

Editorial

Catalysis, Meet the Machine: From Models to Meaning

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In recent years, machine learning (ML) has expanded beyond specialized fields in informatics and physical sciences to become a part of our everyday lives — from personalized recommendations on streaming platforms to image generation and video synthesis using simple text prompts on Generative Pre-trained Transformer (GPT) architecture, in platforms like ChatGPT and other artificial intelligence (AI) tools [1]. While the potential of ML in many fields is already well recognized, its application in the natural sciences, including chemistry and physics, is still in a relatively early stage. Encouragingly, the results so far are impressive, and the next decade promises even greater advances.

This is especially true in catalysis, a field marked by complexity at every level — from the atomic structure of active sites to the large-scale design of industrial reactors. Catalysis plays a pivotal role in enabling a sustainable chemical industry, being integral to the production of over 90% of industrial chemicals [2]. Thus, innovations in catalyst design, process optimization, and system modeling are critical to reshaping how we produce fuels, materials, and fine chemicals.



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Traditionally, catalytic systems have been studied through mechanistic understanding, empirical exploration, and first-principles computational modeling [3-5]. While these approaches have generated profound insights, they often face limitations when dealing with the high dimensionality, nonlinear behavior, and multiscale interactions inherent in real-world systems [6, 7]. ML offers a complementary pathway — one that does not require full mechanistic knowledge to make robust predictions. From estimating adsorption energies [8] and reaction barriers [9] to optimizing operating conditions and reactor configurations [10], ML is reshaping catalysis research across scales. The recent surge in publications on ML in catalysis reflects this growing interest (Figure 1).

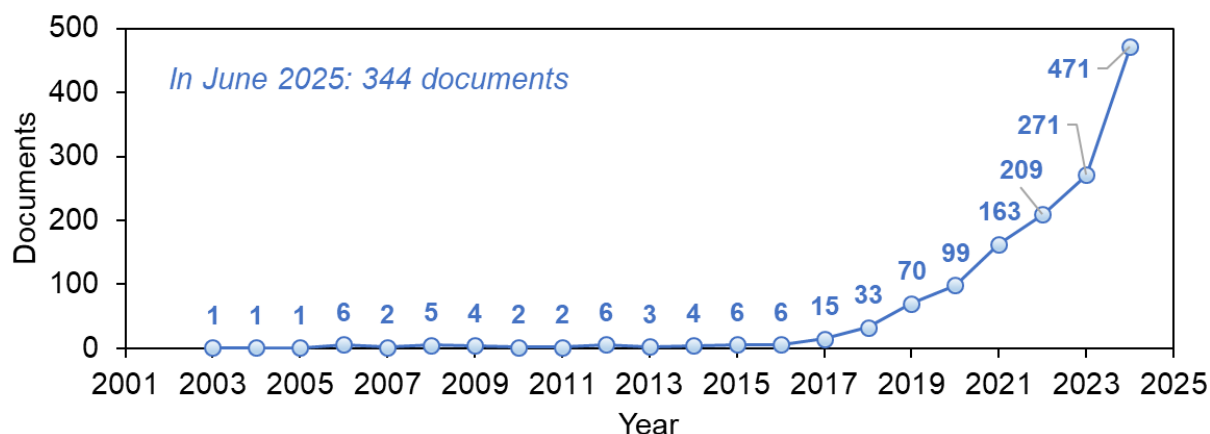


Figure 1 Number of publications per year combining the keywords “machine learning” AND “catalysis” using data from Scopus. Language: English. Data retrieved on 24 June 2025.

This Focus Issue, *Machine Learning in Catalysis: From Data to Discovery*, brings together contributions that highlight how ML is accelerating the discovery of new materials and improving catalytic processes. However, the story goes beyond speed; it is also about interpretability, hybridization, and the generation of insights.

