AQCat

Accelerated Catalyst Discovery Powered by Quantitative AI

Designing, optimizing, and manufacturing new catalysts is hard, slow, and expensive. Worse, failures in R&D and testing can lead to costly failures and delays during pilots and scale-up.

AQCat is SandboxAQ's catalysis platform that combines quantum chemistry, machine learning, and multiscale physics to rapidly discover and optimize novel catalyst materials. Using our proprietary Large Quantitative Models (LQMs), AQCat dramatically reduces the time and human effort required to identify catalysts that are active, selective, stable, and synthesizable, cutting discovery cycles from years to months and reducing risks during scale-up. Whether you want to discover new materials or improve existing products, AQCat can help.

Why AQCat? Why Now?

Catalysts used to be designed by chemists laboring over benches, using trial-and-error experimentation guided by chemistry expertise and intuition. These days, demand for new, specialized chemistries and materials is surging. Whether it is to combat global warming, reduce supply chain risks, or compete more aggressively with international business threats, traditional methods and R&D budgets simply can't keep up.

Enter quantitative AI. Catalyst R&D is moving from benchtop to laptop. Breakthroughs in computing allow us to translate abundant experimental and real-world data into actionable insights. By expanding the scope of AI through physics-based techniques, SandboxAQ guides customers through the vast possibilities in chemical space, towards the winning formulations.

We have long known that quantum chemistry and AI hold the keys to understanding the chemical world. But until recently, the computations necessary to conduct these calculations at scale were not feasible. Now, with improvements to GPUs and other scientific advances, SandboxAQ has developed software that can solve catalysis and process design problems repeatedly and at scale.

Working with Sandbox allows you to focus your R&D efforts on short-term gains while SAQ develops the next generation of products.

How Does It Work

No quantum computer needed. SandboxAQ's cloud-native software runs on classical hardware, combining the accuracy of quantum mechanical predictions with the speed of AI-driven insights.

Our world-class scientists and engineers leverage cutting-edge techniques (ML, tensor networks, quantum chemistry, generative AI, and others) to achieve unprecedented speed and accuracy. Moving R&D from trial-and-error experiments to in silico physics-based simulations dramatically accelerates product innovation cycles to minimize dollar and time costs. It also reduces reliance on experimental data (no need to train large models based on confidential and proprietary data) and is generalizable across reaction types and catalyst classes.

Catalysis Use Cases

AQCat supports discovery in mission-critical industrial sectors:

- **Energy:** Gas-to-liquids, CO_2-to-fuel, flare gas conversion
- **Plastics:** Polyolefin production, depolymerization
- **Electrification:** Green hydrogen, fuel cells, electrochemical [illegible]

Quantitative AI Solutions for Catalysis Use Cases

Our proprietary data generation workflows are purpose-built for high-throughput discovery. By combining active learning, enhanced sampling techniques, and automated DFT pipelines, we generate diverse and chemically rich datasets tailored to each use case—heterogeneous catalysis or homogeneous catalysis. These datasets power specialized ML force fields (MLFFs) that retain quantum accuracy while enabling simulations at a massive scale. This approach not only minimizes the cost of data generation but also ensures high extrapolation performance across wide chemical spaces. AQCat is trained using AQCat25, a high-fidelity, magnetism-aware dataset of over 10 million sample structures, generated using NVIDIA DGX clusters. These models power industrial use cases in collaboration with partners like **Aramco**, **Grace**, and others seeking to accelerate discovery in complex reaction systems.

SandboxAQ - Your Innovation Partner

SandboxAQ is your innovation partner, committed to ensuring that you retain full ownership of all material and molecular IP, because your success is our success. We structure projects around clear, milestone-based goals, giving you flexibility without ongoing obligations. And from atomic-scale modeling to experimental handoff, we provide end-to-end support throughout the entire discovery journey.

Purpose-Built by Experts in Physics, Chemistry & AI

SandboxAQ is a company built on deep expertise in physics, chemistry, and AI, with a team of over 250 specialists. Their capabilities span quantum and computational chemistry, multiscale physics, prescriptive and descriptive AI modeling, and software engineering with cloud computing.

Let's Transform Catalyst Discovery Together

To learn more about how SandboxAQ can help you, visit us at www.sandboxaq.com/catalysis.

Contact Us Today

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