

# ROCK-IT: TAILOR-MADE DIGITAL SOLUTIONS FOR OPERANDO CATALYSIS RESEARCH

Remote, operando controlled, knowledge-driven, IT-based catalysis research at BESSY II

**ABSTRACT:** Insights into "catalysts at work" are of high interest to academic and industrial users, prompting the ROCK-IT project partners DESY, HZB, HZDR and KIT to enhance capabilities for in situ and operando experiments by optimizing workflows through common remote access protocols, data management standards, automation, robotics, experiment and beamline control software including AI aspects and real-time evaluation. The results of the project will allow for a more effective catalyst development and an increased attractiveness for non-expert users as well as users from industry. Ultimately, access barriers are lowered and innovation cycles accelerated.

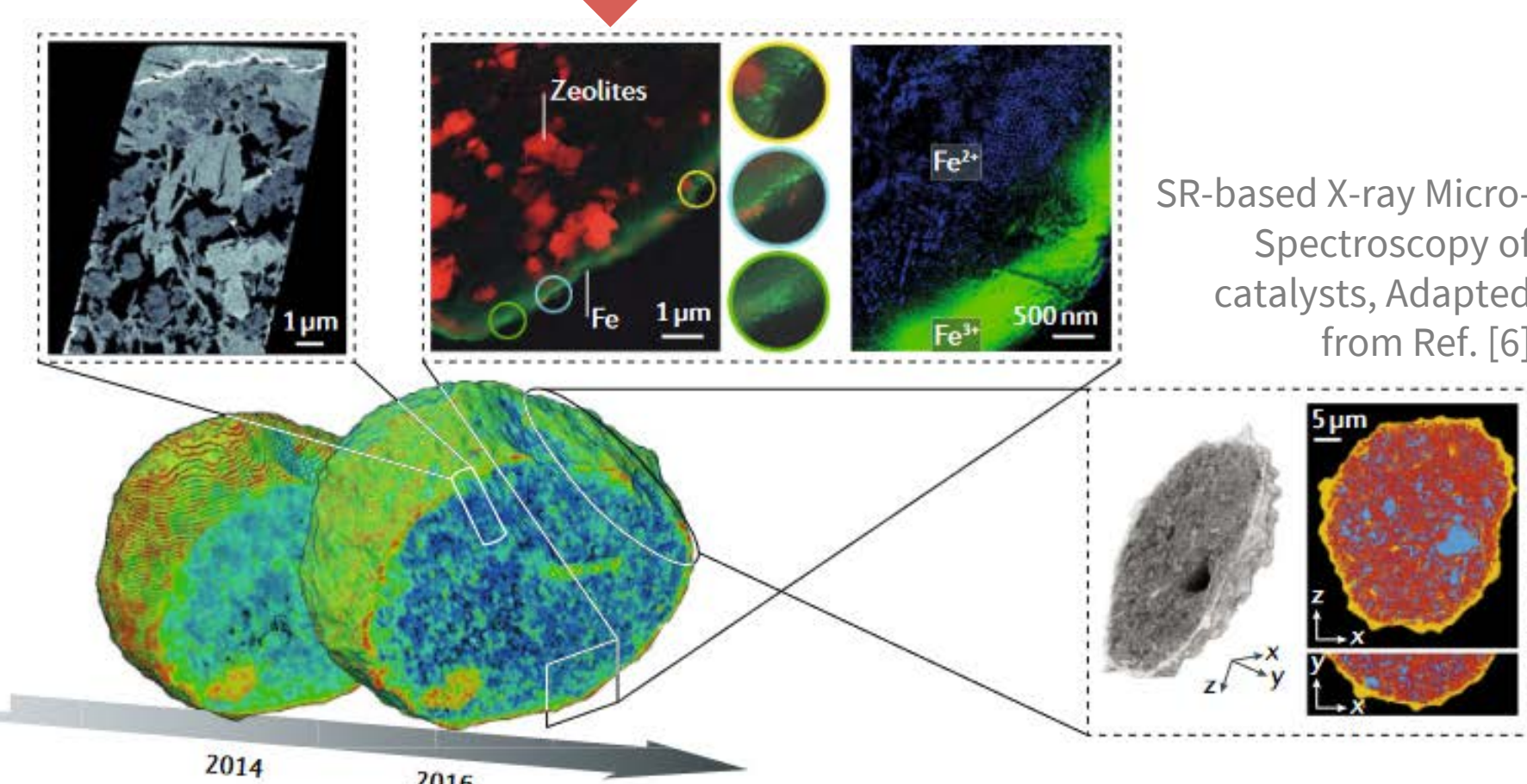
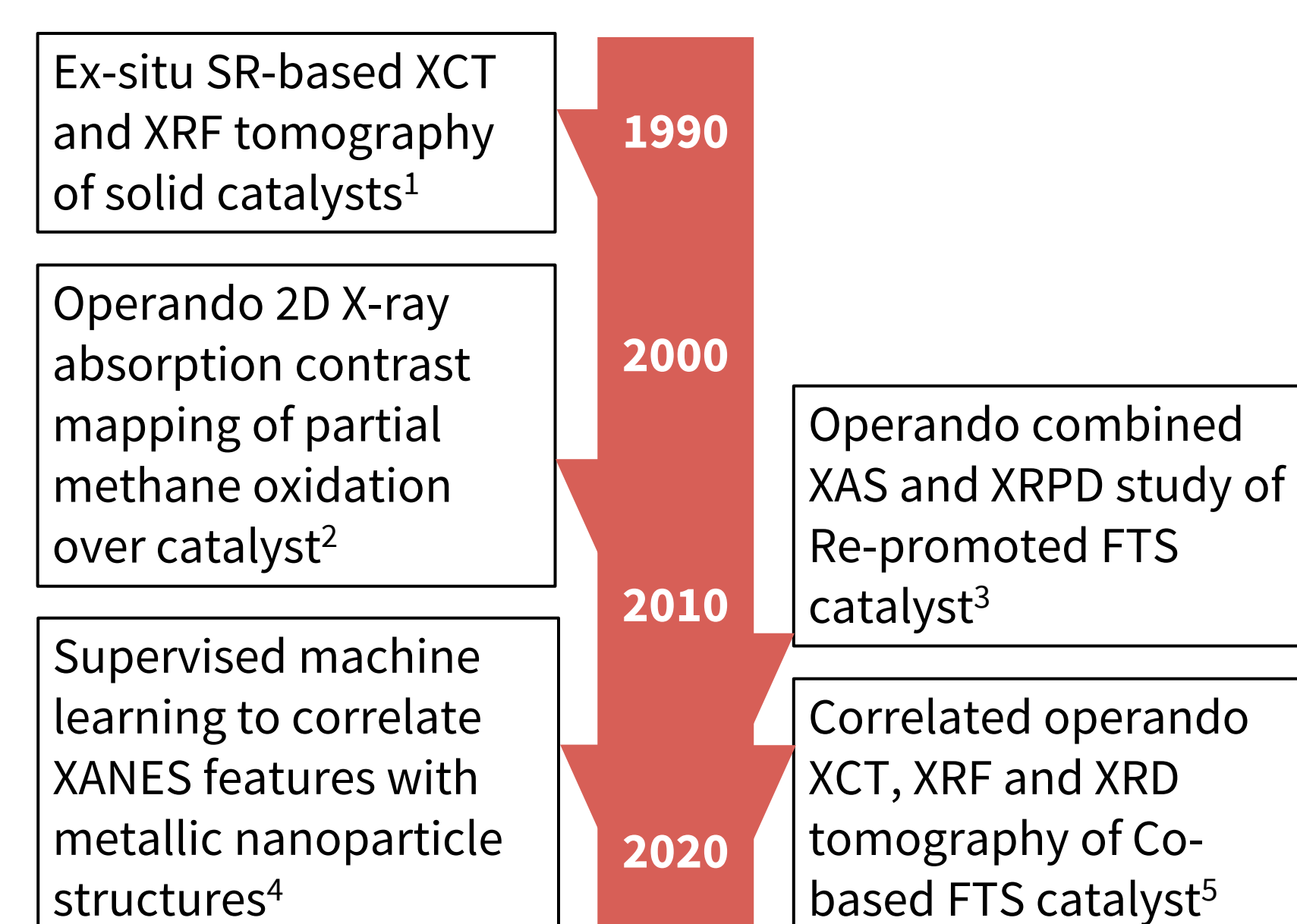
Alexander Dillmann, Ana Velazquez, Aniket Phutane, Anil Badarinarayan, Antonin Sulc, Ants Finke, Athar Khodabakhsh, Britta Höpfner, Chen Zhengyu, Daniel Tomecki, David Meier, Dirk Wallacher, Felix Möller, Gerrit Günther, Gina Ruland, Gregor Hartmann, Gudrun von der Waydrink, Heike Görzig, Heiko Kreth, Jens Viehhaus, Katherine Rial, Klaus Kiefer, Luca Porzio, Marcel Bajdel, Mario Meier, Max Gisel, Mezzio Bertrand Donack, Olaf Schwarzkopf, Peter Feuer-Forson, Peter Wegmann, Roland Müller, Rolf Krah, Sebastian Gerischer, Sebastian Sachse, Simone Vadilonga, Sonal Patel, Sven Erdem, William Smith.

