

Electronic Lab Documentation at HZDR

From Small Experiments to Large-Scale Research Facilities

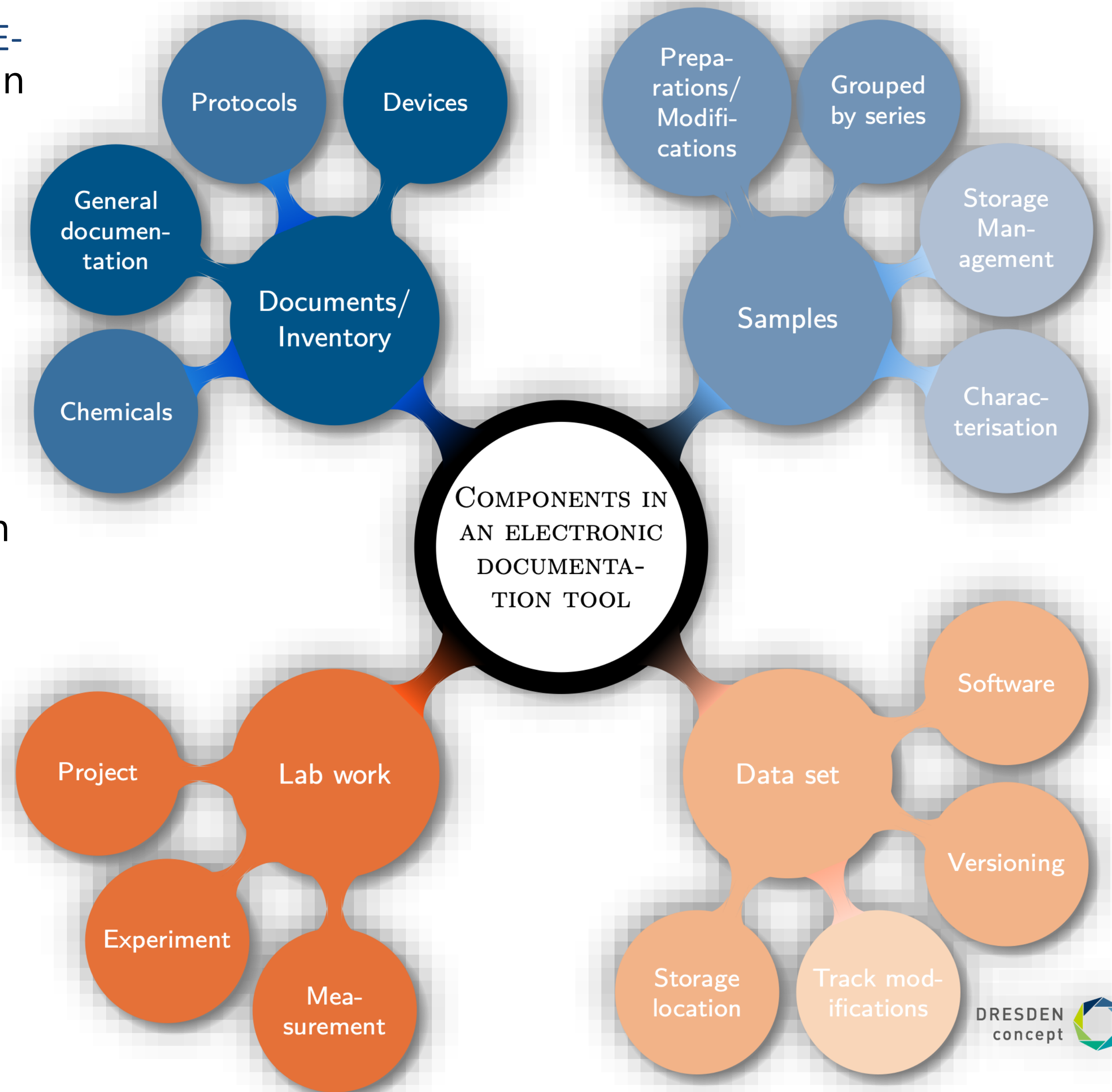
Workshop on FDM in Core Facilities, B CUBE, 6. November 2023

