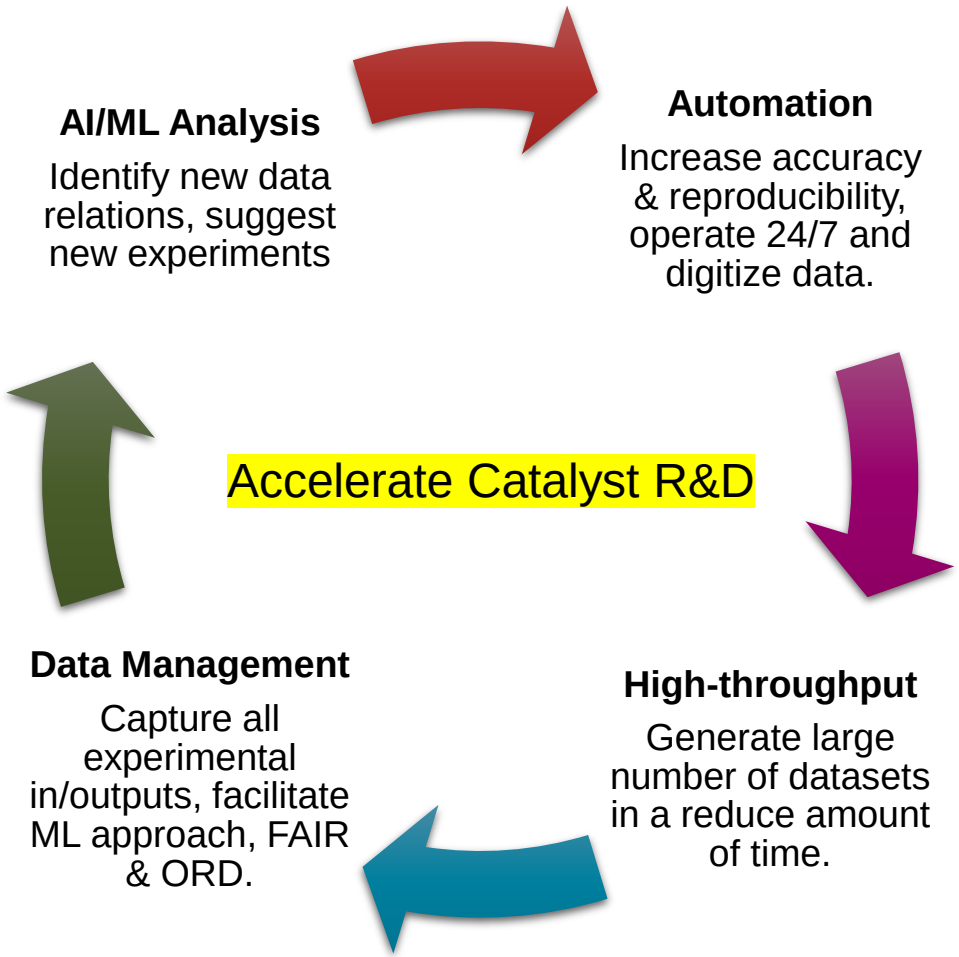
# SWISSCAT+ EAST

# ETHZ Data-Driven Automated High-Throughput Experimentation Facility

P. Laveille

# SWISSCAT+ PROJECT

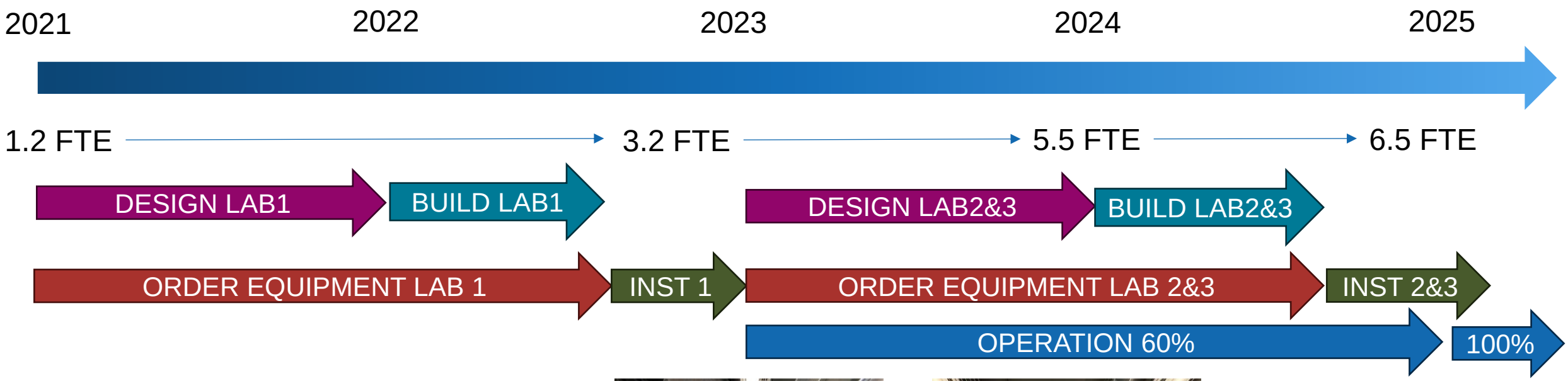
## *A service hub open to all academic and private research groups*




- National initiative co-headed by ETHZ and EPFL.
- 25 MCHF starting fund (2021-2024) from ETH-Domain.
- 8 MCHF (2025-2028)
- Two Hubs:
  - East Hub (ETHZ) focuses on **heterogeneous** catalysis.
  - West Hub (EPFL) focuses on **homogeneous** catalysis
- Under the authority of VPR at ETHZ and VPA at EPFL.

