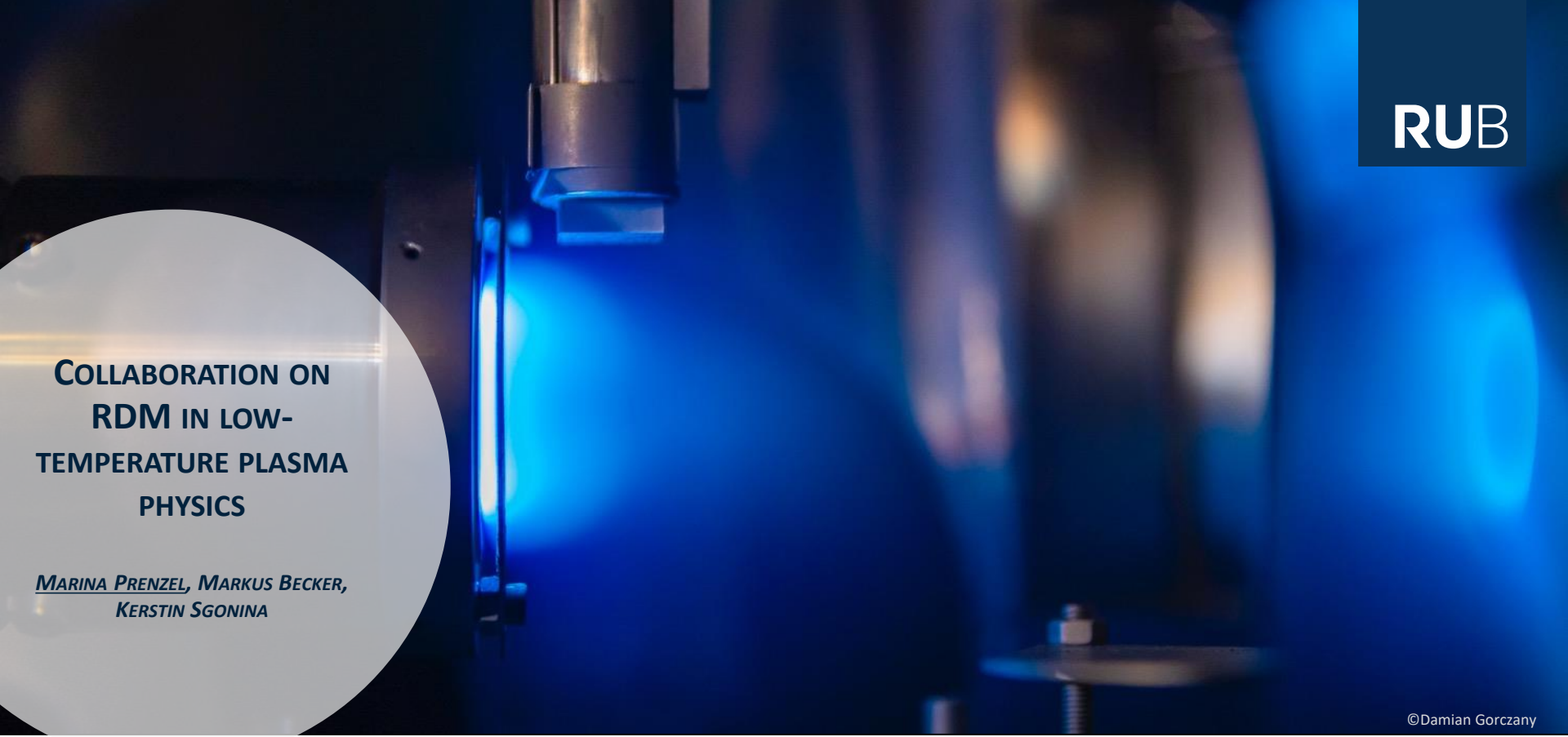


Collaboration on RDM in low-temperature plasma physics

Marina Prenzel, Markus Becker, Kerstin Sgonina

INP

C|A|U Christian-Albrechts-Universität zu Kiel

RUHR UNIVERSITÄT BOCHUM

RUB

LAB SITUATION IN SCIENCE I

Hello, I am the next PhD student in the project. Could you please forward your previous data to me?

Hello, nice to meet you. Sure, please log in to our central repository. There you will find all measurement data according to our metadata standards from my scientific work.

LAB SITUATION IN SCIENCE II

Hello, I am the next PhD student in the project. Could you please forward your previous data to me?

Hello, nice to meet you. I'm very sorry. The lab was flooded by cooling water, so my lab book was destroyed. But yes, the data I collected is on these 10 different CDs. So, help yourself.

RECIPE FOR FAIR DATA

RECIPE FOR FAIR DATA

Is there any recipe to achieve FAIR data?

Unfortunately, there is no single recipe for this. But I'm happy to show you what it's all about and what activities are available so far.

FAIR DATA

Metadata and data should be easily **findable** for both humans and computers.

Data need to be **interoperable** with other data, software or workflows for further processing.

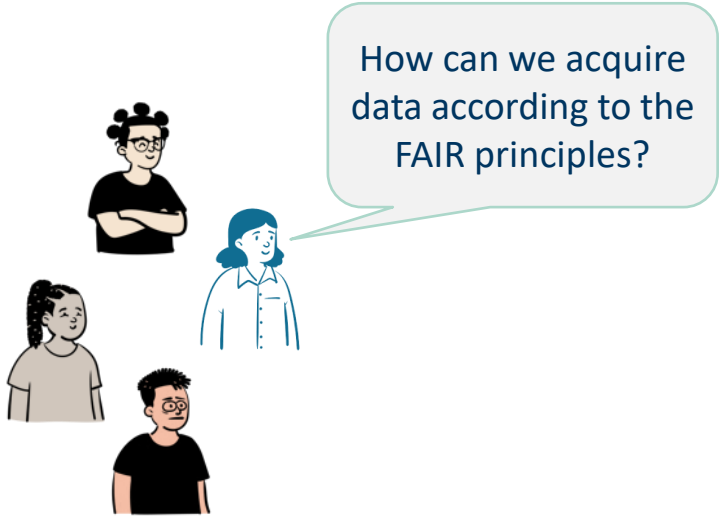
Data must be **accessible**, i.e. users need to know how they can be retrieved.

Metadata and data should be well described so that they are **re-usable** within their scope.

DATA LIFE CYCLE

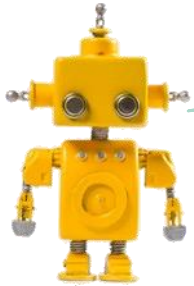
- Six steps define the data life cycle
- Process Scientific data should be handled according to the FAIR principle
- Various aspects of processing are required to find solutions
- Common challenges in the research groups