Thomas Gruber, Oliver Knodel, Stefan E. Müller and Guido Juckeland // contact: t.gruber@hzdr.de



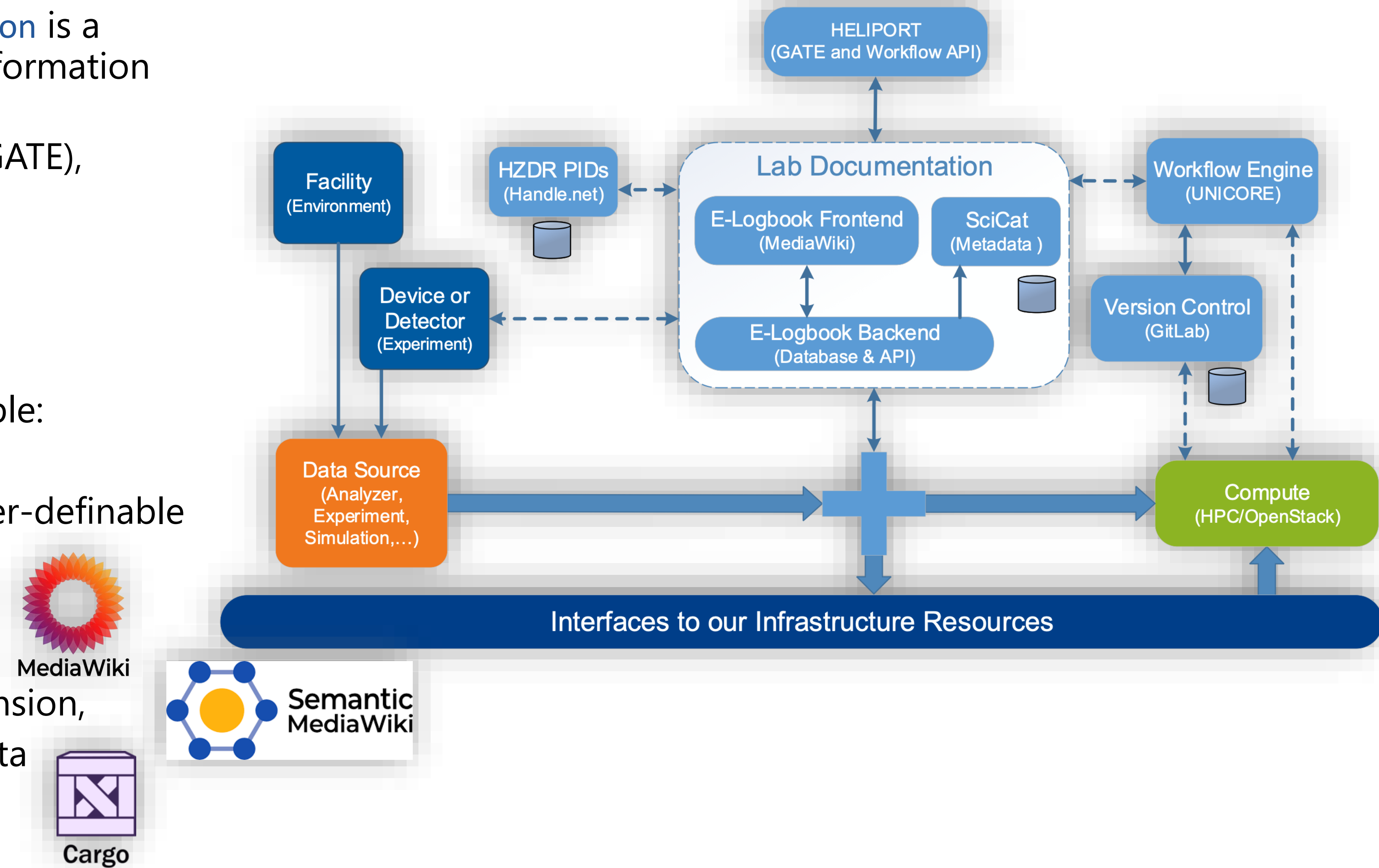
Documentation in our E-Labbook

- The Electronic Lab Documentation (E-Labbook) is an essential component in the experiments lifecycle.
- Metadata from an experiment is generated or stored in different third-party systems or services.
- Various third-party systems can provide additional (meta) data.
- First steps in creating an E-Labbook:
 - Identify essential elements,
 - Define properties describes each element,
 - Access (meta)data in other systems,
 - Define relationships.



