

# *Towards Open Science in the Photon and Neutron Community*



**Oscar Matilla**  
**ALBA Synchrotron**  
**19-09-2023**

# The Photon and Neutron Community



<http://dx.doi.org/10.1016/j.elspec.2013.12.007>

# The European Photon and Neutron Community



## Photon – LEAPS

<https://leaps-initiative.eu>



## CERIC

Central European  
Research Infrastructure  
Consortium



## Neutron - LENS

<https://lens-initiative.org>



# The European Photon Community

## LEAPS key figures:

**19 facilities - 16 institutions - 10 countries**

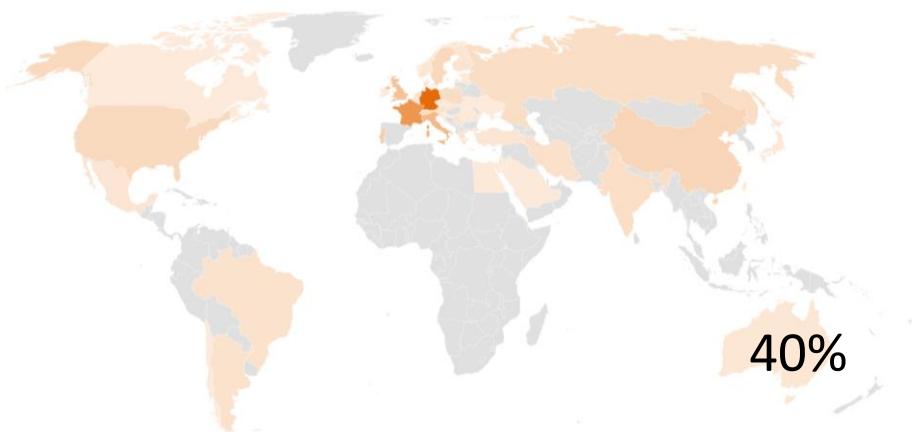
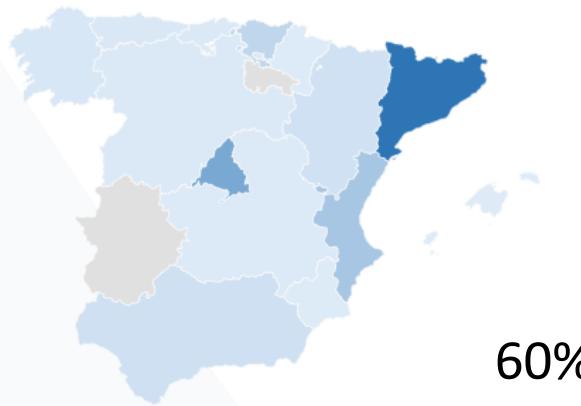
- > 300 operating End Stations
- 1.000.000 h beamtime /year  
Excellence-driven access free of charge
- > 5.000 publications/year
- > 15 spin off companies
- > 35.000 users from all EU & beyond  
researchers from all research area



# ALBA Synchrotron



**National Research Infrastructure** with 50% national + 50% regional funding: Ministerio de Ciencia e Innovación and Departament de Recerca i Universitats.

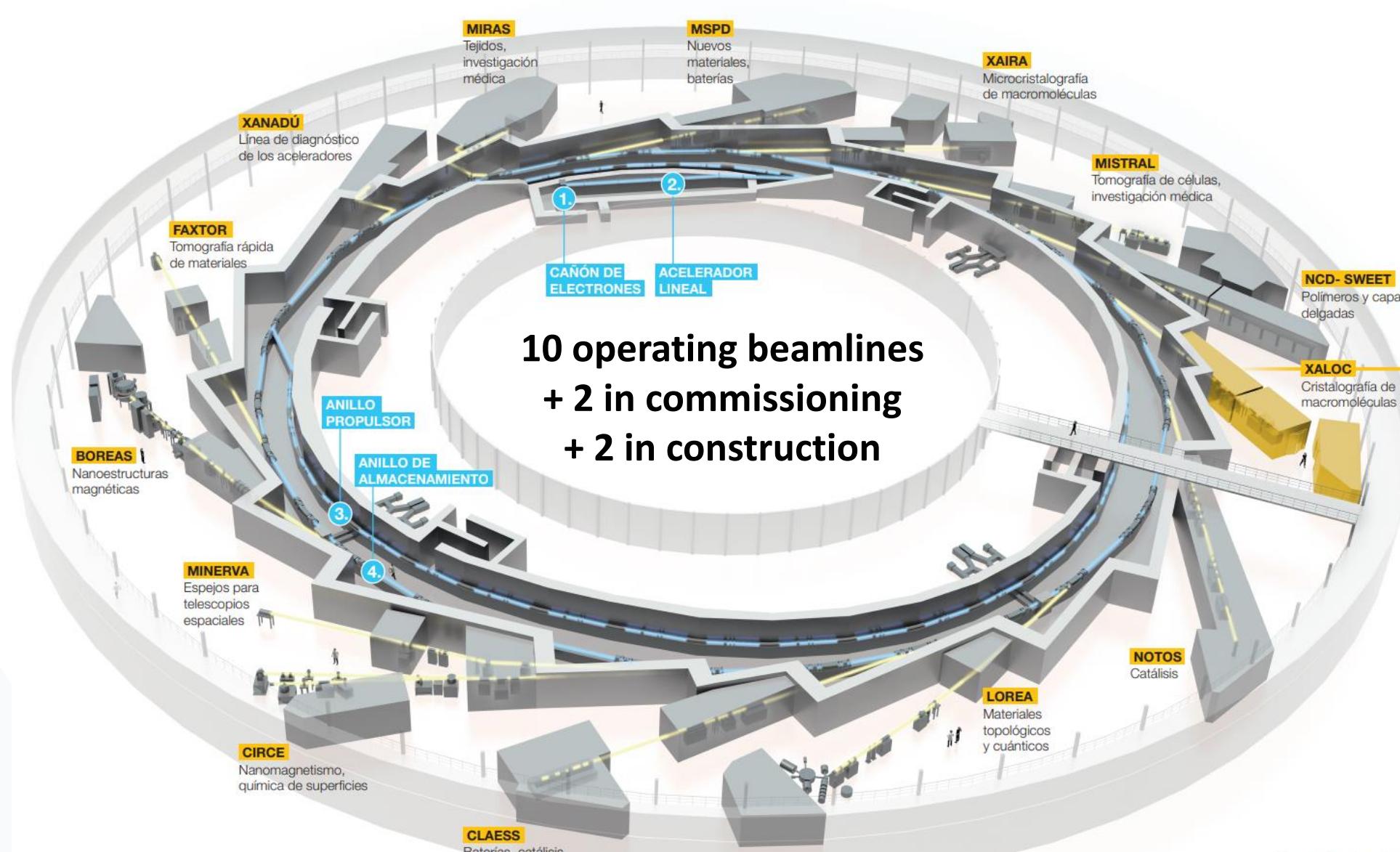


Towards Open Science in PaN - O.Matilla



SR Parameter	Value
Energy	3 GeV
Circumference	269 m
Emittance	4.4 n mrad
Current	250 mA
Rf frequency	500 MHz
# cavities	6
Long straights	4 (8 m)
Short straights	12 (4 m)

# ALBA Synchrotron



Infografia: Fundamentum

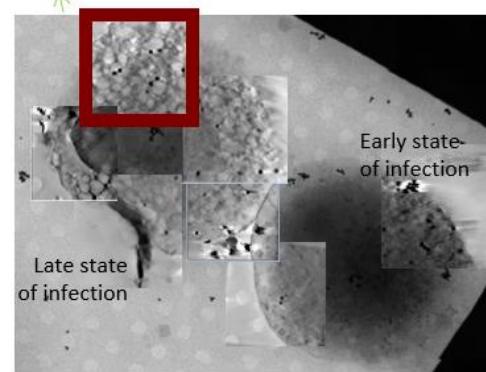
# ALBA Synchrotron Research Infrastructure



