DAPHNE4NFDI@TrackAct

More than 95% of all chemical products have seen a catalyst during their production. The catalyst market is worth three trillion Dollars per year, so it is crucial to develop and optimize catalysts as efficiently as possible.

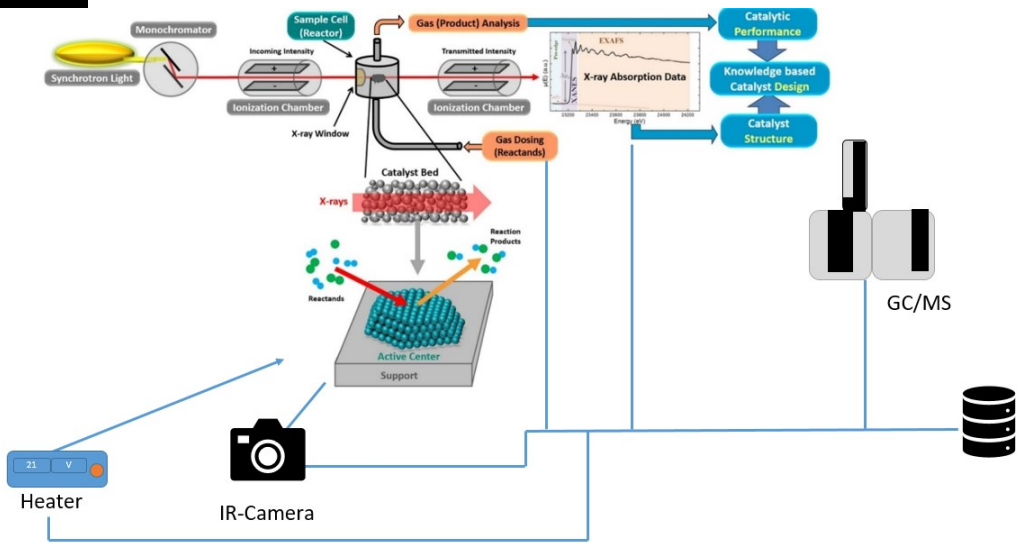
The goal of CRC1441, project TrackAct is to identify and track the nature of the active site of catalysts. Those will be designed to be manipulated from bottom-up, throughout the whole scale-up process. Eventually, as a long-term vision the catalyst's structure and behavior should be predicted and actively controlled during operation.

Within TrackAct, a close collaboration among the NFDI initiatives DAPHNE4NFDI, NFDI4Cat, and NFDI4CHEM and TrackAct's INF project exists.

At this year's **project status meeting**, on October 21st, DAPHNE4NFDI was invited to exchange views about the challenges of catalyst operando XAS measurements.

DAPHNE4NFDI XAS Use Case

Katja Kornetzky presented a typical operando characterization use case at a large-scale facility. As an example of a spectroscopic measurement at a synchrotron-beamline, data recorded at CATACT (KIT light source) have been used. In operando experiments, data are manifold and are usually generated from different sources. These are apart from the spectroscopic data (X-ray absorption, X-ray fluorescence, X-ray diffraction). In our example, a gas dosage unit, a heating element, an infrared camera and a GC/MS system were used, leading to heterogenous datasets. According to FAIR principles, all data must be stored in a single location and must be findable.



Katja also briefly referred to SciCAT, a metadata catalog for experimental data from neutron- or synchrotron sources, which is supported by the University of Tübingen in DAPHNE4NFDI. With SciCAT, data can be easily retrieved and used for machine learning. A laboratory notebook, LabImotion ELN, can also hold XAS, XRD or even tomography data. This was explained and demonstrated in great depth by Nicole Jung. Last but not least, the information pertaining from the gas dosage system with its different components can be tracked by a software named Adacta, providing a fully FAIR and compliant solution for catalysis scientists. This was presented by Olaf Deutschmann und Johannes Riedel, who also gave a hands-on training.

That way researchers obtain all relevant data concerning their measurement in a single repository, making it easy to share results, publish them and use them for further analysis.

Synopsis

The neutron- and synchrotron radiation user community is very diverse, and this was an excellent opportunity to dive in deeply into a specific use case and kindle the discussion. Taking the operando characterization use case, many TrackAct seminar attendees could identify with similar challenges and relate to the solution.
We hope DAPHNE project members will get more opportunities to exchange with the community in the future.

For more information on the use case, contact: Katja Kornetzky.

For further information on the CRC TrackAct go to: www.trackact.kit.edu

Are you interested in project DAPHNE4NFDI and want to be part of it?

Please send a mail to our coordinator, Lisa Amelung: lisa.amelung@desy.de