As shown in Figure 2, applications may include the use of surrogate ML models trained on DFT calculations for catalyst screening [11], graph-based learning for exploring reaction networks [12], reinforcement learning for process optimization [13], and the increasingly prominent use of physics-informed machine learning (PIML) and physics-informed neural networks (PINNs) [14, 15]. These hybrid methods embed scientific laws — such as conservation principles, kinetic expressions, and transport equations — directly into ML architectures. The result is a class of models that can generate reliable predictions while remaining consistent with physical reality.

Examples of Machine Learning Applications in Catalysis

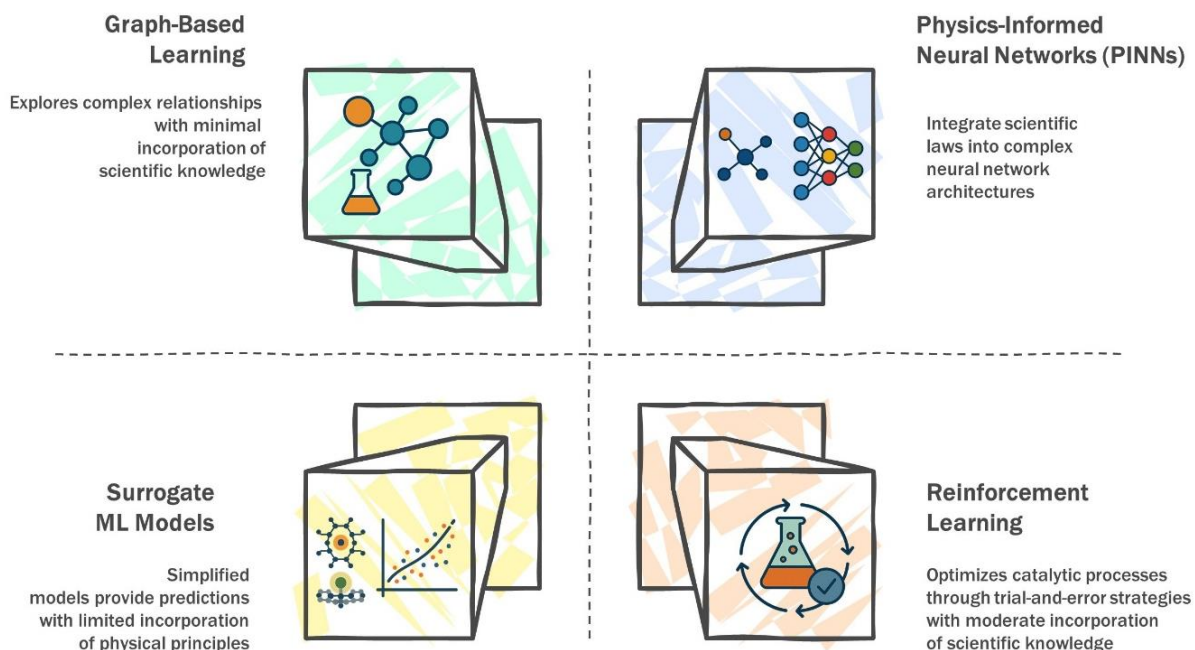


Figure 2 Schematic illustration of examples of machine learning applications in catalysis.

Throughout this issue, the readers may find diverse examples of how ML is being applied across the entire catalytic value chain — from molecular understanding to process-level integration. Still, several challenges persist: limited datasets, bias in reported results, the scarcity of negative data, and the need for standardized benchmarks. Nevertheless, as the catalysis community increasingly adopts open science practices and interdisciplinary approaches, ML is poised to transition from a promising technique to a core tool in scientific discovery.

If catalysis is the science of transformation, then ML is transforming how that science is practiced. We hope this special issue captures the breadth, depth, and dynamism of this evolving field — and encourages researchers to see not just patterns in data, but pathways to discovery.

Author Contributions

The author did all the research work for this study.

Competing Interests

The author declares no conflict of interest.

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