AI ADVANCES IN CATALYST AND MATERIALS DESIGN: PRACTICALITIES AND MYTHS

Multi-Client Study Proposal

"For the Industry, By the Industry"

November 2025

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ABSTRACT

Catalysts drive efficiency and innovation across various industries, including fuels, pharmaceuticals, and the energy materials sector. The energy and chemistry transition requires accelerating the discovery of new catalytic materials. Their immense diversity makes discovery both fundamental and difficult to automate with advanced Artificial Intelligence (AI) and Machine Learning (ML) methods. Utilizing Design of Experiments (DOE) to augment High-Throughput Screening (HTS) for R&D is a step towards the long-term goal of developing Autonomous Laboratory (AL) systems. Progress will come from integrating advanced computing, data resources, and IP protection, while closing existing gaps and promoting collaboration to improve accessibility. Understanding this complexity is key to developing new business and research strategies in the discovery of catalytic materials. This report presents an industrial perspective on achieving this progress, providing future roadmaps and business models while emphasizing practical implementation and dispelling common myths.

I. BACKGROUND

Since the mid-2000s, the emergence of companies such as Avantium (from Shell), Chemspeed, and hte (from BASF) has made high-throughput screening tools and services a core component of catalyst development, now widely embedded in industrial R&D. Now, AI coupled with HTS has accelerated catalyst discovery by enabling rapid screening of new compositions. Yet, it still depends heavily on each company's internal "Design of Experiments" expertise, driven by proprietary knowledge and manual innovation.

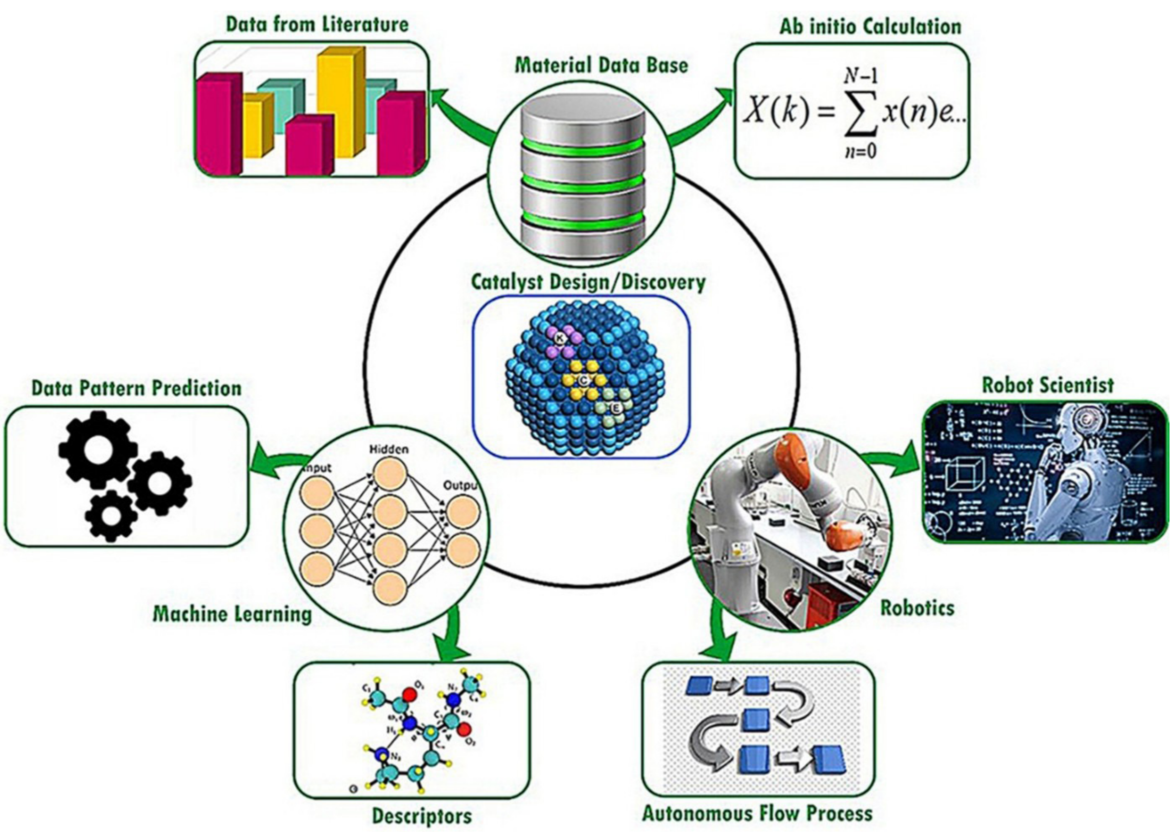

Figure 1. Integrated Data-Driven and Robotic Workflow for Accelerated Catalyst Discover, (Moses et al., 2021)

