NOMAD: a federated data infrastructure transforming materials-science laboratories

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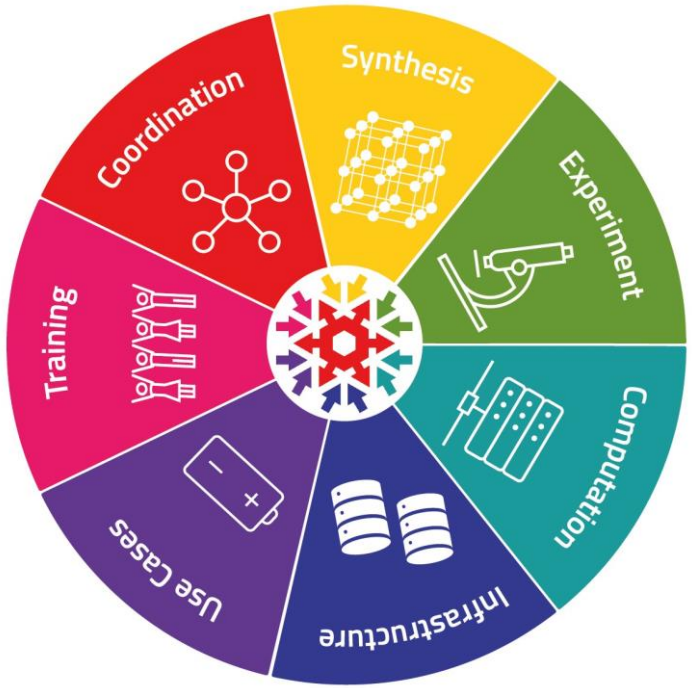
HU Berlin | FAIRmat | NOMAD

