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# Swiss CAT+, a Data-driven Infrastructure for Accelerated Catalysts Discovery and Optimization

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*Abstract:* The Catalysis Hub – Swiss CAT+, is a new infrastructure project funded by the ETH Domain, co-headed by EPFL and ETHZ. It offers the scientific community a unique integrated technology platform combining automated and high-throughput experimentation with advanced computational data analysis to accelerate the discoveries in the field of sustainable catalytic technologies. Divided into two hubs of expertise, homogeneous catalysis at EPFL and heterogeneous catalysis at ETHZ, the platform is open to academic and private research groups. Following a multi-year investment plan, both hubs have acquired and developed several high-end robotic platforms devoted to the synthesis, characterization, and testing of large numbers of molecular and solid catalysts. The hardware is associated with a fully digitalized experimental workflow and a specific data management strategy to support closed-loop experimentation and advanced computational data analysis.

**Keywords**: Automation · Catalysts · Data-driven · Research infrastructure

***Paco Laveille*** holds a PhD in Materials Chemistry from ENSCM, France (2009). After a post-doc at the Institut Français du Pétrole – Energies Nouvelles, he worked as a Research Engineer at the KAUST Catalysis Center in Saudi Arabia, overseeing the high-throughput experimentation platform and participating in the design of various heterogeneous catalysts in the group of Prof. J-M Basset. In 2015, he joined the Abu Dhabi National Oil Company in the UAE as Senior Scientist and led projects related to hydroprocessing catalyst technology and sustainable fuels production. He was appointed Managing Director of the ETH Zurich Catalysis Hub – Swiss CAT+ in January 2021.

***Pascal Miéville*** started his career as an apprentice laboratory technician at the University of Geneva, then moved to pharmaceutical development in industry before completing his studies with a Bachelor's degree in Chemistry at the University of Geneva, a Master's degree in Physical Chemistry at EPFL and a PhD in Nuclear Magnetic Resonance hyperpolarization in Prof. G. Bodenhausen's group at EPFL. In 2012, he took over the management of the NMR platform at EPFL where he developed the automation and piloted the acquisition and installation of the 900 MHz ss-DNP system. In parallel, he obtained an MPA from IDHEAP at the University of Lausanne. In September 2020, he was appointed Executive Director of the EPFL Catalysis Hub – Swiss CAT+.

## 1. The Catalysis Hub – Swiss CAT+ project

Data is the essence of science. By gathering more data in a shorter amount of time, scientists can verify their hypothesis or build models faster and more accurately. The development of automated liquid handlers in the 80s, associated with microplates and computers, initiated a new area for chemical sciences, allowing to generate and screen the properties of hundreds of compounds in a fraction of time compared to traditional manual laboratory methods. The continuous improvement of robotic and analytical equipment brought ever more performant tools on the market, increasing reaction parallelization, automation, as well as the quantity and quality of the data generated. In addition, the decreasing cost of data storage and computing power have led to more efficient computational data analysis methods, with Artificial Intelligence (AI) and Machine Learning (ML) models already significantly accelerating discovery and optimization in various fields of chemistry and chemical engineering.[1,2] So far, the high cost of robotic and high-throughput tools has restricted their acquisition to large industrial research laboratories.[3] Most chemistry laboratories in universities continue to perform research with a traditional one-at-a-time experiment approach and limited digitization. Providing such tools and expertise to universities could significantly help research groups to screen their chemical space and shorten time to discovery.

The Catalysis Hub project – Swiss CAT+ aims to establish a facility, open to the entire academic and industrial scientific community, devoted to data-driven, high-throughput and automated

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discovery and optimization of homogeneous and heterogeneous catalysts.[4] Funded by the ETH Domain, the technology platform hosts state-of-the-art robotic and parallelized tools to synthesize, characterize and evaluate the performance of libraries of solid and molecular catalysts. This equipment allows for digitizing complete experimental workflows, eliminating manual inputs and capturing every process and analytical parameters into databases. In addition, advanced computational data analysis using AI/ML methods will be provided to identify hidden chemical descriptors and suggest new sets of experimental conditions, targeting closed-loop experimentation.

For an efficient dissemination within Switzerland, the Catalysis Hub – Swiss CAT+ is split across the two Swiss federal institutes according to specific expertise: the East Hub at ETH Zurich focuses on heterogeneous catalysis technology, whereas the West Hub at EPFL targets homogeneous catalysis. Users will be able to request services to the respective hub. Their request will be evaluated, validated technically and implemented by a team of experts in close collaboration with the applicant research group.