*Three Scientific Sections, three main research lines*

## Life Science

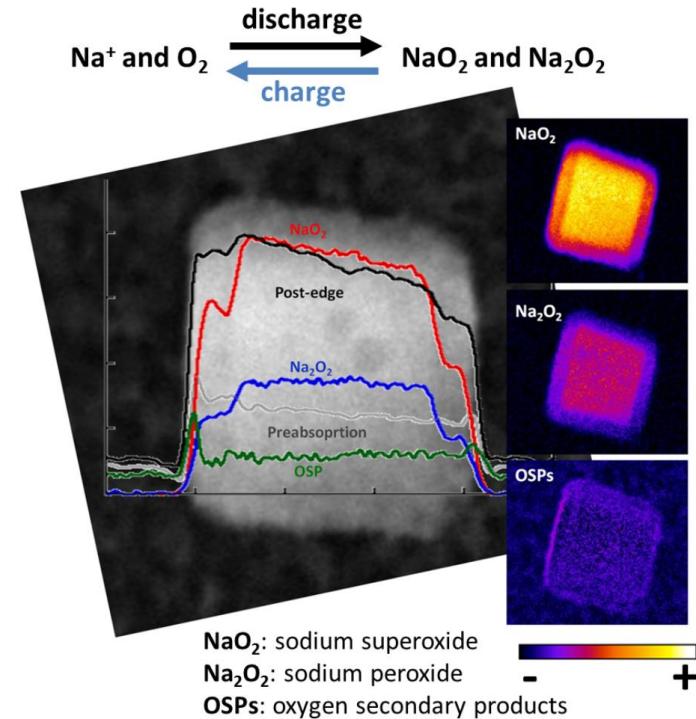
From the protein, to cell, to tissues



*Cell infected by covid-19*

## Chemistry and Material Science

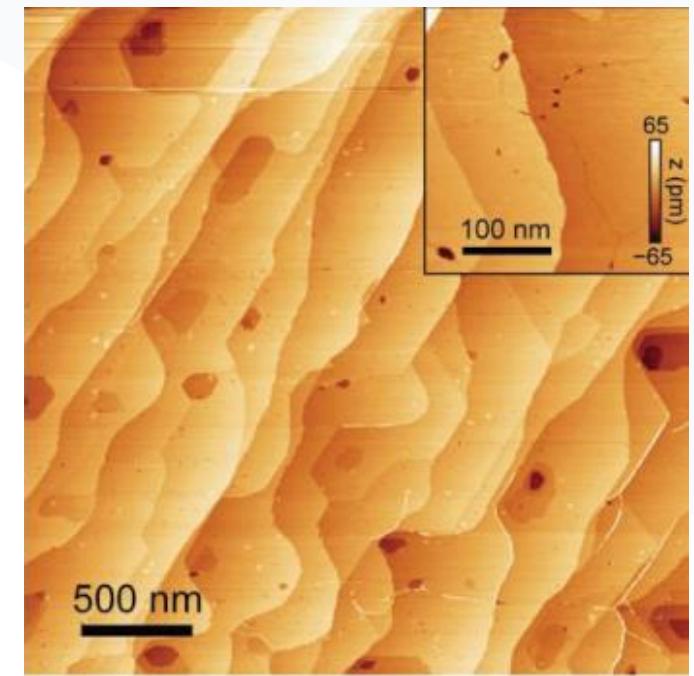
Energy material, catalysts, environment



*Battery developments*

## Electronic and Magnetic Structure of Matter

Advanced materials



*Nanomaterials for data storage*

# ALBA Synchrotron



TABLE 2-1: MAIN TECHNIQUES OFFERED BY ALBA BEAMLINES

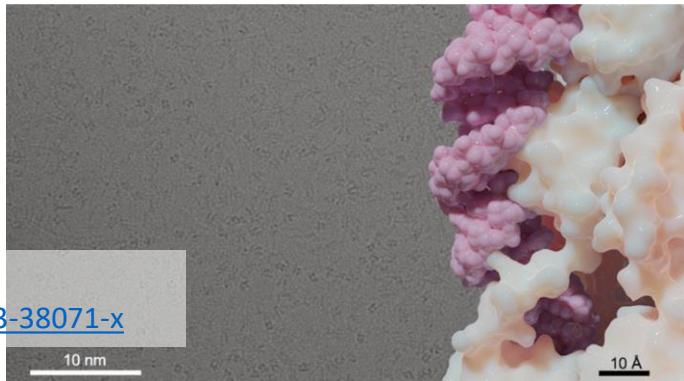
PORT AND NAME	SCIENTIFIC SECTION	MAIN TECHNIQUES AND STATUS
<b>BL01 - MIRAS</b>	Life Science	Infrared Spectroscopy & Microscopy – in operation
<b>BL06 - XAIRA</b>	Life Science	Macromolecular Microcrystallography – in commissioning; in operation in 2024
<b>BL09 - MISTRAL</b>	Life Science	Soft X-ray Microscopy - in operation
<b>BL13 - XALOC</b>	Life Science	Macromolecular Crystallography - in operation
<b>BL31 - FAXTOR</b>	Life Science	Fast X-ray Tomography and Radioscopy Beamline - being installed; starting operation in 2024
<b>BL20 - LOREA</b>	Electronic & Magnetic Structure of Matter	Angle Resolved Photoemission Spectroscopy – in operation
<b>BL24 - CIRCE</b>	Electronic & Magnetic Structure of Matter	Photoemission Spectroscopy and Near Ambient Pressure Photoemission – in operation
<b>BL29 - BOREAS</b>	Electronic & Magnetic Structure of Matter	Resonant Absorption and Scattering – in operation
<b>BL04 - MSPD</b>	Chemistry & Material Science	Materials Science and Powder Diffraction – in operation
<b>BL11 - NCD-SWEET</b>	Chemistry & Material Science	Non-Crystalline Diffraction – Small/wide Angle X-ray Scattering – in operation
<b>BL15 - 3SBAR</b>	Chemistry & Material Science	Surface Spectroscopy and Structure at 1 bar – in construction; starting operation in 2026
<b>BL16 - NOTOS</b>	Chemistry & Material Science	Absorption, Diffraction, Instrumentation innovation and development – in operation
<b>BL22 - CLÆSS</b>	Chemistry & Material Science	Core Level Absorption & Emission Spectroscopies – in operation
<b>BL25 - MINERVA</b>	Instrumentation & optics	Metrology and instrumentation – in operation in 2023

# Joint Electron Microscope Center at ALBA (JEMCA)

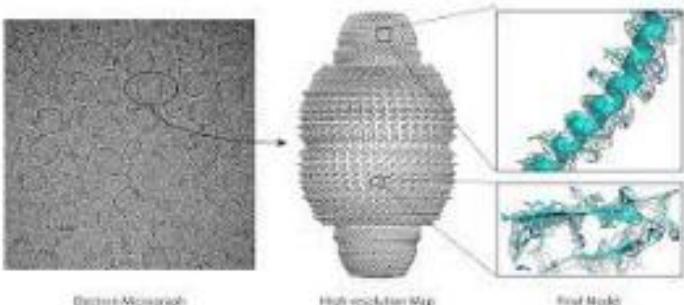
50% Funded through Catalan ERDF and 50% co-funded by different partners

## Life science Cryo-EM

- 200 kV Glacios cryo-TEM
- In operation . Receiving users (overbooking >2)



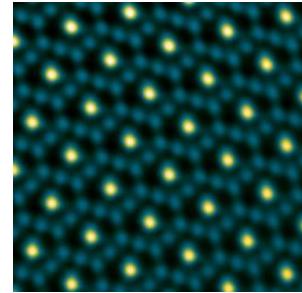
Nature Commun  
. DOI: [0.1038/s41467-023-38071-x](https://doi.org/10.1038/s41467-023-38071-x)



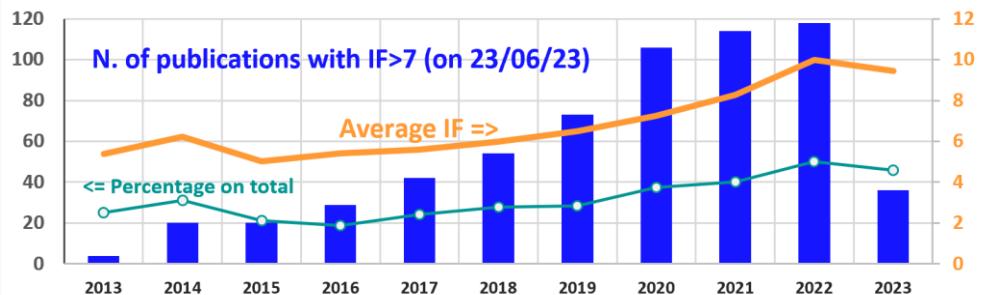
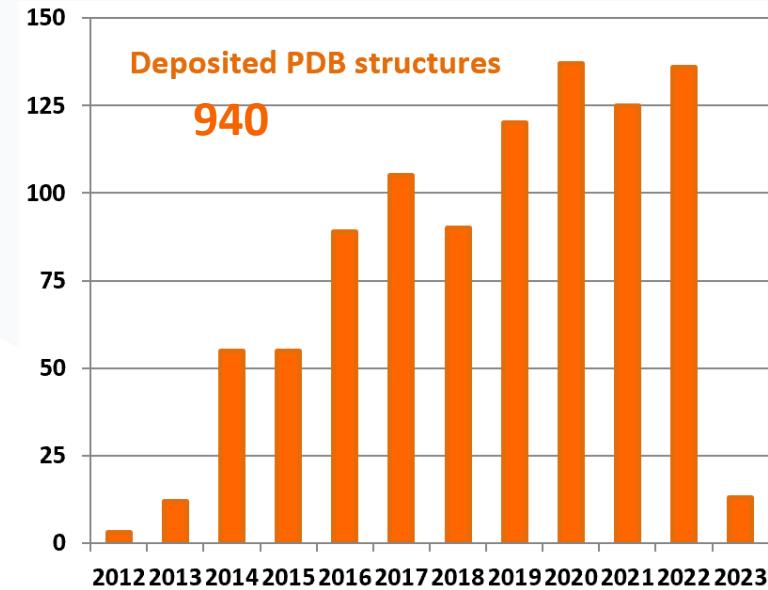
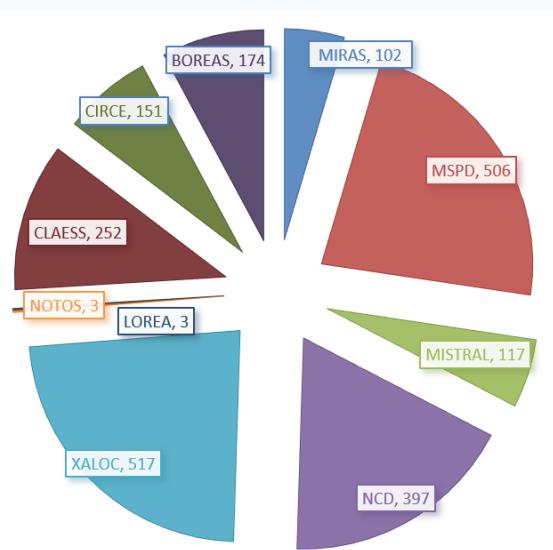
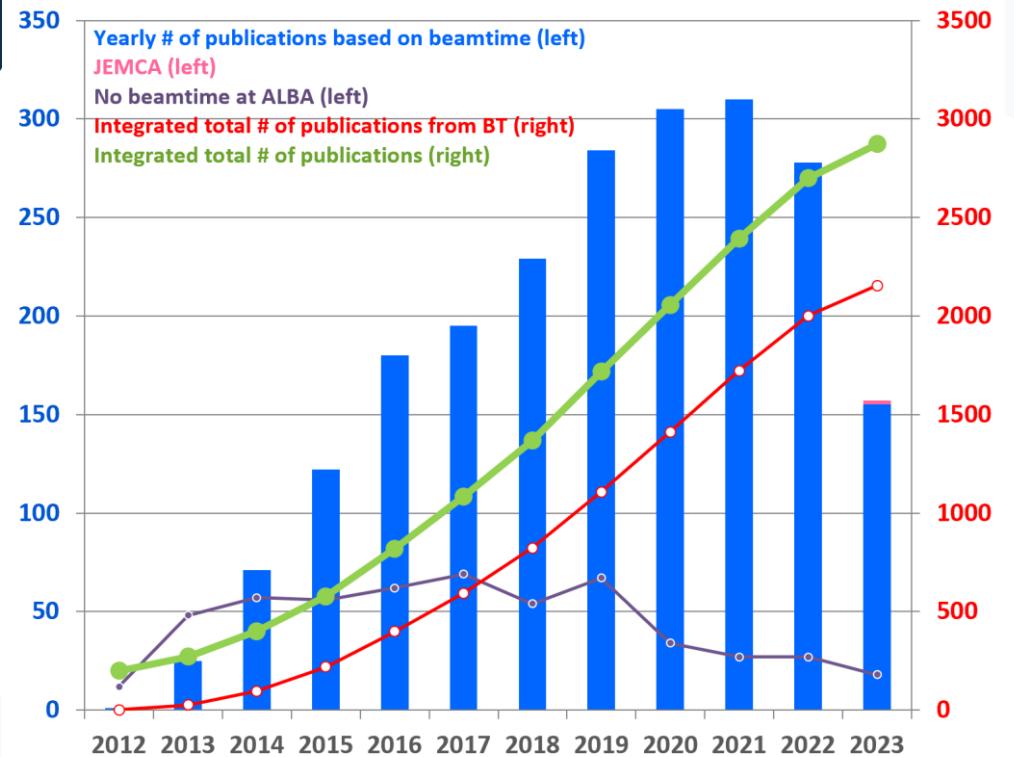
## Material Science TEM

- 60-300 keV Spectra (S)TEM + New EM to be installed in 1 year (InCAEM project)
- First external users in following weeks

Atomic resolution aberration corrected HAADF STEM images of one of the catalyst nanoparticles and a zoom out of the  $\text{Co}_2\text{FeO}_4$  cubic spinel structure