DATA ACQUISITION



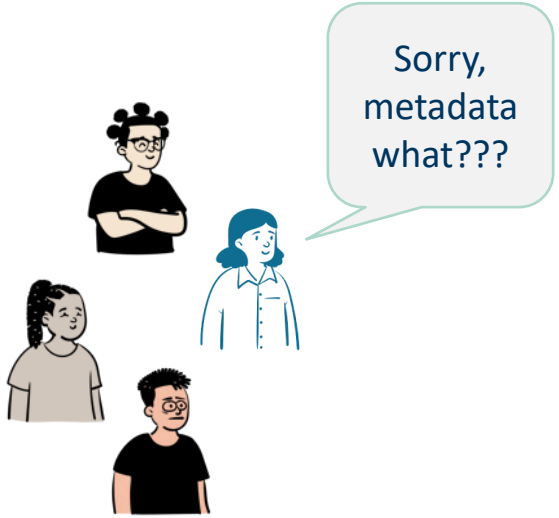
DATA ACQUISITION

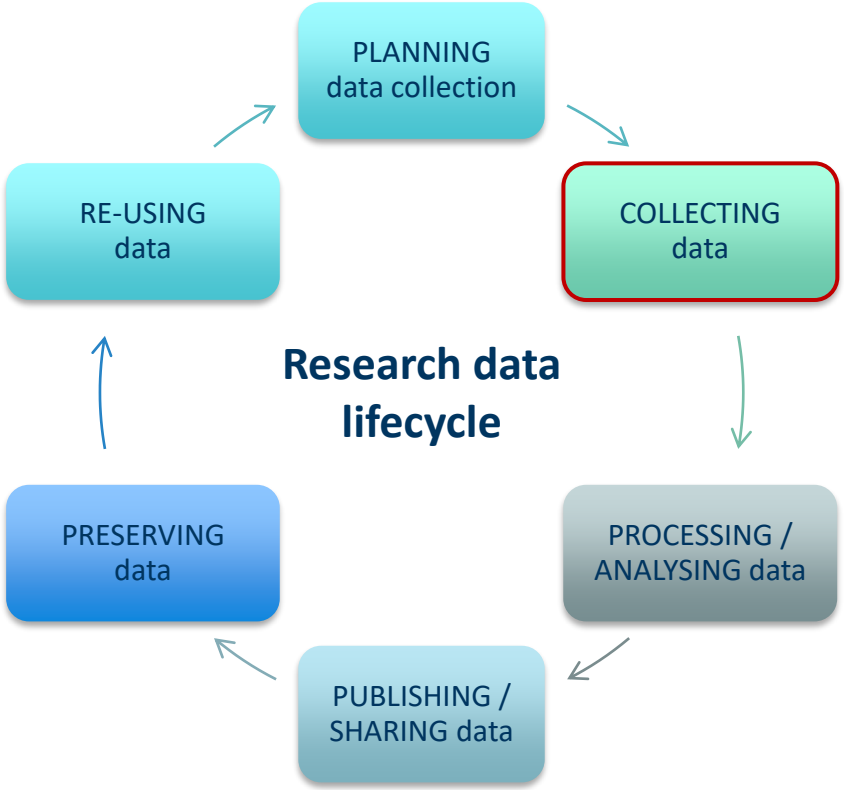
How can we acquire data according to the FAIR principles?



Using an electronic lab book with uniform metadata schemas is the common way.

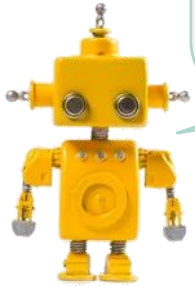
DATA ACQUISITION





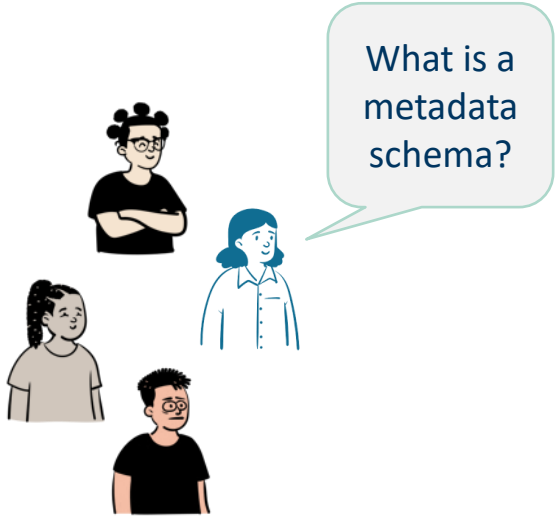
DATA ACQUISITION

Sorry, metadata what???

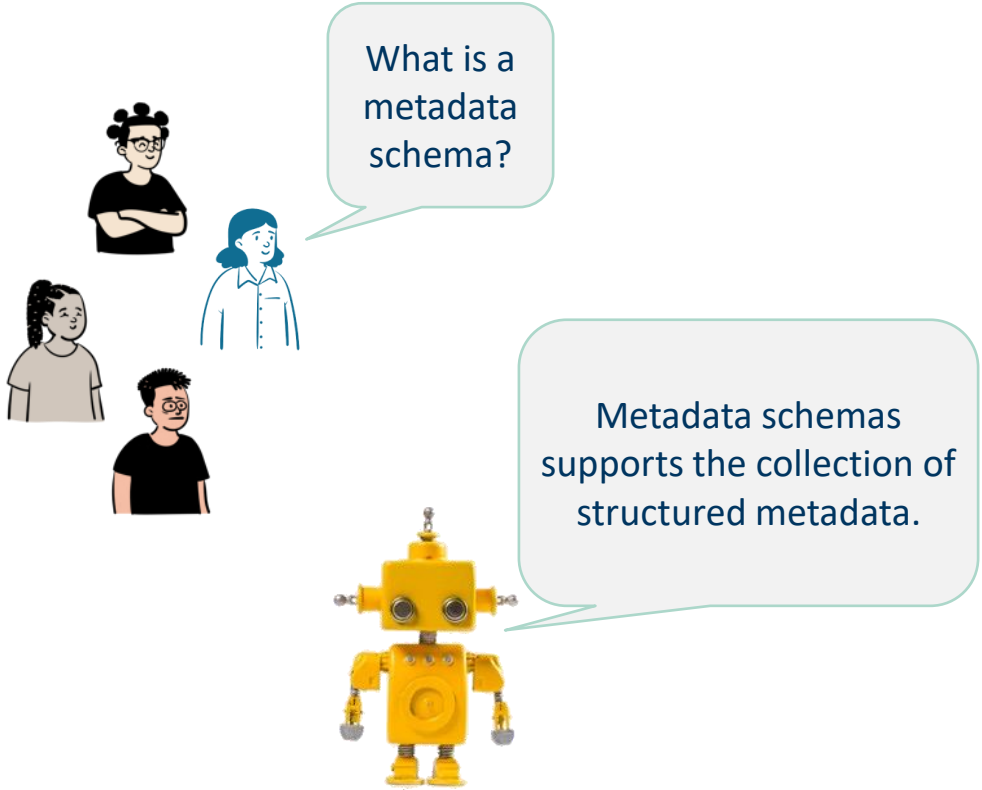


Metadata are structured information that describe, explain, locate and thus make it easier to retrieve, use or manage an information resource.