### 1.1 *Project Schedule and Funding*

The Catalysis Hub – Swiss CAT+ project, initiated by Profs. C. Copéret and N. Cramer in 2019, was approved by ETH Domain in 2020 with an initial budget of CHF 25M for the first four years (Phase I: 2021–2024). In addition, the respective institutes agreed to provide the project with adequate infrastructure and specialized platform support. Since 2021, expert teams have been assembled and work on preparing the laboratories to host state-of-the-art equipment. In 2022, the hubs started to receive and install the first pieces of equipment. Machines and experimental workflow will be validated in 2023, targeting full operation in 2024 (Table 1).

Table 1. Catalysis Hub - Swiss CAT+ schedule

| | |
|---|---|
| Project Design | 2019–2020 |
| Preparation | 2021–2022 |
| Implementation | 2023 |
| Service operations | 2024 onwards |
| Continuous development | until 2028 |

A second round of funding is currently being requested for 2025–2028. During the second phase, in parallel to the service operations, the development of further automation capabilities as well as the data-driven tools (optimization tools, automated data analysis, chemical space exploration, closed-loop experimentation) is foreseen. Swiss CAT+ is a research infrastructure project with a long-term objective. The future evolution will depend on the success of the hubs raising interest within the community and providing researchers with innovative strategies and tools for the discovery and optimization of catalyst libraries.

### 1.2 *Governing Structures*

Catalysis Hub – Swiss CAT+ is a key project of the ETH Domain. It is therefore directly subordinated to the ETH Domain through local administrations at both hub locations. A steering committee involving the two founding PIs and both hub directors is in charge of suggesting and validating the project strategy, as well as reporting to the school and ETH Domain managements. The steering committee also coordinates the Advisory Board and the User Assembly. The two directors of the hubs are in charge of the day-to-day developments and operations of their respective hubs. This structure is depicted in Fig.1.

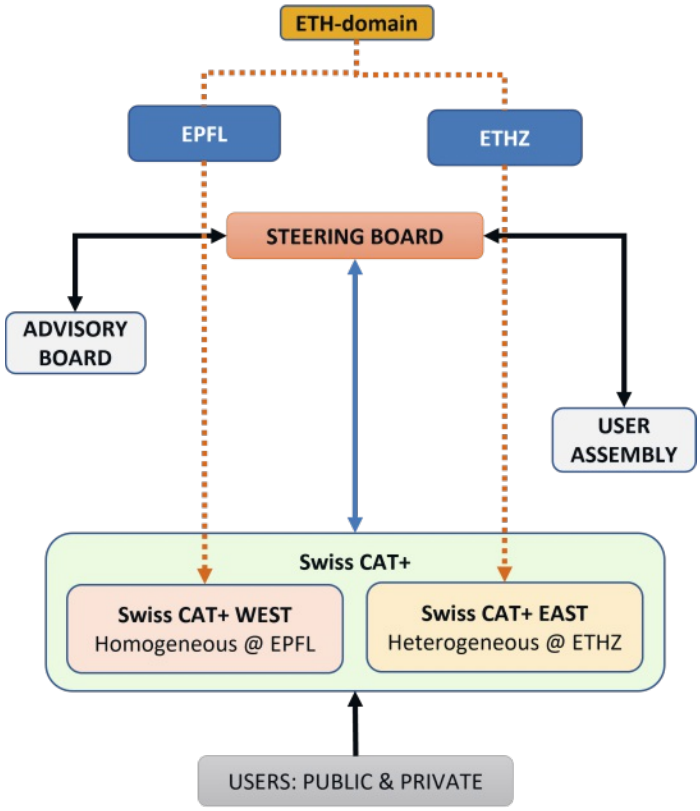


Fig. 1. Swiss CAT+ governing structures.

The Catalysis Hub – Swiss CAT+ Advisory Board is composed of recognized experts from academia and industry spanning the catalysis field at large. It has the role of maintaining close contact between the project and the state-of-the-art in this fast-moving research area.

## 2. ETHZ – East Hub

The ETHZ Catalysis Hub focusses on data-driven high-throughput and automated heterogeneous catalyst synthesis, characterization and performance evaluation. However, the inherent flexibility of the tools allows for accommodating studies beyond heterogeneous catalysis, including the synthesis of functional materials and the evaluation of catalysts in homogeneous phases. Two laboratory units, with a total of 150 $m^2$, located in the HCI building of the ETH Hönggerberg campus, where the Department of Chemistry and Applied Biosciences is located, have been secured for the first phase of the project. Additional laboratory space is being identified to plan for the foreseen extension in 2025. At the end of 2022, the East Hub counted three scientific experts and an administrative assistant (3.2 FTE) among its staff. The platform plans to hire additional staff members as the activity ramps up. Interested users can request services on the dedicated website Catalysis Hub | ETH Zurich (https://swisscatplus.ethz.ch).

