

# Public data from Photon and Neutron Reflectometry: Introducing the PaN Reflectivity Database

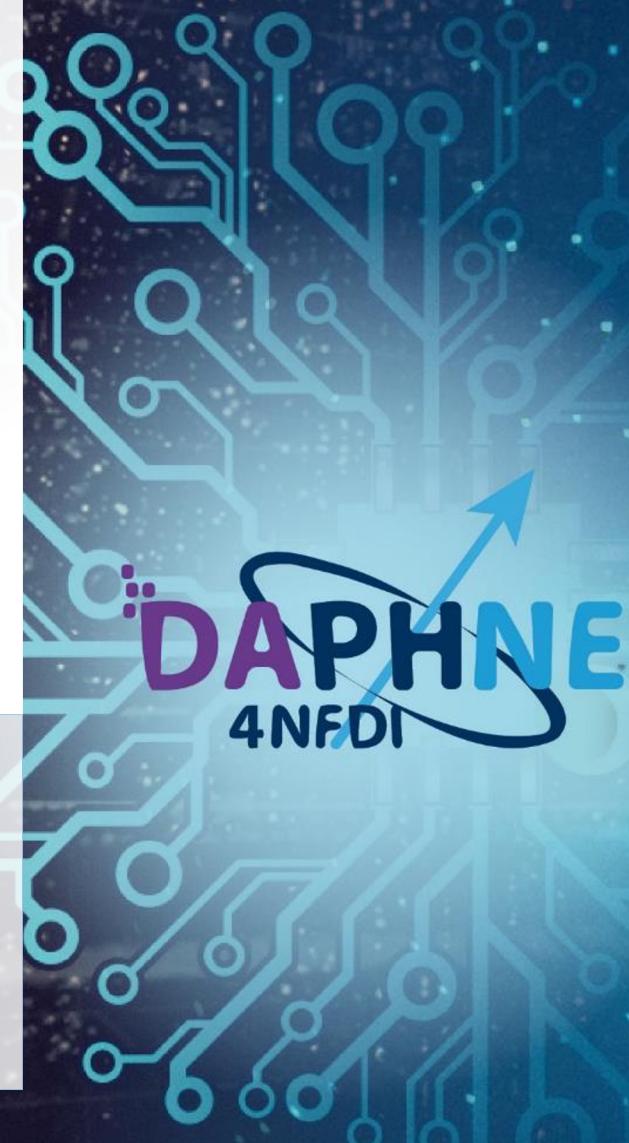
Julia Kobus<sup>1</sup>, Linus Pithan<sup>2</sup>, Tim Wetzel<sup>2</sup>, Bridget Murphy<sup>1</sup>