DATA ACQUISITION

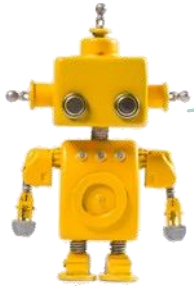


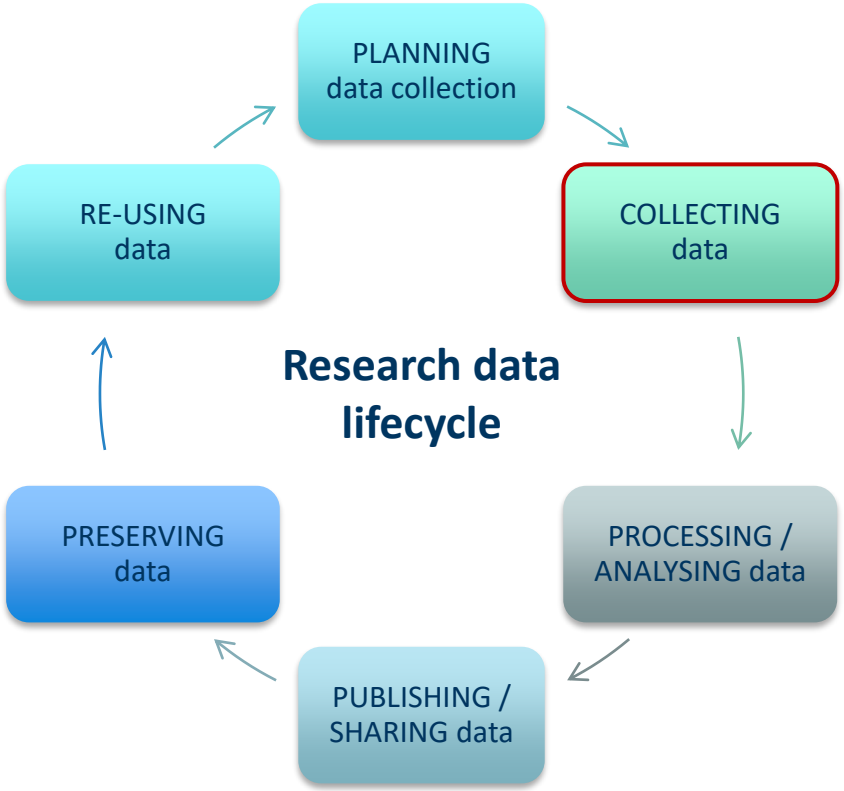
DATA ACQUISITION



DATA ACQUISITION

DATA ACQUISITION



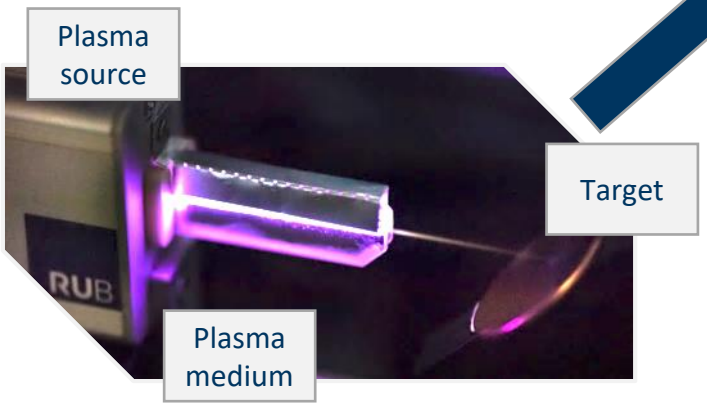


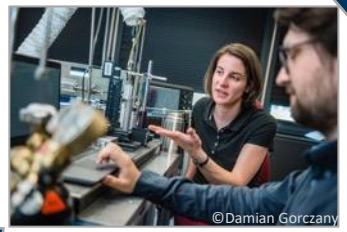
METADATA STANDARDS

Example dinosaur game

- The dinosaurs are compared with each other
- Comparison needs to be defined by a defined description of the length, weight....

METADATA SCHEMA DEVELOPMENT INP, CAU, RUB





every 3rd Friday in month

Plasma source

description of name and/or type of the plasma source including application the plasma source is applied for

Plasma medium

medium name the plasma source is operated in or acting on and properties of the medium the plasma source is operated in or acting on

Target

name of the target the plasma source is acting on, either directly or mediated by a medium and properties of the target the plasma source is acting on

METADATA SCHEMAS IN PLASMA SCIENCE

Example for metadata of APPJ device:

Id	Title	Unit	Description
1	Name		Name of the plasma source device
2	Serial number		Serial number of the plasma source device
3	Commercial product		Is the plasma source commercially available?
4	TRL		Technology Readiness Level (TRL)
5	Developer		Name of the institution / group where the plasma source has been developed
6	Documentation		Publication or other report describing the plasma source
7	Geometry		Description of the electrode configuration
8	Min. power	W	Minimum power dissipated in the plasma

METADATA SCHEMAS IN PLASMA SCIENCE

Example for metadata of APPJ device:

Id	Title	Unit	Description
9	Max. power	W	Maximum power dissipated in the plasma
10	Reflected power	%	Part of the input power which is reflected and not coupled to the electrode
11	Min. voltage (p-p)	V	Minimum peak-to-peak voltage
12	Max. voltage (p-p)	V	Maximum peak-to-peak voltage
13	Min. frequency	Hz	Minimum frequency of the voltage signal
14	Max. frequency	Hz	Maximum frequency of the voltage signal
15	Min. current (p-p)	A	Minimum peak-to-peak current
16	Max. current (p-p)	A	Maximum peak-to-peak current

METADATA STANDARDS IN PLASMA SCIENCE

Github for metadata documentation

- https://github.com/plasma-mds/plasma-metadata-schema

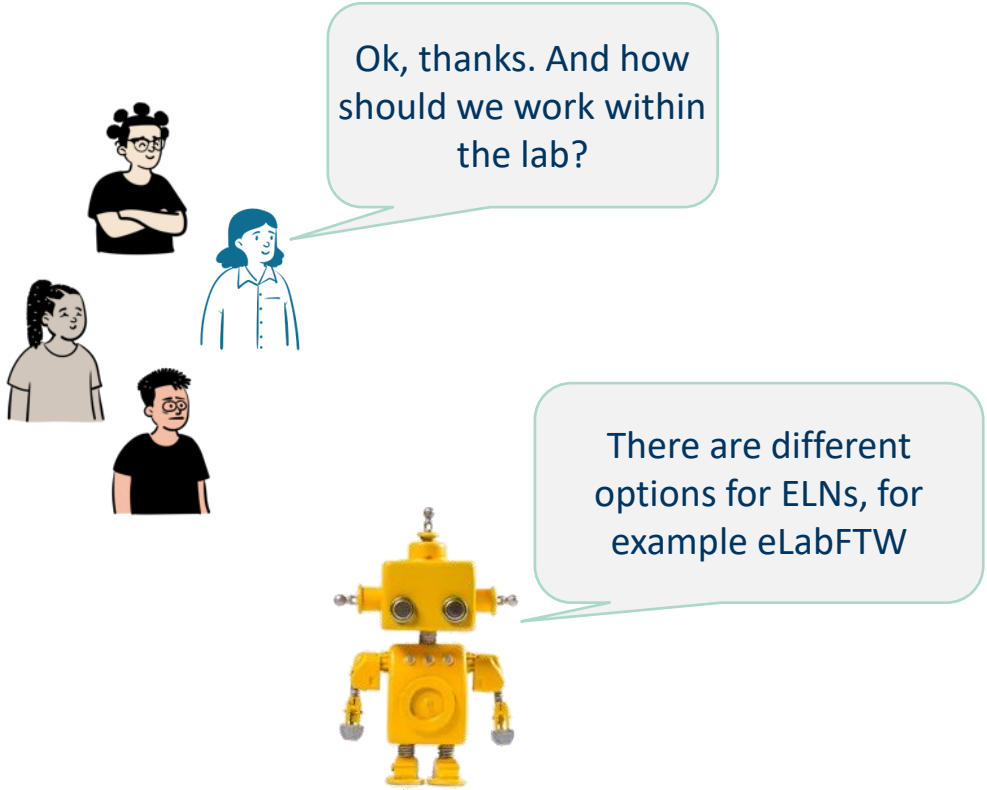
Meetings are announced here

- https://www.plasma-mds.org/ws-metadata.html

We look forward to an exchange and participation from you!