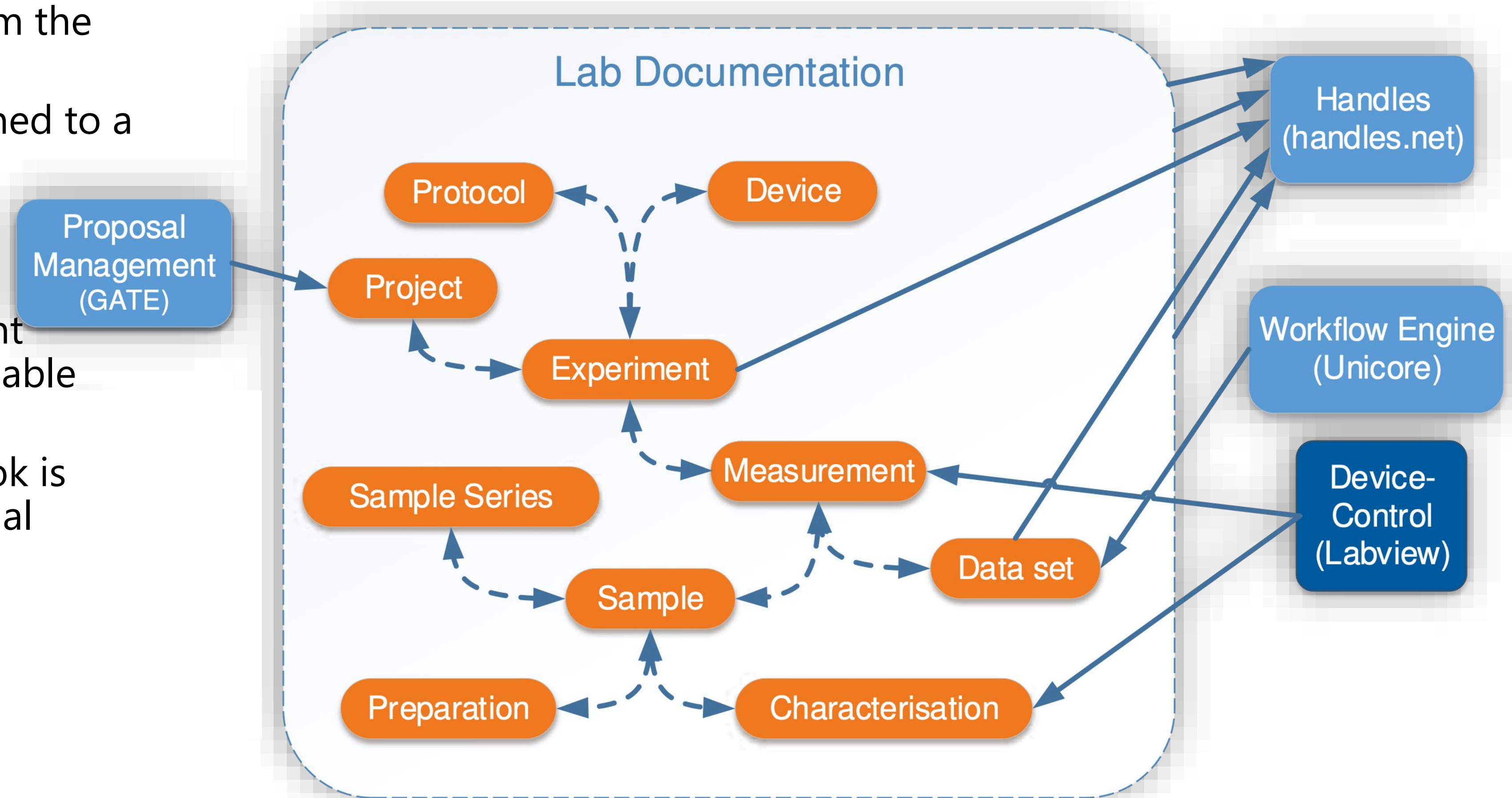
Surrounding Documentation Ecosystem at HZDR

