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MAX-PLANCK-GESSELLSCHAFT

FAIRMAT - A CONSORTIUM OF THE GERMAN RESEARCH-DATA INFRASTRUCTURE (NFDI)



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National Research Data Infrastructure

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In Germany, an initiative for a Research Data Infrastructure has been started.

What Is the NFDI?

The aim of the national research data infrastructure (NFDI) is to systematically manage scientific and research data, provide long-term data storage, backup and accessibility, and integrate the data both nationally and internationally. The NFDI will bring multiple stakeholders together in a coordinated network of consortia tasked with providing science-driven data services to research communities.

 DFG – German Research Foundation

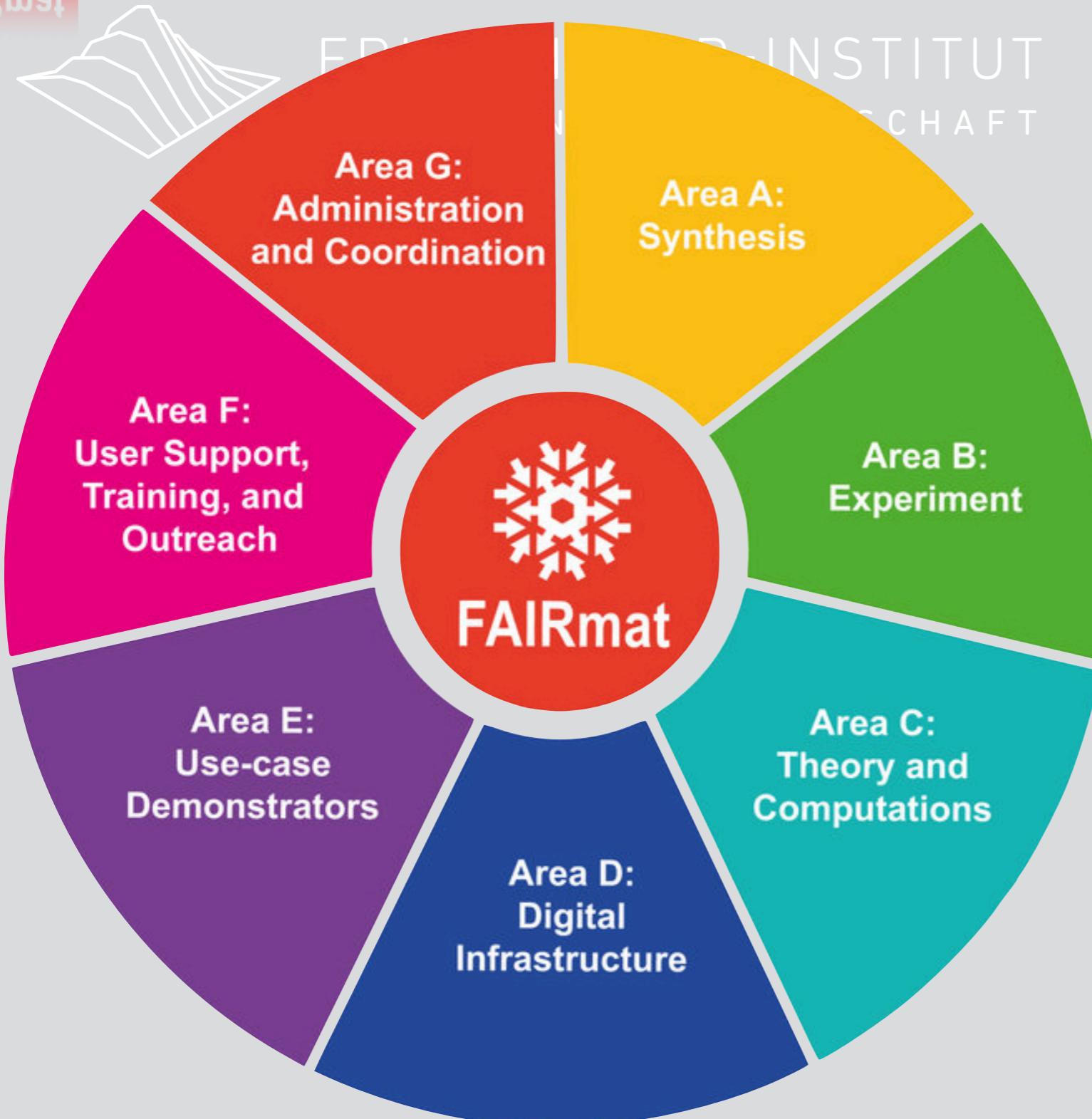


FAIRmat consortium

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- FAIRmat (FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids) will build a FAIR research-data infrastructure for the noted fields.