ELECTRONIC LAB NOTEBOOK (ELN)

ELECTRONIC LAB NOTEBOOK (ELN)



ELECTRONIC LAB NOTEBOOK (ELN)

eLabFTW

- Open-source ELN system with increasing popularity at research institutions in Europe
  - In productive use at INP, CAU and RUB
- ➢ Statistics: >150 members >1,000 Experiments
- Next step: Replacement for hand-written lab books or other digital solutions, such as Excel, Word, MS Notes

RESEARCH DATA LIFECYCLE

Measures within RDM adapted to research data lifecycle

- From planning of data collection to re-use of the data
- Storage and processing needs to be supported

XPS METADATA SCHEMA

Measurement data schema available

- Community activity
- Iterations between meetings
- Now in testing phase
- Publication in GitHub

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	name	Name		Name of the XPS device	string	1	
2	sn	Serial number		Serial number of the device	string	0-1	
3	developedBy	Developer		Name of the company	string	1	
4	AngleSourceValue	Angle between source and analyser	°	Angle between source and analyser	number	1	
5	Aperture	Aperture of the device		Aperture of the device	string	1	
6	ReferenceScalePE	Reference scale PE	eV	By giving position and FWHM of a ref material at a reference PE	number	1	
6.1	ReferenceScaleAu	Reference scale Au	eV	By giving position and FWHM of a ref material at a reference Au	number	1	
6.2	ReferenceScaleAg	Reference scale Ag	eV	By giving position and FWHM of a ref material at a reference Ag	number	1	
6.3	ReferenceScaleCu	Reference scale Cu	eV	By giving position and FWHM of a ref material at a reference Cu	number	1	
6.4	ReferenceScaleC	Reference scale C	Ev	By giving position and FWHM of a ref material at a reference C	number	1	
7	Detector	Detector type		Type and name of the detector	string	1	
8	MaintenanceDate	Last maintenance date		The date date of maintenance	string	1	

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6.2	ReferenceScaleAg	Reference sc... Ag			number	1	
6.3	ReferenceScaleCu	Reference scale Cu	eV	By giving position and FWHM of a ref material at a reference Cu	number	1	
6.4	ReferenceScaleC	Reference scale C	Ev	By giving position and FWHM of a ref material at a reference C	number	1	
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Device description

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Device description

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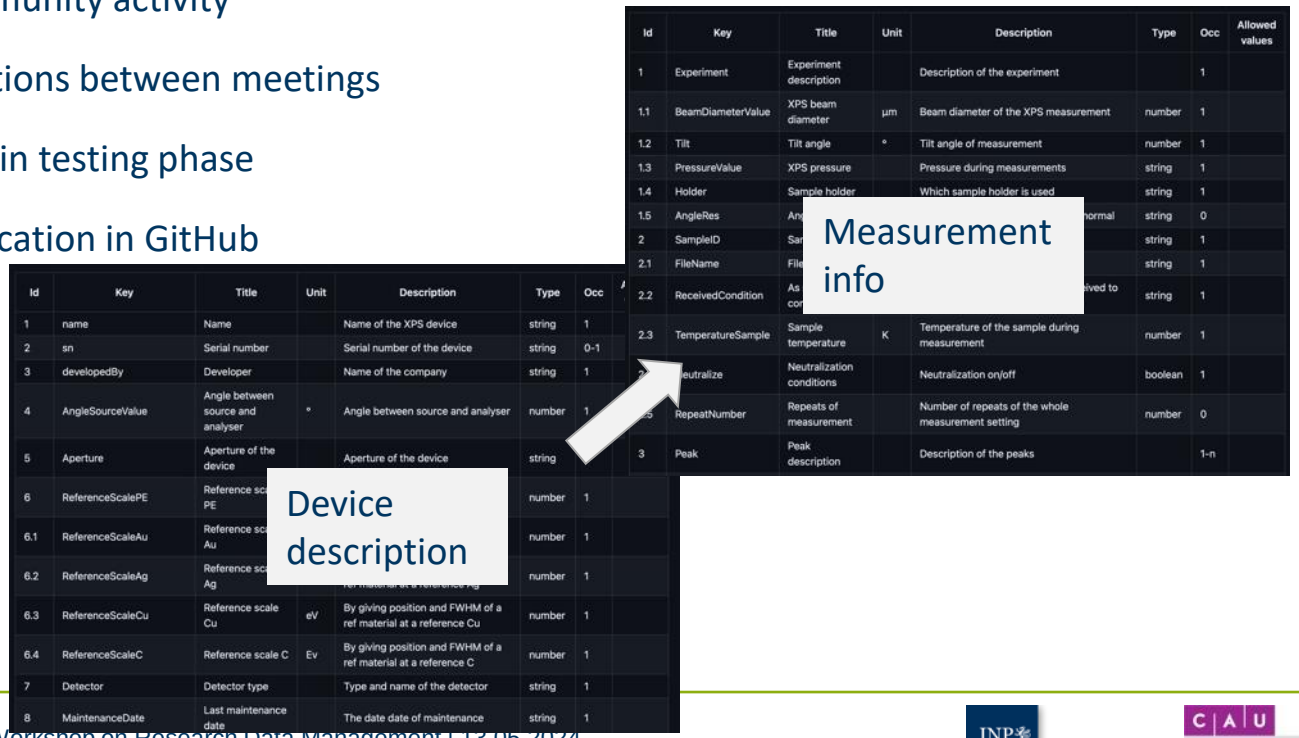

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	Experiment	Experiment description		Description of the experiment		1	
1.1	BeamDiameterValue	XPS beam diameter	µm	Beam diameter of the XPS measurement	number	1	
1.2	Tilt	Tilt angle	°	Tilt angle of measurement	number	1	
1.3	PressureValue	XPS pressure		Pressure during measurements	string	1	
1.4	Holder	Sample holder		Which sample holder is used	string	1	
1.5	AngleRes	An		ormal	string	0	
2	SampleID	Sa			string	1	
2.1	FileName	Fil			string	1	
2.2	ReceivedCondition	As co		ived to	string	1	
2.3	TemperatureSample	Sample temperature	K	Temperature of the sample during measurement	number	1	
		eutralize		Neutralization conditions	Neutralization on/off	boolean	1
		RepeatNumber		Repeats of measurement	Number of repeats of the whole measurement setting	number	0
3	Peak	Peak description		Description of the peaks		1-n	

Measurement info

Id	Key	Title	Unit	Description	Type	Occ
1	name	Name		Name of the XPS device	string	1
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Device description

