



PaNOSC tools for FAIR data handling at ELI-ALPS

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13 September 2022



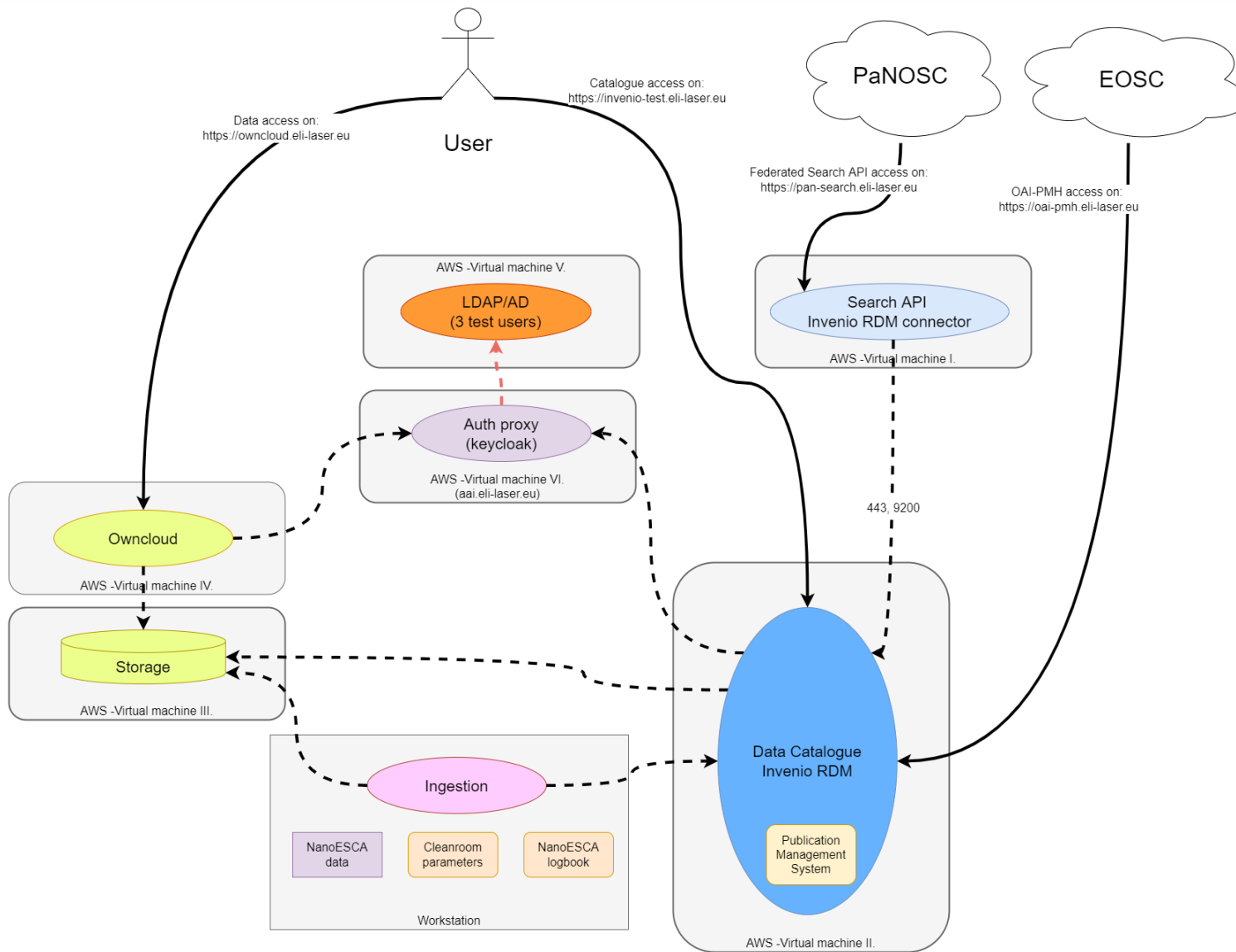
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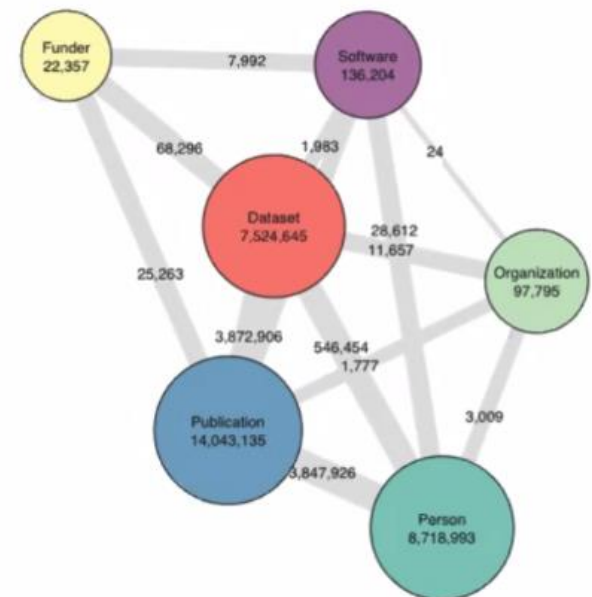
- **Data pilot project**
- **PaNOSC Search API**
 - **Federated service**
- **NeXus Data Format**
 - **HDF5**
 - **Application definitions**
 - **Energy scan with NanoESCA**
- **Photon and Neutron Experiment Techniques (PaNET)**
 - **New techniques for NanoESCA**