### 2.1 *Strategic Approaches*

Automating heterogeneous catalyst synthesis, characterization and evaluation has been a challenge since the 1990s, mostly due to the specific conditions required along the experimental workflow (*e.g.*, fine dispensing of powders with different properties, high-temperature and pressure synthesis/testing, solids sieving/crushing/pelletizing and transfer to specific vessels for thermal treatment/ characterization/testing). Even though several research groups and companies propose solutions to overcome some of those problems, building an automatic experimental workflow for heterogeneous catalyst discovery and optimization requires making compromises and to identify the potential bottlenecks.[5–7]

For the first phase of ETHZ Catalysis Hub, the laboratory is designed as 'islands' of automated tasks with manual transfer of samples between each equipment. A strong effort is placed on digitizing the whole experimental workflow and removing any manual activity directly impacting the experiment. As depicted in Fig. 2, the typical experimental workflow consists of:

- Computer-assisted experimental design
- Compound library synthesis by robotic platform
- Thermal treatment of the libraries in automated furnaces
- Primary screening of the library microplates in batch mode
- Basic surface characterization of a subset of candidates
- Secondary screening of sub-set of candidates in fixed-bed reactors
- Advanced surface property characterization of a limited number of candidates
- Computer-assisted data analysis

## 2.2 *Hardware and Laboratory Layout*

The initial investment includes automated units for heterogeneous catalyst preparation (a Chemspeed Swing XL, a Hobersal automated furnace, an Unchained Lab Junior robotic platform and a CEM Mars 6 parallel microwave reactor), catalyst testing (a HEL CAT96; an Avantium Flowrence XR and two XD fixed bed units) and characterization (a Netzsch pulse-TGA/DSC-MS and Bruker 263 GHz klystron DNP NMR).

These units will allow the automated simultaneous synthesis of up to 96 heterogeneous materials/catalysts using established preparation methods which includes liquid and solid dispensing, pH and temperature control as well as high temperature post-treatment and calcination.[8] A fingerprint of each material of the prepared libraries will be captured by thermal gravimetric and differential scanning calorimetry analysis (TGA/DSC) coupled to a mass spectrometer,[9,10] and a set of conventional spectroscopy methods (X-ray diffraction, X-ray fluorescence, infra-red, Raman). Detailed characterization will be performed on a limited number of promising candidates by advanced techniques including high resolution solid-state nuclear magnetic resonance (NMR) spectroscopy, X-ray adsorption spectroscopy (XAS) and electron microscopy (TEM/SEM).

Heterogeneous catalyst testing will be performed in either batch or fixed-bed flow reactors, allowing the simultaneous measurement of 96 or 16 reactions, respectively. Reactions can be performed at up to 100 bar and 925 °C, depending on the reactor configuration.[11–13] Gaseous products will be characterized by online gas chromatography and liquid products by off-line gas chromatography-mass spectrometry equipped with an autosampler. In addition, eight fixed-bed reactors are integrated in a glovebox, allowing the simultaneous testing of multiple air- and moisture sensitive materials.

## 2.3 *Data-driven Strategy*

One of the main objectives of the Catalysis Hub is to digitize all the input/output of the experiments and use advanced computational tools (AI/ML) to support closed-loop experimentation and identify chemical descriptors leading to a given catalytic activity/reaction mechanism. To this end, all the individual databases generated by each hardware described above are automatically copied and aggregated to a physical server, and backed-up on a cloud service for ease of manipulation and visualization.

The first requirement for a suitable data-driven approach is to apply statistical experimental design methods to reduce the number of experiments needed to screen a given parameter space (*e.g.*, Design of Experiment, Genetic Algorithms, Bayesian Optimization).[14–17] To kick-start the activity of the ETHZ Catalysis Hub, we have partnered with Atinary (https://atinary.com), a start-up active in the field of Bayesian experimental optimization and laboratory automation.[18–20]. In a first demonstration attempt, their software will be specifically adapted to the Swiss CAT+ experimental workflow to perform closed-loop Bayesian optimization of heterogeneous catalyst composition applied to $CO_2$ conversion. In addition, we will also train and benchmark the experimental data with popular ML algorithms such as Random Forest, Support Vector Machine and Gaussian Process Regression, to name a few.[21,22] Other potential use of the database and application of AI/ML tools will be implemented and presented at a later stage.