Today, this expertise remains fragmented across different industrial, academic, governmental, and AI software stakeholders (**Table 1**). Bridging these silos, or selectively integrating the most effective approaches, is critical to advancing industrial-computational collaboration toward a unified roadmap for automated catalyst design.

Table 1.
Examples of Stakeholders, by Silo, Invested in Automated DOE Functions. Source: TCGR

Industry	Universities	Governments	AI Developers
Refining	DTU Denmark	U.S. National Labs	Google
Chemicals and Plastics	Berkeley	EU Programs	Meta
Agrochemicals	Amsterdam	China Programs	Microsoft
Pharmaceuticals	Tsinghua	National Programs	IBM
Electrolyzers	Carnegie Mellon	Gov. Consortiums	Nvidia

Since 2020, efforts have focused on automating experimental design through data-driven and machine learning methods, with LLMs (Large Language Models) emerging mainly as tools for semantic data interpretation and research support (**Figure 2**). While progress has been made, key challenges remain. Despite the introduction of many new models and datasets, no approach has yet yielded a viable pathway to proving the large expectations.

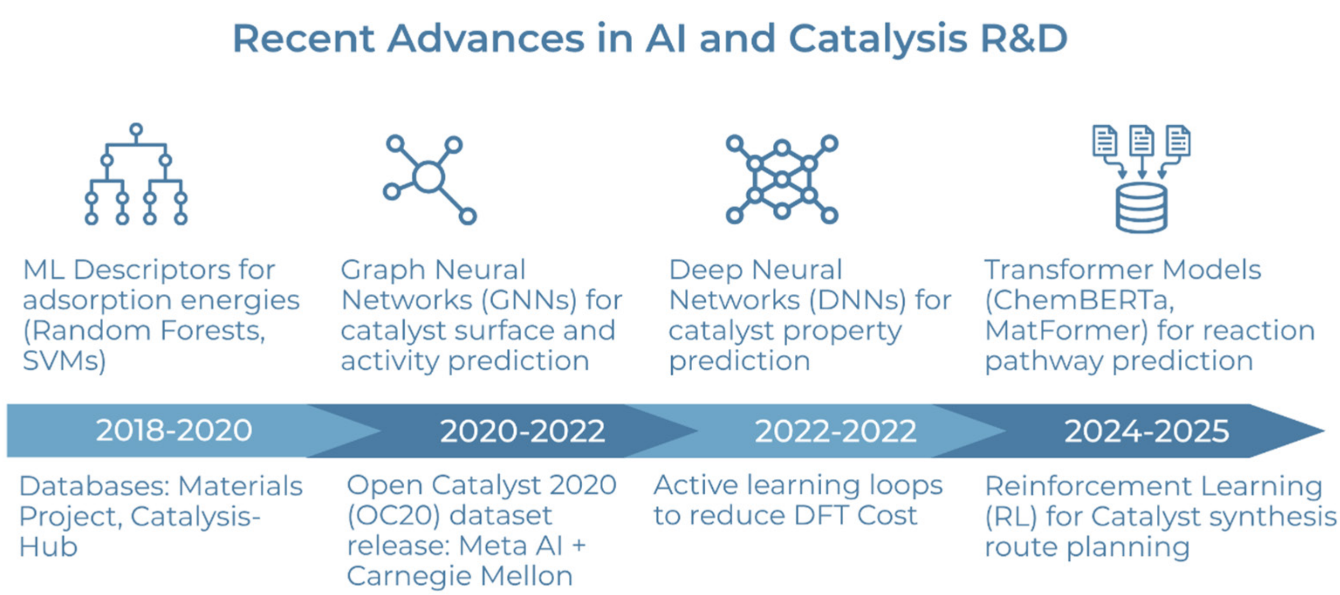

Figure 2. AI in Catalysis R&D 2018-2025. TCGR (2025)

A key issue is that each DOE catalyst design algorithm is specific to its industrial context, making commonalities difficult to define and leading to thousands of unique formulations. Moreover, while high-throughput experimentation (HTE) can identify promising catalysts, scale-up using real feedstocks often alters selectivity, conversion, and yield due to process engineering constraints. Both DOE and HTE methods require knowledge of the space field, i.e., the variables and their relationships. AI and ML methods help identify these aspects in areas such as the exploration of unknown regions (e.g., new catalysts, reactions, or products). These factors impede commercial viability and remain a major hurdle even for hybrid ML systems designed for reaction- or product-specific applications.