## REFERENCES

- 1 Conner, W. C. et al. doi: 10.1021/ma00224a002
- 2 Grunwaldt, J.-D. et al. doi: 10.1021/jp060371n
- 3 Tsakoumis, N. E. et al. doi: 10.1016/j.jcat.2012.04.018
- 4 Timoshenko, J. et al. doi: 10.1021/acs.jpcllett.7b02364
- 5 Price, S. W. et al. doi: 10.1126/sciadv.160283
- 6 Meirer, F. et al. doi: 10.1038/s41578-018-0044-5
- 7 Wilkinson, M. D. et al. doi: 10.1038/sdata.2016.18

## SHINING A LIGHT ON CATALYSIS:

### PROGRESS OF SR-BASED RESEARCH



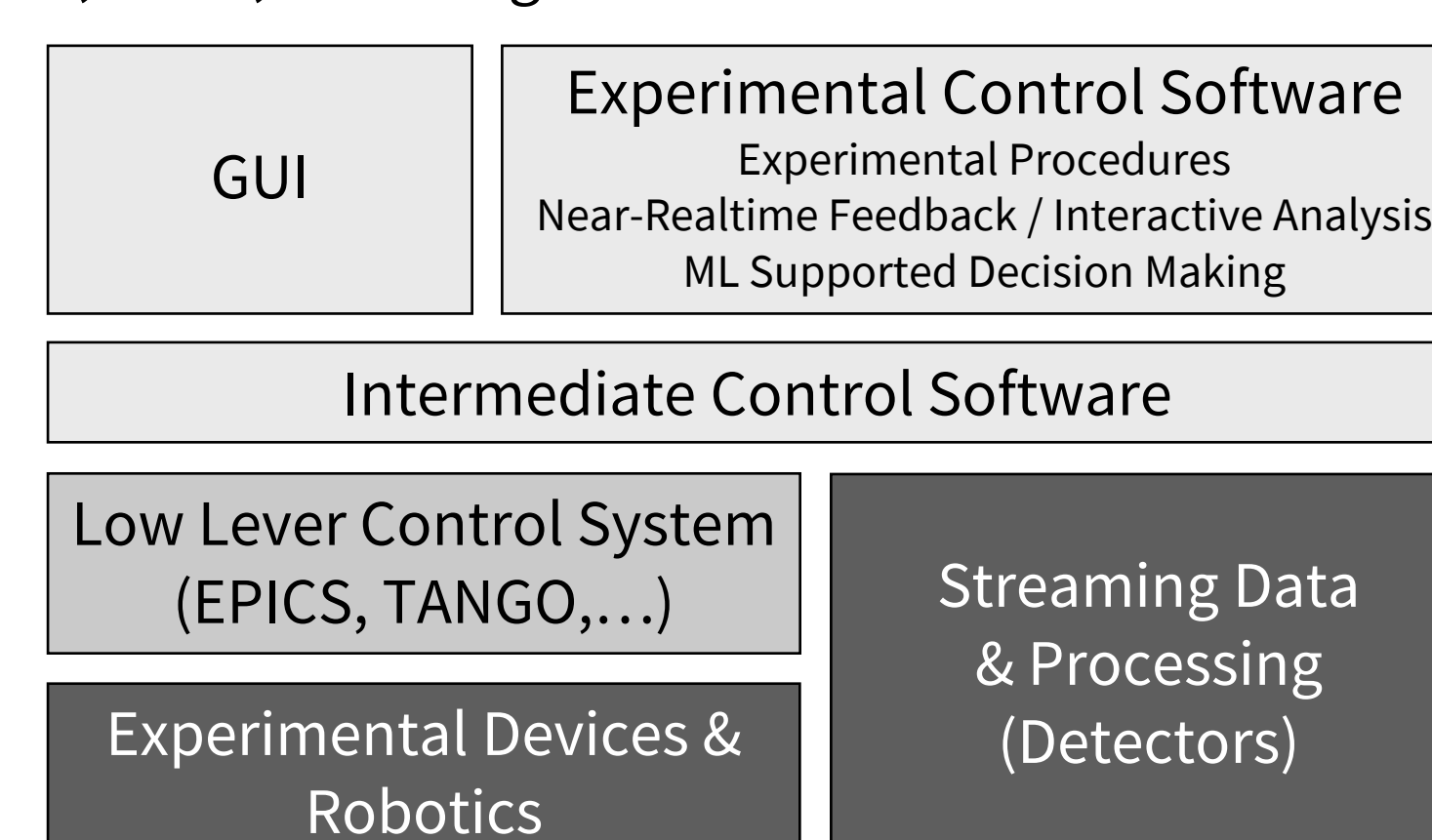
- Unravelling the complex mechanisms of catalysts needs a better understanding of material dynamics under reaction conditions
- SR sources (BESSY II, PETRA III, KARA) provide advanced capabilities for operando characterization at atomic and molecular level