## 2.4 *Development and Challenges*

In a second phase, the ETHZ Catalysis Hub plans to purchase additional robotic platforms for synthesis, characterization and

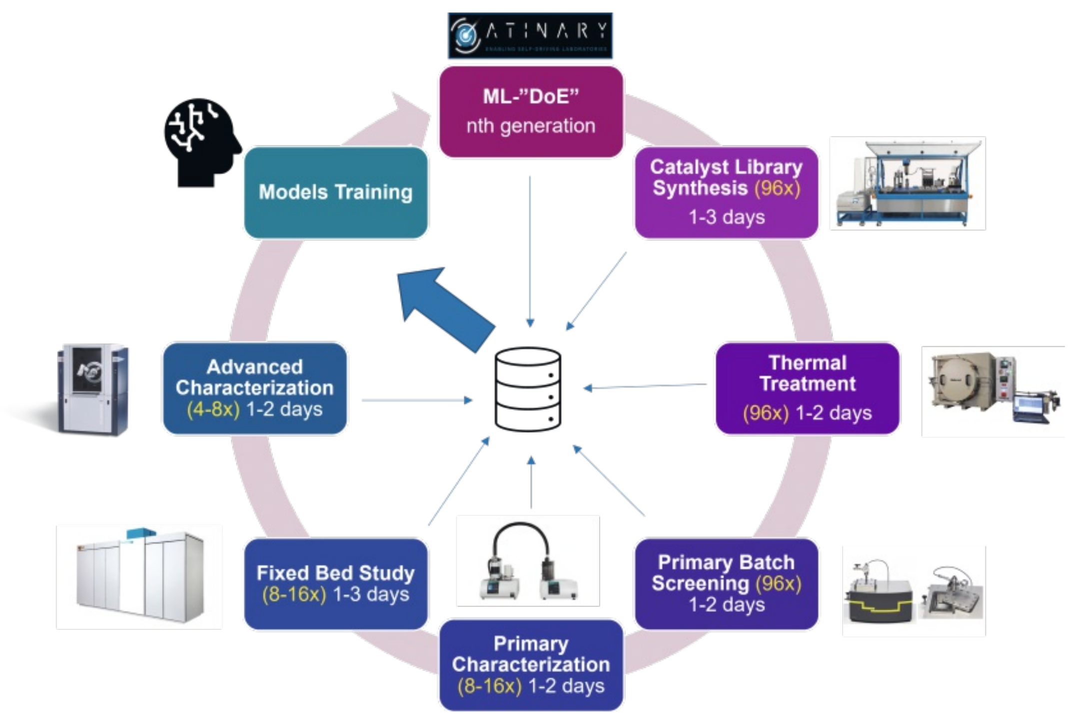


Fig. 2. Scheme depicting the ETHZ Catalysis Hub experimental workflow with the expected throughput (x96, x24..) and step duration.

testing of heterogeneous catalysts. The range of catalytic applications will be extended to include screening capabilities for Fischer-Tropsch, bio-feedstocks upgrading, olefins polymerization, photo- and electrocatalysis. Similarly, more heterogeneous catalyst characterization techniques will be offered, targeting their automation and parallelization. Significant effort will be placed on standardizing experimental methods and benchmarking key reactions, as well as developing relevant data analysis and visualization scripts.

## 3. EPFL – West Hub

The Swiss CAT+ West Hub is located in the CH building at EPFL in Lausanne. In the context of the Swiss CAT+ project, this hub addresses homogeneous catalysis and is presently composed of 6.5 FTE including scientists, robotic engineers, IT developers and administrative staff.

### 3.1 *Strategic Approaches*

Considering the goal of developing an automated[23] and progressively autonomous[24–26] laboratory for homogeneous catalysts discovery and optimization, we defined the following drivelines:

- Building a high-quality experimental data generator
- Organizing a complete sample and data integration
- Preserving data integrity
- Adopting constantly a machine point of view
- Garbage in – garbage out[27]

These drivelines being established, we identified the chemical strategies we will apply in the view of achieving catalysts discovery and optimization (Fig. 3). Then we converted this chemical discovery and optimization strategy into an experimental workflow constituting the base for the laboratory conception and material acquisition.

