Towards FAIR Data in Heterogeneous Catalysis Research

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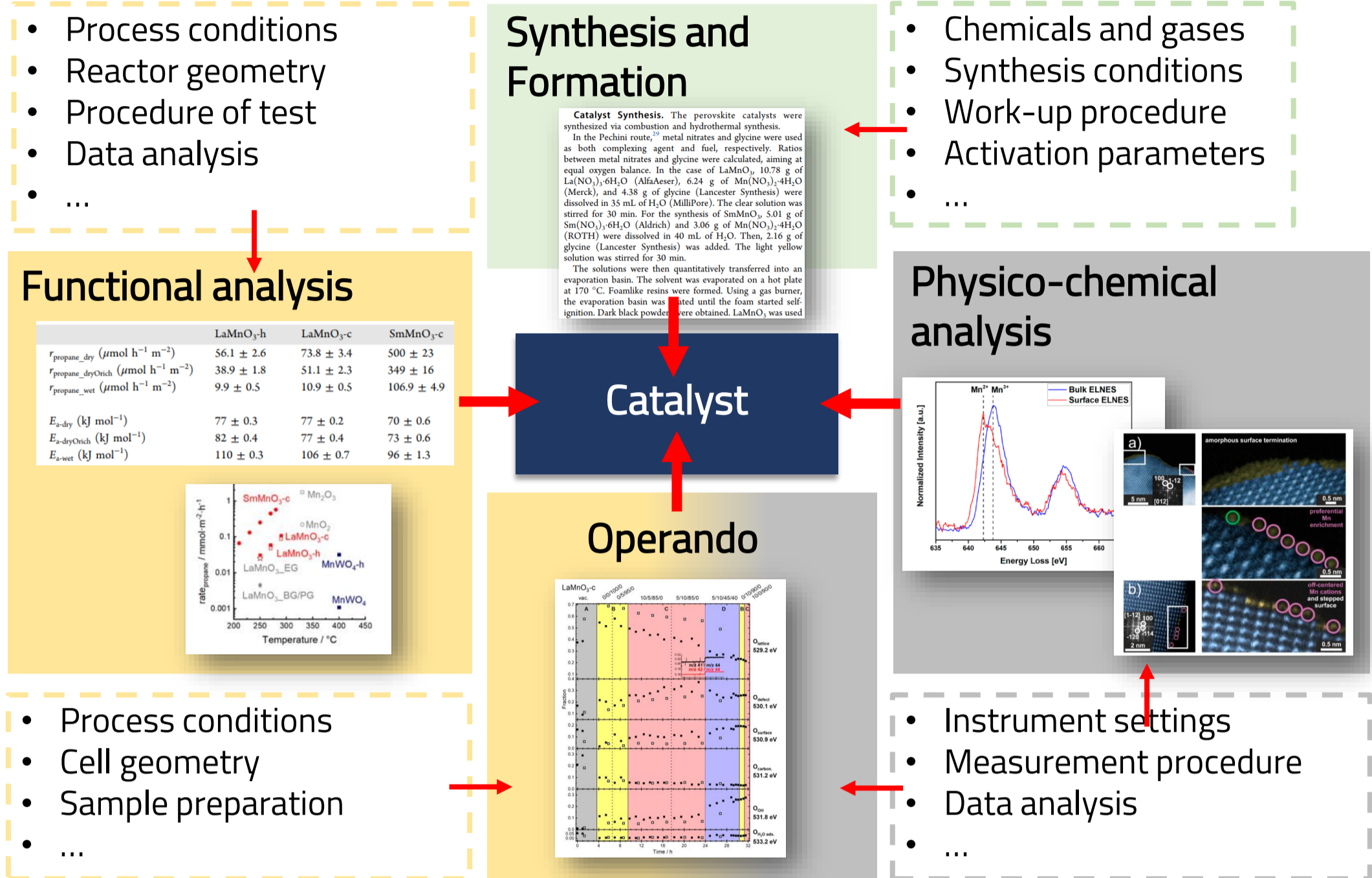[1]Physics Department and IRIS Adlershof, Humboldt Universität zu Berlin;
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Catalysis Data is Complex

- Process conditions
- Reactor geometry
- Procedure of test
- Data analysis
- …

Synthesis and Formation

- Chemicals and gases
- Synthesis conditions
- Work-up procedure
- Activation parameters
- …

Functional analysis

Physico-chemical analysis

Catalyst

Operando

- Process conditions
- Cell geometry
- Sample preparation
- …

- Instrument settings
- Measurement procedure
- Data analysis
- …

* C. Marshall, J. Schumann, A. Trunschke, *Angew. Chem. Int. Ed.*, **2023**, https://doi.org/10.1002/anie.202302971

