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Digital Data Management in Catalysis: Funding for the NFDI4Cat Consortium is Extended

The digital data management projects within the NFDI4Cat catalysis consortium as part of the National Research Data Infrastructure (NFDI) will continue to be funded in the coming years. In a corresponding decision, the German Research Foundation (DFG) has approved a good 8.5 million euros for the second funding phase until the end of 2028. The Leibniz Institute for Catalysis in Rostock will receive 600,000 euros of this.

The NFDI e.V. was founded in October 2020 by the federal and state governments with the aim of coordinated data management, especially digitization in the field of research data. Catalyst-related research was also to be promoted from the outset, which is why the NFDI4Cat consortium was founded, coordinated by DECHEMA.

Complete digital documentation possible

LIKAT was already awarded a contract for its projects in the first round of tenders. Under the leadership of Dr. David Linke, programs and data models were developed that enable practically any laboratory to make its catalysis research data available in digital form, i.e. machine-readable. This data is referred to as FAIR data, which stands for its properties: Findable, Accessible, Interoperable, Reusable. They are provided in an NFDI4Cat data space and are used, for example, to train AI models.

Entering the second funding phase with NFDI4Cat: David Linke. (Photo: LIKAT)

David Linke: "This data is of great benefit to everyone in the scientific community. They fully document the procedure for all experiments, which can run into the hundreds for a single

publication." So far, catalysis researchers have only published a fraction of this data in their scientific articles, as the chemist explains further. "But there is ten to 50 times the amount of data behind it. For example, on experiments that were unsuccessful even though they were carried out correctly. And this is precisely what an AI model needs to learn in order to become more reliable."

One of the tasks was to develop a precise machine-readable vocabulary. David Linke received the "NFDI4Cat - Digital Chemist Award" in 2024 for his work on this project.

Second funding phase

In the next funding phase, NFDI4Cat will expand the data space-based cooperation between science and industry. "Ongoing training, community feedback, a sustainable organizational model and the further development of interoperable tools will ensure long-term transfer to research, teaching and industry," says Dr Linke.

With an AI-compatible pool of research data, scientific work will be much more effective than before. "I can create comprehensive cross-connections to my topic and see, for example, where other laboratories have left experimental gaps that could become interesting with my level of knowledge." The pool of globally usable knowledge is simply getting bigger.

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