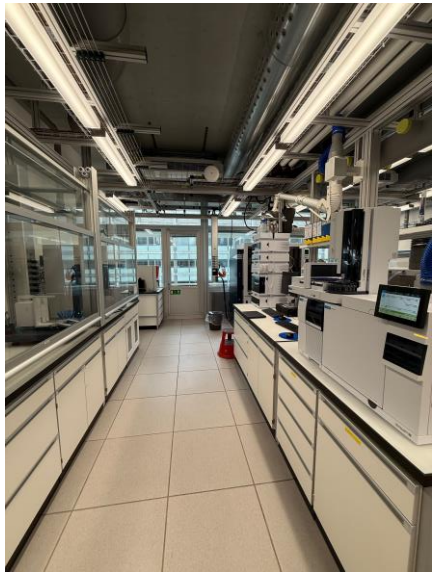
Laveille *et al., Chimia*, **2023**

# TIMELINE, HR & COSTS




- Lab refurbishment: **1 MCHF** (in-kind)
- Equipmemnt: **10 MCHF** (80%)
- OPEX (**1.2 MCHF/yr**):
  - FTE: **0.8 MCHF/yr**
  - Maintenance: **0.3 MCHF/yr**
  - Chemicals/Consumables: **0.1 MCHF/yr**

LAB1 – 60m2



LAB2 – 80m2

LAB3 – 40m2

# HARDWARE

- 3 Synthesis Robots
- Multi-position microwave oven
- High-temperature furnace

**Synthesis**
(30%)

**10 MCHF**

- 52 fixed bed reactors
- 4 units for batch testing
- GCMS + HPLC/GPC

**Testing**
(50%)

**Characterization**
(20%)

- XRD
- LA-ICPMS
- BET
- TGA-DSC
- DNP-NMR

# AUTOMATION STRATEGY

- Not full self-driving lab
  - Islands of automated activities with manual transfer of sample plates
  - No manual activity impacting the experiment
  - All input and output parameters are digitalized

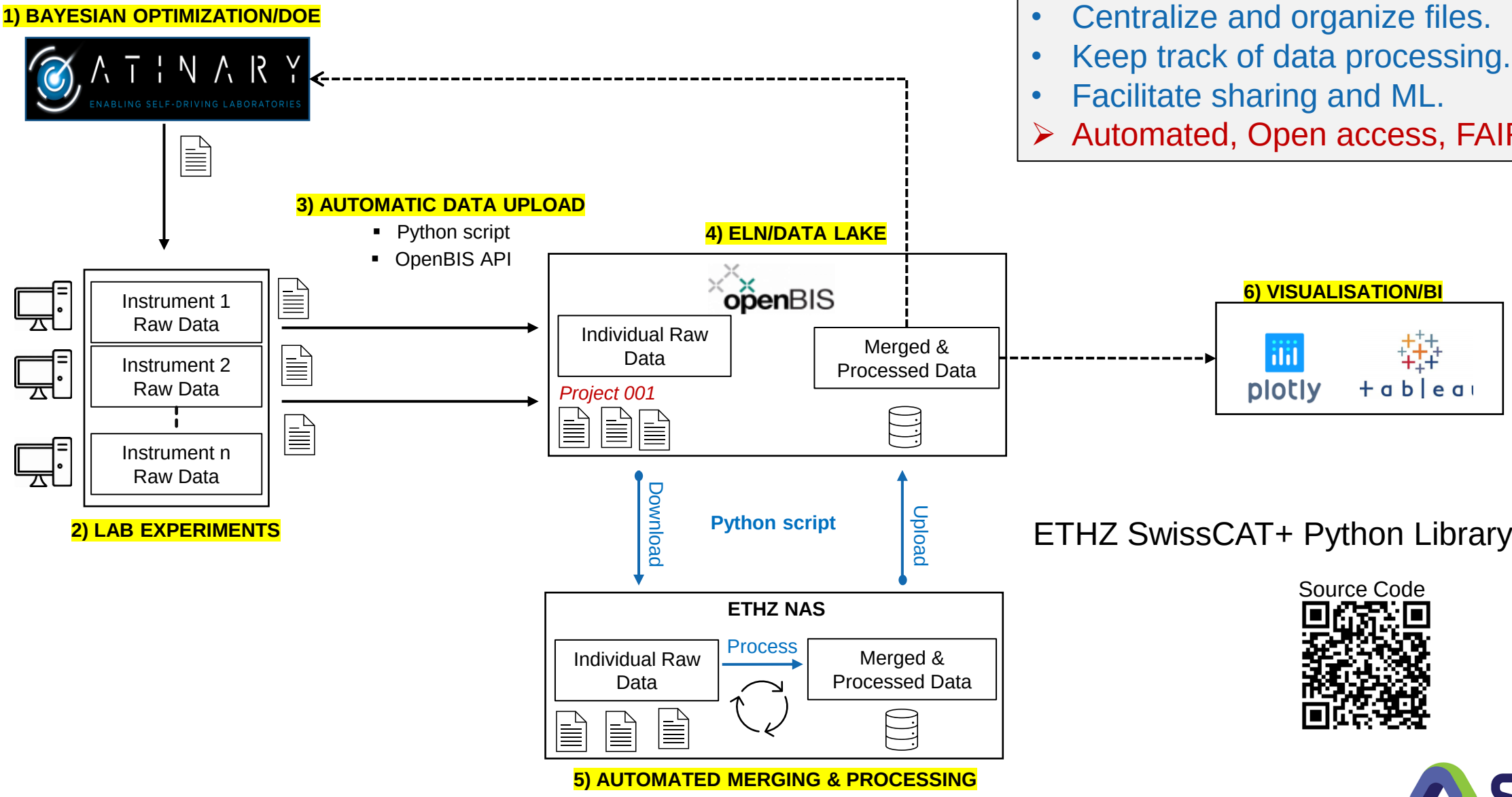
- Why?
  1. Difficult to automate activities:
     - Transfer of powders to specific vessels/non automated machines.
     - Working with high-temperature/high pressure equipment (opening/closing, cleaning…).
  2. Throughput not limited by sample transfer:
     - 24-96 samples per day.
  3. Always a human in the lab to program/maintain equipment.
  4. 3 labs at different levels

➢ High cost & complexity for limited benefits.
➢ Working with suppliers to bridge the gaps in the coming years.