# ALBA scientific productivity



## Publications per BL

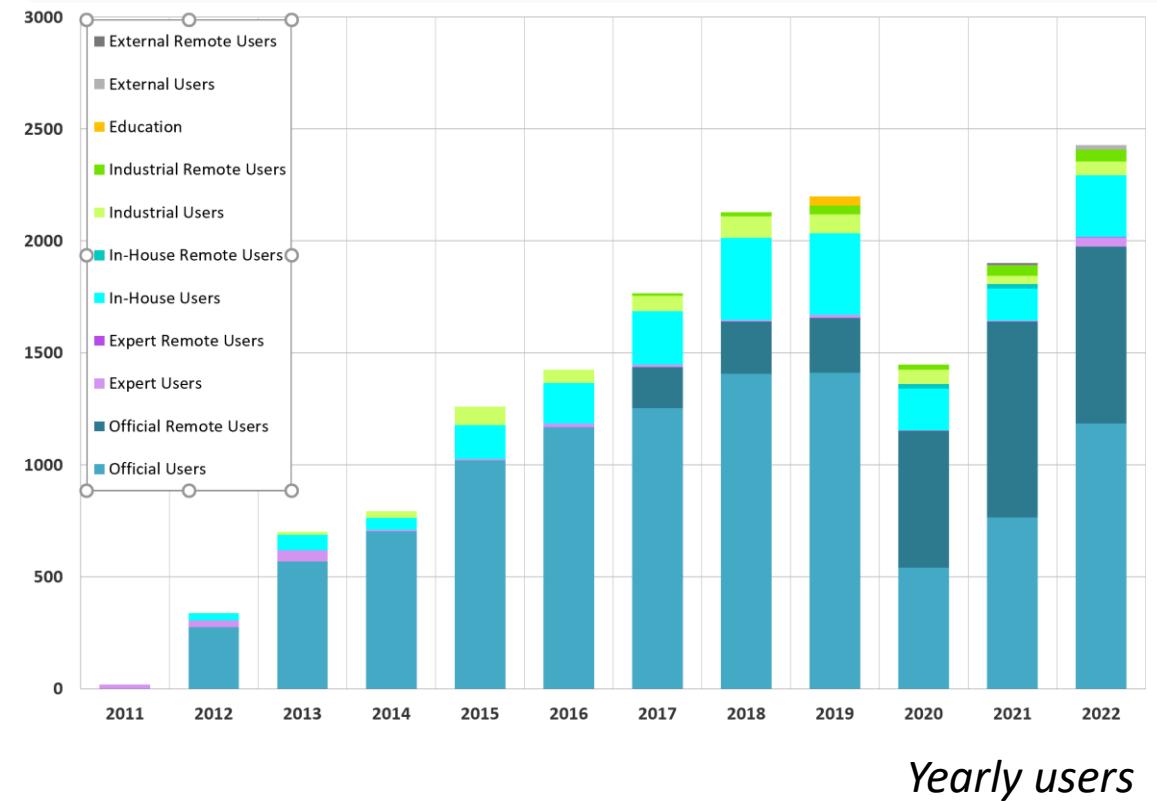
2020/2021: average # of publications per op. BL > 38  
 2021:  $\langle \text{IF} \rangle = 8.3$ ; 41% of publications with  $\text{IF} > 7$   
 2022:  $\langle \text{IF} \rangle = 10$ ; 50% of publications with  $\text{IF} > 7$

# ALBA scientific productivity

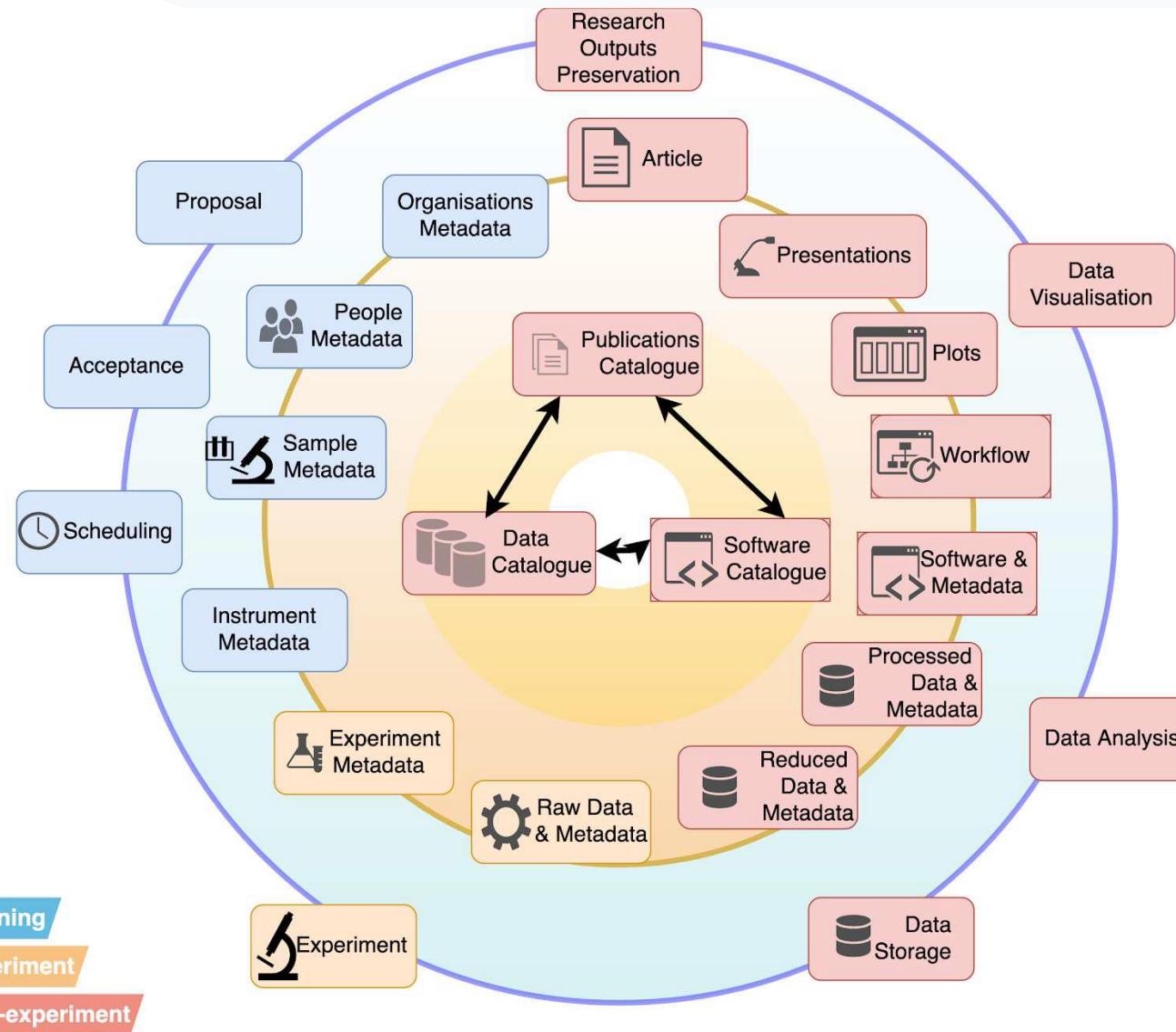


## ALBA key figures:

- +450 yearly experiments
- +2800 publications
- <IF>2022 = 10
- +900 Proteins in PDB
- + 2400 yearly user visits
- +500 industrial experiments



# Life Cycle of a PaN experiment



Planning  
Experiment  
Post-experiment

# Life Cycle of a PaN experiment



- There are many steps between the user sending a first proposal and achieving publication.
- Ensuring the data FAIRness requires data access and data integrity of every step.
- This role cannot be delegated to our users.
- RIs have to take a step forward and assume not only the custodian role as until now, but also data stewardship.
- Our users (scientists) must keep always the ownership and the IP of the data.

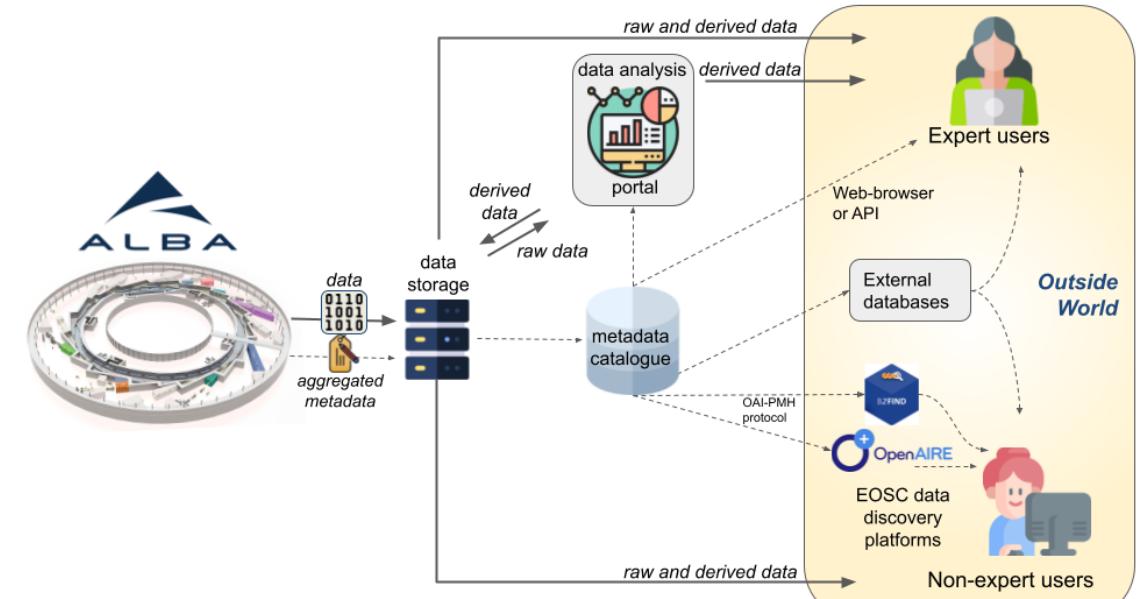
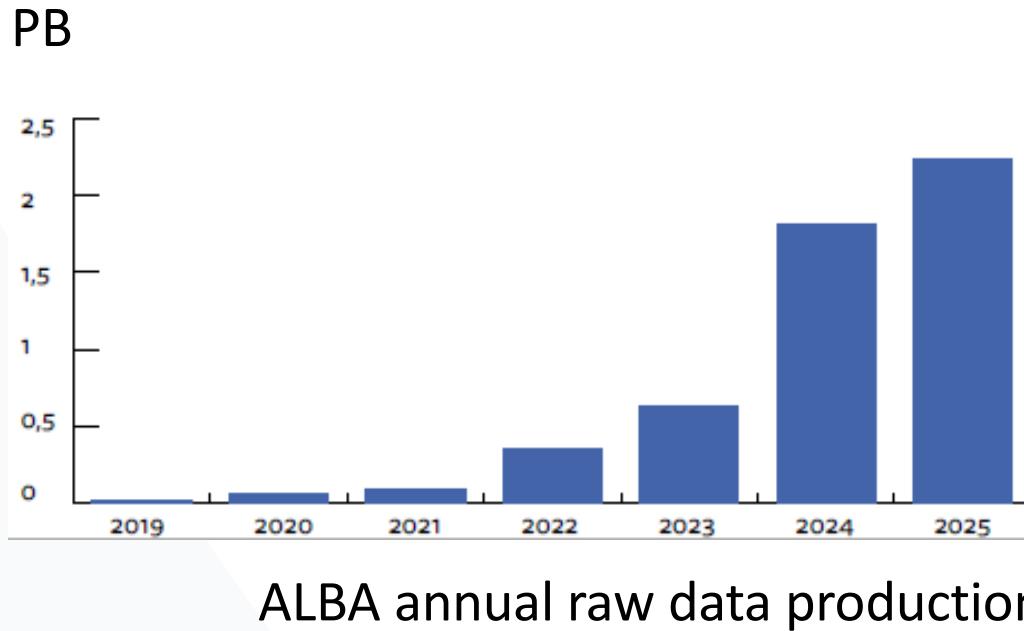
# Life Cycle of a PaN experiment



# Life Cycle of a PaN experiment



- ... But things are becoming more challenging.
- The volume of data generated by new data-intensive beamlines is too large for users to handle at their premises.