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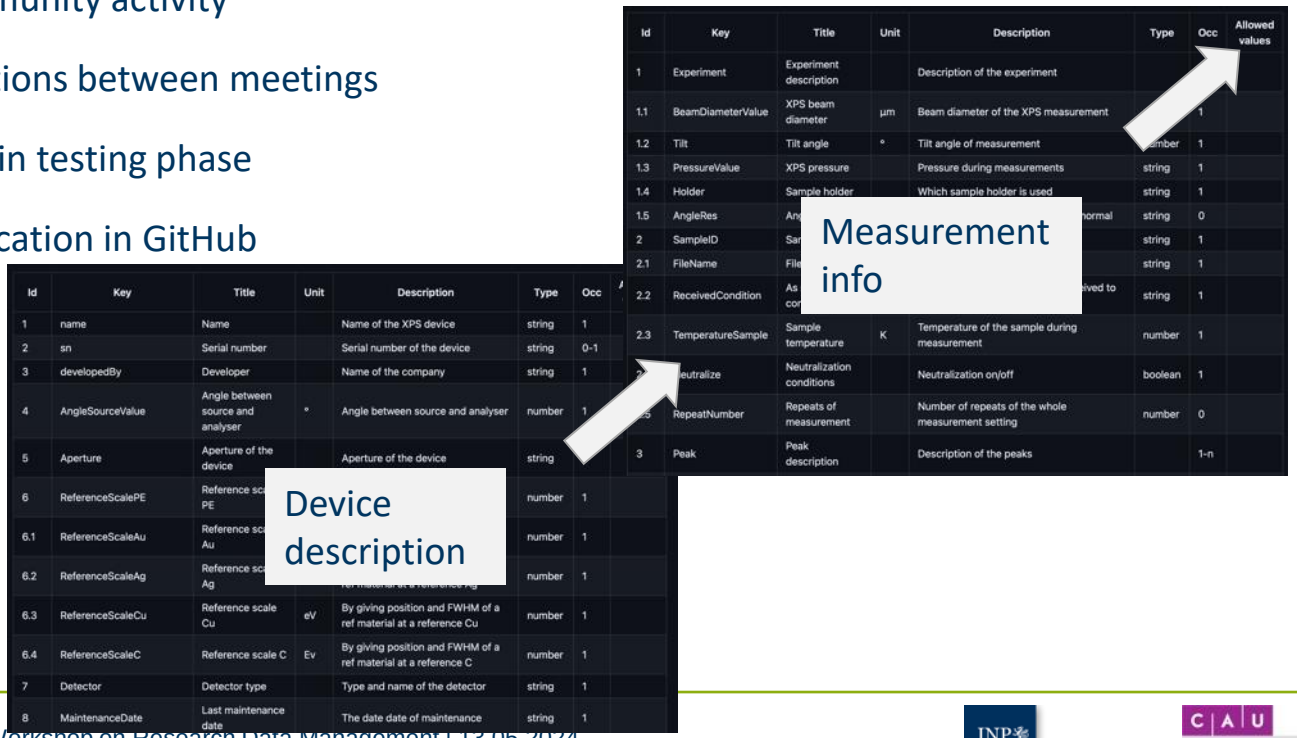

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1.3	PressureValue	XPS pressure		Pressure during measurements	string	1	
1.4	Holder	Sample holder		Which sample holder is used	string	1	
1.5	AngleRes	An		normal	string	0	
2	SampleID	Sa			string	1	
2.1	FileName	Fil			string	1	
2.2	ReceivedCondition	As co		ived to	string	1	
2.3	TemperatureSample	Sample temperature	K	Temperature of the sample during measurement	number	1	
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Device description

XPS METADATA SCHEMA

Measurement data schema available

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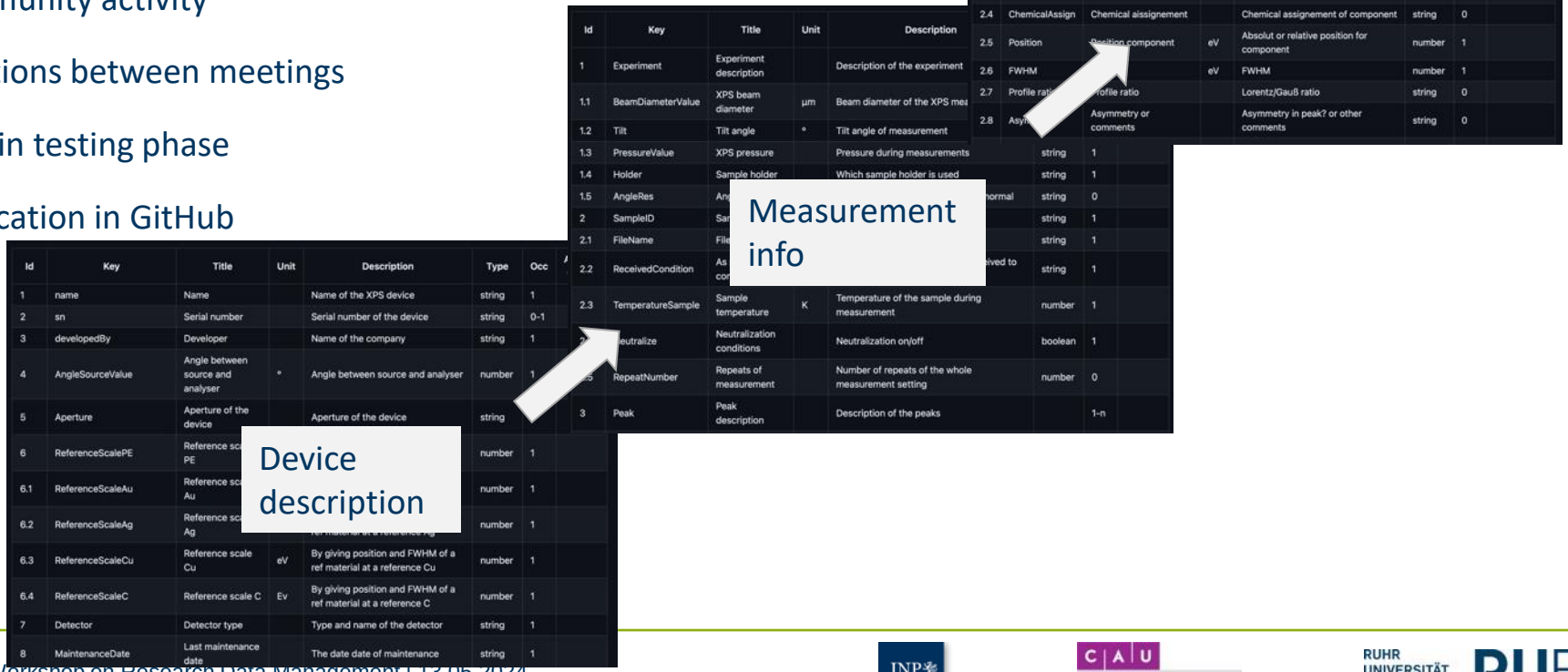

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	General	General information		General information for processing the fit	string	1	
1.1	Normalization	Normalization		Normalization (reference for fit)	string	1	
1.2	IntensityFactor	Intensity factor		Intensity factor (name/storage)	string	1	
1.3	ReferencePaper	Reference paper		Information about the reference	string	0	
2	Component	Analysed com				1-n	
2.1	Background	Background				1	
2.2	Fit type	Fit type				1	singlet; doublet
2.3	Profile	FitProfile		Fit profile	boolean	1	Voigt; Lorentzian
2.4	ChemicalAssign	Chemical aissignement		Chemical assignement of component	string	0	
2.5	Position	Position component	eV	Absolut or relative position for component	number	1	
2.6	FWHM		eV	FWHM	number	1	
2.7	Profile rati	Profile ratio		Lorentz/Gauß ratio	string	0	
2.8	Asy	Asymmetry or comments		Asymmetry in peak? or other comments	string	0	

Id	Key	Title	Unit	Description	Type	Occ
1	Experiment	Experiment description		Description of the experiment		
1.1	BeamDiameterValue	XPS beam diameter	µm	Beam diameter of the XPS mea		
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7	Detector	Detector type		Type and name of the detector	string	1
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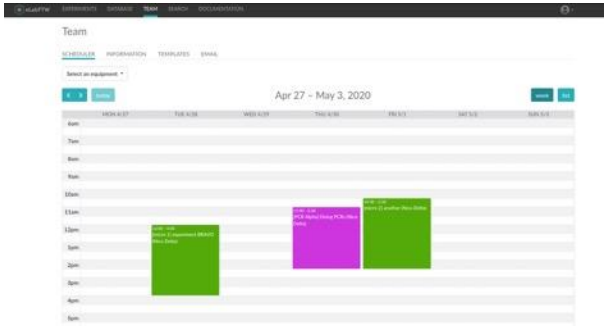
STEP 1 – APPOINTMENT BOOKING

