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# LabIMotion Electronic Lab Notebook as Research Data Management tool in Catalysis

Paolo Dolcet[1], Mariam L. Schulte[1,2], Florian Maurer[1], Nicole Jung[3], Rinu Chacko[1], Olaf Deutschmann[1,2], and Jan-Dierk Grunwaldt[1,2]

[1] Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Germany

[2] Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology, Germany

[3] Institute of Organic Chemistry, Karlsruhe Institute of Technology, Germany

**Abstract .** In the field of heterogenous catalysis, Electronic Lab Notebooks (ELNs) are only rarely employed, due to complex data structure and different needs of the community with respect to the typical features provided by wide-spread ELNs. On the contrary, LabIMotion, an extension of the open-source ELN Chemotion, adapts to the characteristic complex workflows in heterogenous catalysis; these encompass catalyst synthesis, adaptation of devices and testing rigs, activity measurements, material characterization (possibly also *in situ/operando*, at large scale facilities) and are complemented by mathematical modelling and simulation. Direct links to metadata catalogues like SciCat (for synchrotron/neutron characterizations) and advanced research data management tools like Adacta (for improved traceability of catalytic data, experimental setups and related resources) are envisioned. The adaptability of LabIMotion in the catalysis field is presented via the topical examples of Cu-based catalysts for methanol synthesis and noble metal-based emission control catalysts.

**Keywords:** Electronic Lab Notebook, Catalysis, Metadata

## Extended abstract

From both an academical and an industrial point of view, Research Data Management (RDM) tools are nowadays of prime importance for efficient usage and optimal reusability of research data, and Electronic Lab Notebooks (ELNs) play a key role in this, since they allow all data concerning an experiment to be stored electronically and be easily accessible.

In the (heterogenous) catalysis development environment, proper RDM practices coupled with big data science have the potential to be of great impact in the rational design of new and/or improved catalysts. Up-to-date, on the other hand, ELNs have found only limited permeation in the catalysis research field. This is due to the fact that the development of a catalyst follows a complex and intertwined workflow, leading to a rich data structure that is not well captured in currently available ELNs. For example, a typical workflow usually includes processes of catalyst synthesis and preparation, material characterization (which might include *in situ* characterization also at large scale facilities, like synchrotrons and neutron sources), activity measurements (also in this case possibly at large scale facilities, with data registered under *operando* conditions) coupled with adaptation of experimental reactor configuration, and finally complemented by mathematical modelling and numerical simulations. The currently available solutions are ill-suited to efficiently represent such a manifold system and no clear-cut solution is available.

We present here LabIMotion, an extension of the open-source ELN Chemotion [1] used in the NFDI4Chem community. This ELN extension, on the contrary, efficiently addresses the specific needs of the catalysis development environment. To achieve this goal, LabIMotion provides the possibility of creating detailed research plans and it is structured into defined functional areas, covering aspects such as catalyst synthesis, characterization and activity testing. For advanced characterizations performed at synchrotron and neutron facilities, LabIMotion will also provide linkage to the metadata catalogue SciCat [2], widely employed in the DAPHNE4NFDI consortium [3]. Devices management tools are also integrated in the platform, additionally offering a direct link to advanced tools like Adacta [4], supported by the NFDI4Cat project [5] and leading to improved traceability of all data and metadata related to kinetic performance studies, including therefore device-related resources. All these different areas are interlinked via a unique sample ID, and combined in a streamlined workflow that help the users in efficiently creating a traceable "digital twin" of their experimental catalyst environment.

Topical examples (e.g., Cu-based catalysts for methanol synthesis and noble metal-based emission control catalysts) are presented to guide through the typical data entry scenario (as shown in Figure 1) and to illustrate the capabilities and adaptability of LabIMotion, also with respect to logging, tracking and sharing of (meta)data.

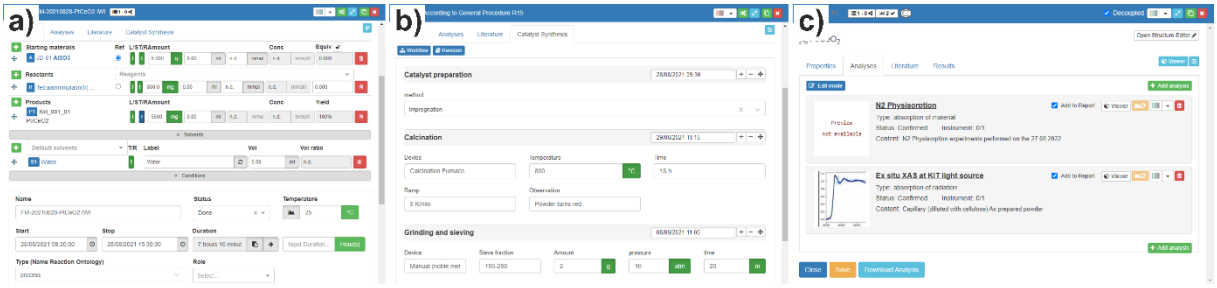


**Figure 1**. LabIMotion is organized in functional areas dedicated, e.g., to a) chemical information about the reactants, b) detailed synthesis procedure and c) material characterization.

LabIMotion is currently under advanced testing in the Collaborative Research Center 1441 "Tracking the Active Site in Heterogeneous Catalysis for Emission Control" [6] and in the Priority Programme 2080 "Catalysts and Reactors under Dynamic Conditions for Energy Storage and Conversion" [7], running at Karlsruhe Institute of Technology.

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