- Within FAIRmat the acronym FAIR is interpreted in a forward-looking way: Research data should be Findable and Artificial-Intelligence Ready.

FAIRmat consortium



FAIRmat consortium

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A universal and easy-to-configure software environment for measurement data acquisition and documentation is to be developed in Task D5 of the FAIRmat consortium.

In the field of Applied Physics, measurement setups with numerous specific measurement devices are often required in each case adapted to the experimental problem. The diversity requires adaptable and easy-to-configure software for experiment control and data acquisition.



Area D: Digital Infrastructure
H.-J. Bungartz, W. Nagel

D1: Metadata, Ontologies, and Workflows
R. Ritz, L. Ghiringhelli / M. Scheffler

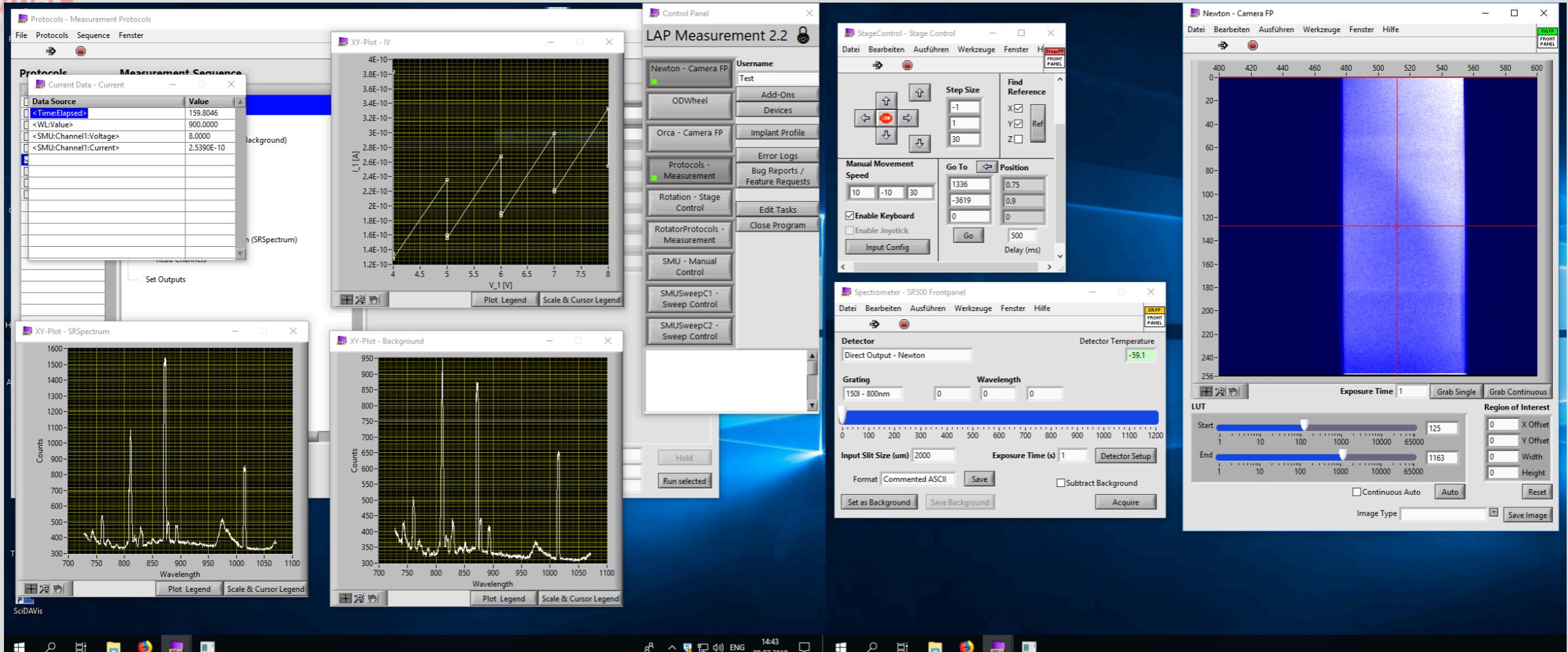
D2: Processing, Storage, and Compute Concept
W. Nagel, H.-J. Bungartz, H. Lederer, G. Sutmann

