

# Implementation of PIDs for Instruments at HZB

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PID Network Deutschland: “Online-Seminar zu PIDs für Instrumente“

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[www.helmholtz-metadaten.de](http://www.helmholtz-metadaten.de)



# Motivation

for implementing PIDs for instruments at HZB





# Implementation of DOIs for Instruments at HZB

- adding nodes and edges in the PID graph -



# DOIs for Instruments at HZB

- HZB minting DataCite DOIs through DataCite API.
  - Alternative to using B2INST with handles.net.
- Started with DataCite 4.4.
  - using PIDINST mapping to DataCite schema.
- Update to DataCite 4.5.
  - HZB updated all records for instruments and data.
- Reference for schema usage:
  - PIDINST: DataCite cookbook [4]
- DataCite records for HZB Instruments: → **resourceType:**
- **resourceTypeGeneral:**
- Data PIDs linked to Instrument PIDs: → **relationType:**

## 3.1. Mapping of PIDINST metadata onto DataCite

[4]

Based on the mapping provided by DataCite, we want to give in the following additional hints and discuss how the metadata describing the instrument can be best represented in the DataCite Schema:

### Identifier

The DOI that you are going to create. Add as DataCite property *Identifier* with *identifierType=DOI*.

### LandingPage

The URL of the landing page that the PID resolves to. The DataCite Schema does not have a property for this, but you'll register the URL along with the metadata when creating the DOI.

### Name

The name by which this instrument is known. Add as DataCite property *Title*.

### Owner

The organization or individual that manages the instrument. Add as DataCite property *Contributor* with *contributorType=HostingInstitution*. Consider also to add an identifier for the owner in the *nameIdentifier* subproperty of *Contributor*.


"BER II Beamline"

"Instrument"

"IsCollectedBy"

```

graph LR
    A(( )) -- "datacite : IsDescribedBy" --> B(( ))
    B -- "datacite : IsCollectedBy" --> C(( ))
  
```



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## E2

### Flat-Cone Diffractometer

**Instrument description**

A 3-dimensional part of the reciprocal space can be scanned in less than five steps by combining the "off-plane Bragg-scattering" and the flat-cone layer concept while using a new computer-controlled tilting axis of the detector bank. Parasitic scattering from cryostat or furnace walls is reduced by an oscillating "radial" collimator. The datasets and all connected information is stored in one independent NeXus file format for each measurement and can be easily archived. The software package TNeXus deals with the raw data sets, the transformed physical spaces and the usual data analysis tools (e.g. MatLab). TNeXus can convert to various data sets e.g. into powder diffractograms, linear detector projections, rotation crystal pictures or the 2D/3D reciprocal space.

For **single crystal** work the multi detector bank (four 2D detectors 300x300 mm<sup>2</sup>) and the sample

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&lt;HMC&gt; | 6

# Connecting HZB nodes in the DataCite PID graph



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## PEAXIS: A RIXS and XPS Endstation for Solid-State Quantum and Energy Materials at BESSY II

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Abstract

PEAXIS (Photo Electron Analysis and resonant X-ray Inelastic Spectroscopy) is a dedicated endstation installed at the beamline U41-PEAXIS that offers high resolution soft X-ray spectroscopy measurements with incident photon energies ranging from 180 – 1600 eV.

## PEAXIS

### Combined RIXS and XPS

The station PEAXIS (PhotoElectron Analysis and X-ray Inelastic Spectroscopy) is a fixed station installed at the U41-PEAXIS beamline. It is dedicated to studies of angle-resolved RIXS (Resonant Inelastic X-ray Scattering) and PES (PhotoElectron Spectroscopy) on solids. As shown in the Schematic figure below, the station is equipped with an electron energy analyzer (violet) and a RIXS spectrometer (blue). Various sample manipulators (red) can be installed in the sample chamber (green). The RIXS arm is continuously rotatable on a supporting rail in a range of 106 degrees.

### Selected Applications:

- Magnetic, d-d and charge transfer excitations in model quantum materials and functional energy materials
- Dispersive excitations in quantum materials (e.g. plasmons and excitons)
- Electron-phonon coupling in solid-state materials
- Reaction mechanisms in battery materials

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Email Business card

## U41-PEAXIS

### PEAXIS - Combined RIXS and XPS

U41-PEAXIS beamline is one of the highest flux beamlines at BESSY II. It provides highly focused soft X-rays, thanks to the ellipsoidal refocusing mirror. The beamline is connected to a fixed endstation PEAXIS that is dedicated to studies of angle-resolved RIXS (Resonant Inelastic X-ray scattering) and PES (PhotoElectron Spectroscopy) on solids.