Database requirements:

➤ One data entry for each state of the catalyst sample (e.g. precursor, calcined, reduced)

➤ One data entry for each activity, i.e. a process, characterization, or activity measurement, needs to be linked to a sample entry

➤ Key information is extracted and accessible through general summary and search pages

➤ Detailed information accessible by browsing through the data entries and also through an application programming interface (API)

➤ NOMAD uniquely suited to process and store different data formats

Summary

No overarching, general catalysis database exists currently

FAIR data requires:

➤ **Digitalization** of lab notes, facilitated by work according to standardized operating procedures and experiment automation

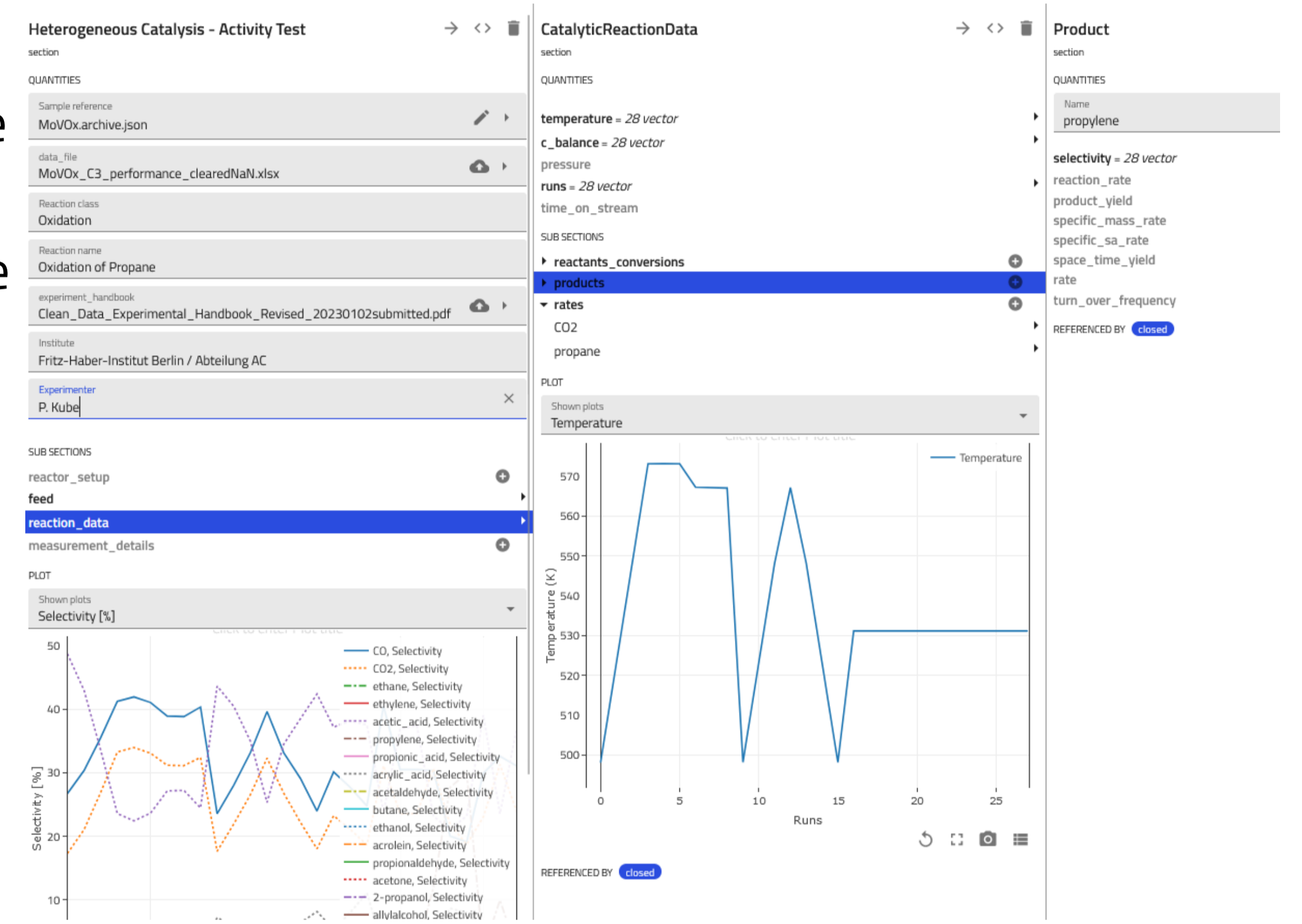➤ **Unified vocabulary** and agreement on key metrics used to compare catalysis performances

Overarching portals need:

➤ **Easy to use** data storage templates for experimentalist

➤ Provide easy access and improved capabilities for **data visualization**, **search** and **summarize** released data

NOMAD a powerful platform for which first templates and datasets are prepared
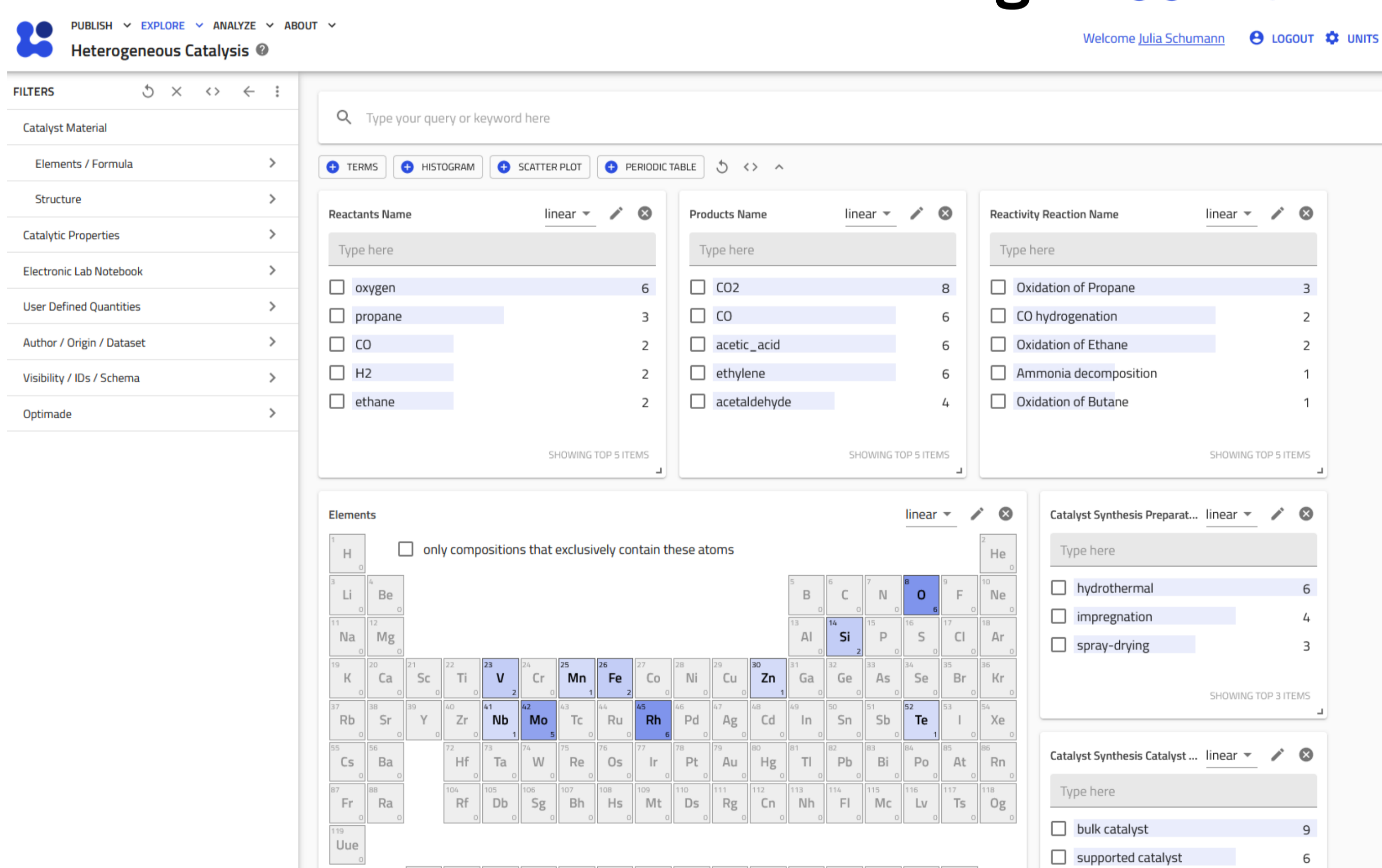
NOMAD Schemas for Catalysis

➤ Entry schemas for sample and activity test[a]

➤ Example of a collaborative project in oxidation catalysis[b]

➤ Automatic parsing of .csv or excel files into subsections

➤ Generation of plots directly from data file

[a] https://github.com/schumannj/nomad-schema-plugin-fhi-catalysis
[b] L. Foppa, *et al.*, *J. Am. Chem. Soc.* **2023**, *145*, 3427, https://doi.org/10.1021/jacs.2c11117.