# Users + Facilities feel the weight of data

## Users

- Huge data volumes  
**Tera → Petabytes**
- Sample metadata
- Raw data quality
- Data processing
- Data exporting
- FAIR data

## Facilities

- Huge data volumes  
**Peta → Exabytes**
- Data acquisition
- Metadata collection
- Data curation
- Data archiving
- FAIR data



# LEAPS Data Strategy



Home > The European Physical Journal Plus > Article

## LEAPS data strategy

Regular Article | Open Access | Published: 17 July 2023 | 138, Article number: 617 (2023)

[Download PDF](#) You have full access to this open access article

### Three pillars:

1. Increasing efficiency of experiments
2. Open Science
3. Sustainability of solutions



THE EUROPEAN  
PHYSICAL JOURNAL PLUS

Eur. Phys. J. Plus (2023) 138:617  
<https://doi.org/10.1140/epjp/s13360-023-04189-6>

Regular Article



### LEAPS data strategy

Andy Götz<sup>1,a</sup>, Erwan le Gall<sup>2,b</sup>, Uwe Konrad<sup>3</sup>, George Kourousias<sup>4,c</sup>, Oliver Knodel<sup>3,d</sup>, Salman Matalgah<sup>5,e</sup>, Oscar Matilla<sup>6</sup>, Darren Spruce<sup>7,f</sup>, Ana Valceril Ortí<sup>8</sup>, Majid Ounsy<sup>9</sup>, Thomas H. Rod<sup>9</sup>, Frank Schluenzen<sup>10</sup>

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<sup>3</sup> Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

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<sup>5</sup> SESAME, Allan, Jordan

<sup>6</sup> ALBA Cerdanyola del Vallès, Spain

<sup>7</sup> MAXIV Laboratory, Lund University, Lund, Sweden

<sup>8</sup> SOLEIL, Saint-Aubin, France

<sup>9</sup> European Spallation Source ERIC, Copenhagen, Denmark

<sup>10</sup> DESY, Hamburg, Germany

Received: 17 December 2022 / Accepted: 14 June 2023

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**Abstract** The continuous evolution of photon sources and their instrumentation enables more and new scientific endeavors at ever increasing pace. This technological evolution is accompanied by an exponential growth of data volumes of increasing complexity, which must be addressed by maximizing efficiency of scientific experiments and automation of workflows covering the entire data lifecycle, aiming to reduce data volumes while producing FAIR and open data of highest reliability. This paper briefly outlines the strategy of the league of European accelerator-based photon sources user facilities to achieve these goals collaboratively in an efficient and sustainable way which will ultimately lead to an increase in the number of publications.



# ExPANDS & PaNOSC outcomes

## Photon – LEAPS

<https://leaps-initiative.eu>



**CERIC**

Central European  
Research Infrastructure  
Consortium

## Neutron - LENS

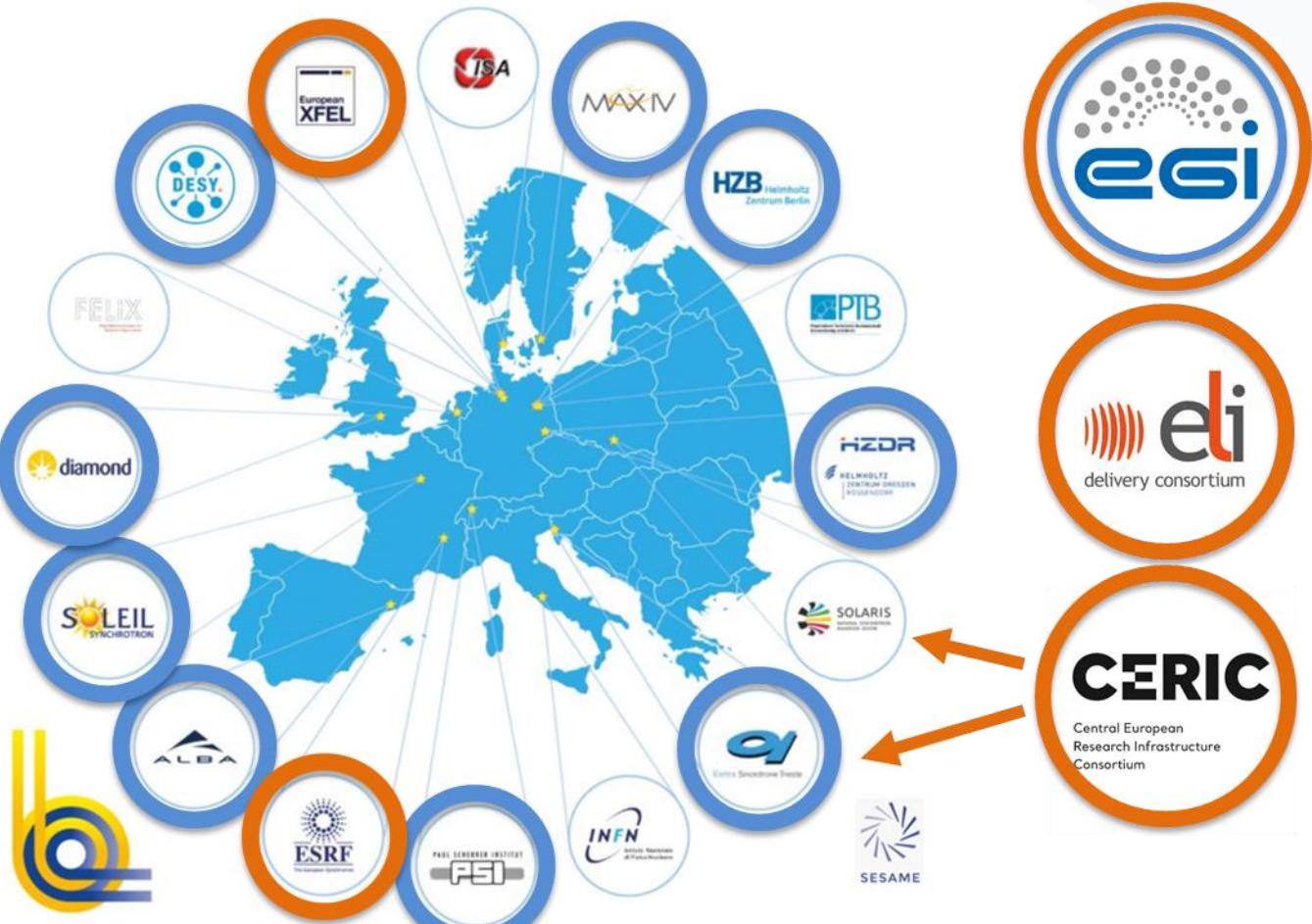
<https://lens-initiative.org>



# ExPANDS & PaNOSC outcomes

## Photon – LEAPS

<https://leaps-initiative.eu>



## Neutron - LENS

<https://lens-initiative.org>



 PaNOSC  
 ExPaNDS

PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.



# PaNOSC + ExPaNDS - 10 Main Achievements



## 1. FAIR data policy and Data Management Plan (DMP)

- We will use Active DMP:
  - An automatic DMP will be generated for every proposal
  - 50 of the 82 questions are automatically filled in.
  - Users can use the DMP to satisfy funders requirements.
  - DMP is the way to ensure that users can manage their data.

## 2. Standardised metadata ([Nexus/HDF5](#))

## 3. Guidelines for FAIR data self-evaluation



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Towards Open Science in PaN - O.Matilla

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## 4. Federated search API for PaN data catalogues

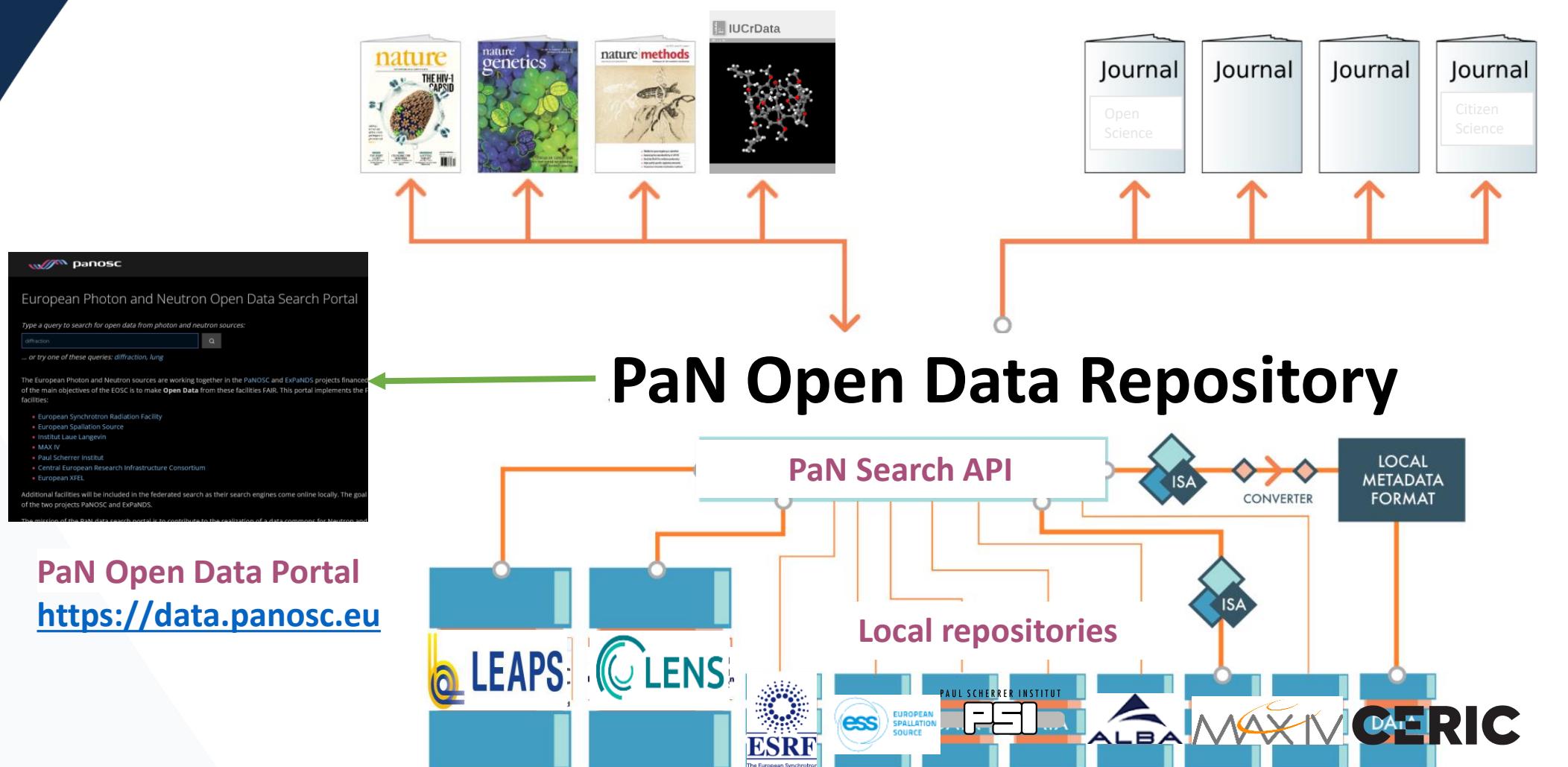
## 5. Open Data portal for searching + downloading data



PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

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# Open Data from federated PaN Repositories



PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.



