytic future. As understanding of electrocatalysis advances, the field is progressing into a transformative phase characterized by the integration of quantum mechanical insights, dynamic interface modeling, and AI-assisted discovery, which are reshaping classical theoretical frameworks. The road ahead promises not only scientific breakthroughs but also a future where cleaner energy and smarter chemical manufacturing are within reach, enabling cleaner energy through efficient water splitting, CO_2 reduction, and nitrogen fixation; driving the sustainable synthesis of high-value chemicals and pharmaceuticals; and unlocking complex multistep reactions with remarkable control.

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DECLARATION OF INTERESTS

The authors declare no competing interests.