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Local solutions for data acquisition and storage in heterogeneous catalysis

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A great potential in catalysis research is seen in an increasing integration of theory and experiment and the broader application of data science methods to experimental and calculated data.1 The data exchange necessary for this requires progressive digitalization. Experimental data must be generated reproducibly and with sufficient diversity, and must be available in machine-readable form. At the Department of Inorganic Chemistry of the Fritz-Haber-Institut (FHI) der Max-Planck-Gesellschaft (MPG), we have developed and implemented a concept for a local data infrastructure during the past years. This work is integrated in our activities in FAIRmat, Use Case Demonstrators E2, "Heterogeneous Catalysis" in coordination with NFDI4Cat and in the BMBF project CatLab. The software solutions were developed in collaboration with the computer support group of the FHI and were initially based on a database that has been used intensively by the department for more than 20 years. The database was upgraded to a modern, flexible electronic laboratory notebook that meets the requirements of research in heterogeneous catalysis and enables data exchange via an Application Programming Interface (API).2 For research projects, handbooks (Standard Operating Procedures (SOP's)) are developed, preferably in machine-readable form, detailing how experimental data are obtained, including the definition of benchmark catalysts. To facilitate the implementation of the handbook concept, automated systems for data acquisition and storage have been designed in the framework of a research project focused on the investigation of innovative catalysts for the efficient conversion of chemical energy into electrical energy and vice versa (CatLab).3 Such systems consist of (i) EPICS for communication with devices and data acquisition, (ii) the database (archive), (iii) an archiving appliance for storing time series, (iv) Phoebus for creating graphical user interfaces, (v) Python/Bluesky/Jupyter notebooks for creating automation and data evaluation, and (vi) a S3 storage for long-term storage. The concept is explained using the examples of an automated reactor for catalyst testing and the automated storage of electron microscopy data.
(1) Marshall, C. P.; Trunschke, A., Achieving Digital Catalysis: Strategies for Data Acquisition, Storage, and Use. Angewandte Chemie International Edition 2023, submitted.
(2) Archive FHI MPG, https://github.com/fhimpg/archive.
(3) Automation solutions FHI MPG, https://gitlab.fhi.mpg.de/fhi-ac/ertl; https://gitlab.fhi.mpg.de/fhi-ac/haber; https://gitlab.fhi.mpg.de/fhi-ac/velox; https://gitlab.fhi.mpg.de/fhi-ac/json-scripte; https://gitlab.fhi.mpg.de/fhi-ac/gaswarnanlage; https://gitlab.fhi.mpg.de/fhi-ac/berty.
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