Searching in NOMAD - the "Explore App"

Search entry data by

➤ Catalytic Test Reaction (Reactants, Product, Reaction Name)

➤ Catalyst sample composition (elements) and synthesis

Refine results by

➤ Temperature, pressure, space velocity

➤ Characterization properties (e.g. surface area)

Display

➤ Visualization of results in histograms and scatterplots

An Ontology for Catalysis

➤ Development in close coordination with Alexander S. Behr and Hendrik Borgelt from **NFDI4Cat** (NFDI for Catalysis-Related Sciences)

➤ Follows the Basic Formal Ontology (BFO, top-level)

➤ Separation into occurrent, i.e. planned process and continuant

➤ Mid-level Ontology: Chemical Methods Ontology (CHMO)

https://gitlab.mpcdf.mpg.de/nomad-lab/catalysis-ontology/-/raw/main/catalysis.owl
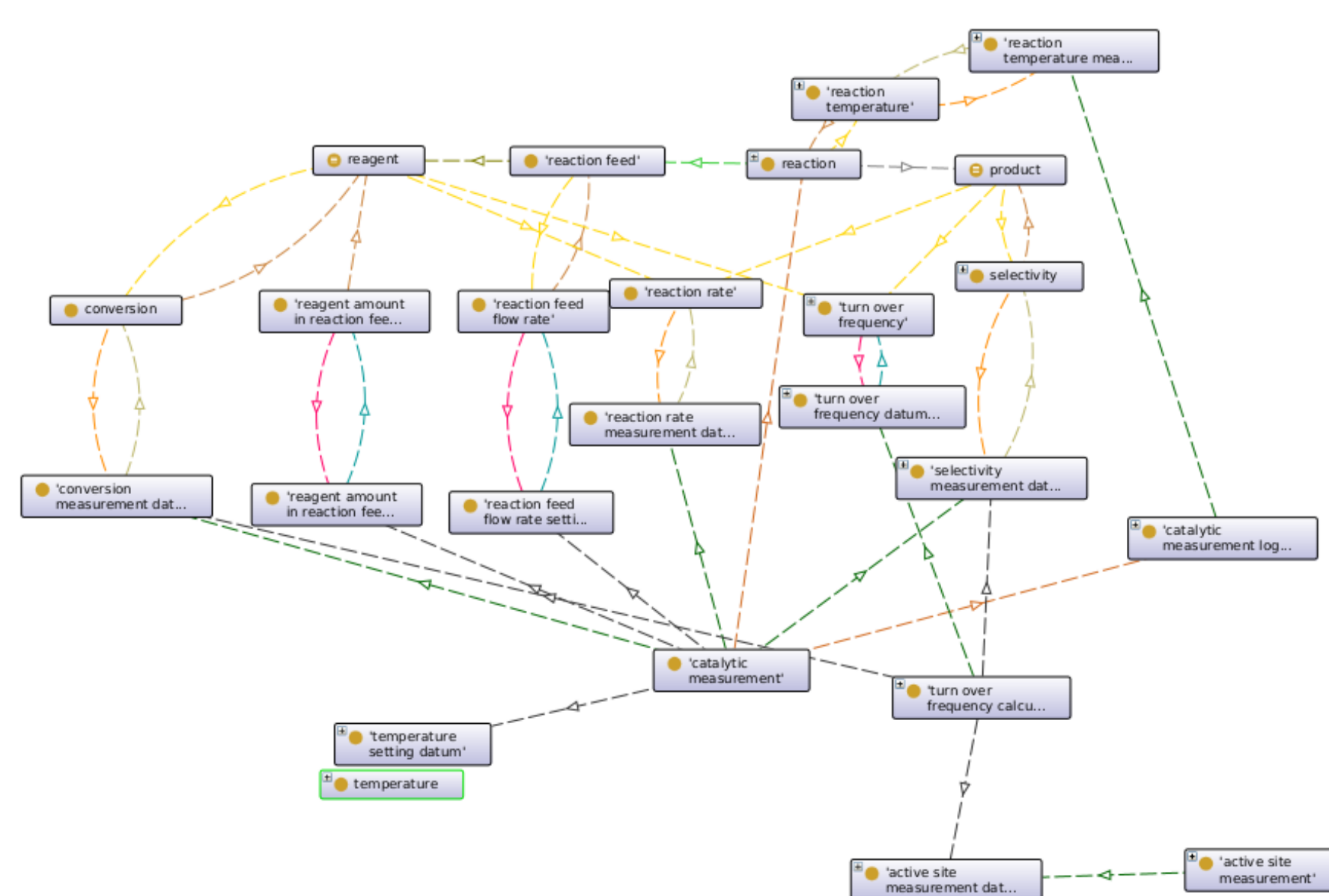
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