Laveille *et al.*, *Chimia*, **2023**

# DATA MANAGEMENT STRATEGY

- Centralize and organize files.
- Keep track of data processing.
- Facilitate sharing and ML.
- ➢ Automated, Open access, FAIR/ORD.



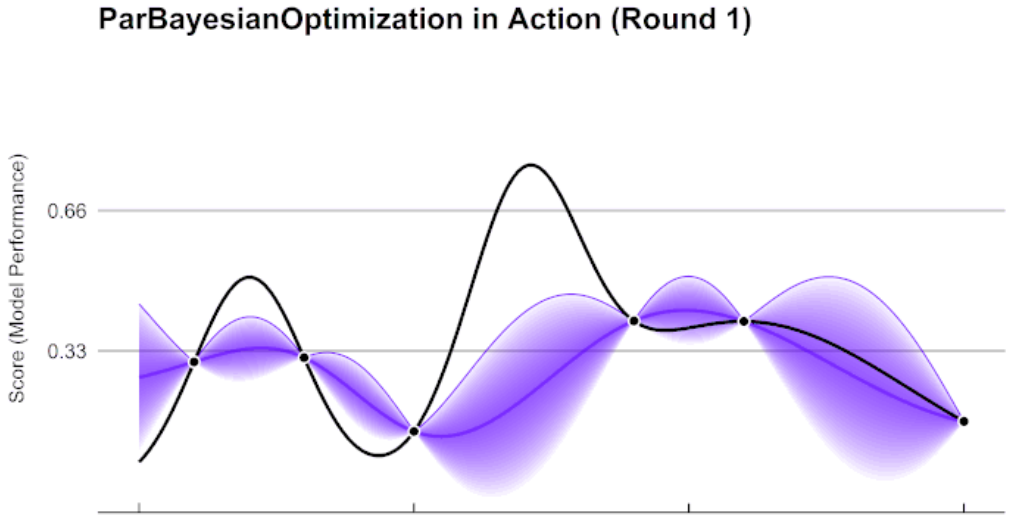

ETHZ SwissCAT+ Python Library (PyCatDat):

Source Code

E. Lam *et al.*, *Digital Discoveries*, **2025.**

# MACHINE LEARNING STRATEGY

- Which catalyst to synthesize out of millions possibilities?
- LLM to mine data on the web -> Data/model quality?
- Deep Learning model and Computational modeling-> large training set / unknown synthesis pathway?
- Experimentally-guided Bayesian Optimization:
  - Probabilistic model significantly reducing the number of experiments.
  - Combines exploration of unknow regions and exploitation of positive signals
  - Multi-parameters, multi-constrains and multi-objectives optimization.
- Atinary SDLabs -> No code software




# ACTIVITY OVERVIEW

- 52 Projects:
  - 75% for ETH-domain
  - 20% for private users
- Catalyst Synthesis:
  - Metal-supported catalysts
  - Zeolites
  - High Entropy Oxides
  - Carbon-based Materials
  - Organometallic catalysts
- Catalyst Testing:
  - Fixed Bed testing:
    - $CO_2$/CO hydrogenation
    - Propane dehydrogenation
    - CH4 Steam/Dry Reforming
  - Batch testing:
    - Hydrogenation
    - Hydrodeoxygenation
    - $CO_2$ mineralization
  - Chemical Sensing

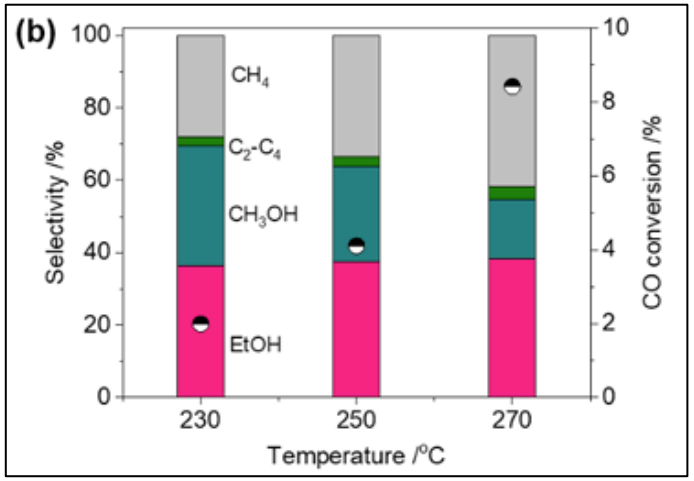
DAPHNE TECHNOLOGY

FORGE MINERALS

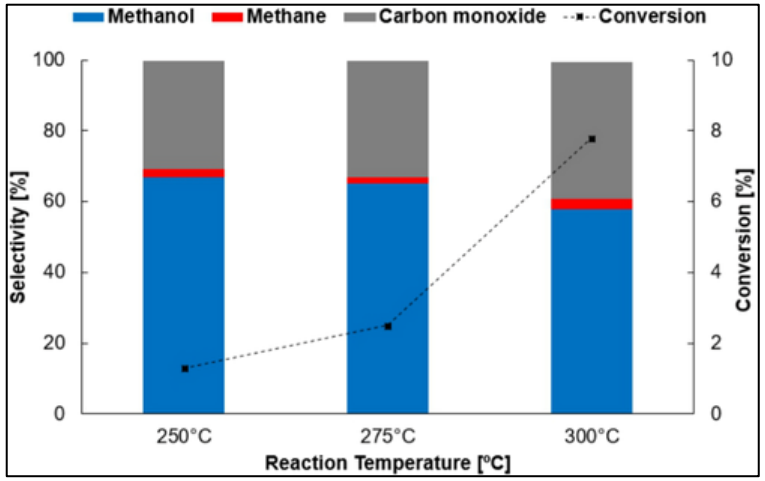
METALOR® TANAKA A member of TANAKA

積智研究院合同会社 Wisdom Pool Research Institute G.K.