Data pilot project



- Purpose of the API
- Data model
- Metadata
 - Bibliographical information
 - Domain specific information
- Persistent identifiers (PID)
 - DOI (publications, data)
 - ORCID (researchers)
 - ROR (Institutes)

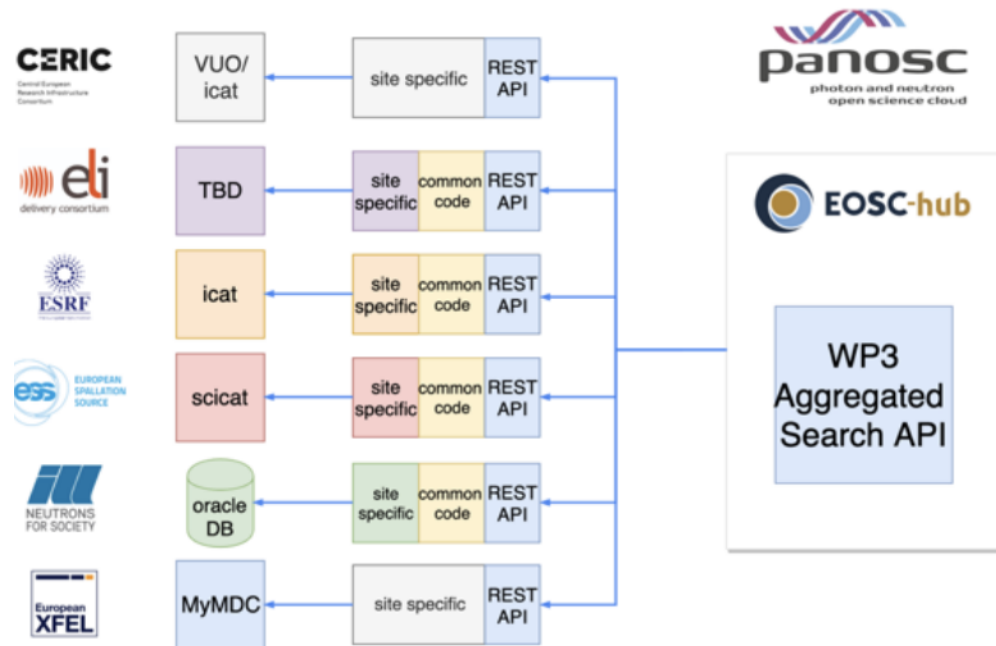
Graph



Federated Service I.



- Local API providers
- Federated API



Federated Service II.