A 2024 Oak Ridge National Laboratory (ORNL) workshop, "Shaping the Future of Self-Driving Autonomous Laboratories" (**Figure 3**), identified specific challenges in autonomous research and provided key gaps and recommendations, particularly in data integration and algorithmic interoperability. A global context for this study was developed through interviews with leading international scientists from academia and industry. Recent advances in reinforcement learning (RL), Bayesian optimization, and closed-loop learning systems, combined with the rapid expansion of large AI platforms and frameworks in China, demonstrate strong potential to consolidate current approaches. Incorporating this collective global knowledge, particularly from China, is essential to this study's methodology (Wang et al., 2023).

This report will examine, challenge, and docuent the current state of the art (SoA) in automated DOE, alongside providing insights and recommendations for practitioners to address key challenges and accelerate internal programs. It focuses on major industrial applications, e.g., polymers, chemicals, and hybrid heterogeneous/homogeneous DOE systems.

KEY INSIGHTS/RECOMMENDATIONS

- Establish a national consortium for self-driving laboratories that leverages DOE facilities as foundational anchors while integrating academia, industry partners, and other federal agencies to build a sustainable ecosystem for advancing autonomous research and fostering cross-sector innovation.
- Develop software, hardware, digital twin, and networking solutions for sustainable ecosystems with diverse scientific instruments and computing systems across mutli-domain access controls and firewalls.
- Develop hybrid AI systems that combine data-driven learning with fundamental scientific principles, ensuring automated decisions remain grounded in core physical and chemical understanding.
- Address the critical timescale mismatch between human decision-making and modern instrumentation capabilities through strategic automation while preserving essential human insight and oversight.
- Create standardized interfaces and protocols for laboratory equipment and data management to enable seamless integration across facilities and institutions.
- Transform scientific education and workforce development by integrating AI/ML training with traditional scientific curricula while maintaining an emphasis on fundamental principles and critical thinking.

Figure 3. Key Insights/Recommendations from ORNL Autonomous Lab Workshop. (ORNL, 2024)

II. THE NEED FOR THE STUDY

In particular, this report will help define the boundary regions between practicalities and myths, thus identifying priorities and feasible paths, as well as the track to specific business-oriented R&D within the framework of large research initiatives.

AI and digitalization are transformative in catalysis and process engineering because these technologies enable data-driven optimization, predictive modeling, and real-time process control. AI accelerates catalyst discovery through machine learning, reducing experimental cycles and costs. Digital twins and advanced simulations enable the virtual testing of processes, enhancing efficiency and sustainability. These technologies create competitive advantages by enabling faster innovation, reducing downtime, and optimizing resource utilization, all of which are critical in an industry where precision, scalability, and environmental compliance define success.

> "Catalysts are the microchips of modern molecular processes."

We recognize the complexity of this landscape and the significant rewards that come with advancing toward a future of a "Self-Driving Autonomous Catalysis Laboratory." Over the past two decades, this effort has attracted billions of dollars in R&D investment from governments and industry, creating high expectations. Still, the challenge remains translating this effort into business opportunities and creating precise innovation strategies. This timely study warrants close attention because it aims to provide information on the following:

1. Reduction of the high cost and time requirements of catalyst development from synthesis to industrial-scale screening, generating substantial efficiency gains.

2. Expansion of the limited parameter space traditionally explored by chemists due to time and material constraints, enabling the discovery of catalysts that may otherwise remain hidden.

3. Explore more efficiently the new opportunities created by the electrification of production, the use of renewable energy sources, and carbon circularity. They require new catalytic technologies that expand on the approaches currently in use in catalysis.

4. Integration of expertise across industries, academia, and AI domains, along with development in robotics, to identify cross-sector solutions that individual organizations may overlook.

