The ROCK-IT project

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The development of novel, highly efficient catalysts is based on knowledge-driven insights into their functioning. Synchrotron radiation can provide *operando* information on “catalysts at work” that is difficult or even impossible to obtain by other means. However, the parameter space of experimental conditions to be explored can be enormous.

Catalysis experiments are currently not highly digitized nor automated when compared to other fields such as macromolecular crystallography, where the potential of automation and digitization of measurements is already successfully exploited. This has been mostly due to complexity of the sample environments, the large and complex parameter space, which must be explored, and the need for multimodal measurements. However, there is significant scope for improvement. The digitalization of experiments will increase our knowledge of complex processes through increased sample throughput, improved data quality, and efficient exploration of complex parameter spaces.

The ROCK-IT project (remote, *operando* controlled, knowledge-driven, IT-based), addresses these challenges by the intention to provide solutions to improve the efficiency of catalysis research, tailor-made, yet composed of generic building blocks portable enough to be applicable to a wide range of measurements. The building blocks – partly interfacing to other ongoing projects in the field of data handling and science – include standardized and interchangeable data formats, standardized metadata collection, interfaces to electronic lab books, sample tracking and handling, machine learning based experiment control and data evaluation, and automation of experiments under remote control. Here, standardization and automation are prerequisites for making the solutions developed available to a broad user base and industry via remote-access modes, providing a consistent "look & feel" at different sources, and thus removing barriers to access and thereby potentially accelerating innovation cycles. As a greater integration of digital technologies is accompanied by higher attack potential in the digital space, cybersecurity considerations play an important role within ROCK-IT.

The ROCK-IT core partners Deutsches Elektronen-Synchrotron DESY, Helmholtz-Zentrum Berlin HZB, Helmholtz-Zentrum Dresden-Rossendorf HZDR, and Karlsruher Institut für Technology KIT, together with key users from science and industry, have the expertise required to achieve real progress enabling automated high throughput measurements for catalysis research. Beyond catalysis research, which serves to provide a concrete focus, ROCK-IT generates added value for Helmholtz as a whole: the interfaces, tools, and standards developed in ROCK-IT will be designed to be portable to other techniques and application domains so that they serve the needs of other research fields.

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