- ELI provider – Invenio RDM

The screenshot displays the ELI Invenio RDM interface. The top navigation bar is orange with the ELI logo, a search bar, and links for Communities, My dashboard, and a user profile (admin@eli...). Below the navigation bar, there's a sidebar on the left with filters for Versions, Access status, Status, Resource types, and Help. The main content area shows search results for 'XUV spectroscopy with PG2 at 60.0 mm'. The first result is highlighted, showing its title, author (Bago, Balazs), and a brief description. The right sidebar contains details for the selected record, including its version (v1), keywords (spectroscopy), and resource type (Dataset). The bottom of the page features an orange banner with the text 'Powered by InvenioRDM'.

Federated Service III.



- Federated portal



StrongLoop API Explorer

Token Not Set

accessToken

Set Access Token

panosc-federated-search-api

Dataset : Information about an experimental run, including optional File, Sample, Instrument and Technique.

Document : Represents a scientific proposal or publication.

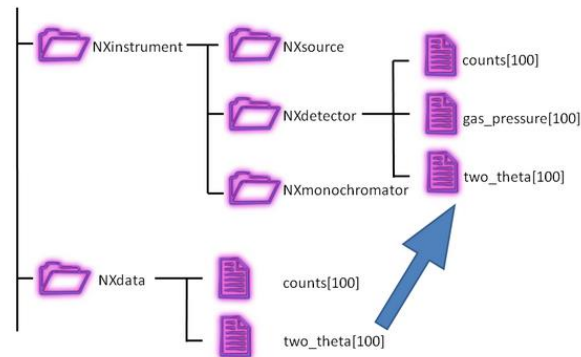
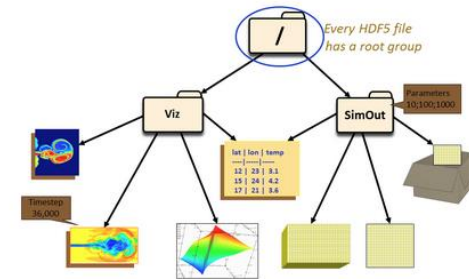
Instrument : Beam line where experiment took place.

[BASE URL: /api , API VERSION: 1.0.0]

The screenshot displays the panosc federated search API interface. On the left, a sidebar contains search filters: Type (proposal, publication), Technique (Select a technique...), Incident Wavelength (min, max, nm), Incident Photon Energy (min, max, eV), Chemical Formula, Temperature (min, max, K), and Pressure (min, max, Pa). The main panel shows search results for 'diffraction', with 50+ documents found. The results list includes:

- 10.15151/ESRF-E5-59848051: Austrian Crystallographic Diffraction Consortium (AC-DC), Released on July 23rd 2021 by the ESRF.
- 10.15151/ESRF-E5-120104269: Austrian Crystallographic Diffraction Consortium (AC-DC), Released on December 10th 2021 by the ESRF.
- 10.15151/ESRF-E5-143436284: Nanobeam diffraction tomography, Released on November 9th 2021 by the ESRF.
- 10.15151/ESRF-E5-405766966: We aim at studying the internal structure of ferroelastic domains in GeTe thin films and their dynamics unde..., Released on April 17th 2024 by the ESRF.
- 10.15151/ESRF-E5-88836881: Austrian Crystallographic Diffraction Consortium (AC-DC), Released on July 23rd 2021 by the ESRF.

- Common data exchange format
- HDF5
- Structured hierarchical data
 - Groups; Fields; Attributes; Links



- Standardization
- Application definitions
 - Base classes
 - NXDL files
 - NeXus International Advisory Committee (NIAC)

```
<definition name="NX_template__" extends="NXobject" type="group"
  category="application"
  xmlns="http://definition.nexusformat.org/nxdl/3.1"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation="http://definition.nexusformat.org/nxdl/3.1 ../nxdl.xsd"
>
  <doc>template for a NXDL application definition</doc>
</definition>
```

NXdirecttof

This is a application definition for raw data from a direct geometry TOF spectrometer

NXfluo

This is an application definition for raw data from an X-ray fluorescence experiment

NXindirecttof

This is a application definition for raw data from a direct geometry TOF spectrometer

NXiopro

Application definition for any $I(Q)$ data.