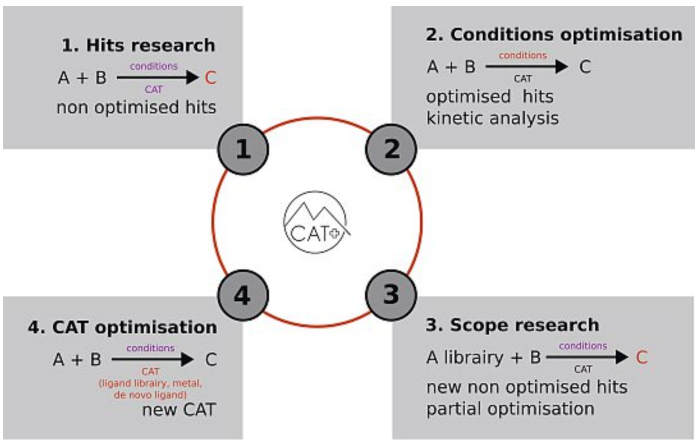


Fig. 3. Discovery and optimization strategies for new homogeneous catalyst at Swiss CAT+ West Hub.

### 3.2 *Hardware and Laboratory Layout*

The above strategy has been turned into a laboratory layout (Fig. 4) containing all automated sampling and storage (DEC Group, HEIG.VD, EPFL), synthesis (Chemspeed Swing XL) and analysis instruments (Agilent LC, SFC, MS & Bruker FT-IR, NMR). The envelope of the 160 m$^2$ laboratory with the distribution of all energies as well as the support infrastructures, more than 150 m$^2$ of laboratory, offices and workshop, was entirely renewed and financed (CHF 1.5M) by the EPFL-DII. The laboratory was handed over in March 2022 and is currently equipped with the instruments. The analytical area is already installed. All synthetic and sample preparation equipment should be installed and qualified by the end of 2023. Service operations are expected to start in early 2024. In parallel, the developments of the overall automation should continue until 2026 and the design of the driving and data processing algorithms until 2028 to reach a complete data-driven laboratory by that time.

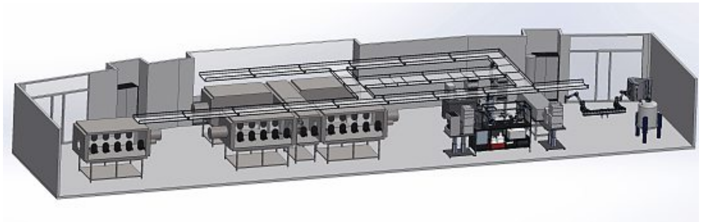

Fig. 4. Swiss CAT+ West Hub laboratory layout. The glove boxes on the left correspond to the optimization and discovery setup. The central setup is the fast analysis line (LC, SFC, MS) and on the right, we see the high-resolution setup with HR-NMR and the IM-Q-TOF. On top we see the 2D-drone swarm sample transfer system track.

### 3.3 *Development and Challenges*

Developing a fully-autonomous laboratory brings many challenges. Among these, the particularly critical ones on the hardware and software side are:

- Transferring samples between instruments
- Establishing a centralized control for all instruments, a scheduler
- Managing solids and viscous liquids automatically
- Standardizing data formats
- Establishing a reliable and efficient database for use in the AI/ML application

We have already carried out internal developments, in particular concerning the transfer of samples between equipment with a swarm of mini robots moving in a ceiling track (Fig. 5) as well as the configuration of several Universal Robots 6-axis cobots. These cobots are necessary to carry out the transfer of samples between the circuit and machines. We have also carried out a number of developments in collaboration with the Haute Ecole d'Ingénieurs d'Yverdon (HEIG-VD, Prof. Marc Kunze) in the field of automated solids handling. Concerning the centralized management of the equipment as well as the standardization of formats, we have established privileged development partnerships with our main suppliers (Agilent, Bruker, Chemspeed and MestreNova). Finally, we work with several academic groups as well as the Swiss Data Science Center (https://datascience.ch/) to develop dedicated data treatment and prediction algorithms specifically adapted to the Swiss CAT+ West Hub data structure.

Another challenge specific to a project of this type is its highly multidisciplinary nature. This involves finding people who are ready to step out of their comfort zone and above all, ready to learn a new commentary of language including computational, robotic, mechanical and chemical dimensions.

## 4. Conclusion

The ETH Domain Swiss CAT+ project is on track to set up a state-of-the-art automated and high-throughput technology platform in the field of catalysis R&D. Combined with advanced computational data analysis, it aims to support users from academia and industry to accelerate catalyst discovery and understand the chemistry guiding the materials' performances. Furthermore, considering the ongoing research activities in catalysis and sustainable chemistry in Switzerland, there are plenty of opportunities for the Swiss Cat+ to support the research landscape by offering such advanced tools and services. In particular, the Swiss CAT+ foresees a strong collaboration with the NCCR Catalysis, which, among others, funds research projects aiming to develop sustaina-

Fig. 5. A detail of the 2D drone swarm system for sample transfer

ble (catalytic) processes and drive the emergence of digital chemistry and data-driven discovery.

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