Kiel University  
Christian-Albrechts-Universität zu Kiel



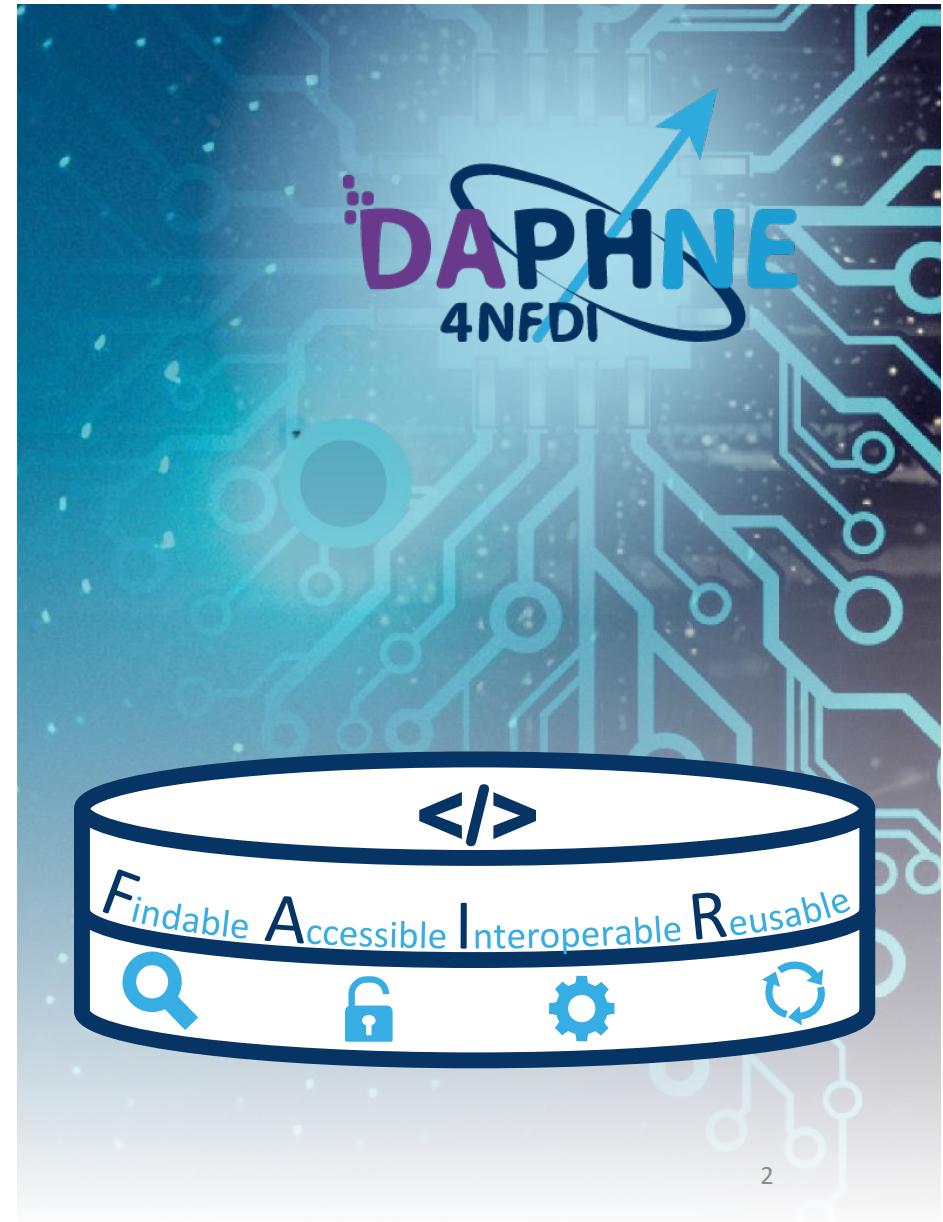
**DAPHNE**  
4NFDI



## DAPHNE4NFDI Task Area 2: **(Meta)data repositories and catalogues**

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- FAIR-compliant catalogs for X-ray and neutron research
- From raw data to final result:
  - All processing and analysis steps
  - Detailed sample description
- Raise transparency and thus quality, trustworthiness and reusability



# PaN Reflectivity Database



Already published high-quality  
PaN reflectometry  
→ best practice reference

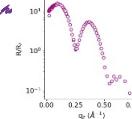
Data and metadata in a standardized format  
→ Compatible with standardized community  
software for evaluation and visualization  
→ Machine readable for AI applications

Interactive use: Integrated data visualization  
and online re-analysis capabilities  
→ Education platform: Easy entry into  
reflectometry analysis.

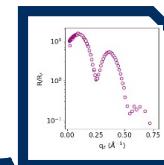
## Publication

X-ray studies of bidirectional structural changes induced by photoswitching in phospholipid membranes

X-ray studies of bidirectional structural changes induced by photoswitching in phospholipid membranes



Make FAIR & Improve Reach



PaN Reflectivity Database



# SciCat

Manage and annotate your scientific data



## Ingest

Automate data importing



## Annotate

Enrich your data



## Find

Browse and search your data



## Publish

Add DOI and share



EUROPEAN  
SPALLATION  
SOURCE

[European Spallation Source](#)