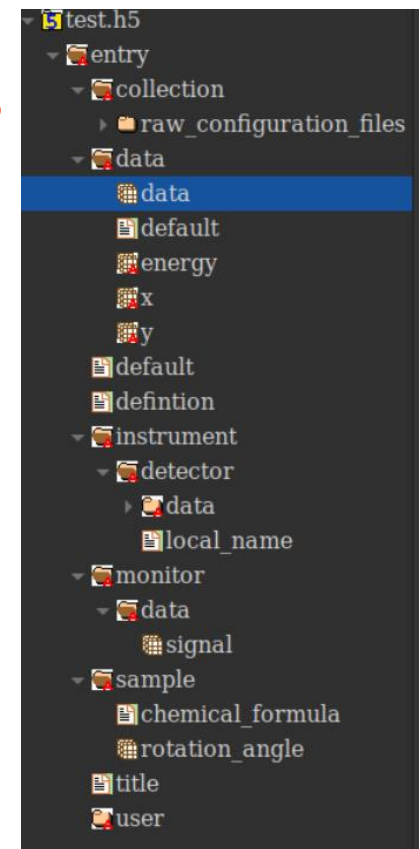
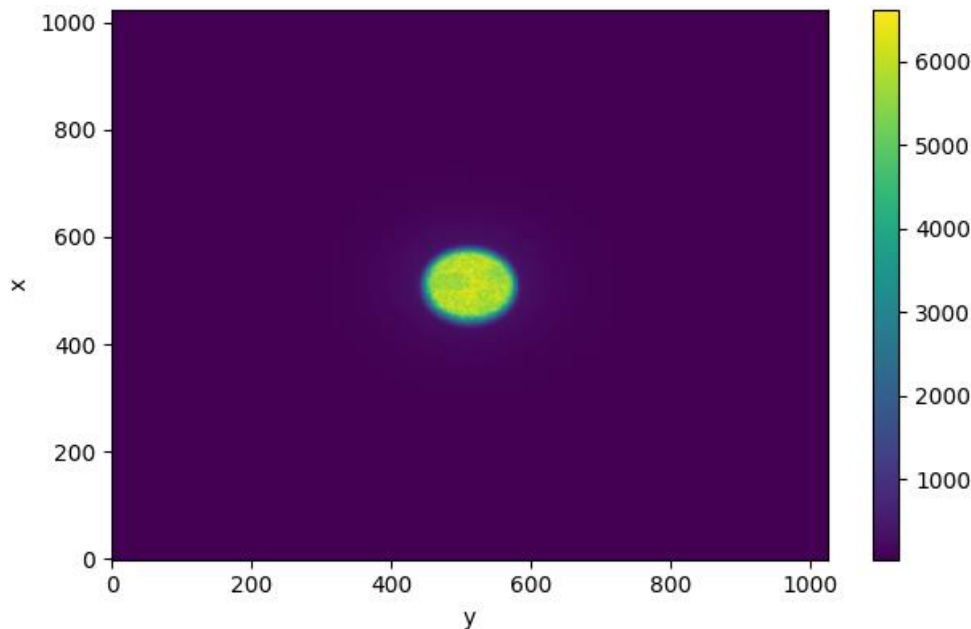
NXlaue