- ROCK-IT aims to accelerate catalysis research and lower access barriers by focusing on automation, remote-access, operando experiments

## WP1: REMOTE CONNECTION & SECURITY

- Modular concepts with defined, secured, and certified interfaces
- Compatibility with existing infrastructures, services (such as FAIRmat, DAPHNE4NFDI,...) and security policies
- Focus on usability in the development of remote-access software so that graphical interfaces are intuitive and easy to use for different types of users with different experiences and backgrounds

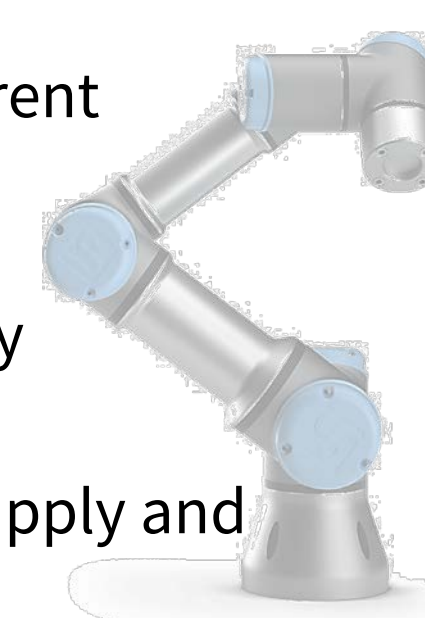
## WP2: CONTROLS & AUTOMATION

- Experimental control software including a graphical user interface and providing the highest degree of automation
- Providing consistent "look & feel" at the SR sources BESSY II, PETRA III, KARA, removing access barriers