- Our **Electronic Lab Documentation** is a central database gathering information from various systems:
 - Proposal management (GATE),
 - Environmental data,
 - Devices (e.g. Labview),
 - Workflows,
 - (Meta)data databases.
- Different frontends are available:
 - SciCat (metadata only),
 - MediaWiki (structured user-definable views).
- The backend is based on:
 - Mediawiki,
 - Semantic MediaWiki extension,
 - Cargo tables for (meta)data and API requests.



Example of an E-Labbook Structure

- For a well structured (E-Labbook), experience and feedback from the community is required.
- Every lab book page is assigned to a category ([template](#)).
- An optimal structure allows:
 - Collaborative work,
 - Information from different sources and reusing available data,
 - Search within the Labbook is also possible from external applications (e.g. Jupyter notebooks).

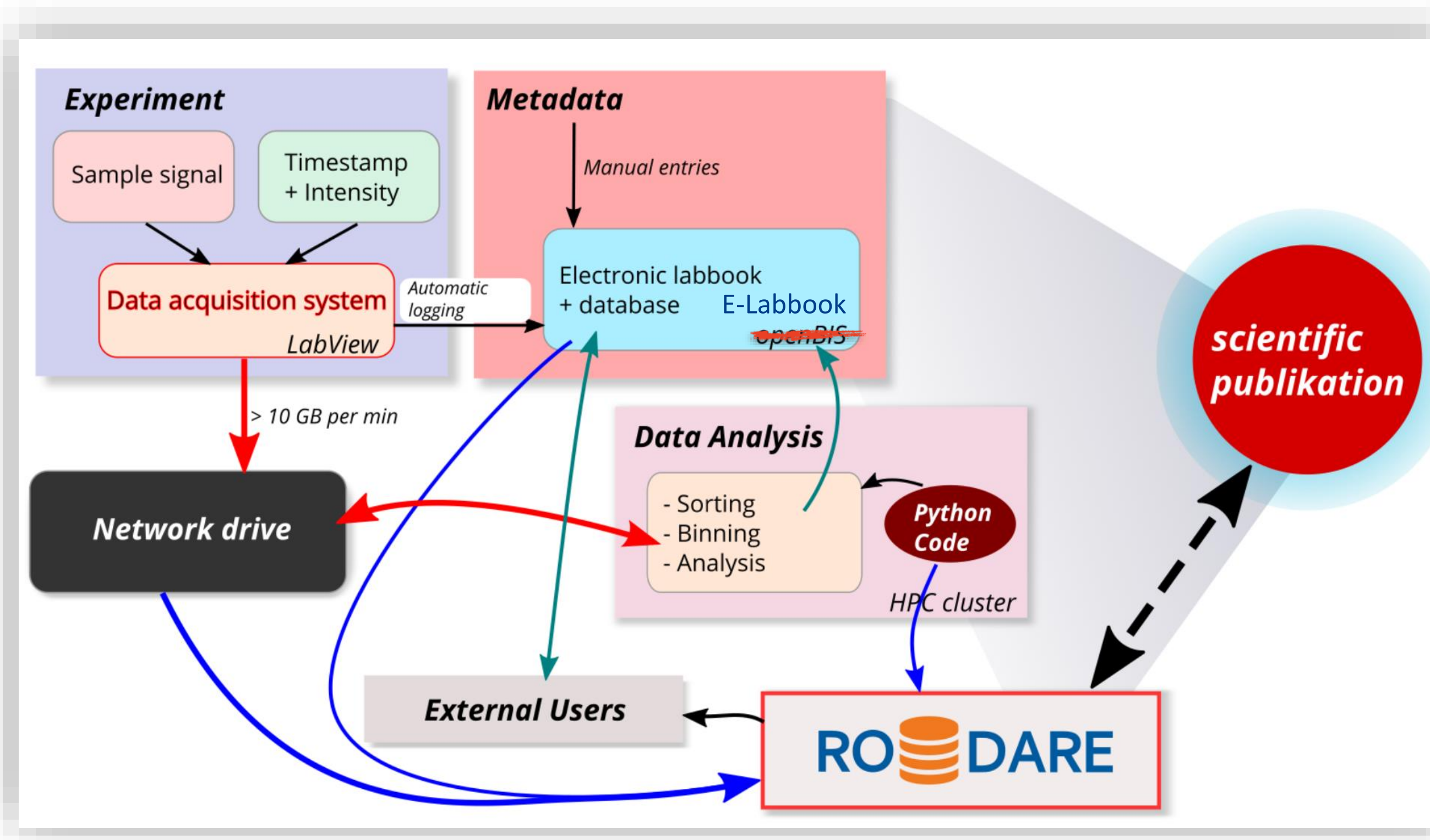




Example: Terahertz facility at the ELBE center for High-Power Radiation Sources

Data Management View of the TELBE Experiment

- Terahertz facility with a sophisticated data management process.
- The data acquisition system (LabView) transfers metadata to the E-Labbook API and starts an analysis job on the HPC Cluster.
- Once the job has been completed the results (metadata and images) are stored in the E-Labbook.



Overview Page of The TELBE Group

- The entry point provides an structured view on all resources such as:
- Projects,
 - Beamtime,
 - Sample,
 - Detectors and additional devices

Special page

Create FWKP:Sample

* Marks mandatory fields

SampleName*:

ProposalNumber:

SampleType*:

SampleOrigin*:

DetailedDescription:

Save page Show preview Show changes Cancel

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FWKP Discussion Read Edit Edit source View history More Search Test-Wiki

FWKP:Main Page

See: https://athene.fz-rossendorf.de/fwk/FWKP:Main_Page

FWKP:Projects

Create new FWKP Project

Recent Projects:

Beamtime Name	Department	Principle Investigator	Start	End
Graphene TPOP	FWKP	Arshad, Atiqa	1 November 2023	
Time-Resolved Dynamics of the Protein Hydration Shell	FWKP	Ilyakov, Dr. Igor	14 September 2023 16:00:00	18 September 2023 04:00:00
Competing or co-operative interaction between superconductivity and charge order: electron-doped cuprate versus hole-doped cuprate	FWKP	Hao Chu	17 March 2023	21 March 2023
Probing the Free Energy Landscape of Multiferroic NiI2 with Strong Field THz Driving	FWKP	Deinert, Dr. Jan-Christoph	9 March 2023	
Transient Weyl states in Dirac semimetal Cd3As2	FWKP	Germanskiy, Semen	12 March 2022	14 March 2022
... further results				

Deprecated ELN Projects:

Beamtime Name	Department	Principle Investigator	Date
TestProject	FWKP	Böse	24 August 2022
THz-induced structural phase transition in hybrid perovskites	FWKP	Kovalev, Dr. Sergey	10 March 2022 08:55:54
THz-light driven spin-lattice coupling under high static magnetic fields	FWKP		10 February 2022 05:54:35


FWKP:Sample DB

Create new Sample → New Sample

Recent Samples:

Sample Name	Proposal Number	Sample Origin
Cuprate Superconductor 001	18101124	Via Stefan Kaiser
Cuprate Superconductor 002	18101124	Via Stefan Kaiser

Measurement Contains Summary and Metadata



HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

Main page

ELN (public)