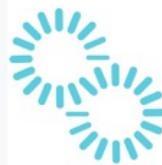
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The Rosalind  
Franklin Institute

[Rosalind Franklin Institute](#)

MLZ

Heinz Maier-Leibnitz Zentrum

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ADVANCED LIGHT SOURCE

[Advanced Light Source](#)



Deutsches Elektronen-Synchrotron DESY

SOLEIL

SYNCHROTRON

[Synchrotron SOLEIL](#)

DAPHNE

4NFDI

[DData from PHoton and Neutron Experiments](#)

## Datasets /

Items per page: 25

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Name	Source Folder	Start Time	Type
LactoseLipid	...8517968076	2024-07-08 Mon 18:55	raw
DPPC	...5144900025	2024-07-08 Mon 18:51	raw
Water	...02770	2024-07-08 Mon 18:51	raw
FeCo/TiN Multilayer Reflectivity			

Reflectometry curves (XRR and NR) and corresponding fits for machine

<https://public-data.desy.de>



Datasets / [undefined/65918bcf-f274-436b-a127-13a5f0668d6b](#) /

≡ Details

⬇ Datafiles

📁 Related Datasets

⟳ Lifecycle

Jupyter Hub



#### General Information

**Name** Water

**Description** Water Reflectivity

**PID** [undefined/65918bcf-f274-436b-a127-13a5f0668d6b](#)

**Type** raw

**Creation Time** 2024-07-08 18:33

**Keywords**

## Keywords



### Creator Information

**Owner** Svenja Hövelmann; Bridget Murphy

**Principal Investigator** Svenja Hövelmann

**Contact Email** [hoevelmann@physik.uni-kiel.de](mailto:hoevelmann@physik.uni-kiel.de)

**Owner Group** ingestor

### Access Groups



### File Information

**Source Folder** /OpenPortal/public-data/SvenjaHövelmannBridgetMurphy-  
I--1748396320277040497



### Related Documents

**Creation Location** DESY/PETRA III/P08/LISA

### Input Datasets



## Scientific Metadata



Search

x



## ▼ Experiment

title I-20200343

instrument P08/LISA Diffractometer

start\_date 2020-10-22

probe x-ray

facility PETRA III

proposalID I-20200343

doi null

## ▼ Sample

name	H2O
category	air/liquid
composition	H2O   air
description	null
environment	Langmuir trough
▶ sample_parameters	
▼ Measurement	
▶ instrument_settings	
▶ data_files	
▶ additional_files	
scheme	angle-dispersive



Datasets / [undefined/65918bcf-f274-436b-a127-13a5f0668d6b](#) /

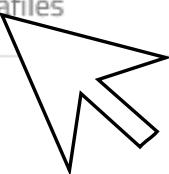
≡ Details

⬇ Datafiles

📁 Related Datasets

⟳ Lifecycle

Jupyter Hub



General Information

Name Water

Description Water Reflectivity

PID [undefined/65918bcf-f274-436b-a127-13a5f0668d6b](#)

Type raw

Creation Time 2024-07-08 18:33

Keywords

[? Help](#)[About](#)[Sign in](#)

Datasets / undefined/65918bcf-f274-436b-a127-13a5f0668d6b /

[Details](#)[Datafiles](#)[Related Datasets](#)[Lifecycle](#)

Maximum allowed download size: 5 GB

Selected: 0 B / 5 GB

21 datafiles.