D3: Central Metadata Repository and Portal
M. Scheidgen / C. Draxl, A. Reinefeld

D4: Connectivity
H.-J. Bungartz, S. Wesner

D5: Configurable Experiment Control System
H. Weber / M. Krieger, H. Junkes

FAIRmat, Task D5, CECS



A prototype software developed at the chair of the Department of Physics at the Friedrich-Alexander-Universität (FAU) Department for experiment control with uniform and documented data output has been using for years



FAIRmat, Task D5, CECS

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This system has proven itself at the FAU-department in research and teaching. However, it does not satisfy the FAIR rules. By using LabVIEW, the system is:

- not open source,
- not operating system independent,
- not platform independent,
- is very poorly scalable.



FAIRmat, Task D5, CECS

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“We will implement the advanced Experimental Physics and Industrial Control System (EPICS) for recording, automatic metadata tagging, storing, archiving and managing research data.” (DFG-Proposal)



Easy to use
configuration

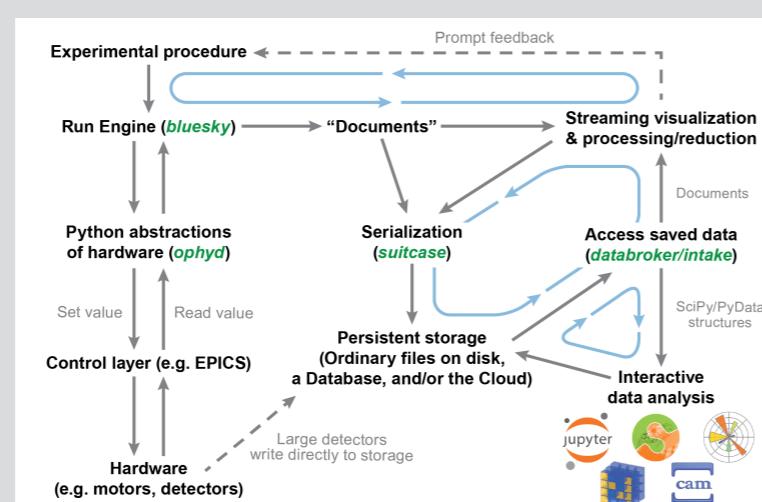


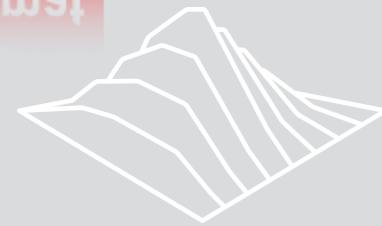
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input



CECS (next step)

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    field(DRVL, "0.0")
    field(DRVH, "359")
    field(PINI, "YES")
}