## European Photon and Neutron Open Data Search Portal

Type a query to search for open data from photon and neutron sources:

... or try one of these queries: [diffraction](#), [lung](#)

The European Photon and Neutron sources are working together in the [PaNOSC](#) and [ExPaNDS](#) projects financed by the European Commission to build the **European Open Science Cloud**. One of the main objectives of the EOSC is to make **Open Data** from these facilities FAIR. This portal implements the F(indable) part of FAIR via a **federated search engine** from the following facilities:

- [European Synchrotron Radiation Facility](#)
- [European Spallation Source](#)
- [Institut Laue Langevin](#)
- [MAX IV](#)
- [Paul Scherrer Institut](#)
- [Central European Research Infrastructure Consortium](#)
- [European XFEL](#)

Additional facilities will be included in the federated search as their search engines come online locally. The goal is to include all photon and neutron facilities who provide open data by the end of the two projects PaNOSC and ExPaNDS.

The mission of the PaN data search portal is to contribute to the realization of a data commons for Neutron and Photon science. The search results provide a link to the landing page of the



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# PaN Data Portal - <https://data.panosc.eu>



panosc

diffraction

50+ documents found

Facility

all

Technique

Select a technique...

Chemical Formula

Incident Wavelength

min max nm

Incident Photon Energy

min max eV

Temperature

10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2 ↗ 0.900

Advances in long-wavelength native phasing at X-ray free-electron lasers

Long-wavelength pulses from the Swiss X-ray free-electron laser (XFEL) have been used for de novo protein structure determination by native single-wavelength anomalous diffraction (native-SAD) phasing of serial femtosecond crystallography (SFX) data. In this work,...

> Details, services ... Released by **PSI** on January 1st 2020

10.22003/XFEL.EU-DATA-700000-00 ↗ 0.900

Example Data

The European XFEL (EuXFEL) example data proposal contains experimental datasets from various original beam-times, currently covering the techniques of serial femtosecond crystallography (SFX), coherent diffraction imaging (single particle imaging, SPI), X-ray powder...

> Details, services ... Released by **EuXFEL** on January 1st 2018

10.5291/ILL-DATA.INTER-368 ↗ 0.900 { ? }

Measurement of 41K's coherent scattering length using powder diffraction

A screenshot of the PaN Data Portal interface. On the left, there is a sidebar with filters for Facility (set to 'all'), Technique (set to 'Select a technique...'), Chemical Formula, Incident Wavelength (min, max, nm), Incident Photon Energy (min, max, eV), and Temperature. The main area displays search results for 'diffraction'. The first result is titled 'Advances in long-wavelength native phasing at X-ray free-electron lasers' (DOI: 10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2), released by PSI on January 1st 2020. The second result is 'Example Data' (DOI: 10.22003/XFEL.EU-DATA-700000-00), released by EuXFEL on January 1st 2018. The third result is 'Measurement of 41K's coherent scattering length using powder diffraction' (DOI: 10.5291/ILL-DATA.INTER-368), with a question mark icon next to its score.



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# PaNOSC + ExPaNDS - 10 Main Achievements



6. Community **AAI UmbrellaId**
  - <https://umbrellaid.org>
7. **JupyterLab notebooks** and **Nexus/HDF5 files** visualisation
8. **Remote data analysis** with VISA + data analysis pipelines



**E x P a N D S**  
European Open Science Cloud Photon  
and Neutron Data Services



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Towards Open Science in PaN - O.Matilla

# VISA - Remote Data Processing/analyses platform



VISA  
[Home](#)  
[Help](#)

## New compute instance

Please fill in the details below to create a new compute instance

### Experiments

Select the experiments you wish to associate with your compute instance

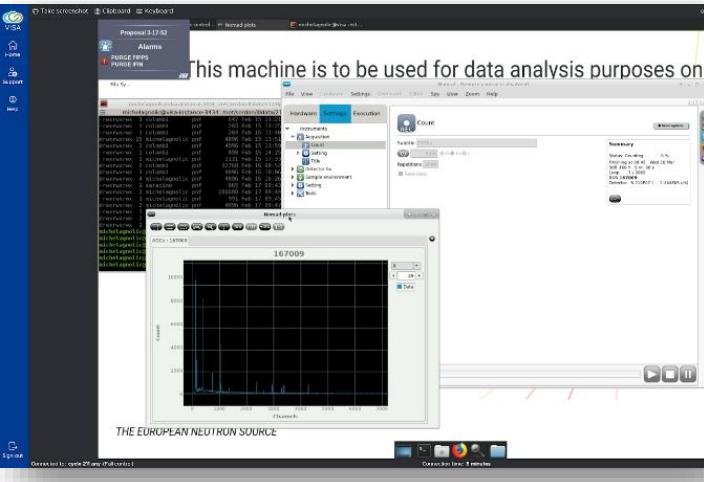
Instance not associated to any specific experiments

### Computing Environment

Choose an environment



Desktop staging



Desktop



Bliss

Choose hardware requirements

4 Cores

4GB memory

esrf.medium

8 Cores

16GB memory

esrf.large

16 Cores

32GB memory

esrf.gpu.a40

32 Cores

128GB memory

esrf.gpu.a40.xlarge

**Infrastructure for remote data processing / analysis**

**Users dedicated VM**

**Access to data**

**Access to Provisioning of scientific SW using CVMFS and Containers**

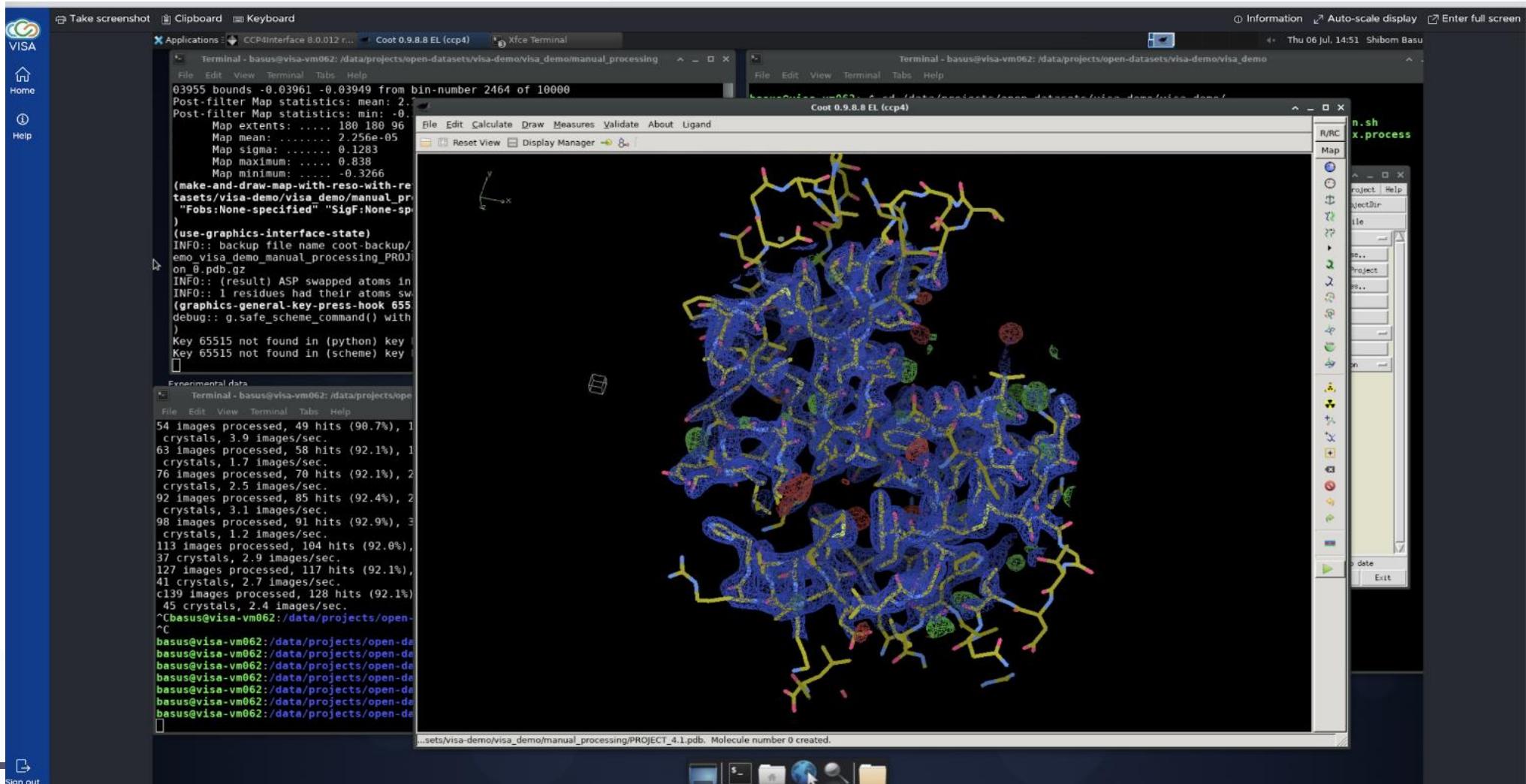
**Access to the GPUs, HPC cluster**

**Infrastructure based on OpenStack**

**Development led by ILL in the scope of the PaNOSC project**



# Example of DaaS using VISA



# PaNOSC + ExPaNDS - 10 Main Achievements



6. Community **AAI UmbrellaId**
  - <https://umbrellaid.org>
7. **JupyterLab notebooks** and **Nexus/HDF5 files** visualisation
8. **Remote data analysis** with VISA + data analysis pipelines
9. **Simulation** software for simulating experimental data (ViNYL)
10. **PaN-learning** platform ([pan-learning.org](http://pan-learning.org))