How To

Recent changes

Random page

Help about MediaWiki

FWCC group

FWC

FWCA

FWCB

FWCC

FWCI

FWCS

Tools

What links here

Related changes

Upload file

Special pages

Printable version

Permanent link

Page information

Browse properties

Cite this page

Page values

FWKP

Discussion

Read

Edit

Edit with form

Edit source

View history

☆

More ▾

Search Test-Wiki

Q

FWKP:Measurement Day March 13 2022

Back to FWKP:Main Page

Logs

[edit source]

> Add log

Measurement Day March 13 2022

Measurement Day Name

Measurement Day March 13 2022

Belongs to Project Name

Transient Weyl states in Dirac semimetal Cd3As2

Belongs to Proposal Number

21202633

Participants

User:

Measurement Day

2022/03/13

Frequency THz

0.7 THz, 2 THz

Log Name	Start Date	End Date	Sample Name	Frequency THz	Sample Temperature	BDA Power	Polarizer Angle
20 DAQ CdAs 120degs WP 40degs SHG V polar 01	31 May 2023 14:44:29	31 May 2023 14:45:22	GFP	2 THz	23.2 K	45 mW	10 °
22 DAQ CdAs 120degs WP 45degs SHG V polar 01	13 March 2022 00:00:00						
23 DAQ CdAs 120degs WP 35degs SHG V polar	17 May 2023 18:01:02	17 May 2023 18:01:10	GFP	0.7 THz		113 mW	
23 DAQ CdAs 120degs WP 35degs SHG V polar 01	13 March 2022 00:00:00						
24 DAQ CdAs 120degs WP 30degs SHG V polar 01	23 May 2023 15:15:30	23 May 2023 15:16:10	TestSample	0.7 THz	2 K	1 mW	
24 DAQ CdAs 120degs WP 30degs SHG V polar 02	23 May 2023 16:11:24	23 May 2023 16:12:07	TestSample	0.7 THz	2 K	1.01 mW	

Description

[edit | edit source]

Category: FWKP:MeasurementDay

This page was last edited on 10 August 2023, at 09:52.

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Semantic MediaWiki



Typical Labbook Entry of a Single Run at TELBE



HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

Main page

ELN (public)