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| Station data      |  |
|-------------------|--|
| Temperature range | 20 – 1000 K                              |
| Pressure range    | 10 <sup>-8</sup> – 10 <sup>-9</sup> mbar |

## Instrument description in JLSRF.

→ “Legacy” PIDs for PaN instruments.

doi: [10.17815/jlsrf-7-177](https://doi.org/10.17815/jlsrf-7-177)

## HZB instrument data base (landing page).

→ Curated with / by instrument scientists.

doi: [10.5442/ni000024](https://doi.org/10.5442/ni000024)

## HZB beamline (landing page).

→ Attached to the referenced HZB instrument.

doi: [10.5442/ni000023](https://doi.org/10.5442/ni000023)

# Outlook and Conclusions





# Outlook

- Data findable through PID- or knowledge graphs.

- PID graph (FREYA, DataCite) [1]
- OpenAIRE Research Graph? [5]
- Helmholtz Knowledge Graph [6, 7]
  - Use case: Instrument PIDs.

- Cultural change with many stakeholders.

- Publishers and PID registries
- Data infrastructures and curators
- Research communities

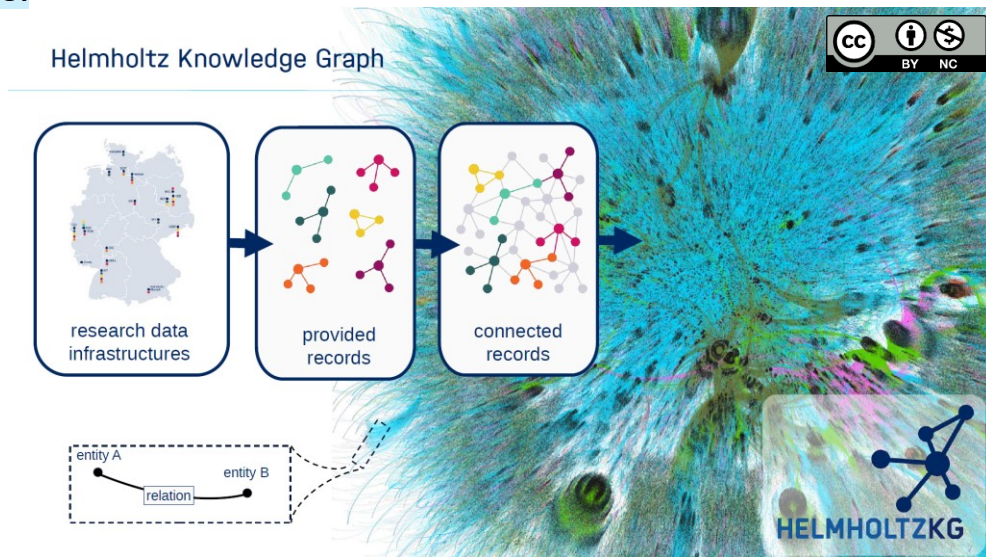


Image source: V. Hofmann [7]

[1] Fenner et al., 'Introducing the PID Graph', (2019). <https://doi.org/10.5438/JWVF-8A66>

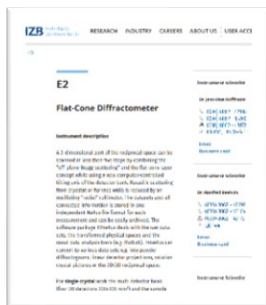
[5] Manghi et al., The OpenAIRE Research Graph Data Model (1.3). Zenodo (2019). <https://doi.org/10.5281/zenodo.2643199>

[6] [https://helmholtz-metadaten.de/en/unhide\\_helmholtz-kg](https://helmholtz-metadaten.de/en/unhide_helmholtz-kg) (accessed 2024/04/26)

[7] Hofmann, V., PIDs in the Helmholtz Knowledge Graph. Online Seminar zu PIDs für Forschungsdaten. Zenodo. (2024) <https://doi.org/10.5281/zenodo.10723293>.

# Conclusions

- HZB mints DOIs for scientific instruments and data publications using the DataCite API.
- HZB links data publications to related instruments via instrument DOIs.
- Adding qualified links for PID- or knowledge graphs requires a multi-stakeholder cultural change.



HZB instrument



HZB data publication

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