

Optimizing Catalyst Formulation for CO₂ to Methanol Conversion

Sector

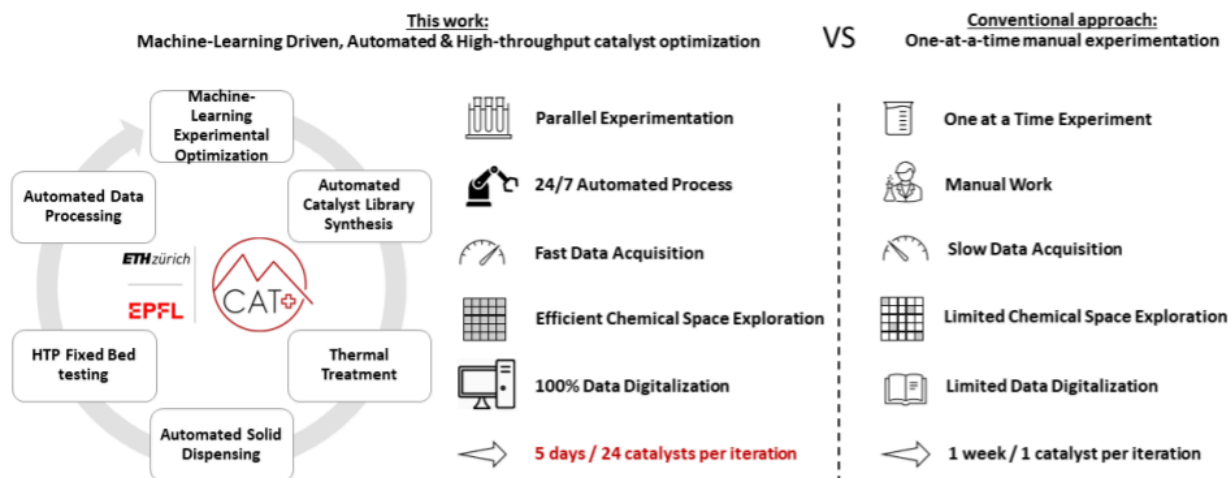
Catalysis, Carbon Capture Use and Sequestration (CCUS), Energy

Impact

Green Chemistry, Renewable Resources

Overview

The collaboration between Atinary and the Swiss national initiative for catalysis known as SwissCat+, based in ETH Zurich, demonstrates the transformative power of AI-driven experimentation. Envisioned by Prof. Christophe Copéret and executed and managed by Dr. Paco Laveille and his team, ETH Zurich's AI-Driven R&D Lab utilizes Atinary's SDLabs platform, which guided the AI-driven process to find the optimal catalyst for the conversion of carbon dioxide (CO₂) into methanol. This project demonstrates the power of augmenting humans with AI and robotics to solve complex R&D challenges, significantly enhancing efficiency, productivity and success rates while minimizing raw material use and costs.

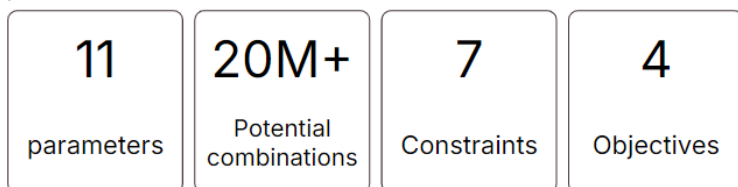


From Figure 1 of our publication, overview of the presented method workflow and benefits in our use-case in comparison with a conventional approach.

Challenge

Find the best catalyst for the conversion of CO₂ to fuels (methanol, MeOH).

By the numbers

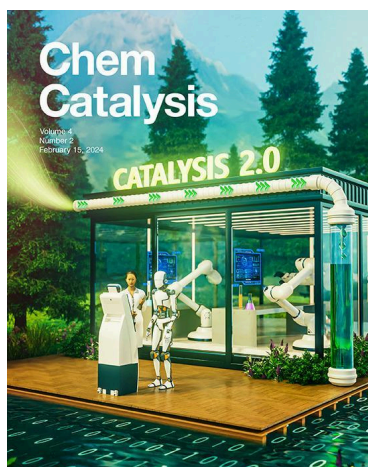


Outcome

In just 30 days (and 120 catalysts), we replicated major development stages that spanned a century.

Resources

- [Link](#) to Atinary-IBM Research Europe Partnership **Press Release**
- [Link](#) to **Publication**: Ramirez et al. Accelerated exploration of heterogeneous CO₂ hydrogenation catalysts by Bayesian-optimized high-throughput and automated experimentation. *Chem Catalysis*. 2024 <https://doi.org/10.1016/j.checat.2023.100888>
- [Link](#) to **Research Highlight** in *Nature Catalysis*
- [Link](#) to **Atinary Webinar**
- More about [ETH Zurich Swiss CAT+](#)
- [Link](#) to **Video** of Atinary-ETH Zurich Project Overview



Our joint article was featured on the cover of Cell Press' *Chem Catalysis* February issue: Illustration of the new generation of chemistry laboratories where humans interact with robots and artificial intelligence to accelerate the discovery of catalysts that convert pollutants into high-value renewable fuels and chemicals. For more information, see the article by Laveille and co-workers. Art by INMYWORK Studio.