J&J




CO to Ethanol with supported nanoparticles [3]



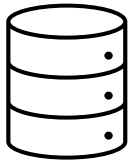

$CO_2$ to Methanol with high entropy alloys [7]

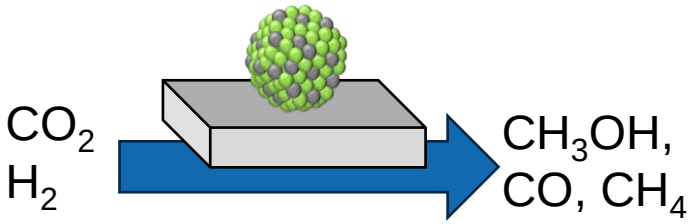
1) P. Laveille *et al. Chimia*, **2023**. 2) Ramirez et al., *Chem. Catal.* **2024**. 3) W. Zhou *et al., JACS.* **2025. 4**) E. Lam *et al., Digital Discoveries*, **2025.** 5) Z. Zhang *et al.*, *Angew. Chem., Int. Ed. Catal.* **2024**.
6) M. Mielniczuk *et al., ChemPlusChem* **2024**. 7) C. Hansen *et al.*, *Chem. Sci,* **2024**

# CASE STUDY

- 1 support among 4 ($Al_2O_3$, $SiO_2$, $TiO_2$, $ZrO_2$).
- Up to 4 elements among 7 (Ce, Co, Cu, Fe, In, Zn. K).
- Total metal loading up to 6wt%.
- > 20 M possibilities.
- Maximize $CO_2$ conversion & MeOH selectivity.
- Minimize $CH_4$ selectivity and metal cost.

- Automated data upload to ELN.
- Automated data analysis & merging via barcode & python script.






6 iterations (144 catalysts).
5 days per generation.

- 24 catalysts per batch.
- 500mg per catalyst.

- 24 reactors simultaneous
- 50mg catalyst per reactor
- $CO_2/H_2$ = 1/3 (8ml/min/re
- 32 bars, 275ºC.

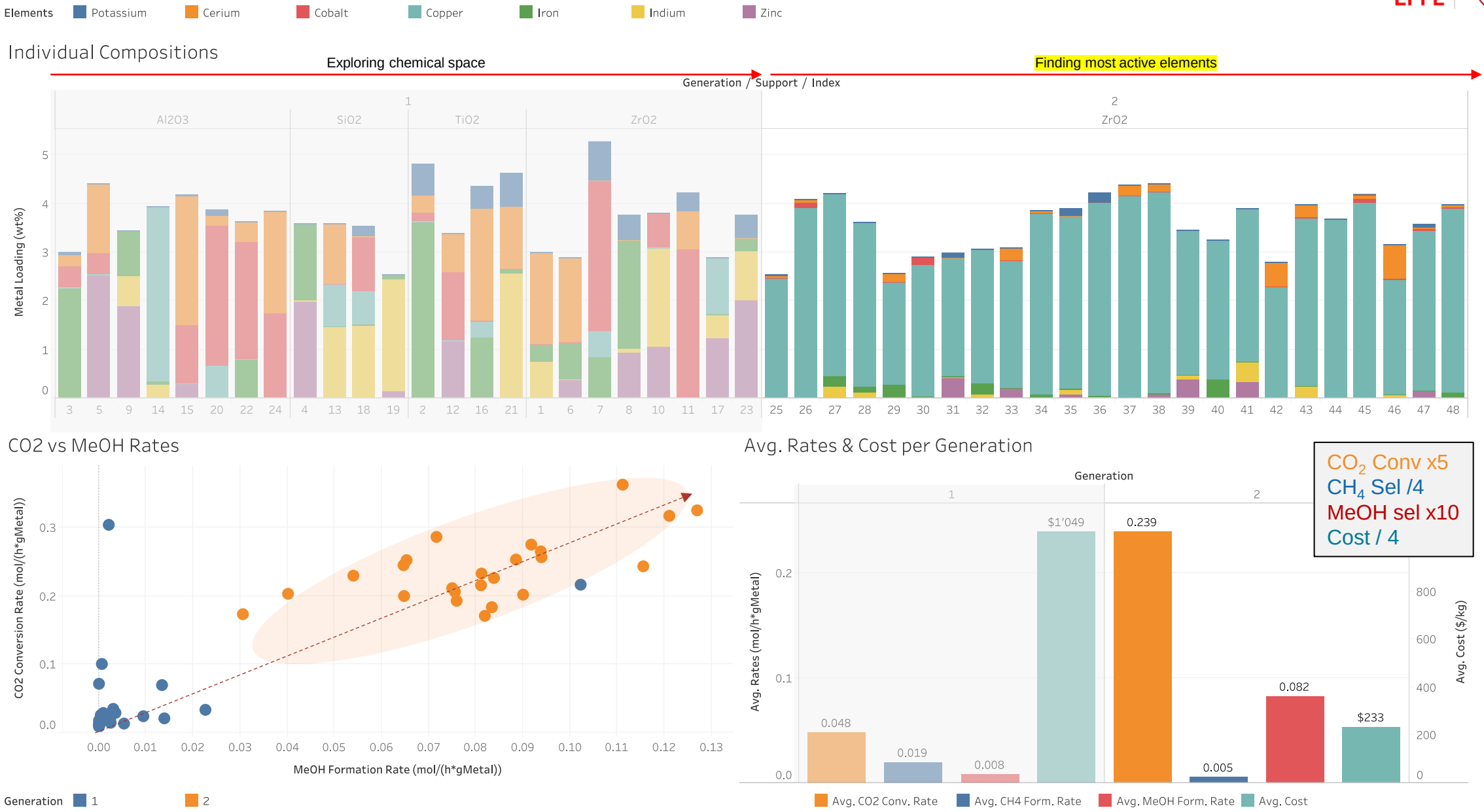
- 24 catalyst simultaneously.
- 4h at 550 C.