This is the application definition for a TOF laue diffractometer

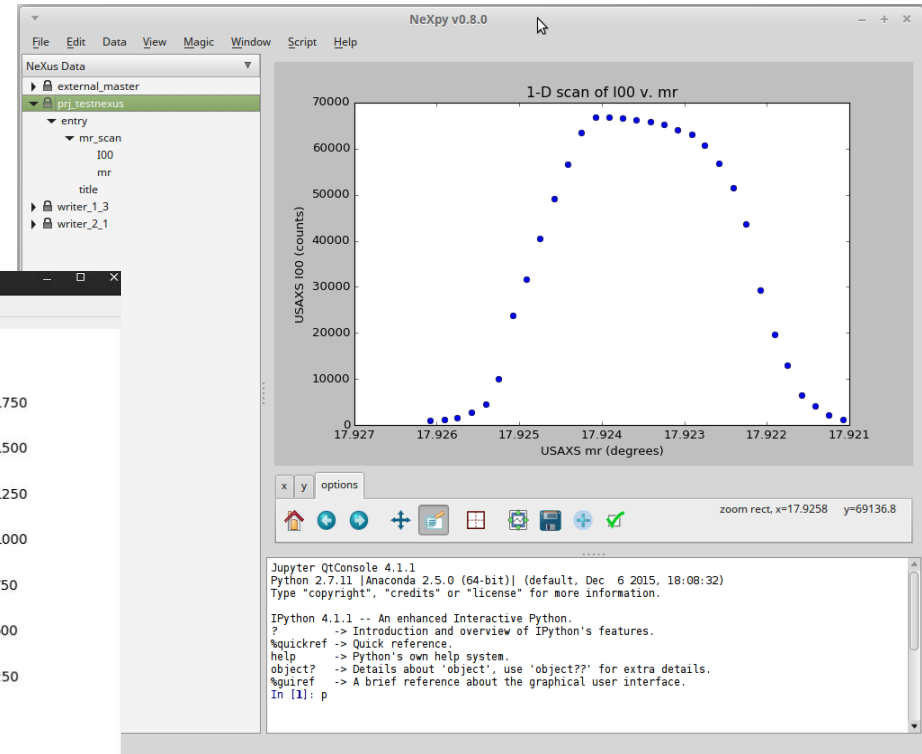
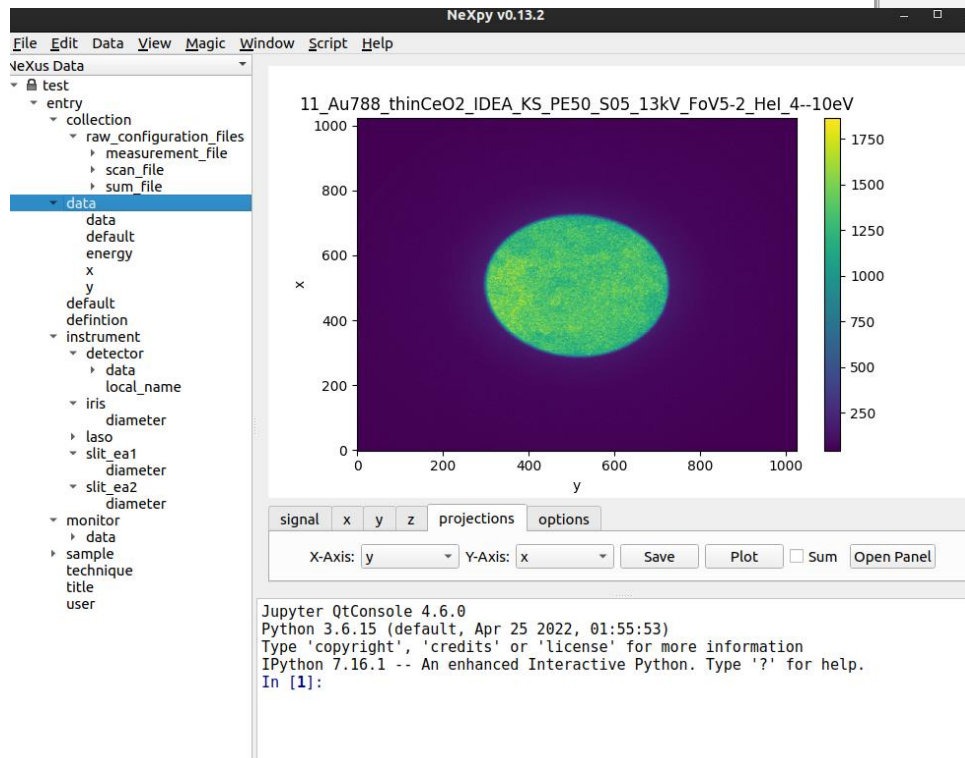
NXmonopd

Monochromatic Neutron and X-Ray Powder diffractometer

- NanoESCA
 - IDEA Mode kinetic energy scan
- Configuration ASCII files and TIFF images
- NXscan