**E x P a N D S**  
European Open Science Cloud Photon  
and Neutron Data Services



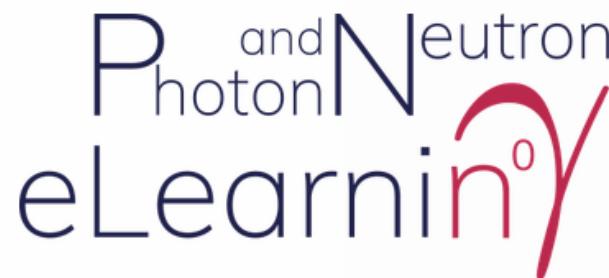
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## Achieving 100% Open Educational Resources:

1. Publish training material on pan-training.org
2. Develop learning material on pan-learning.org

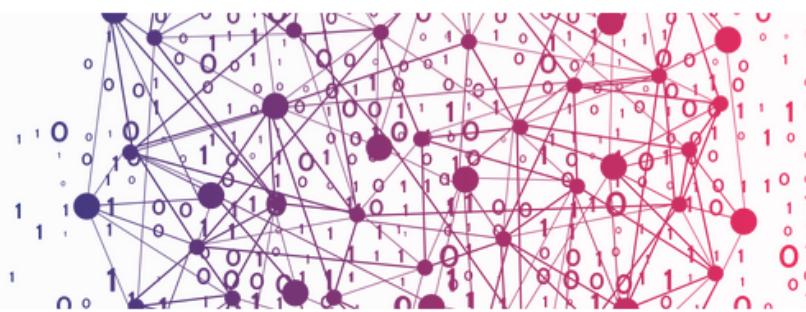
The screenshot shows a dark blue header bar with a white navigation menu. On the left is a red stylized logo. To its right are the menu items: Catalogue, e-Learning, Events, About, and You are not logged in. (Log in).



### Welcome to the e-Learning platform

This e-Learning platform hosts free education and training for scientists and students.

Below you will find courses on both the theory of photon and neutron scattering  
and how to use python code or software for data reduction and modelling.



Login

Username

Password

**E x P a N D S**  
European Open Science Cloud Photon  
and Neutron Data Services



<https://e-learning.pan-training.eu/moodle/>

# Workshop on leveraging Open Data for ML

<https://indico.synchrotron-soleil.fr/event/67/>

A blue-toned background image featuring a stylized profile of a human head containing a glowing yellow circuit board brain. To the left, there are two yellow padlocks, one open and one closed, set against a backdrop of hexagonal binary code and data points.

Leveraging open data from PaN facilities for machine learning

Oct 17 – 18, 2023  
Europe/Paris timezone

Enter your search term

During the last decade, most European Photon and Neutron (PaN) facilities have adopted **open data policies**, making data available for the benefit of the entire scientific community. At the same time, **machine learning** (ML) is seen as an essential tool to address the exponential growth of data volumes from PaN facilities.



# Evolution of Synchrotron Radiation Sources



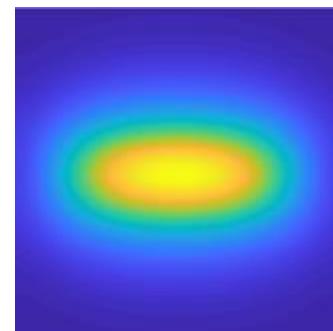
Increase in Brilliance

Increase in Resolution Power

Increase in Coherence

Increase in Data management capacity

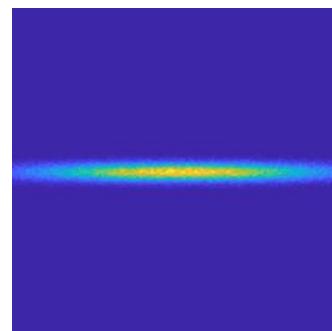
*Representation of  
photon beam on  
sample* →



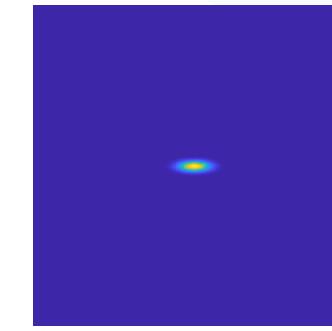
1960

1<sup>st</sup>  
Gen

1970



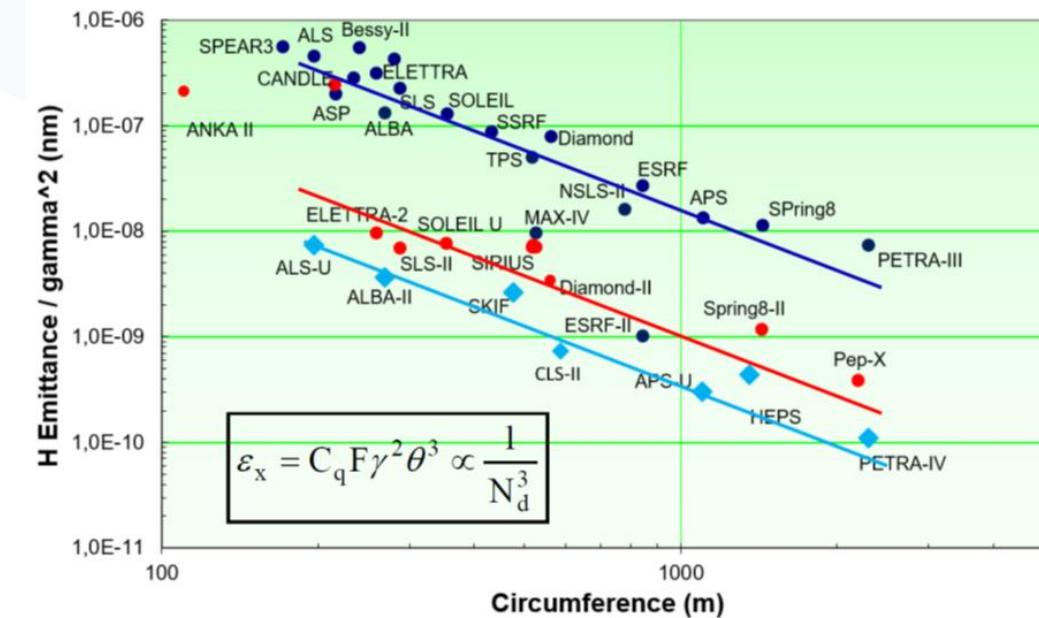
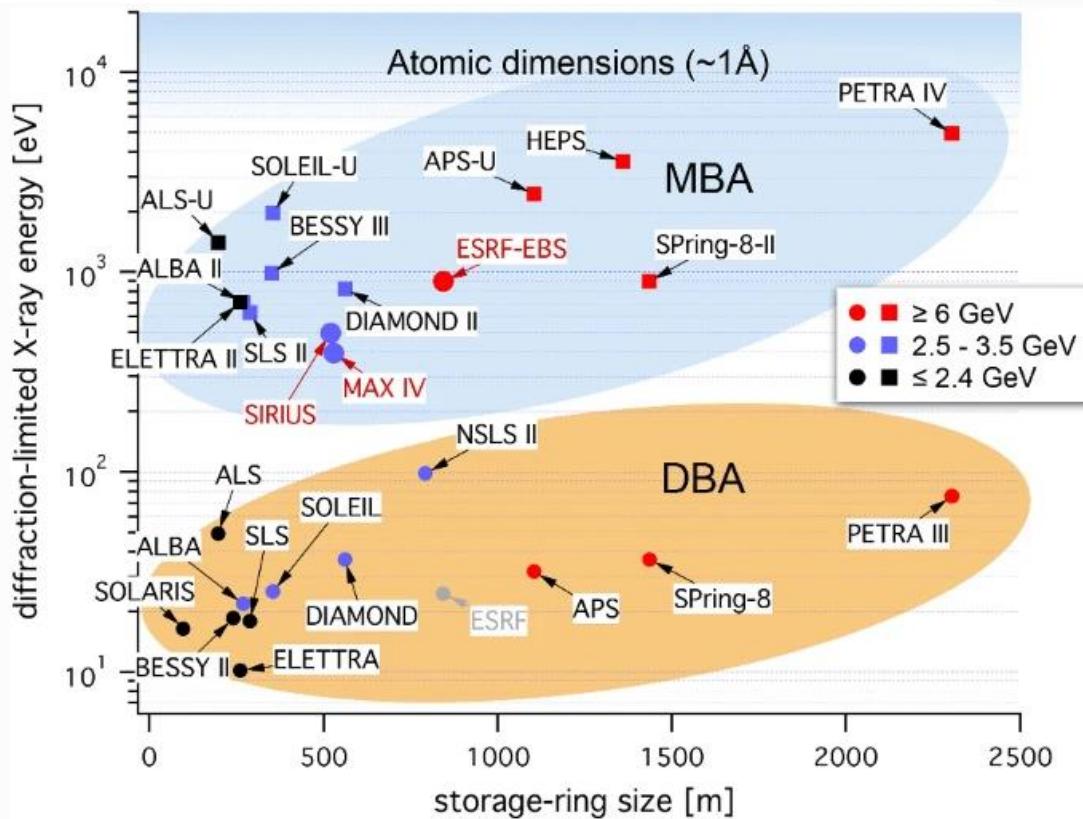
1990



2020

4<sup>th</sup> Gen

# Towards 4<sup>th</sup> Generation light sources

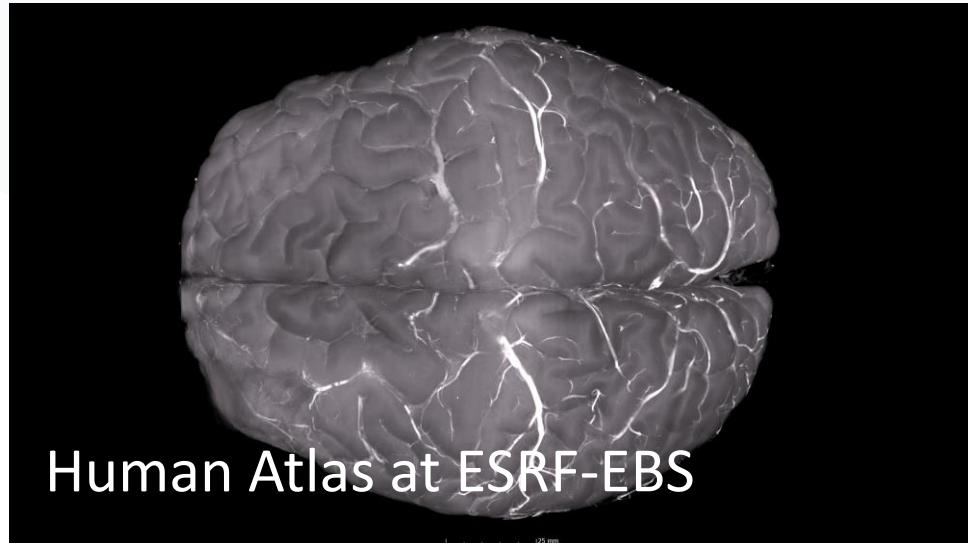


Abela, R., Biscari, C., Daillant, J. et al. The European strategy for accelerator-based photon science. *Eur. Phys. J. Plus* **138**, 355 (2023).  
<https://doi.org/10.1140/epjp/s13360-023-03947-w>