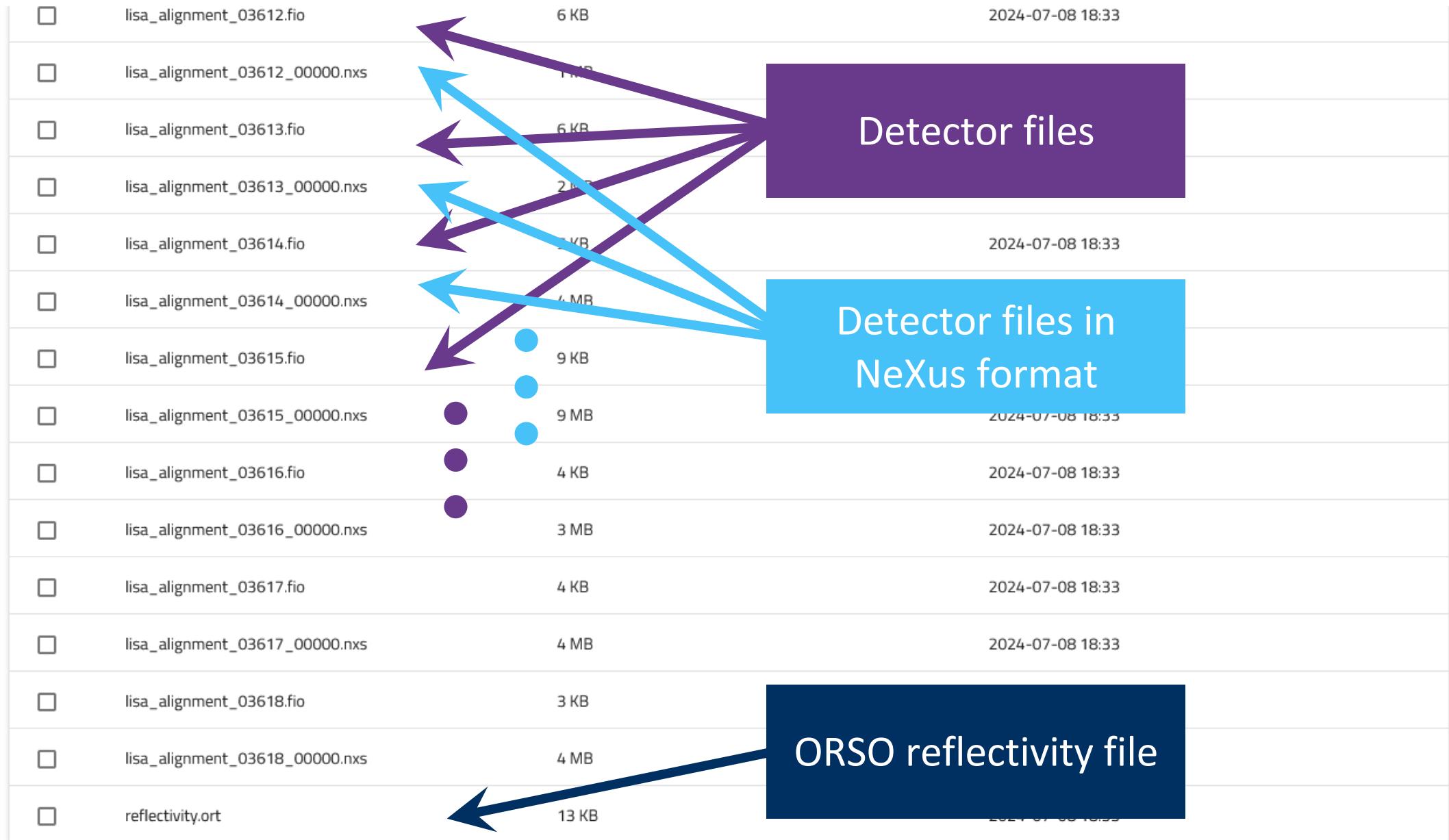
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1 – 21 of 21