Ramirez *et al., Chem Catalysis,* **2024**

# CASE STUDY


Ramirez *et al.*, *Chem Catalysis*, **2024**

# CASE STUDY




Ramirez *et al.*, *Chem Catalysis*, **2024**

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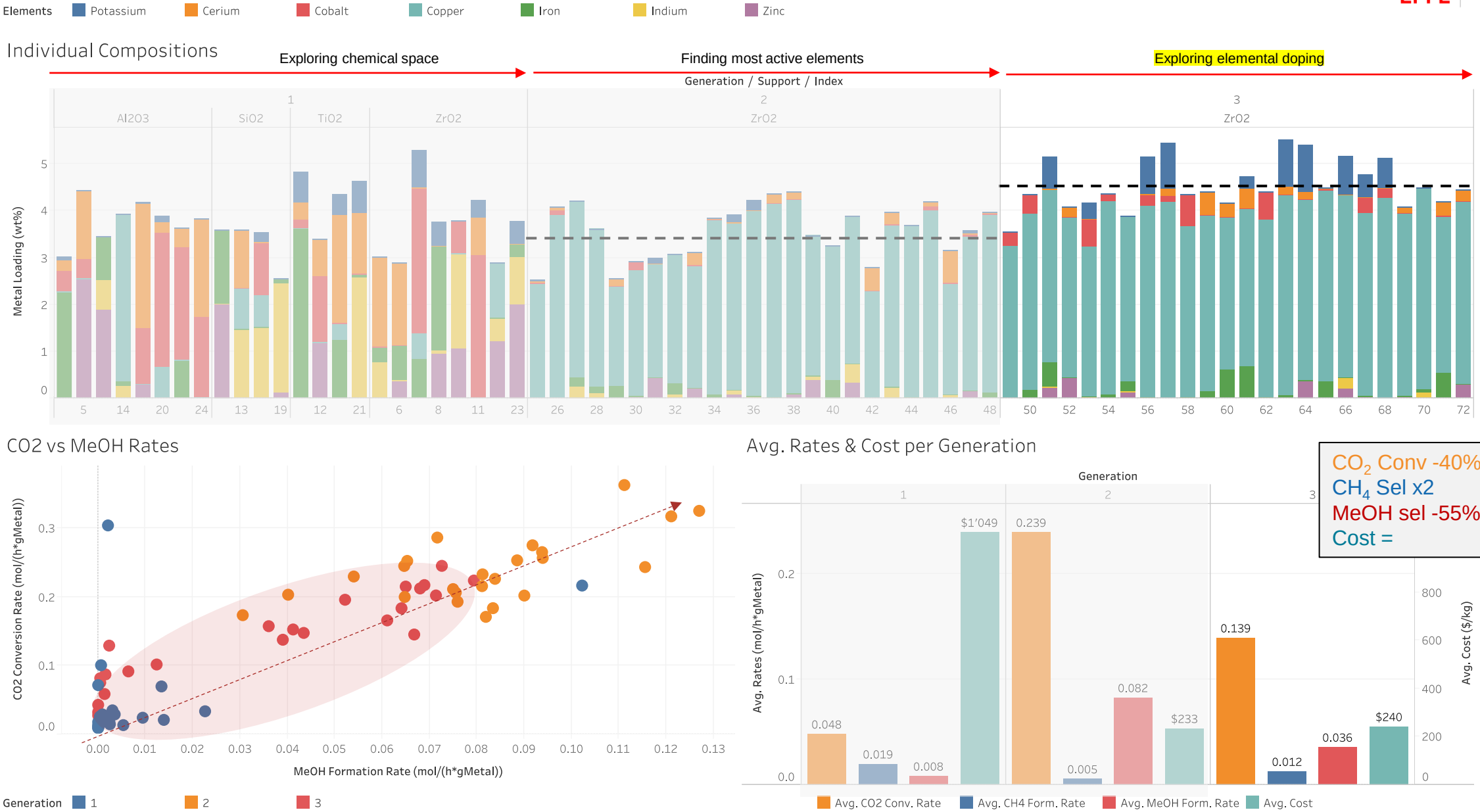


Ramirez *et al., Chem Catalysis*, **2024**

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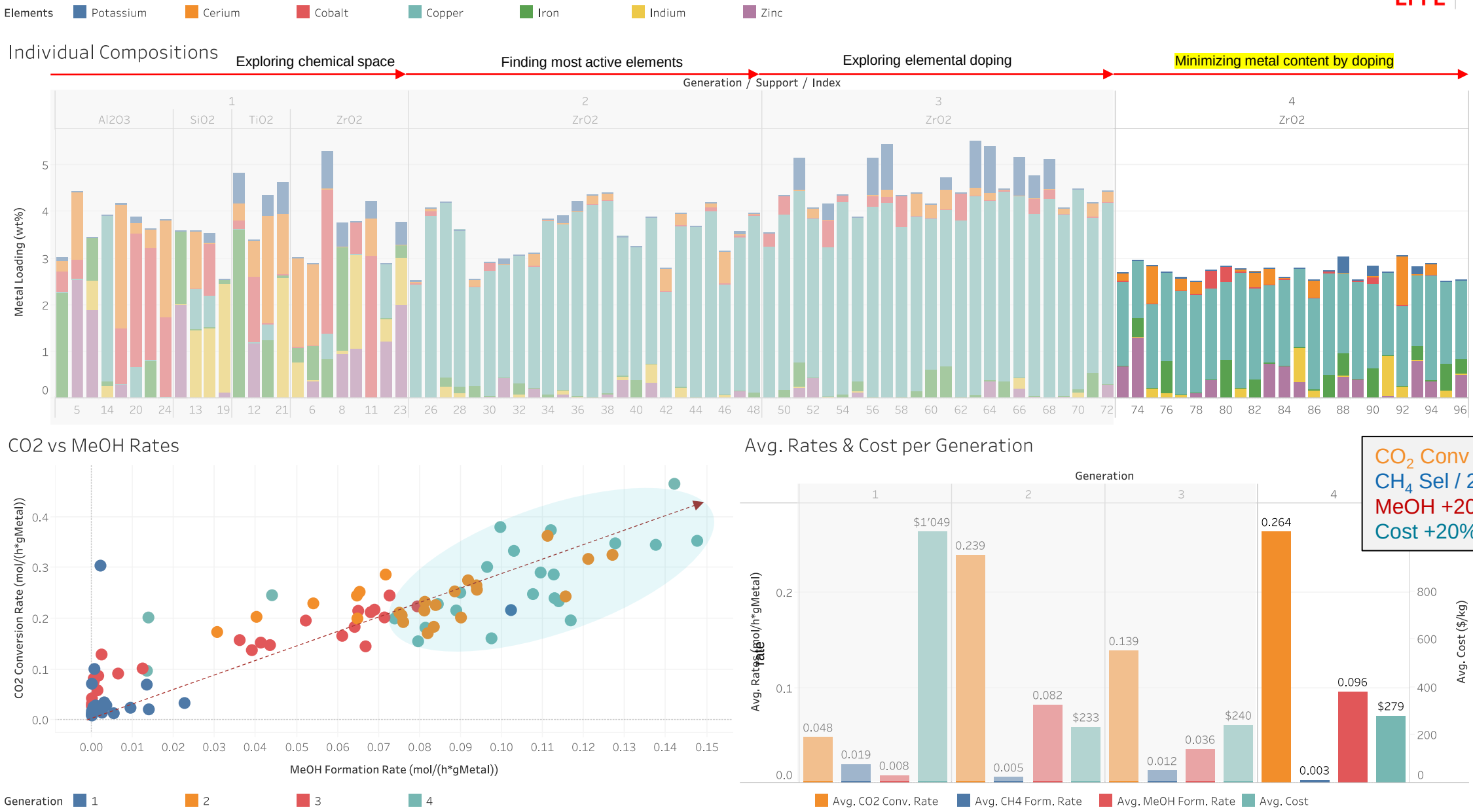