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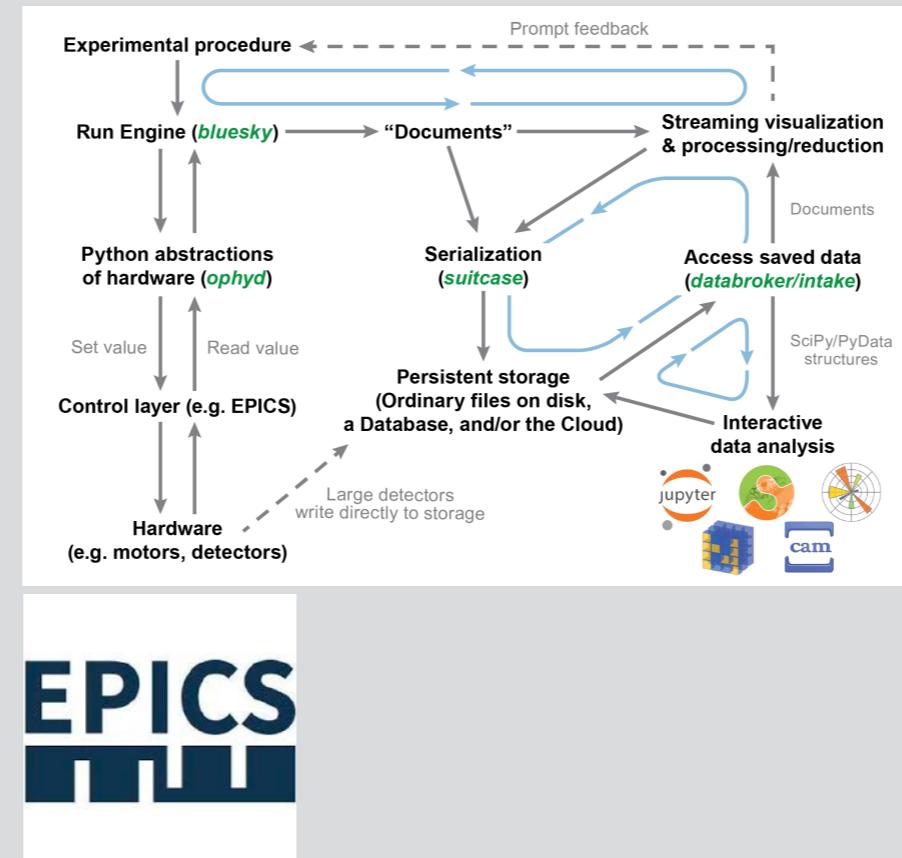
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    field(INPD, "360")
    field(DESC, "Angle")
    field(EGU , "deg")
    field(LOLO, "45")
    field(LOW , "135")
    field(HIGH, "225")
    field(HIHI, "315")
    field(LLSV, "MAJOR")
    field(LSV , "MINOR")
    field(HSV, "MINOR")
    field(HHSV, "MAJOR")
    field(CALC, "C:=A+B;(C>=D)?C-D:C")
    field(FLNK, "$(user):circle:x")
    field(PREC, "3")
    info(Q:group, {
        "$(user):circle": {"angle": {+channel:"VAL"}},
        "$(user):line": {"a": {+channel:"VAL"}}
    })
    alias("$(user):line:a")
}
...

```

generates



input

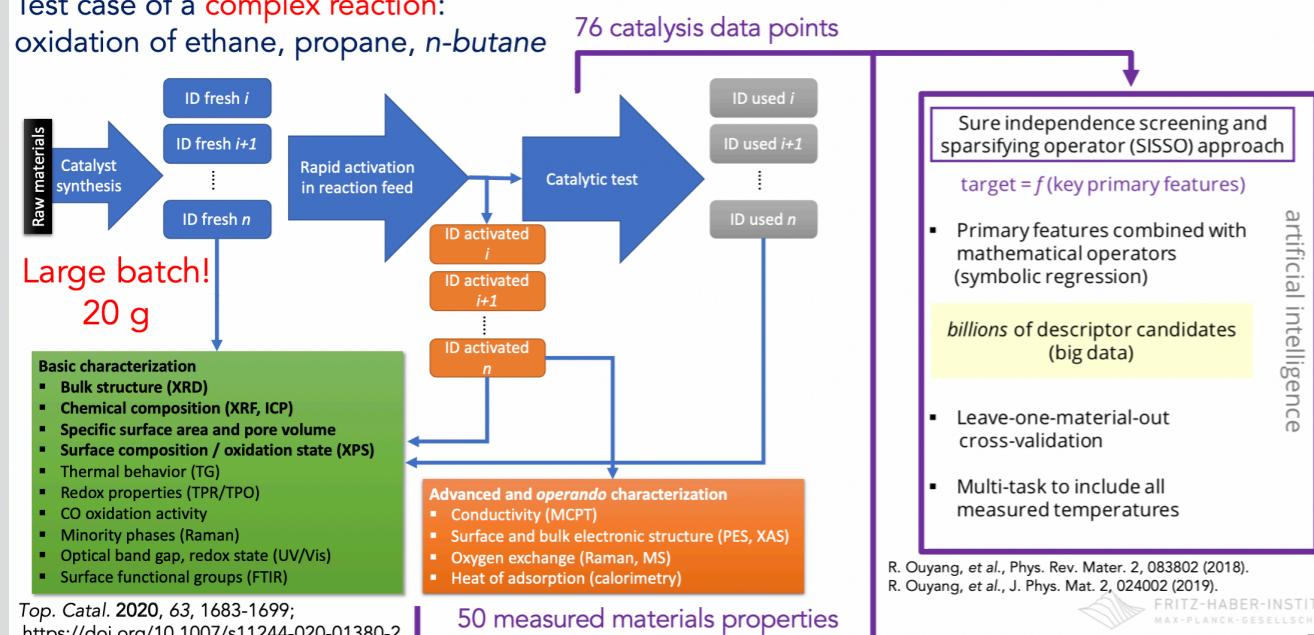


CECS (for our chemists)