| < < > > |

<input type="checkbox"/>	Path	Size	Time
<input type="checkbox"/>	lisa_alignment_03609.fio	9 KB	2024-07-08 18:33
<input type="checkbox"/>	lisa_alignment_03609_00000.nxs	640 KB	2024-07-08 18:33
<input type="checkbox"/>	lisa_alignment_03610.fio	6 KB	2024-07-08 18:33
<input type="checkbox"/>	lisa_alignment_03610_00000.nxs	422 KB	2024-07-08 18:33
<input type="checkbox"/>	lisa_alignment_03611.fio	7 KB	2024-07-08 18:33
<input type="checkbox"/>	lisa_alignment_03611_00000.nxs	674 KB	2024-07-08 18:33



```
# # ORSO reflectivity data file | 1.1 standard | YAML encoding | https://www.reflectometry.org/
# # I-20200343 | 2020-10-22 | H2O | R(Qz)
# license: CC-BY
# data_source:
#   owner:
#     name: null
#     affiliation: null
#     owner: "Svenja Hövelmann; Bridget Murphy"
#     contactEmail: hoevelmann@physik.uni-kiel.de
#     datasetName: Water
#     principalInvestigator: "Svenja Hövelmann"
#     creationLocation: DESY/PETRA III/P08/LISA
#     type: raw
#     creationTime: '2024-07-08T16:33:58'
#     ownerGroup: ingestor
#     sourceFolder: /OpenPortal/public-data/dataset_id
# experiment:
#   title: I-20200343
#   instrument: P08/LISA Diffractometer
#   start_date: 2020-10-22T00:00:00
#   probe: x-ray
#   facility: PETRA III
#   proposalID: I-20200343
# sample:
#   name: H2O
#   category: air/liquid
```

```
# data_set: 0
# columns:
# - {name: Qz, unit: 1/angstrom, physical_quantity: Normal momentum transfer}
# - {name: R, unit: '1', physical_quantity: Reflectivity}
# - {error_of: R, error_type: uncertainty, value_is: sigma}
# - {error_of: Qz, error_type: resolution, value_is: sigma}
# # Qz (1/angstrom)      R (1)          sR          sQz
1.8061414316384899e-02 1.0168648125592998e+00 1.0268767438248770e-01 nan
1.8823626592257000e-02 1.0119312587138705e+00 1.0219241734361410e-01 nan
1.9557435974092999e-02 1.0124946091274163e+00 1.0225043204203710e-01 nan
2.0313384799493898e-02 1.0000000000000000e+00 1.0099229420682709e-01 nan
2.1056880677038300e-02 9.4089176056280199e-01 9.5050976706056903e-02 nan
2.1791431218294199e-02 6.8430700017274881e-01 6.9251609883111395e-02 nan
2.2530764177529701e-02 3.9483490839404650e-01 4.0109050294710402e-02 nan
2.3273463026900299e-02 2.3835962411875050e-01 2.4320765851725001e-02 nan
2.4018643092771200e-02 1.6664893742052941e-01 1.7072799802283600e-02 nan
2.4764062896027599e-02 1.2722019263095979e-01 1.3077106002505600e-02 nan
2.5479753813939899e-02 1.0178254330461650e-01 1.0497318676486600e-02 nan
2.6218849954409901e-02 8.1601261309097797e-02 8.4459177885130004e-03 nan
2.6959673654095101e-02 6.7046878237287805e-02 6.9640854697610999e-03 nan
2.7707883332418901e-02 5.6777388476264103e-02 5.9153401441304999e-03 nan
2.8451136713687701e-02 4.7289252544830900e-02 4.9462772173201001e-03 nan
2.9126645431800501e-02 3.9931521255725598e-02 4.0513461404416999e-03 nan
2.9184137813541001e-02 4.0701010118705402e-02 4.2704261363153001e-03 nan
2.9925750394786600e-02 3.5504072884883602e-02 3.7381835883993999e-03 nan
3.0666154957699601e-02 3.0264688850005699e-02 3.2002045796629000e-03 nan
3.1341645127650100e-02 2.8200751402250200e-02 2.8600271007201000e-02 nan
```

## First FAIR high-quality PaN reflectometry datasets

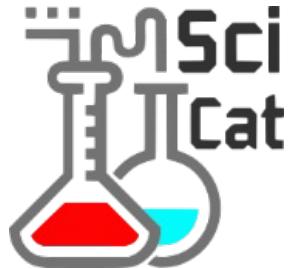


- Metadata following ORSO specifications
- Reflectivity data in ORSO format
- Raw data (detector images)
- PID