Ramirez *et al.*, *Chem Catalysis*, **2024**

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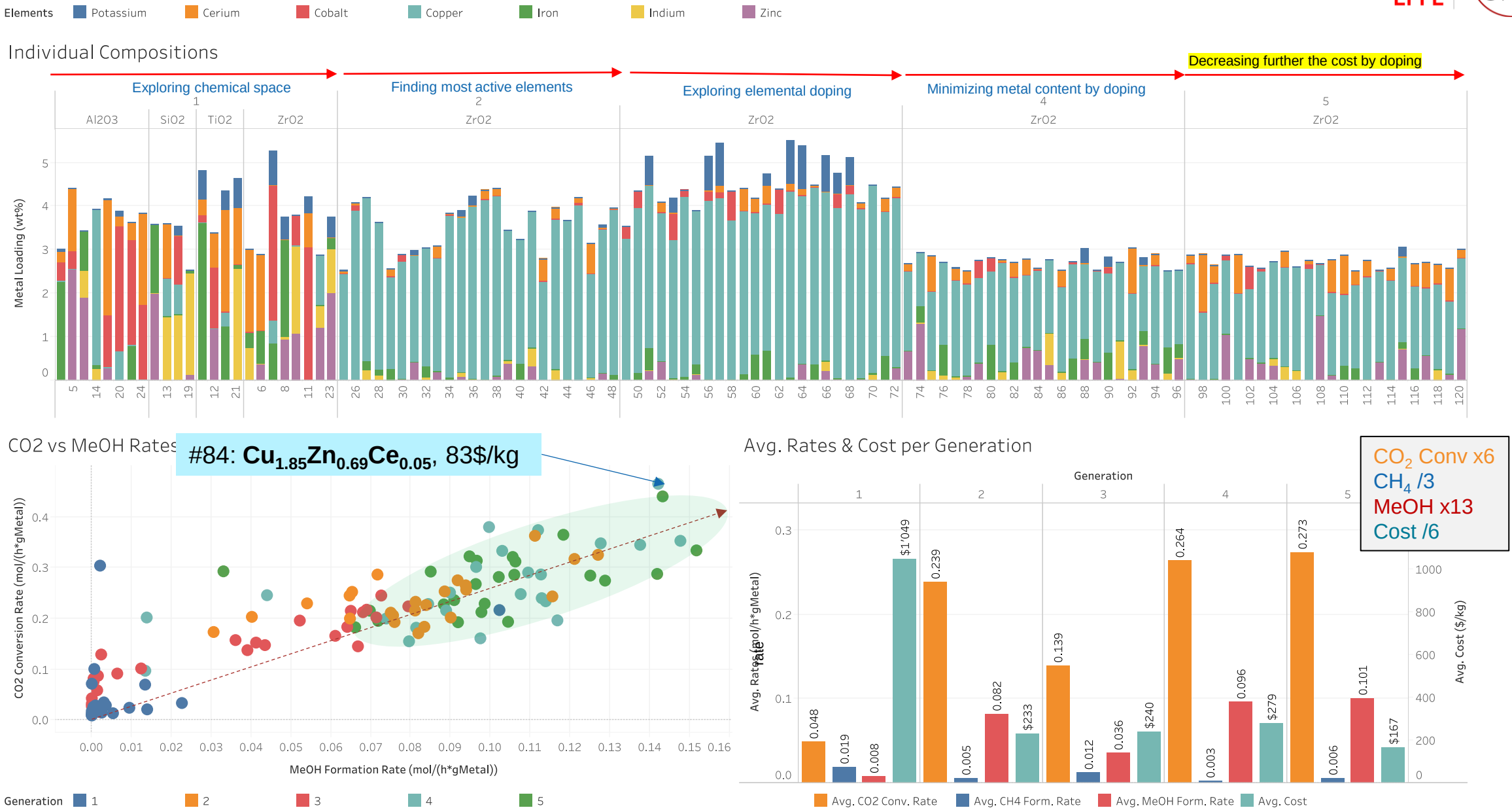
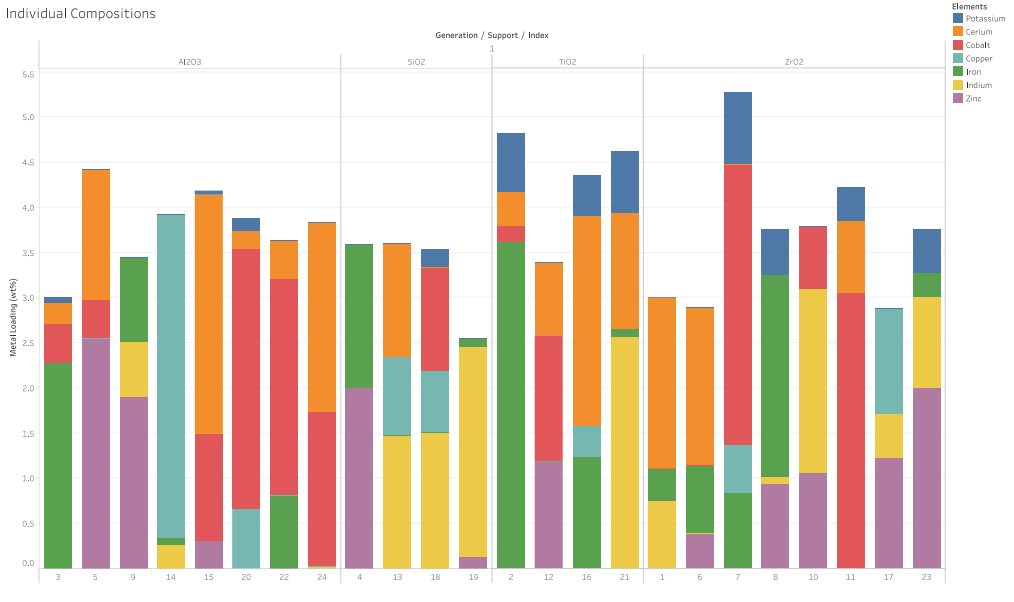
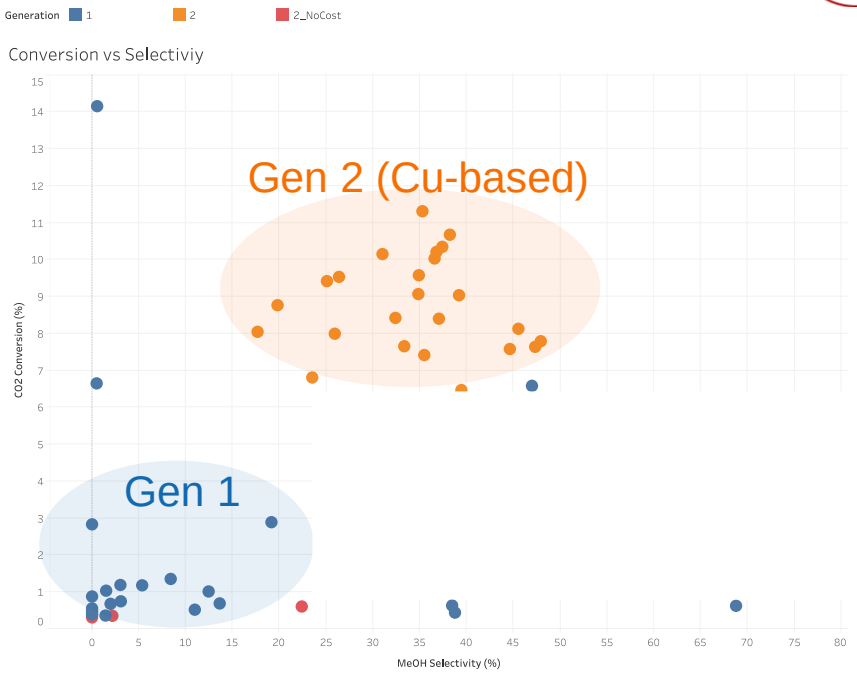