Each of these objectives is compelling on its own. Combined with the unique international expertise of The Catalyst Group and an international team including esteemed professionals such as Stephan Schunk and his team from hte-company (BASF), Dr. Vegge (DTU Denmark) on materials and scale up, Prof. Gabriele Centi (President ERIC - Eur. Res. Inst. of Catalysis) as project manager, along with a team of Chinese experts, this study offers an unparalleled opportunity to guide strategic investment in AI-driven catalyst R&D and benchmarking. The EU has also established the AI Office and RAISE, the Resource for Artificial Intelligence Science in Europe. Meanwhile, Germany has initiated the second phase of the National Research Data Infrastructure (NFDI), a national initiative that advances data-driven and AI-enabled research across scientific disciplines.

Assimilating AI and digitalization in catalysis and process engineering is no longer optional; it is a strategic imperative. At the strategic level, these technologies enable companies to lead in innovation, accelerate catalyst discovery, and meet sustainability targets. Through optimized resource use they also provide agility to adapt quickly to market and regulatory changes, creating a clear competitive edge. Tactically, AI-driven predictive models and digital twins enhance operational efficiency by minimizing downtime, improving yields, and reducing waste. Real-time monitoring and adaptive control strengthen safety and compliance while lowering costs. Together, these elements transform traditional workflows into intelligent, data-driven ecosystems, ensuring faster development cycles, resilient operations, and long-term profitability in an increasingly demanding and competitive environment.

III. SCOPE AND METHODOLOGY

Every TCGR study delivers competitive, strategic insights for industrial and financial investors, highlighting key trends, challenges, expectations, and actionable conclusions. With more than 40 years of experience, TCGR is recognized for providing sound, data-driven strategic guidance. Leveraging its extensive global Dialog Group® network, TCGR brings unmatched expertise to this study. The team will draw on seasoned specialists in catalyst design, DOE, and HTS to provide insights grounded in real-world experience and informed by engagement with global innovation leaders that go beyond the reach of other organizations lacking real-world industrial depth and perspective.

The following tentative Table of Contents, issued for pre-publication orders, will be refined based on collective subscriber input before the study's initiation and completion. The numbers in brackets indicate the anticipated page count for each section. Most chapters will have a dedicated topic presenting the status of the area in China and Asian countries.

Table of Contents* [TENTATIVE]

Each of these subtitles will have expanded a, b, c, etc., with references.

The total page count is anticipated to be 160-175, excluding appendices.

IV. QUALIFICATIONS

The Catalyst Group's main mission has been to accelerate advanced catalysis, materials science, and biocatalysis since the early 80's. During the early 2000s, TCG was instrumental in identifying and transferring High Throughput Experimentation2000s from the fine chemical/pharmaceutical industry into the refining and chemical industries. Many will remember TCGR's COMBICAT Conference Series, as highlighted in **Figure 4** below.

Figure 4. High Throughput Experimentation with COMBICAT Meetings. (TCGR, 2020)

Since then, we have remained deeply engaged in catalysis R&D and completed numerous consulting assignments. Notably, we completed a Catalytic Advances Program (CAP) report, "Advances in Digitalization of Catalysis" (2020), as an update to prior work and supported the U.S. DOE in formalizing its own programs.

Drawing on our in-depth knowledge of molecular structures, process systems, and commercial applications, we provide a unique combination of business insights and technology skills through a range of "for the industry, by the industry" client-focused services. Often working as an extension of our clients' teams, we combine our knowledge of cutting-edge technology. We have built our consulting practice on long-term client relationships, dedication, and a commitment to integrity.

> **"We Provide the "Catalysts" for Business Growth, Linking Technology Innovation with market opportunity"**

V. CONFIDENTIALITY

TCGR's report is based on technology evaluations, commercial/market assessments, and interviews with key players, and goes beyond public-domain information. This report is both timely and strategically important to industry participants and observers, as it facilitates informed monitoring and investment decisions. As a result, subscribers are requested to complete and sign the "Order Form and Secrecy Confidentiality Agreement" on the following page.

VI. DELIVERABLES AND PRICING

The study, "***AI Advances in Catalyst and Materials Design: Practicalities and Myths***" is expected to be available 6 months after launch.

PARTICIPATION	DEADLINE	PRICE
"Charter" subscribers*	January, 2026	$28,500
Post-launch subscribers	After June, 2026	$32,500

*Charter subscribers (those who sign up for the study before others) will have the opportunity to work with TCGR to further refine the scope of the report by delineating areas of particular interest for inclusion in the assessment.

ORDER FORM & CONFIDENTIALITY AGREEMENT

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