How To

Recent changes

Random page

Help about MediaWiki

FWCC group

FWC

FWCA

FWCB

FWCC

FWCI

FWCS

Tools

What links here

Related changes

Upload file

Special pages

Printable version

Permanent link

Page information

Browse properties

Cite this page

Page values

FWKP

Discussion

Read

Edit

Edit with form

Edit source

View history

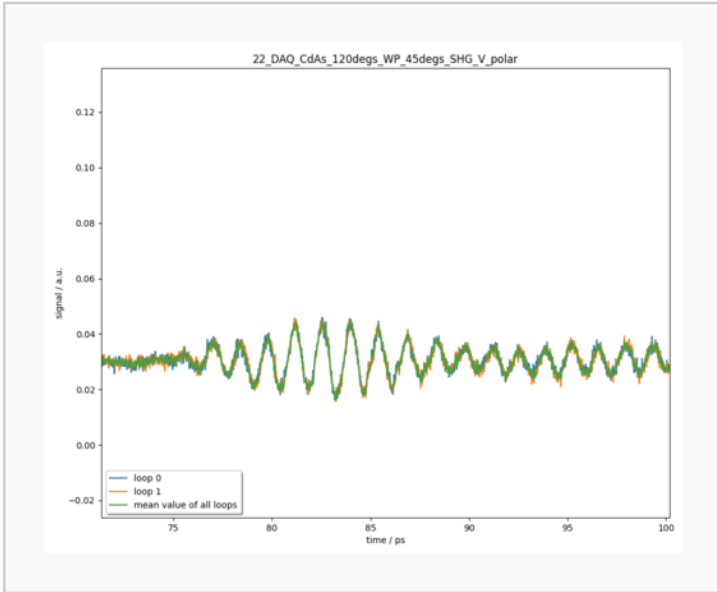
More

Search Test-Wiki

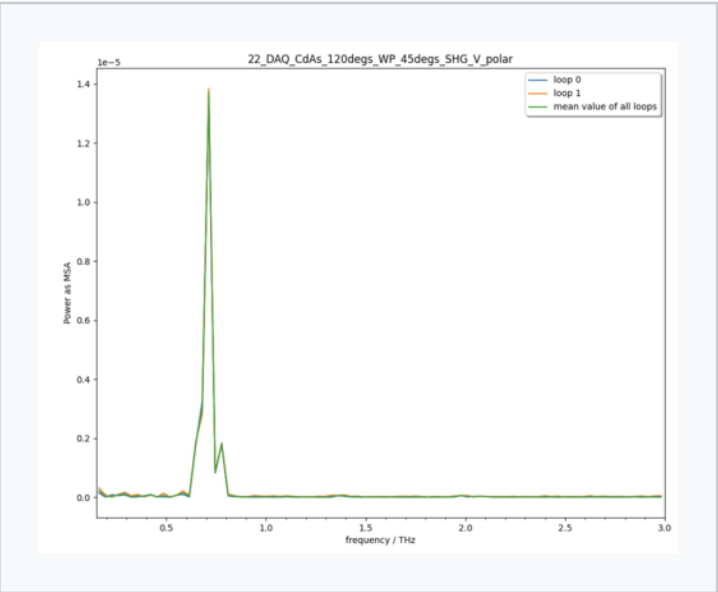
FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar 01

Back to [FWKP:Main Page](#)


Dataset [\[edit \]](#) [\[edit source \]](#)



FWKP:direct plot of 22 DAQ CdAs 120degs WP 45degs SHG V polar



FWKP:fft power linscale plot of 22 DAQ CdAs 120degs WP 45degs SHG V polar



FWKP:fft power logscale plot of 22 DAQ CdAs 120degs WP 45degs SHG V polar

Data Files	File:FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar all loops.dat
Workflowhub URL	https://workflowhub.eu/workflows/459/ro crate?version=1
Workflowhub Version	1
Repetition Rate	50000 Hz
time on single step measurement	1
points measured by ADC	192
CDD ADC Offset	-1
Pixel to ps Conversion	0.0042
Stage position at Start	50 mm

Category: FWKP:Log

22 DAQ CdAs 120degs WP 45degs SHG V polar 01

Log Name

22_DAQ_CdAs_120degs_WP_45degs_SHG_V_polar

Start Date

2022/03/13 00:00:00

Belongs to

Measurement [Measurement Day March 13 2022](#)

Day Name

BDA Power

mW

Frequency

THz

Polarizer

°

Angle

Filter Used

No

Al2 Three

No

Switch

Pyro Channel

No

Stage1 Start

mm

Pos

Stage1 Step

mm

Size

Path binned

/bigdata/telbe/Sorted_data/2022/2022-March_datasorting/2022-03-13/binned

file

Scicat Export

No



Individual Configuration and Customisation

wiki-dev.fz-rossendorf.de/wiki/FWIN:Main_Page

HZDR
HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

FWIN

Discussion

Read

Edit

Edit source

FWIN:Main Page

FMR TEAM

FWIN:ElectronicLabNotebook and LIMS (Trial version)

Workflow: Register a project → register new sample series → enter new sample (→ create measurement - automatically c

Search

Enter values below; this search is case-sensitive.

SampleID contains:

Sample Series ID contains:

Project ID contains:

Operator contains:

Owner contains:

Measurement Name contains:

Search

Sample Database

→ Register a new sample

→ Register a new sample series

→ List of unknown sample IDs

→ List of unknown sample series

Recent Samples:

Entry Date ↕	Sample ID
Sample-00004	2021-2
2022/08/26 09:30:00	RM-SensorStack14-A1 JexMultiturnSensorStack Multilayer
2022/08/26 09:29:00	RM-SensorStack13-A1 JexMultiturnSensorStack Multilayer
2022/08/26 08:33:00	RM-SensorStackWafer-slot4 JexMultiturnSensorStack Multilayer
... further results	