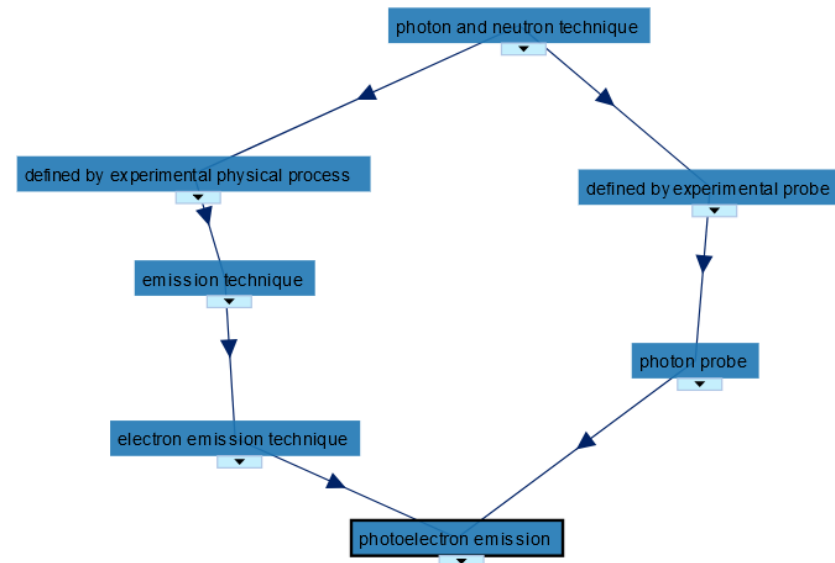


- GUI tool



- Ontology for photon and neutron science
- Graph structure
- Name; Definition; Alternative names; PID

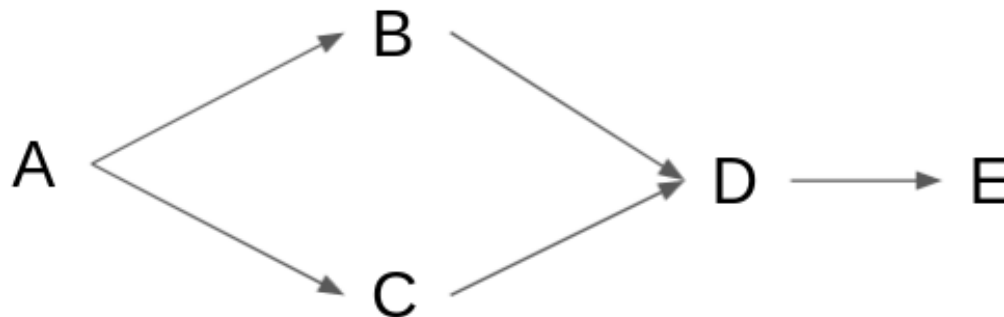
dataset
 Person
 photon and neutron technique
 + defined by experimental physical process
 + defined by experimental probe
 + microfocussed probe
 + muon probe
 + neutron probe
 + photon probe
 + dichroism
 + ellipsometry
 + ion imaging
 + IR photon probe
 + magnetic circular dichroism
 + magnetic linear dichroism
 + magnetochiral dichroism
 + natural circular dichroism
 + **photoelectron emission**
 + photoelectron spectroscopy
 + photoemission microscopy
 + raman spectroscopy
 + THz photon probe
 + UV visible photon probe
 + versus photon circular polarization
 + versus photon linear polarization
 + x-ray probe
 + pulsed probe
 + scanning probe
 + solid probe
 + defined by functional dependence
 + defined by purpose





- **Expandable**
- **NanoESCA existing techniques**
 - **PEEM**
 - **Photoemission spectroscopy**
- **NanoESCA – sub-graph**
 - **Spectro-microscopy**
 - ...
 - **Momentum microscope**

- Descendants in the graph
- Querying a "general" term
 - $B \rightarrow B, D \text{ and } E$
 - $D \rightarrow E$



THANK YOU FOR YOUR ATTENTION!

SZÉCHENYI 



HUNGARIAN
GOVERNMENT

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