

# 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>



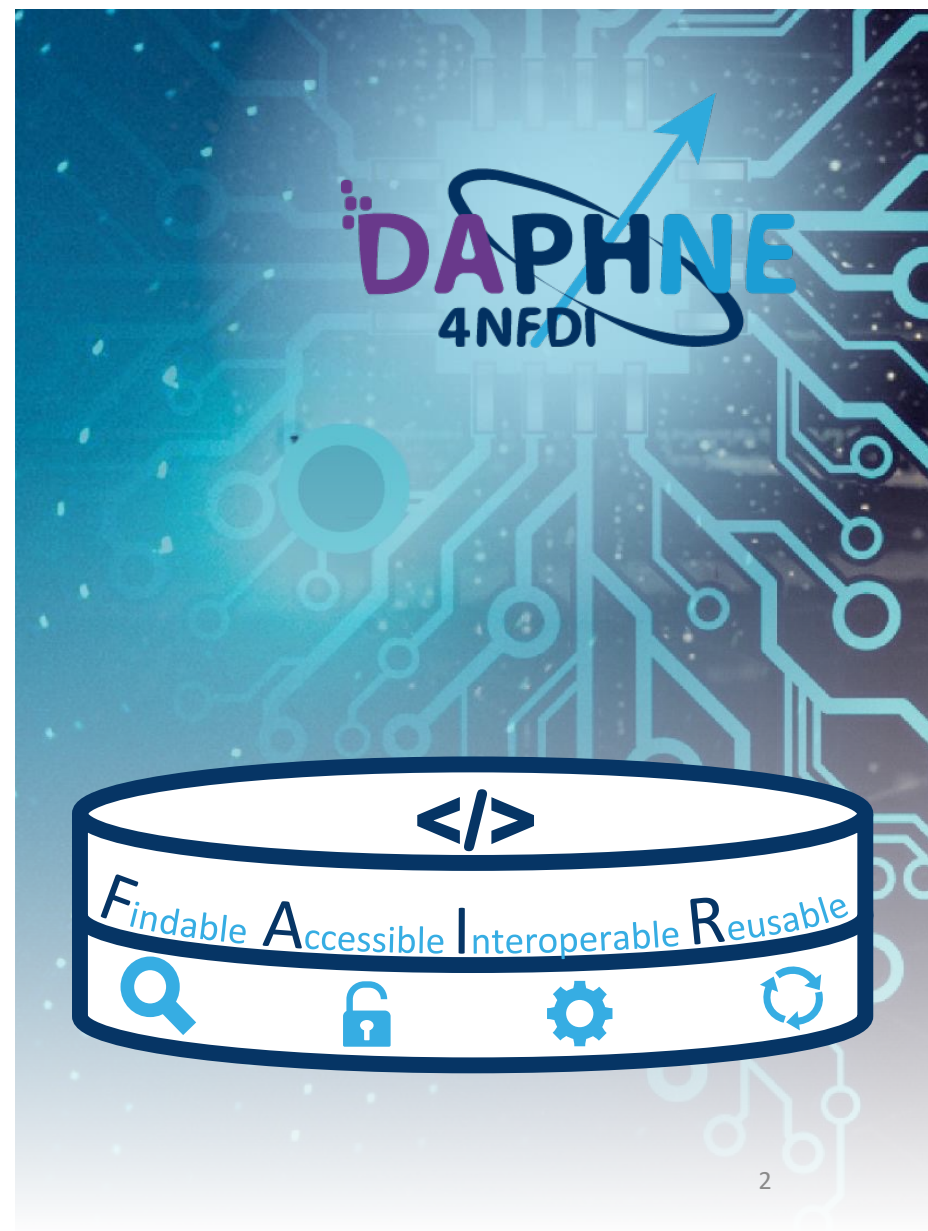
Kiel University  
Christian-Albrechts-Universität zu Kiel



## 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.

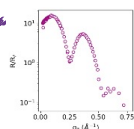
## Publication

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

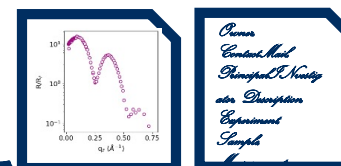
*X-ray studies of bidirectional structural changes induced by photoswitching in photoisoleptid membranes*

*induced by photoswitching in photoisoleptid membranes*

*induced by photoswitching in photoisoleptid membranes*



Make FAIR & Improve Reach



PaN Reflectivity Database



**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



Paul Scherrer Institut



MAX IV



Rosalind Franklin Institute



Heinz Maier-Leibnitz Zentrum



Advanced Light Source



Deutsches Elektronen-Synchrotron DESY



Synchrotron SOLEIL



Data from Photon and Neutron Experiments

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PID

Text Search

Location

Group

Type

Keywords

Start Date – End Date



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

...02778

2024-07-08

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](#) /

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

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21 datafiles.

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<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
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<input type="checkbox"/>	lisa_alignment_03618.fio	3 KB	
<input type="checkbox"/>	lisa_alignment_03618_00000.nxs	4 MB	
<input type="checkbox"/>	reflectivity.ort	13 KB	2024-07-08 18:33

Detector files

Detector files in  
NeXus format

ORSO reflectivity file

```
# # 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 H\xF6velmann; Bridget Murphy"
#     contactEmail: hoevelmann@physik.uni-kiel.de
#     datasetName: Water
#     principalInvestigator: "Svenja H\xF6velmann"
#     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
3.1241645137650100e-02 2.8200751403352300e-02 2.8600321007304000e-03 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

A circular flow diagram consisting of two concentric arrows. The outer arrow is purple and points clockwise. The inner arrow is light blue and points counter-clockwise. The text "Upload your data" is centered within the space between the two arrows.

**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/>

A screenshot of a web browser displaying the 'PaN Reflectivity Database - Upload tool' interface. The browser window has a white background with a blue header bar. In the top right corner of the header, there are icons for 'Deploy', a star, a heart, a share icon, and a menu icon. Below the header, there are three logos: 'DAPHNE 4NFOI' (a blue and purple logo with a stylized 'D' and 'A'), 'DESY' (a blue circular logo with a network-like pattern), and 'ORSO' (a black logo with a stylized 'O' and 'S'). The main content area has a white background. At the top, the title 'PaN Reflectivity Database - Upload tool' is displayed in a bold, black font, followed by a horizontal line. Below the title, there is a paragraph of 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](#).' Below this paragraph, there is a red 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.' At the bottom of the form, there is a label 'owner\*' in a small, black font, followed by a light gray input field. To the right of the input field, there is a small circular icon with a question mark inside.



# 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

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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.

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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  $Q_z$  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 ( $Q_z$ )

Unit of  $Q_z$

1/angstrom



Column 2: Reflectivity ( $R$ )

Unit of  $R$