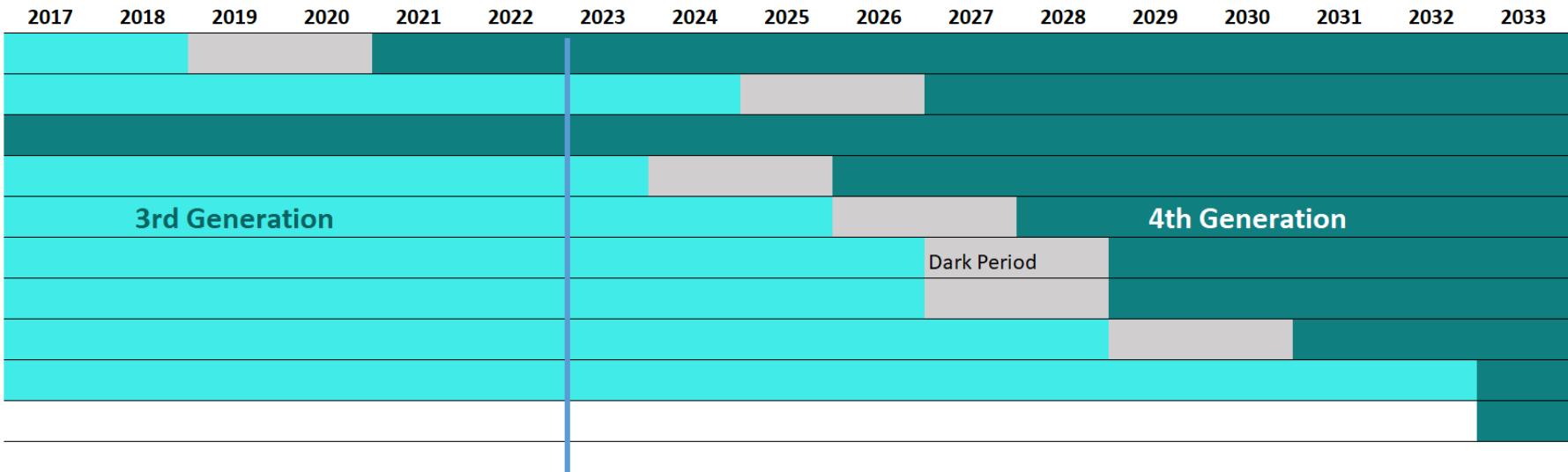
# Evolution from 3<sup>rd</sup> to 4<sup>th</sup> generation in Europe



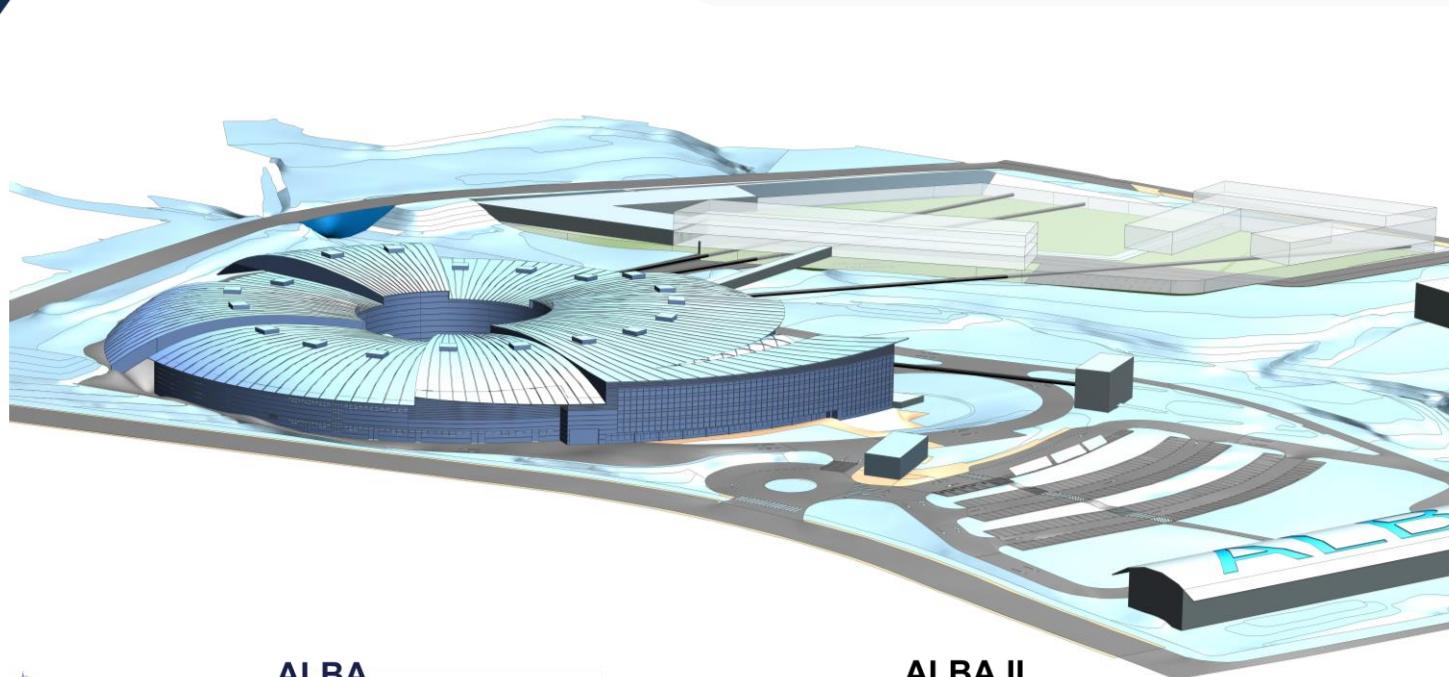
All synchrotrons in Europe (and in America and Asia) are evolving towards the 4<sup>th</sup> generation



ESRF (Europa) - 6 GeV  
PETRA III (Alemania) - 6 GeV  
MAX IV (Suecia) - 3 GeV  
SLS (Suiza) - 2.7 GeV  
ELETTRA (Italia) 2.4 GeV  
Diamond (UK) - 3.5 GeV  
Soleil (Francia) 2.75 GeV  
ALBA (España) 3 GeV  
BESSY II (Alemania) 1.7GeV  
BESSY III (Alemania) 2.5 GeV



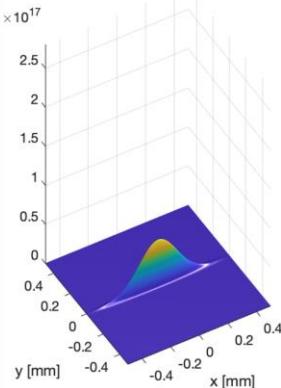
# ALBA II



ALBA

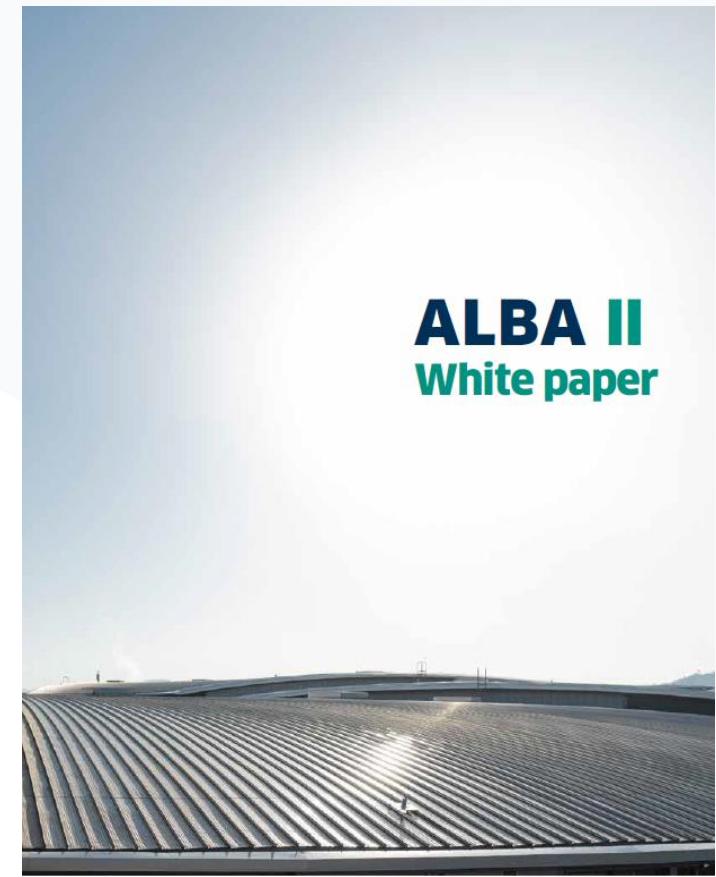
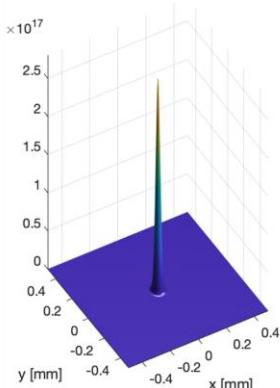
Flux Distr. E=12654 eV

e- beam  
transverse  
dimensions:  
 $50 \mu\text{m}$   
(like the diameter  
of a hair,  
and like the eye  
resolution power)