User acquires XPS appointment in eLabFTW calendar

scientist → XPS expert

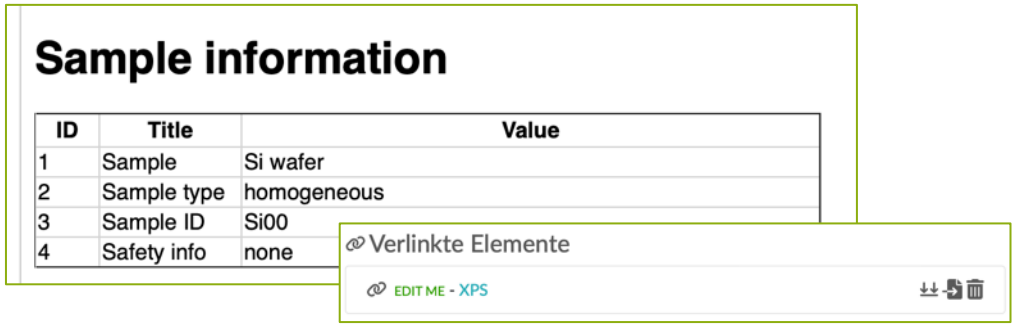


✓ XPS booking within eLabFTW

STEP 2 – XPS SAMPLE TRANSITION

User hands over samples for measurement

scientist → XPS expert



- ✓ XPS booking &
- ✓ device information &
- ✓ sample information
- ➢ directly connected with measurement details

STEP 3 – XPS MEASUREMENT

XPS measurement is done

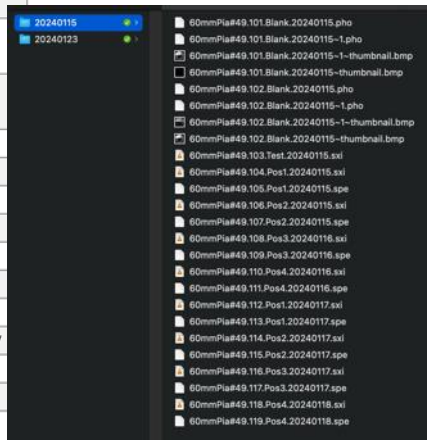
scientist ← XPS expert

✓ XPS acquisition with minimum documentation effort

Measurement details

File name	Pia#49
Position	Pos. 1
Peak name	Surv | O1s| C1s | Si2p
Binding energy	-5/1200 | 523/18 | 273/27 | 90/18
Pass energy	187.85eV | 23.5eV | 23.5eV | 23.5eV
Scan number	1 | 1 | 2 | 3 | 5
Cycles	3

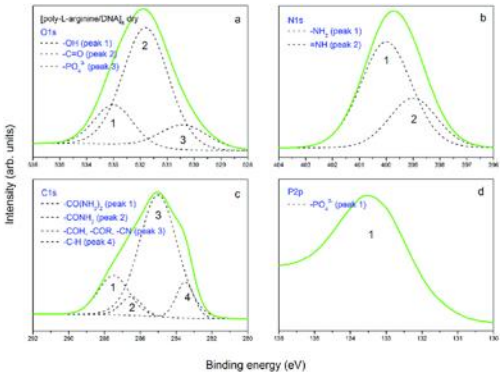
File name	Pia#49
Position	Pos. 2
Peak name	Surv | O1s| C1s
Binding energy	-5/1200 | 523/18
Pass energy	187.85 eV | 23.5 eV | 23.5 eV
Scan number	1 | 1 | 2 | 3
Cycles	3



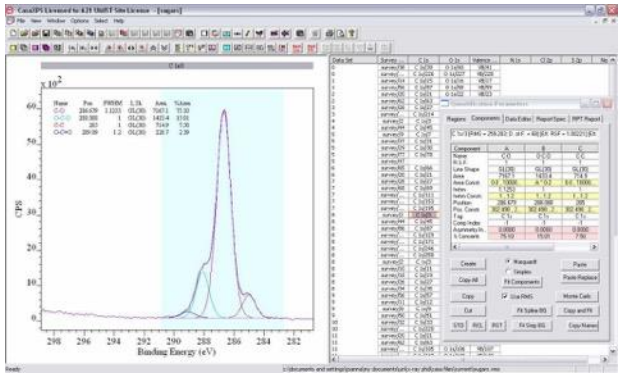
STEP 4 – XPS ANALYSIS

XPS analysis is done

scientist



XPS expert



✓ Publication including all relevant information by extracting eLabFTW information

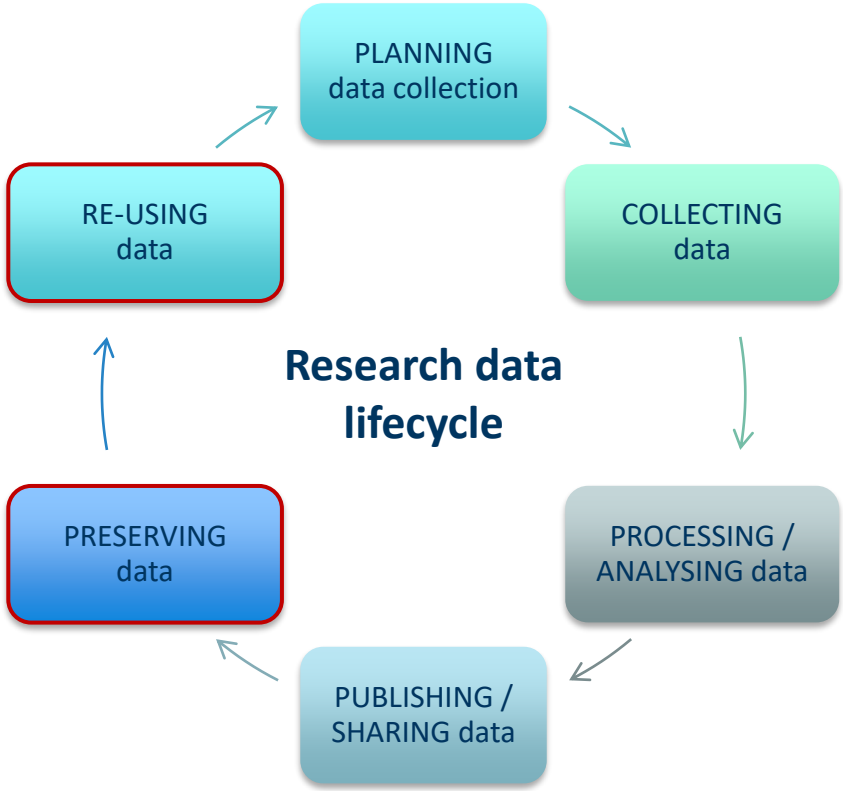
INP

CAU Christian-Albrechts-Universität zu Kiel

RUHR UNIVERSITÄT BOCHUM RUB

RE-USE

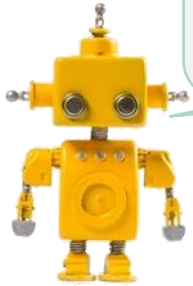

And how can others re-use my scientific data?