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We need firmly agreed experimental workflows: Handbooks

Test case of a **complex reaction**:
oxidation of ethane, propane, n-butane

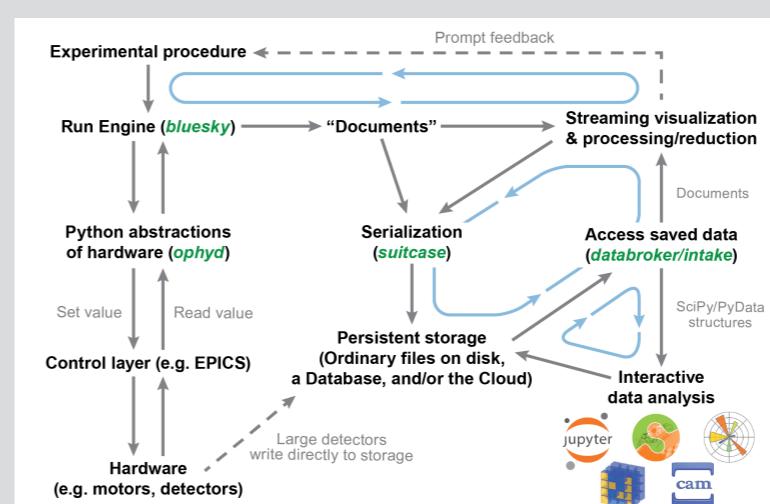


Top. Catal. 2020, 63, 1683-1699;
<https://doi.org/10.1007/s11244-020-01380-2>.

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 "header": {
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generates

input



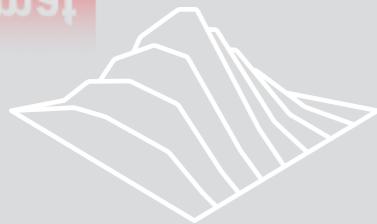


Development

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Thanks to
Abdulrhman Moshantaf (CatLab)

Thanks to
Johannes Lehmeyer
Alexander Fuchs (FAU)



Support

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Thanks to Sven/PP&B for the film studio and the support there.

