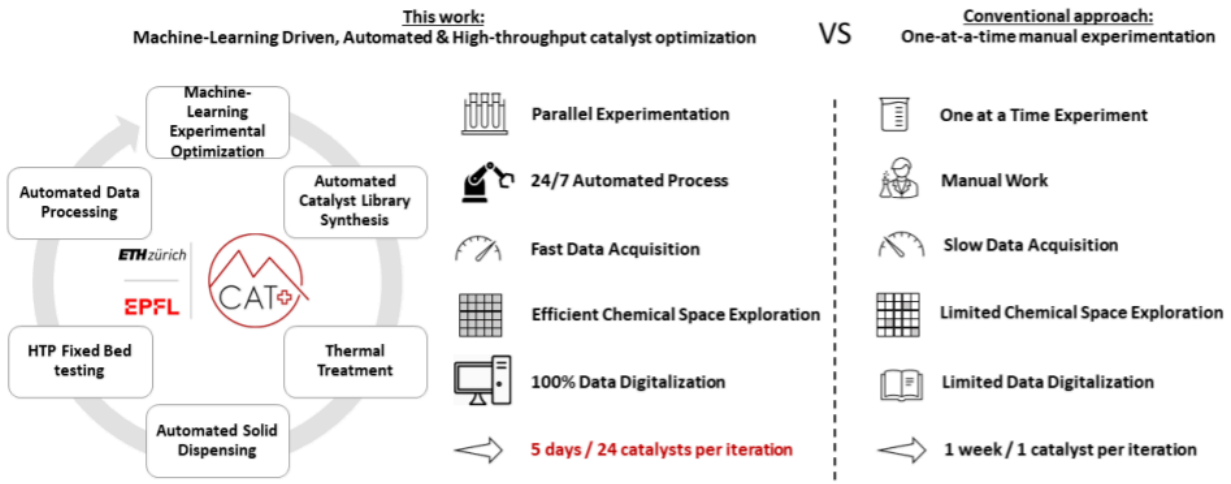
ATINARY
ENABLING SELF-DRIVING LABORATORIES

Optimizing Catalyst Formulation for CO_2 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 (CO_2) 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.

Use Case
We are entering a transformative era in research and development (R&D) with the integration of artificial intelligence (AI), robotics, and cloud computing. At Atinary, we call this the Self-Driving Labs Era. This Self-driving labs technology (SDLabs) accelerates innovation at an unprecedented pace.

Imagine discovering breakthrough molecules and materials in days or weeks, rather than waiting years or even decades. This vision is now becoming reality with Atinary's SDLabs platform. Our collaboration with the SwissCAT+ hub at ETH Zurich is a testament to this groundbreaking potential. The exciting results of our use case in catalyst R&D were published in Chem Catalysis from Cell Press. In this peer-reviewed publication, we demonstrated the compression of 100 years of catalyst R&D in CO_2 to methanol conversion could be achieved in

just 6 weeks, revolutionizing the pace of innovation in this field. This paper was featured in the journal's cover page in February 2024, and was also highlighted in Nature Catalysis.