Ramirez *et al.*, *Chem Catalysis*, **2024**

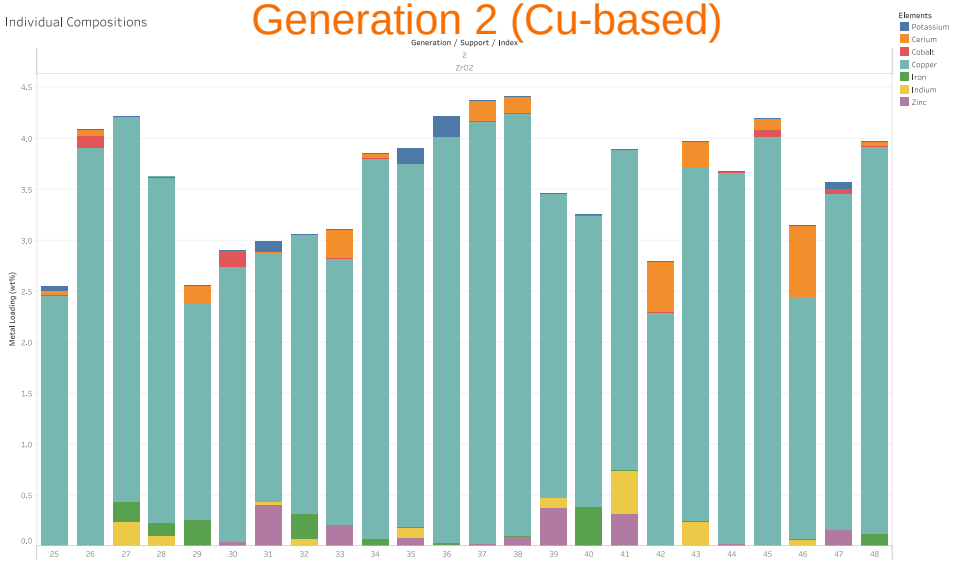
# CASE STUDY

## Generation 1

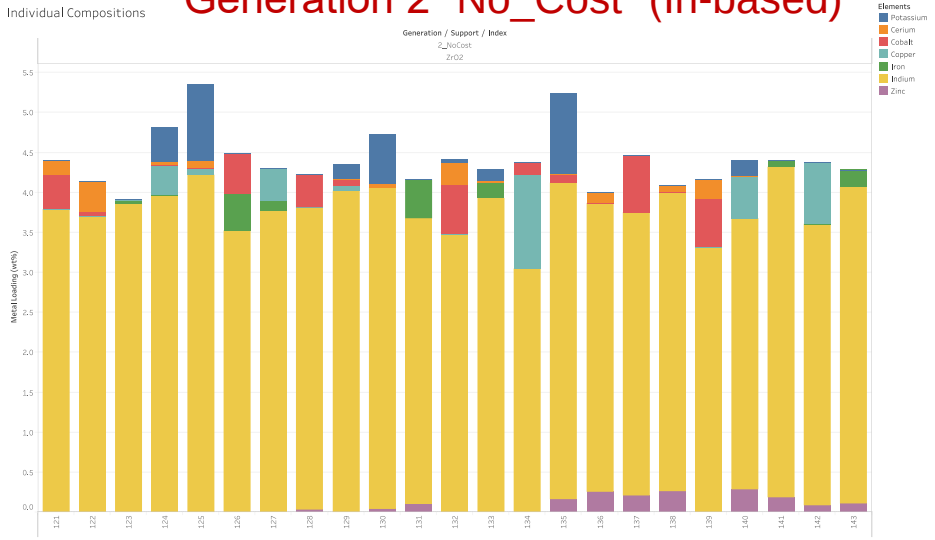



## Generation 2 (Cu-based)




## Generation 2 “No_Cost” (In-based)




Ramirez *et al.*, *Chem Catalysis*, **2024**

# 100 YEARS OF R&D PERFORMED IN 30 DAYS!

**1920s**
- $ZnO-Cr_2O_3$ by BASF

**1940s**
- First Cu-based catalyst $Cu/Al_2O_3$ for $CO_2$-to-MeOH

**1960s**
- $Cu-ZnO/Al_2O_3$ by Imperial Chemical Industries

**1980s**
- $ZrO_2$-based catalyst ($Re/ZrO_2$ and $Cu/ZrO_2$)

**1990-now**
- More in depth investigation on $Cu/ZrO_2$

**2010-now**
- Report and Study of $In_2O_3/ZrO_2$

**Week 1**
Exploring chemical space

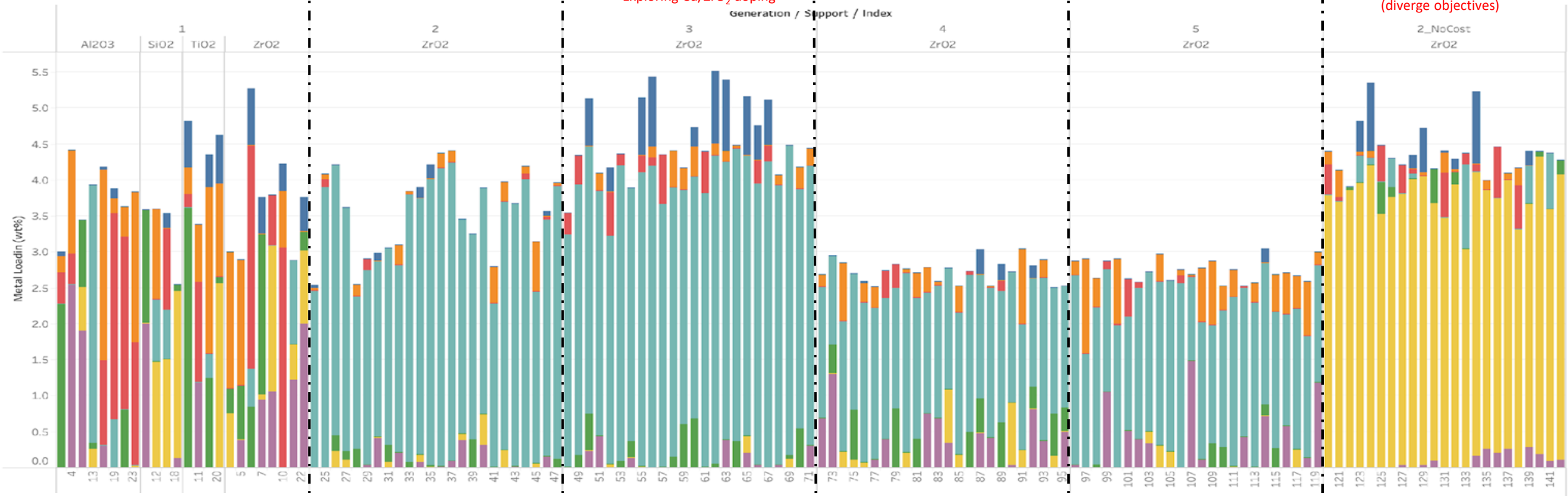
**Week 2**
Identifying $Cu/ZrO_2$

**Week 3**
Exploring $Cu/ZrO_2$ doping

**Week 4**
Identifying $CuCeZn/ZrO_2$

**Week 5**
Pushing doping of $Cu/ZrO_2$

**Week 6**
Identifying $In/ZrO_2$
(diverge objectives)




Ipatieff *et al., J. Am. Chem. Soc.* **1945.** Álvarez *et al., Chem. Rev.* **2017**. Shibata *et al.,* J. Catal. **1985**, Iizuka *et al., J. Chem. Soc., Chem. Commun.*, **1983**, Martin *et al., Angew. Chem., Int. Ed.* **2016**. Sun, *et al., J. CO2 Util.* **2015**

# CONCLUSION & PERSPECTIVES

- ETHZ has an operational state of the art data-driven automated and high-throughput platform.
- Open to academic and private research institutes.
- Broad capabilities in term of catalyst synthesis, testing and characterization.
- Experimentally-guided Bayesian Optimisation to screen of large chemical space
- Next steps:
  - Exploring larger parameter spaces.
  - Adding more chemical knowledge in ML approach (characterization data).
  - Bridging the lab automation gaps.

-> Innovation in hardware and software needed to advance autonomous / self-driving labs.

# Thank you!

P. Laveille