PLANNING data collection
COLLECTING data
PROCESSING / ANALYSING data
PUBLISHING / SHARING data
PRESERVING data
RE-USING data
Research data lifecycle

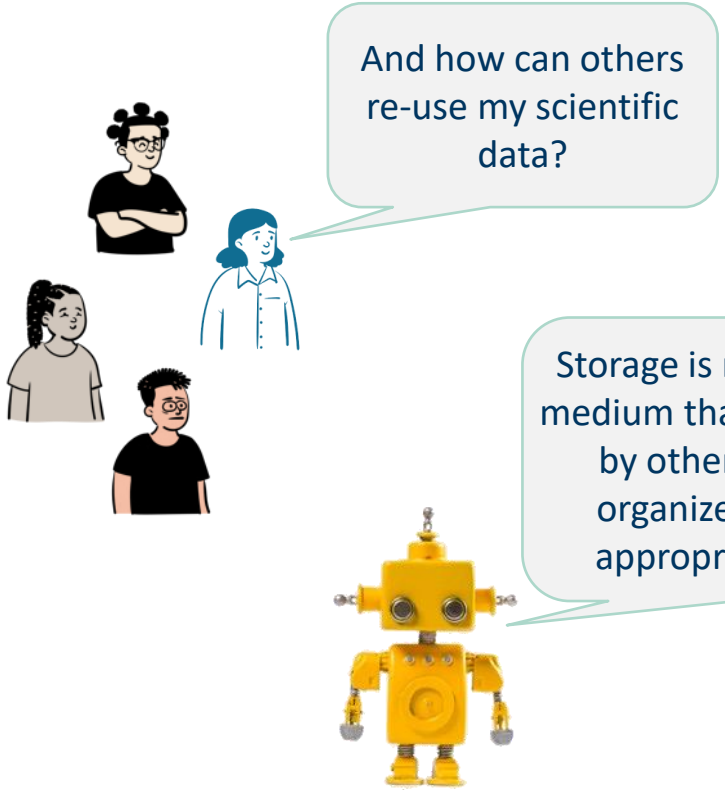
RE-USE

And how can others re-use my scientific data?

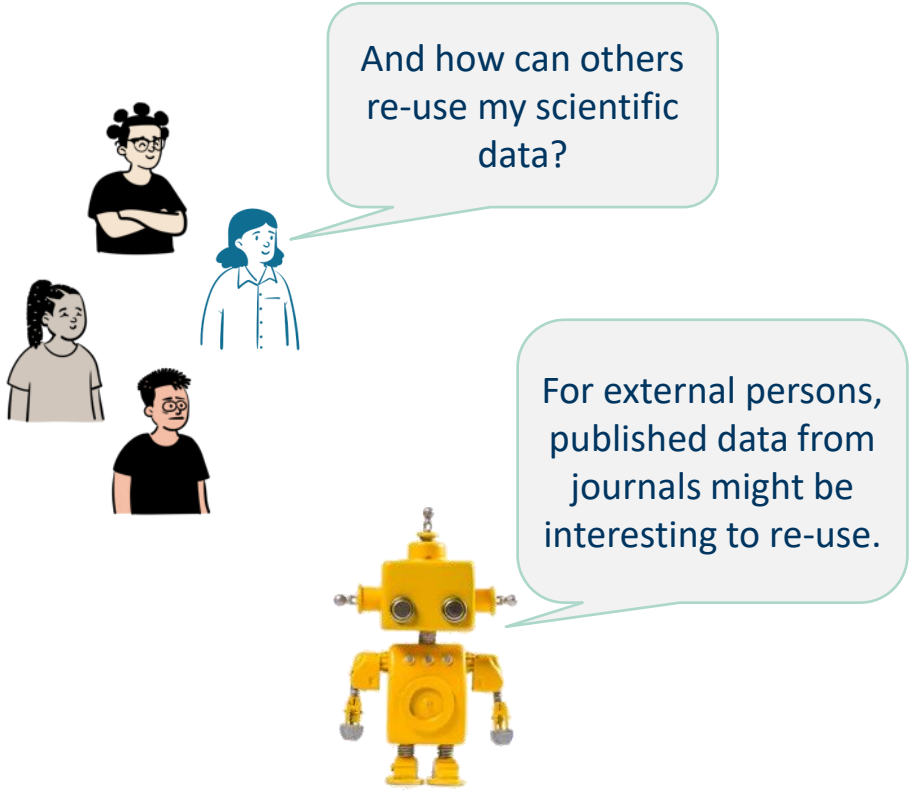
We would like to distinguish between internal and external usage.



RE-USE - STORAGE



RE-USE - REPOSITORY



METADATA SCHEMAS & REPOSITORY

Filter by structured data is possible

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	General	General information		General information for processing the fit	string	1	
1.1	Normalization	Normalization		Normalization (reference for fit)	string	1	
1.2	IntensityFactor	Intensity factor		Intensity factor (name/storage)	string	1	
1.3	ReferencePaper	Reference paper		Information about the reference paper	string	0	
2	Component	Analysed component		Analysed component	string	1-n	
2.1	Background	Background		Background fit	string	1	
2.2	Fit type	Fit type		Fit type	boolean	1	singlet; doublet
2.3	Profile	FitProfile		Fit profile	boolean	1	Voigt; Lorentzian
2.4	ChemicalAssign	Chemical aissignement		Chemical assignement of component	string	0	
2.5	Position	Position component	eV	Absolut or relative position for component	number	1	
2.6	FWHM	FWHM	eV	FWHM	number	1	
2.7	Profile ratio	Profile ratio		Lorentz/Gauß ratio	string	0	
2.8	Asymmetry	Asymmetry or comments		Asymmetry in peak? or other comments	string	0	

METADATA SCHEMAS & REPOSITORY

Filter by structured data is possible

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	General	General information		General information for processing the fit	string	1	
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2	Component	Analysed component		Analysed component	string	1-n	
2.1	Background	Background		Background fit	string	1	
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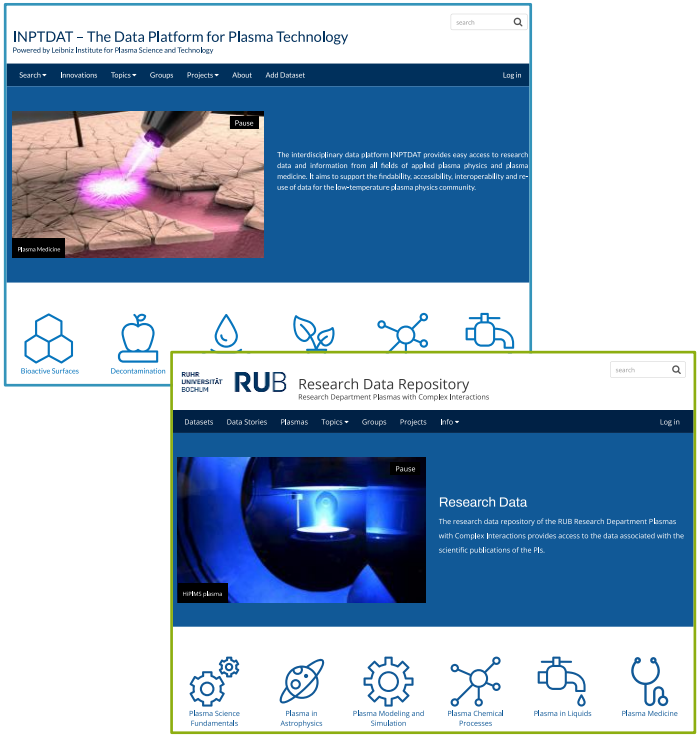
2.6	FWHM	FWHM	eV	FWHM	number	1	
2.7	Profile ratio	Profile ratio		Lorentz/Gauß ratio	string	0	
2.8	Asymmetry	Asymmetry or comments		Asymmetry in peak? or other comments	string	0	