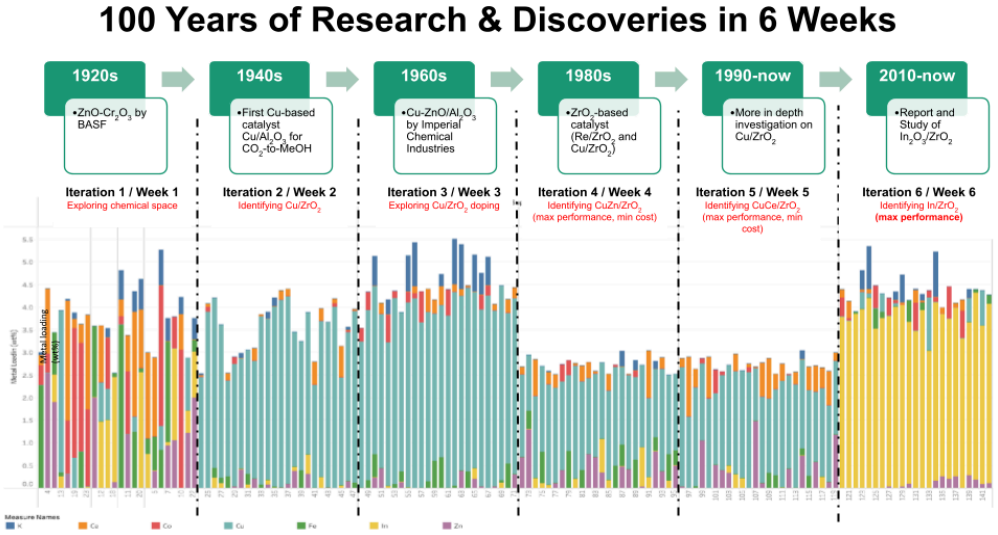
Platform Integration

The AI algorithms were deployed on Atinary's no-code cloud-based platform, SDLabs. In this use-case, a total of 8 experimental parameters, 4 constraints, and 4 objectives were entered into the SDLabs platform. At the end of each experimental cycle, the catalytic results for each of the 24 catalysts (CO_2 conversion, methanol selectivity, methane selectivity, and metal cost) were obtained. These results were uploaded back to the SDLabs platform to retrain the ML algorithm and generate the parameter values for the next iteration.

Results

In this use case with ETHZ, we use ML algorithms, known as Bayesian Optimization (BO), to efficiently navigate the large parameter space that is composed of more than 20 million combinations. The ML algorithms guide the optimization of catalyst compositions for the conversion of CO_2 to methanol, starting from scratch, with no data and within a very limited number of experiments. Following an iterative process the team quickly found the optimal catalyst composition at an unprecedented speed, maximizing performance and reducing unwanted by-products and costs.

These results were recently published in the journal *Chem Catalysis* from Cell Press, highlighting the efficacy of this AI-driven approach in catalyst optimization to identify optimal catalyst compositions with minimal human intervention. Specifically, the teams were able to replicate research results that were achieved over the last 100 years in only 5 iterations, where each iteration took 5 days. Atinary's SDLabs platform enabled the exploration of more than 20 million catalyst combinations for converting CO_2 into methanol. The robots executed the experiments in batches of 24, produced and tested in each iteration for a total of 120 catalysts, achieving significant improvements in CO_2 conversion and yields achieved, while reducing methane selectivity and cost.



From Atinary's Webinar Series Ep01, graphical result of each iterative process as conducted by SwissCAT+ in just 6 weeks in contrast to the decades of catalyst R&D in CO_2 to methanol conversion

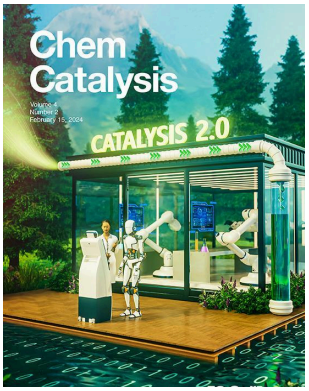
Future Prospects
In just 30 days and starting from scratch, our teams successfully reproduced the best catalyst known today for CO_2 conversion to methanol. This is more than 1,000 times faster compared to traditional methods.

This achievement illustrates the opportunities to revolutionize the energy landscape, address the challenge of reducing greenhouse gas (GHG) emissions, and drive sustainable change globally. Our AI-driven approach can solve larger and more complex challenges, maximize efficiency and minimize waste. Self-driving labs can help us develop the high performance materials that will help accelerate chemical R&D and discovery and the transition to a sustainable and circular future.

The AI-driven lab at ETH Zurich is just the beginning. Self-driving labs hold limitless possibilities for other chemistries and reactions, offering a pathway to discovering new catalysts and advancing sustainable energy research at an unprecedented pace. The synergy between human ingenuity and machine intelligence exemplified by the SwissCAT+ project is paving the way for a greener, more innovative future.

Conclusion
The integration of AI and robotics to augment scientists in R&D labs is reshaping the landscape of chemical optimization and discovery. The collaboration between Atinary and ETH Zurich is a powerful example of how AI-driven experimentation can accelerate breakthroughs and optimize processes, ultimately leading to a cleaner, greener tomorrow. As we continue to explore the vast potential of self-driving labs technology, we are committed to driving sustainable change and unlocking the full potential of renewable energy sources.

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.