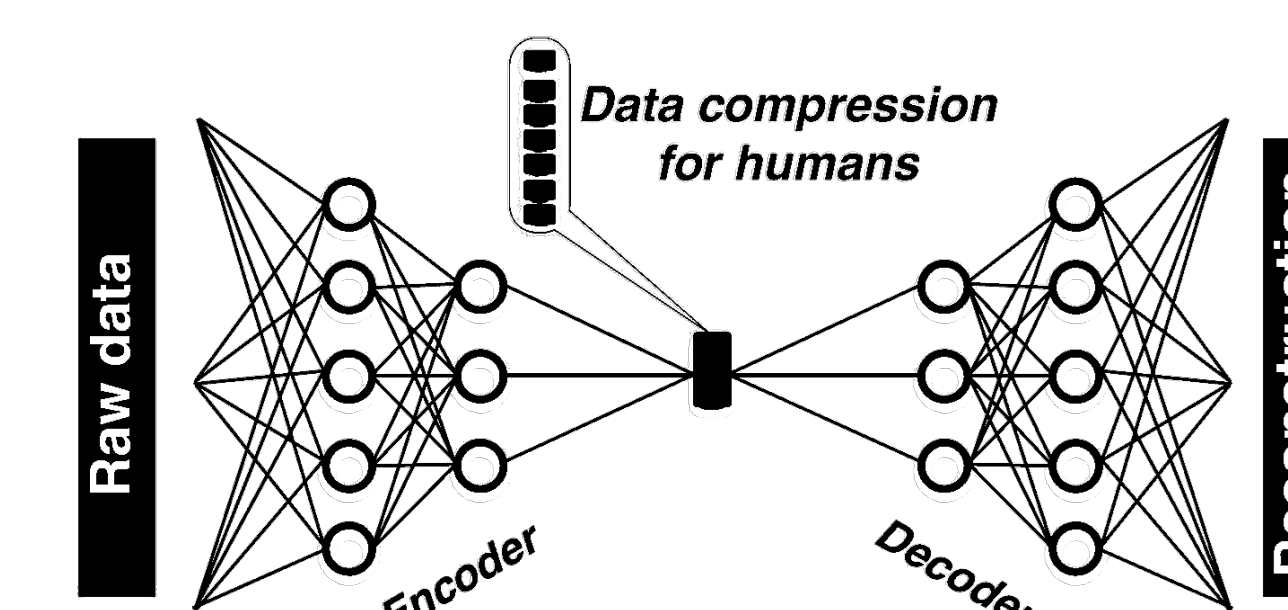


## WP3: EXPERIMENT & ROBOTICS

- Tailored sample environments: Measure catalytic performance and get access to multimodal analytics
- Setup and control of exemplary reactor cells (for different samples and investigation methods) using robotic manipulators, realization of standardized gas supply and analysis infrastructure including quality control by automated reference measurements
- Aim: Full automation (robotic sample handling, gas supply and analysis infrastructure, metadata)