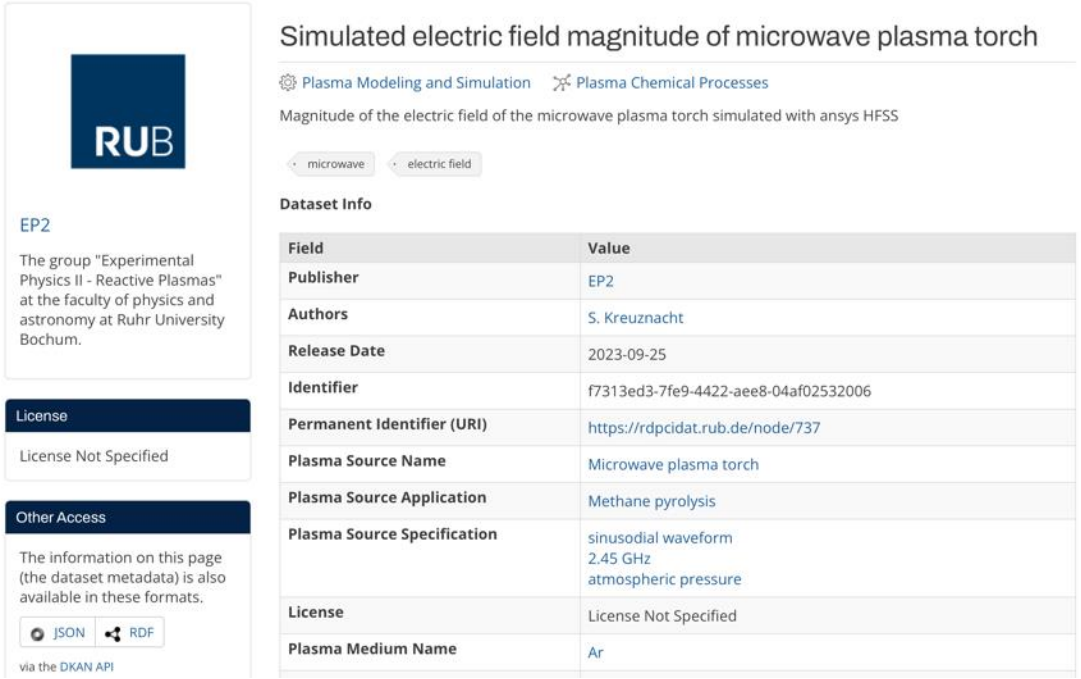
REPOSITORY

- Data platform for the publication and linking of datasets, patents and plasma sources
- Potential to use also as “expert database”
  - In productive use at INP inptdat
  - In productive use at RUB rdpcidat
- Next step: broader use for the publication of plasma sources, technology offers and datasets belonging to scientific publications

  citable DOI for the data



REPOSITORY - EXAMPLE



RUB

EP2

The group "Experimental Physics II - Reactive Plasmas" at the faculty of physics and astronomy at Ruhr University Bochum.

License

License Not Specified

Other Access

The information on this page (the dataset metadata) is also available in these formats.

JSON RDF

via the DKAN API

Simulated electric field magnitude of microwave plasma torch

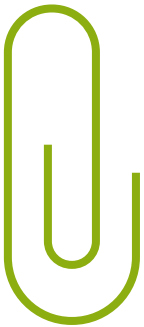
Plasma Modeling and Simulation Plasma Chemical Processes

Magnitude of the electric field of the microwave plasma torch simulated with ansys HFSS

microwave electric field

Dataset Info

Field	Value
Publisher	EP2
Authors	S. Kreuznacht
Release Date	2023-09-25
Identifier	f7313ed3-7fe9-4422-aee8-04af02532006
Permanent Identifier (URI)	https://rdpcidat.rub.de/node/737
Plasma Source Name	Microwave plasma torch
Plasma Source Application	Methane pyrolysis
Plasma Source Specification	sinusodial waveform 2.45 GHz atmospheric pressure
License	License Not Specified
Plasma Medium Name	Ar

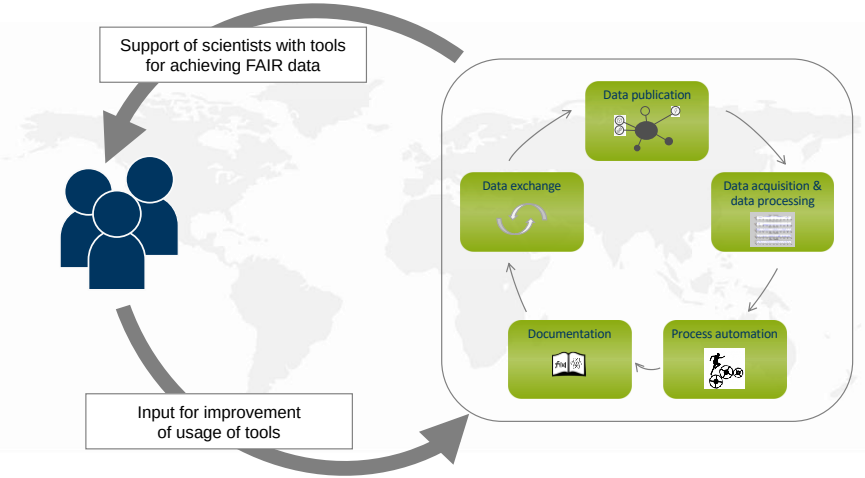


Download of raw data

SUMMARY

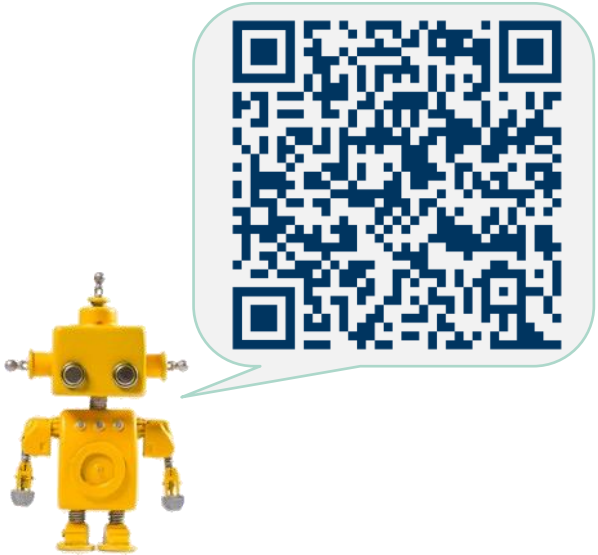
Aim of collaboration between plasma science groups of CAU, INP & RUB

- Development of methods and tools for research data management in low-temperature plasma physics
- Repository usage for data sets of peer-reviewed articles, Plasma-MDS for homogeneous metadata
- Highly addressing the community aspects
- Joint working groups for definition of metadata standards and quality criteria



SUBSCRIBE FOR eMAIL LIST

Mailing list for metadata discussion &
announcement of workshops or other activities



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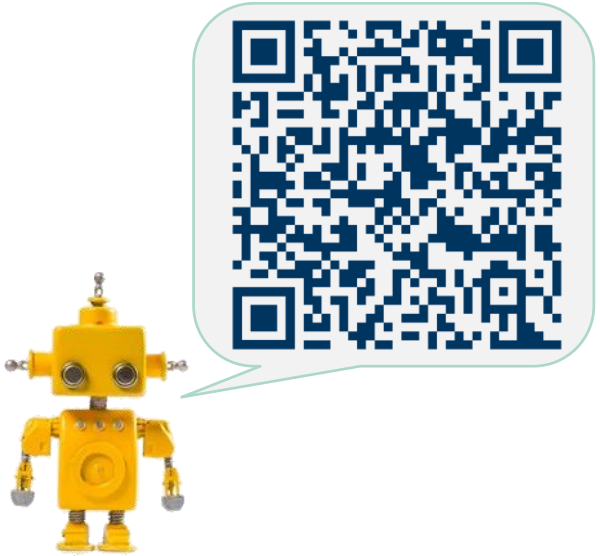

Thank you for your kind attention!