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## Catalysis use case in DAPHNE4NFDI at KIT

In the frame of the collaboration centre “TrackAct” ([www.trackact.kit.edu](http://www.trackact.kit.edu)), the priority program SPP2080 ([www.spp2080.org](http://www.spp2080.org)) and ROCK-IT ([www.rock-it-project.de](http://www.rock-it-project.de)), we have developed a workflow for catalysis experiments in DAPHNE4NFDI. Starting with sample preparation and basic characterization of the samples, documentation based on FAIR principle is needed by established tools such as LabIMotion for synthesis, catalytic performance using LabIMotion (NFDI4Chem) / AdActa (NFDI4CAT) and characterization which is also documented in the electronic lab notebooks. Preferentially, the samples are published in data publications/DOIs. Key to understanding catalysts are operando studies, often conducted at synchrotron radiation facilities [1]. For this purpose a workflow similar to the XAS use case has been set up. On-site we are improving the workflow using the catalysis beamline at KIT Light Source (CatAct), e.g. SciCat has been recently implemented based on collaboration in the DAPHNE4NFDI-initiative. We will discuss the present status using the power of the different tools and recent studies including Pt/CeO<sub>2</sub> catalysts [2] and coated catalysts [3] for emission control as well as Cu/ZnO-ZrO<sub>2</sub> catalysts for the production of green methanol [4]. In all cases, in addition to the main paper, electronic supporting informations and data publications of the raw data have been published (e.g. on KITOpen, Zenodo [5]) Particularly, the format of the data publications will be discussed and how the data are then uploaded into reference databases.

[1] Sarma, B. B.; Grunwaldt, J.-D., CHIMIA 78 (5), 288–296 (2024). doi:10.2533/chimia.2024.288.

[2] Gashnikova, D.; Maurer, F.; Bauer, M. R.; Bernart, S.; Jelic, J.; Lützen, M.; Maliakkal, C. B.; Dolcet, P.; Studt, F.; Kübel, C.; Damsgaard, C. D.; Casapu, M.; Grunwaldt, J.-D.

2024. ACS Catal. 14 (19), 14871–14886 (2024). doi:10.1021/acscatal.4c02077

[3] Rang, F.; Delrieux, T.; Maurer, F.; Flecken, F.; Grunwaldt, J.-D.; Hanf, S., Small Science, 4 (12), 2400345 (2024). doi:10.1002/sssc.202400345

[4] Schulte, M. L.; Truttmann, V.; Doronkin, D. E.; Baumgarten, L.; Nicolai, A.; Beltran, D. A. M.; Summ, F. J.; Kiener, C.; Warmuth, L.; Pitter, S.; Saraçi, E.; Grunwaldt, J.-D., Angew. Chem. Int. Ed., in press, e202423281 (2025). doi:10.1002/anie.202423281

[5] For the KITOpen-raw data publications: <https://doi.org/10.35097/ncym5afk9q64kz8x>; <https://doi.org/10.35097/0k5f6x56uxjs7cw>; <https://zenodo.org/records/14054929>

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