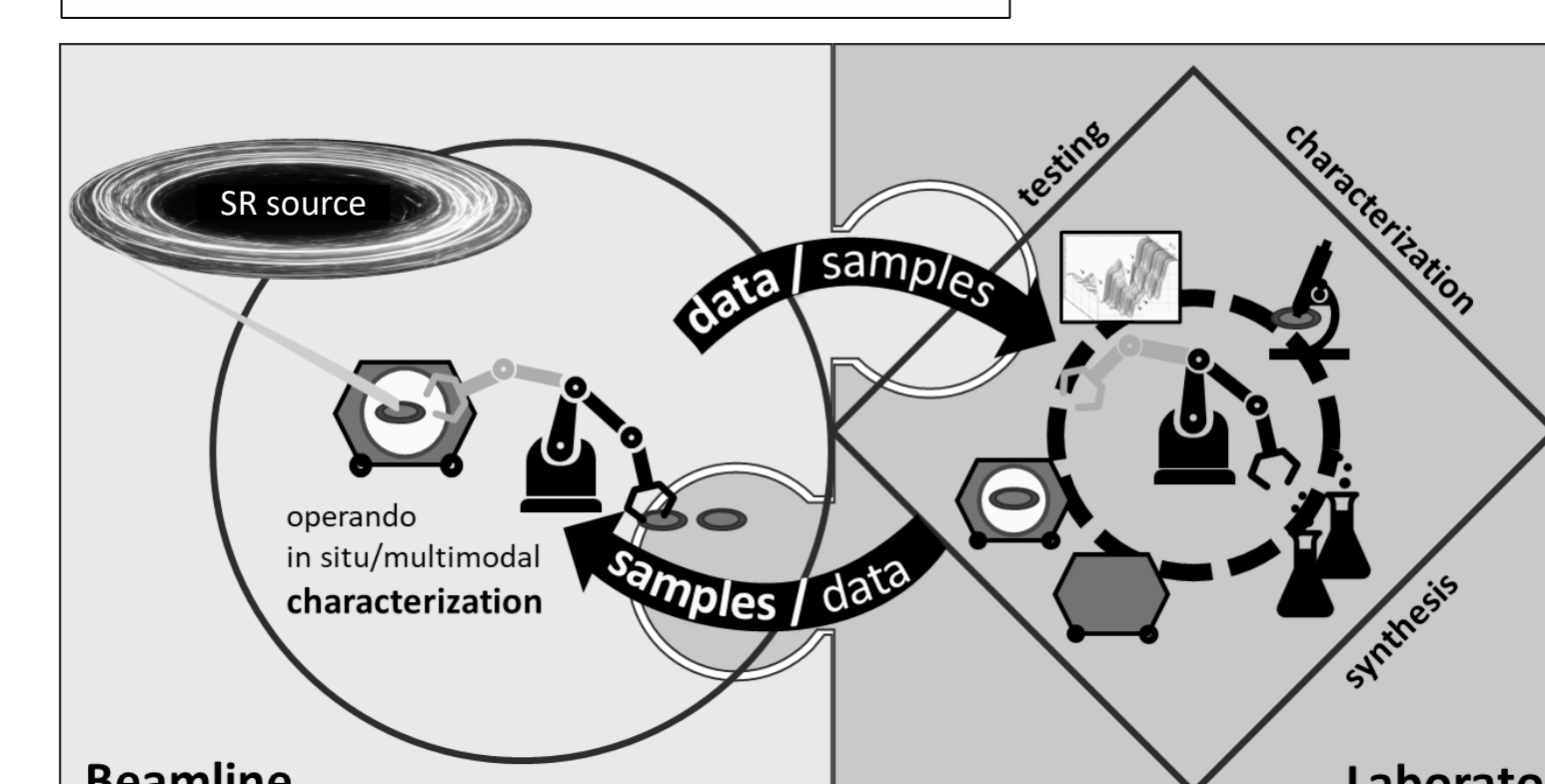
## WP4: NEAR-REALTIME ANALYSIS (ML)



- Near-Realtime analysis: Optimization by looking at experiment outcome, optimizing data quality, allowing for in-transit data reduction, steering experiments towards optimum usage of measurement time and identify outliers
- Increase in efficiency and quality of data enabled through advances in machine learning (ML)

## WP5: DATA LIFECYCLE MANAGEMENT

- Data management based on FAIR principles building on German research data infrastructure (NFDI) projects, including DAPHNE4NFDI, FAIRmat, and NFDI4Cat
- FAIR ≠ Open: Protection of sensitive data
- Focus on standardizing metadata and data generation workflows, and on establishing best practices for electronic lab book usage



## Acknowledgement & Partners

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## KEY POINTS

Synchrotron radiation studies of "catalysts at work" drive their development based on insights into their functioning

ROCK-IT will:

- **increase our knowledge of catalytic processes** via efficient exploration of complex parameter spaces through increased sample throughput, improved data quality and integrated data management
- **accelerate innovation cycles** due to a higher degree of automation by advanced robotics and suitable software tools
- **facilitate user access from science and industry** to multiple German synchrotron sources by a unified workflow
- help **reduce the CO<sub>2</sub>-footprint** of the entire operation due to less travel requirements of users and **enable broader participation** worldwide
- apply advanced cyber security to **safeguard data and infrastructure**