ALBA II

Flux Distr. E=12654 eV

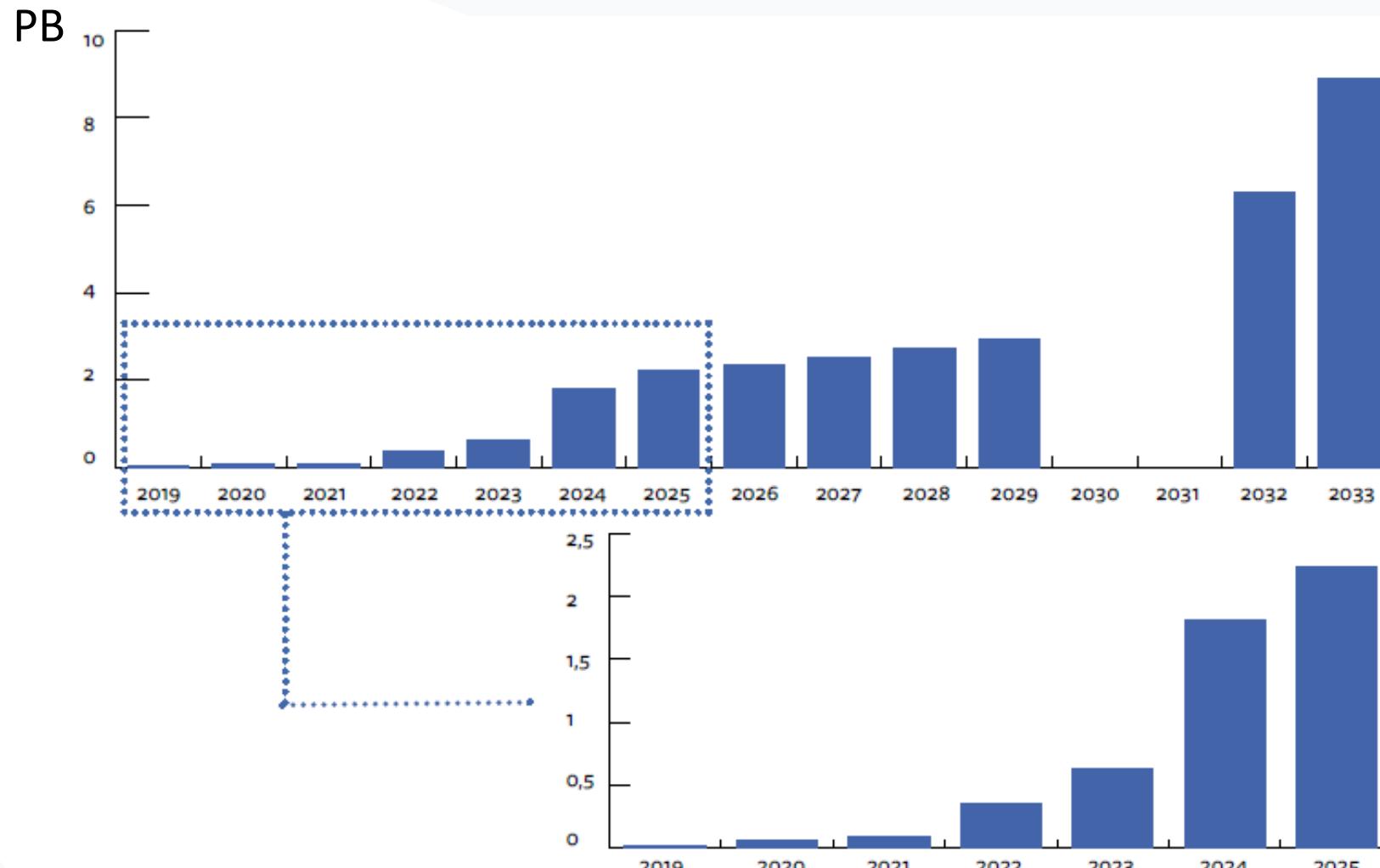


**ALBA II**  
White paper



<https://www.cells.es/en/science-at-alba/alba-ii-upgrade/alba-ii>

# Data Produced in ALBA II



ALBA annual raw data production

# IT infrastructures @ ALBA

Evolución del Sincrotrón ALBA			
	2023 - ALBA	2029 - ALBA	2032 – ALBA II
Aceleradores	3 <sup>a</sup> generación	3 <sup>a</sup> generación ALBA II preparado para la instalación	4 <sup>a</sup> generación Mayor brillanza, resolución, coherencia
Beamlines	10 operativas 4 en construcción	14 operativas 3 en avanzado estado de construcción	17 operativas (dos extra largas). Potencial de ampliar hasta 26 líneas
Otras capacidades experimentales	JEMCA (2 TEM con colaboradores), laboratorio de baterías	JEMCA e InCAEM (3 TEM + 3 microscopios) laboratorio de catálisis	Se añaden capacidades con laboratorios en los nuevos terrenos en colaboración con otros institutos
Infraestructuras almacenamiento y análisis de datos	Almacenamiento: 2 PB Procesado CPU: 500 Procesado GPU: 12.500	Almacenamiento: 18 PB Procesado CPU: 13.000 Procesado GPU: 190.000	Almacenamiento: 34 PB Procesado CPU: 28.000 Procesado GPU: 400.000
Usuarios, experimentos y tiempo de luz de sincrotrón anual	2500 usuarios / 300 experimentos / 46.500 h para usuarios	3500 usuarios / 400 experimentos / 65000 h para usuarios	4250 usuarios / 500 experimentos / 79 000 h para usuarios
Publicaciones	300 / año	400 / año	500 / año
Uso industrial	60 experimentos/año	85 experimentos/año	100 experimentos/año
Impulso innovación	[Hablar de Patentes, contratos mayores con componente innovación]	[Hablar de Patentes, contratos mayores con componente innovación]	[Hablar de Patentes, contratos mayores con componente innovación]

- To provide service to the ALBA II and the JEMCA.
  - Including acquisition, processing and DaaS services to the user.
- EOSC required services are difficult to be seized.

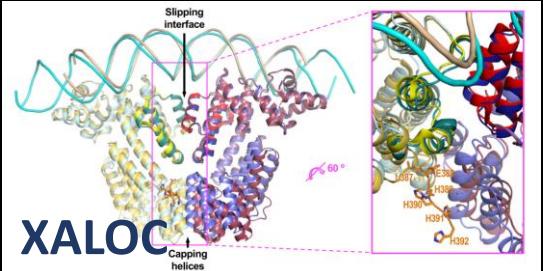
<b>Infraestructuras almacenamiento y análisis de datos</b>	<b>Almacenamiento: 2 PB</b> <b>Procesado CPU: 500</b> <b>Procesado GPU: 12.500</b>	<b>Almacenamiento: 18 PB</b> <b>Procesado CPU: 13.000</b> <b>Procesado GPU: 190.000</b>	<b>Almacenamiento: 34 PB</b> <b>Procesado CPU: 28.000</b> <b>Procesado GPU: 400.000</b>
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- The PaN community is taking important steps towards Open Science.
  - Common Data Catalogues tools (ICAT, SCICAT) have been developed
  - PaN Data Portal is operative (and compatible with Open AIRE and B2FIND)
  - All facilities are in the process of linking their acquired data, creating a federated repository.
  - The Common DaaS platform (VISA) is functional, but it still has a long development roadmap ahead.

- Future challenges:
  - The volume of data is exploding (every facility will generate 10s PB/year).
  - Such volumes will require new techniques for leveraging Open Data or transferring/processing data from various sources.
  - Data Analysis algorithms must be optimized for this new scenario.
  - As of 2023, it appears to be a Herculean task to unify Ontologies, Data formats, and data analysis tools for every field.

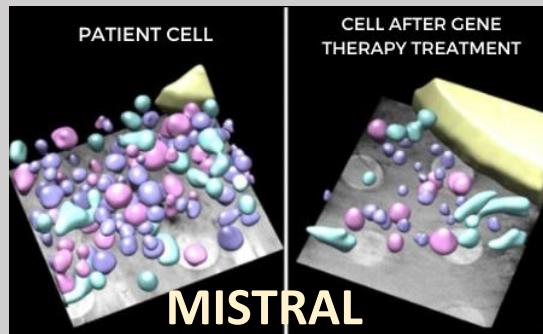
# Some highlights from the scientific results published in the last months

## MECHANISM OF ACTION OF THE ARBITRIUM COMMUNICATION SYSTEM IN SPBETA PHAGES



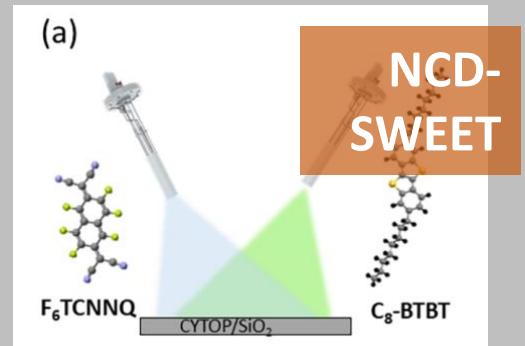
*Nature Communications* volume 13,  
Article number: 3627 (2022)

## GENE THERAPY PROVED AGAINST MUSCULAR DYSTROPHY



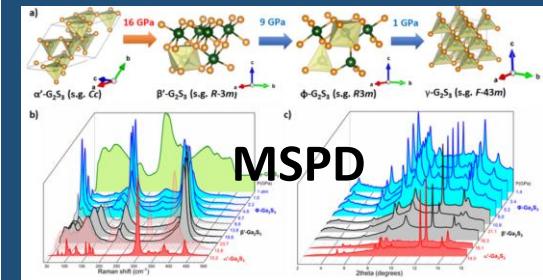
*Int. J. Mol. Sci.* 2022, 23,  
[7651doi.org/10.3390/ijms23147651](https://doi.org/10.3390/ijms23147651)

## CHARGE-TRANSFER COMPLEXES IN ORGANIC FIELD-EFFECT TRANSISTORS



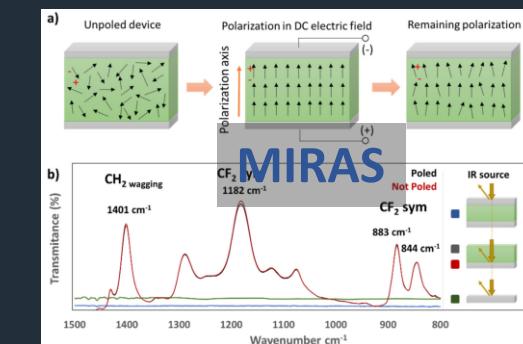
*Applied materials and interfaces*  
10.1021/acsami.2c09168

## PRESSURE-INDUCED PARAELECTRIC TO FERROELECTRIC PHASE TRANSITION



*Chem. Mater.* (2022), 34, 13, 6068–6086. <https://doi.org/10.1021/acs.chemmater.2c01169>

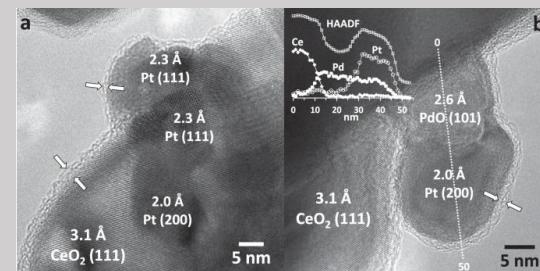
## CONTROLLED POLING OF A FULLY 3D PRINTED PIEZOELECTRIC DEVICE



*J. Mater. Chem. C*, 2022, 10, 11555

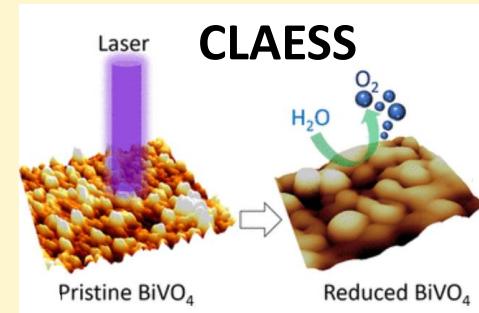
## CATALYST TO REMOVE EMISSIONS OF METHANE

### CIRCE (+CLAESS & MSPD)



*Nat Commun* 13, 5080 (2022).  
[doi.org/10.1038/s41467-022-32765-4](https://doi.org/10.1038/s41467-022-32765-4)

## LIGHT-INDUCED SPIN SWITCHING DEVICE WITH APPLICATIONS IN SPINTRONICS



*ACS Applied Materials & Interfaces*,  
2022, 14, 29, 33200–33210

### BOREAS



*Advanced Materials* (2022).  
[doi.org/10.1002/adma.202202551](https://doi.org/10.1002/adma.202202551)