- Update metadata to DAPHNE specifications

# Metadata schema



owner  
ownerEmail



SciCat  
Data Model



owner:  
- name  
- affiliation  
- contact



ORSO  
file format  
specifications



Principal Investigator  
- Last Name  
- First Name  
- Email  
- Affiliation



DAPHNE4NFDI  
metadata  
white paper

## First FAIR high-quality PaN reflectometry datasets



- Metadata following ORSO specifications
- Reflectivity data in ORSO format
- Raw data (detector images)
- PID



- Update metadata to DAPHNE specifications
- Reflectivity and raw data in NeXus/hdf5 format
- Link to Publication
- DOI
- Data Visualization
- Interactive data analysis

Fill the database with your FAIR data



Upload your data



Give feedback on the upload process and the database contents

Facilitates FAIR compliance for your published reflectivity data by querying the (meta)data, automatically processing it into an ORSO file along with the reflectivity data, and uploading it to the database:

## PaN Reflectivity Database - Upload tool

<https://sisyphos.desy.de/>



The screenshot shows a web browser window with the following elements:

- Header:** A yellow navigation bar with icons for back, forward, search, and user profile.
- Toolbar:** Includes "Deploy" and a three-dot menu icon.
- Logos:** Logos for DAPHNE 4NFOI, DESY, and ORSC.
- Title:** "PaN Reflectivity Database - Upload tool".
- Welcome Text:** "Welcome to our open data community. This tool will guide you through uploading your x-ray and neutron reflectometry data to the PaN Reflectivity Database. Please enter the metadata for your data set below and then upload your reflectometry curve. By submitting your data, you agree to make the data available in accordance with the Creative Commons Attribution (CC-BY) Licence. After submission, the data and metadata are written to the [ORSO file format](#). Following curation, the data set will be published in the [DESY public data catalogue](#).
- Note:** "Note: This upload tool is currently in the alpha version phase. Please contact [jkobus@physik.uni-kiel.de](mailto:jkobus@physik.uni-kiel.de) in case you experience any problems."
- Form Fields:** A form with a "owner\*" label and a text input field.



# Upload your data

Feedback?

<https://sisyphos.desy.de/>

This work was supported by the consortium DAPHNE4NFDI in the context of the work of the NFDI e.V. The consortium is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - project number 460248799





# PaN Reflectivity Database - Upload tool

---

Welcome to our open data community. This tool will guide you through uploading your x-ray and neutron reflectometry data to the PaN Reflectivity Database. Please enter the metadata for your data set below and then upload your reflectometry curve. By submitting your data, you agree to make the data available in accordance with the Creative Commons Attribution (CC-BY) Licence. After submission, the data and metadata are written to the [ORSO file format](#). Following curation, the data set will be published in the [DESY public data catalogue](#).

**Note:** This upload tool is currently in the alpha version phase. Please contact [jkobus@physik.uni-kiel.de](mailto:jkobus@physik.uni-kiel.de) in case you experience any problems.

owner\*



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Note: This upload tool is currently in the alpha version phase. Please contact [jkobus@physik.uni-kiel.de](mailto:jkobus@physik.uni-kiel.de) in case you experience any problems.

owner\*



contactEmail\*



description\*



datasetName\*



# Experiment

title\*



instrument\*



start date\*

 YYYY/MM/DD

probe

x-ray

facility



proposalID



# Sample

name\*



category



composition



description\*



environment



## Reflectivity Data Upload

Please upload your reflectivity data csv-file. The file must contain at least two columns Qz and R. For further columns, please enter the relevant information below.



Drag and drop file here

Limit 200MB per file

[Browse files](#)



example.data 447.0B



Column 1: Normal momentum transfer (Qz)

Unit of Qz

1/angstrom



Column 2: Reflectivity (R)

Unit of R