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Labimotion as a customizable ELN for heterogeneous catalysis workflows

Due to the complex data structures and the unique needs of the community, the design of Electronic Lab Notebooks (ELNs) solutions in the field of heterogeneous catalysis and particularly when including research in large scale facilities[1] is highly challenging. LabIMotion, an extension of the open-source ELN Chemotion[2], is designed to fill the gap between the preparation, testing and characterization of heterogeneous catalytic materials. Within the ELN, the user can work with pre-defined workflows, but also free input fields for e.g. research plans as well as link and share data with other users. LabIMotion envisions direct links to metadata catalogues like SciCat[3] (for synchrotron/neutron characterizations), PID solutions and advanced research data management tools like Adacta (for improved traceability of catalytic data, experimental setups, and related resources). In the presented work, the adaptability of LabIMotion in the catalysis field is demonstrated through examples such as Cu-based catalysts for methanol synthesis[4] and noble metal-based emission control catalysts[5].

DAPHNE4NFDI Deliverables / Categories:

2.2.1 White paper on metadata definition and known metadata

2.3.2 Preliminary specification for use cases minimum metadata

Topics to be (potentially) discussed/addressed in the course of the meeting:

1. Sample PID, DataCite services
2. ELN integration –Integration of Electronic log notebook

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[1] <https://www.tandfonline.com/doi/full/10.1080/08940886.2024.2432265>

[2] <https://chemotion.net/docs/labimotion>

[3] <https://scicatproject.github.io/>

[4] <https://www.spp2080.org>

[5] <https://www.trackact.kit.edu>

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