Recent Projects:

Entry Date ↕	Project ID ↕	Number ↕	Type ↕	Entry Date ↕	PI ↕	Funding Agency ↕
2022/04/25 11:36:18	CoFeB-Toni	n .a.	In-house Research	25 April 2022 11:36:18		in-house Project
2022/04/25 11:33:56	CoFe	n.a	In-house Research	25 April 2022 11:33:56		in-house Project
2022/04/25 11:32:48	Tilted Stripe Domain-Peter	n.a	In-house Research	25 April 2022 11:32:48		in-house Project
2022/04/21 13:36:15	Microresonators	n.a.	In-house Research	21 April 2022 13:36:15		in-house Project

wiki-dev.fz-rossendorf.de/wiki/FWIN-Recipe_of_Sample_MBEoo48AH

KnodeI39

Talk

Preferences

Watchlist

Contributions

Log out

Page Discussion Read Edit Edit source View history More Search Test-Wiki

FWIN-Recipe of Sample MBEoo48AH

Sonic Bath	Creation Date	Solvent
	2022/04/26 15:50:57	Aceton

Sonic Bath	Creation Date	Solvent
	2022/04/26 15:50:57	Aceton

Sonic Bath	Creation Date	Solvent
	2022/04/26 15:50:57	Isopropanol

Drying	Creation Date	Gas	Note
	2022/04/26 15:50:57	Nitrogen	isopropanol blown away with nitrogen

Annealing	Creation Date	Temperature	Heating rate	Cooling rate	Note
	2022/04/26 15:50:57	423.15 K	5 K/min	10 K/min	silver paste degas in UHV-Furnace

Annealing	Creation Date	Temperature	Heating rate	Cooling rate	Note
	2022/04/28 15:50:57	100 °C	5 K/min	10 K/min	heated in ALDI-MBE LoadLock

API Interface

```
▼ cargoquery:
  ▼ 0:
    ▼ title:
      LINK: "FWG:HIF.SampleProject.231005-1-01"
      SampleProject Name: "Example Sample Project"
      Department: "FWGB-A"
      Creation date: "2023-10-05"
      Creation date__precision: "1"
    ▼ 1:
      ▼ title:
        LINK: "FWG:Test test test-01"
        SampleProject Name: "test test test"
        Department: "FWCC"
        Creation date: "2023-10-05"
        Creation date__precision: "1"
    ▼ 2:
      ▼ title:
        LINK: "FWG:Test project name-01"
        SampleProject Name: "test project name"
        Department: null
        Creation date: "2023-10-05"
        Creation date__precision: "1"
    ▼ 3:
      ▼ title:
        LINK: "FWG:Test1-01"
        SampleProject Name: "test1"
        Department: null
        Creation date: "2023-10-06"
        Creation date__precision: "1"
    ▼ 4:
      ▼ title:
        LINK: "FWG:SampleProject.20231117-02"
```

MediaWiki API help

This is an auto-generated MediaWiki API documentation page.

Documentation and examples: https://www.mediawiki.org/wiki/Special:MyLanguage/API:Main_page

action=cargoquery

([main](#) | **cargoquery**)

Runs a query on the Cargo data.

Parameters:

limit:	A limit on the number of results returned
	Type: integer or max
	The value must be between 1 and 5,000.
	Default: 50
tables:	The Cargo database table or tables on which to search
fields:	The table field(s) to retrieve
where:	The conditions for the query, corresponding to an SQL WHERE clause
join_on:	Conditions for joining multiple tables, corresponding to an SQL JOIN ON clause
group_by:	Field(s) on which to group results, corresponding to an SQL GROUP BY clause
having:	Conditions for grouped values, corresponding to an SQL HAVING clause
order_by:	The order of results, corresponding to an SQL ORDER BY clause
offset:	The query offset
	Type: integer
	The value must be no less than 0.
	Default: 0

- This module requires read rights.
- Source: Cargo
- License: [GPL-2.0-or-later](#)