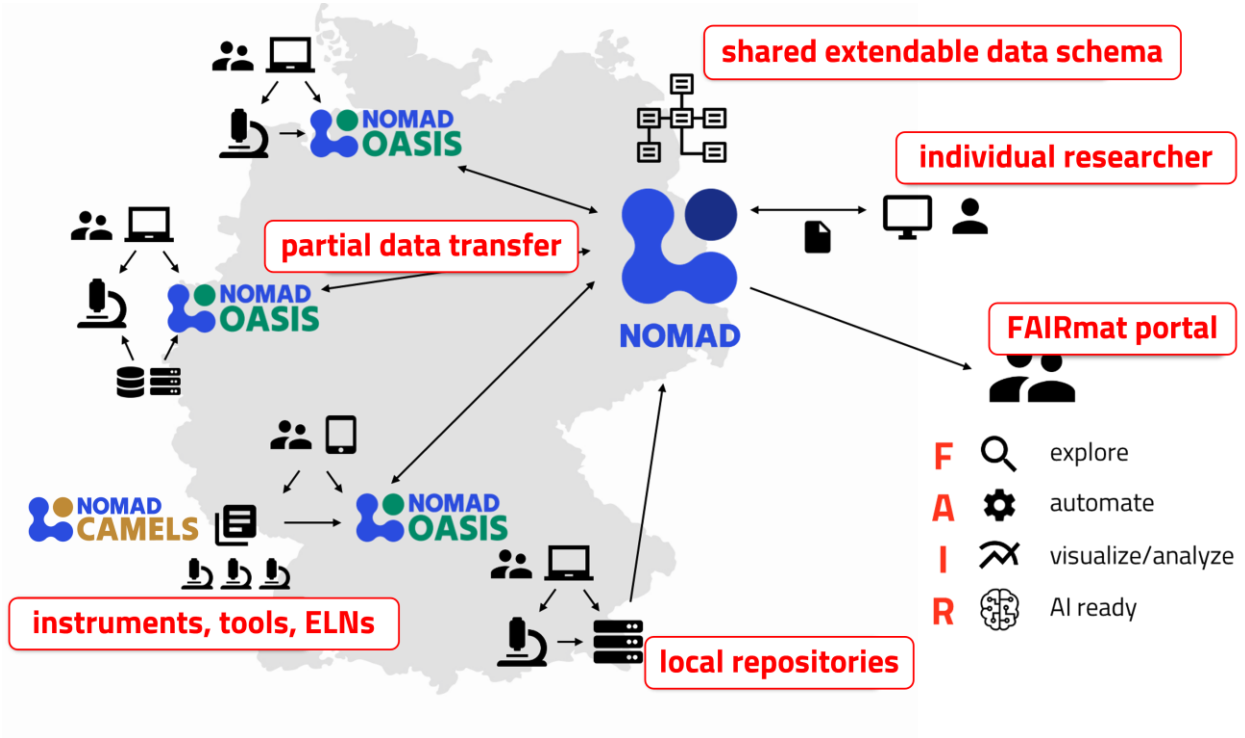
FORSCHUNGSDATEN@RMU
October 30, 2025

FAIRmat

What is FAIRmat

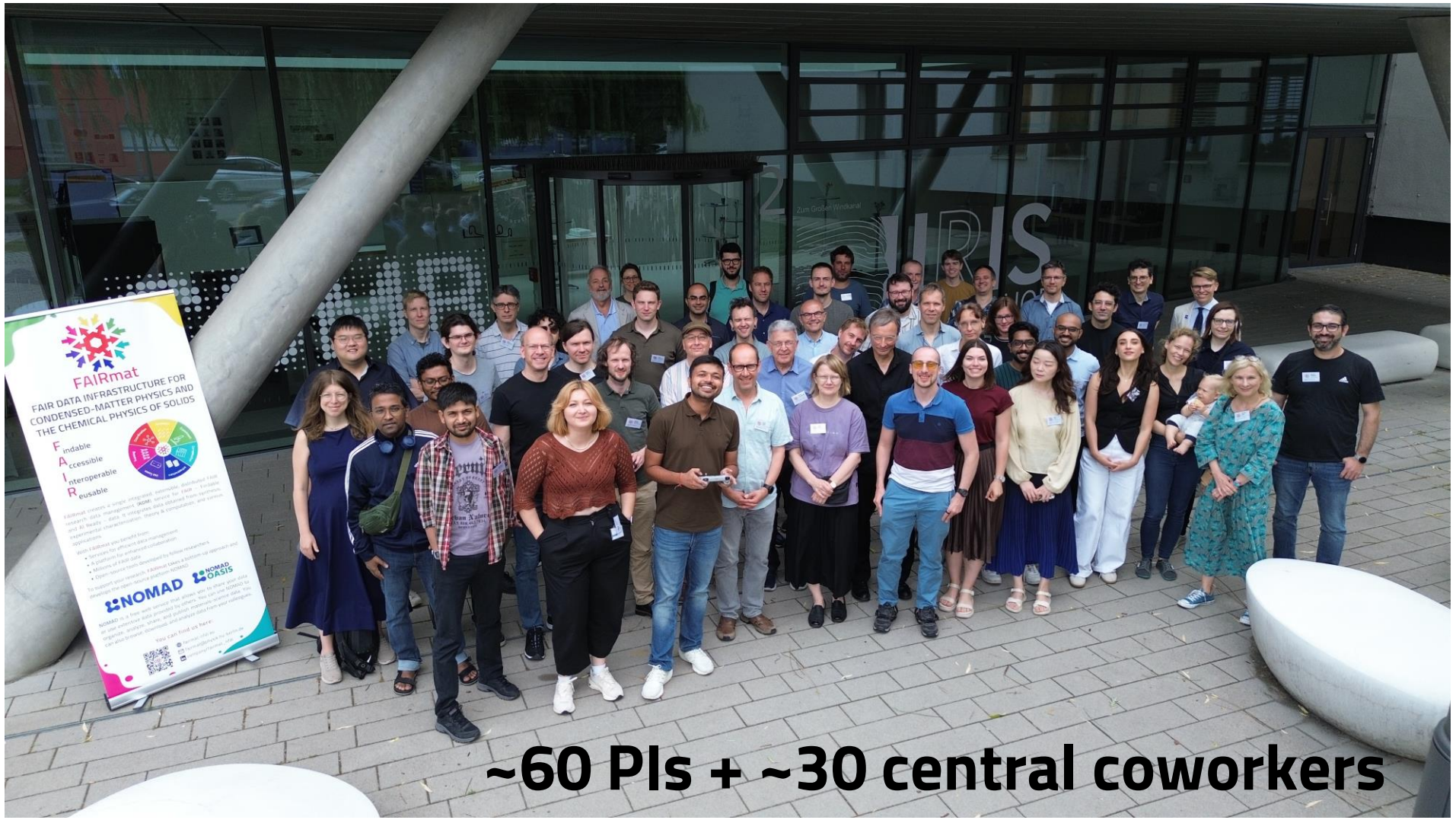
FAIRmat is the NFDI consortium developing a FAIR federated data infrastructure for solid-state physics.





NFDI: National (German) Research Data Infrastructure

The FAIRmat team

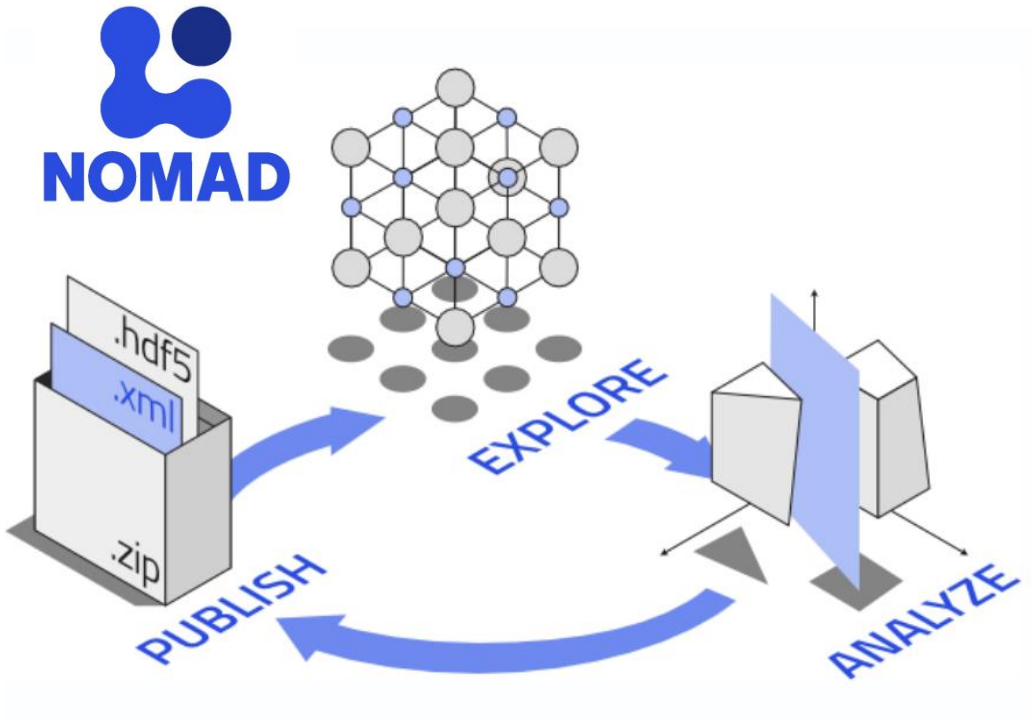


The FAIRmat Hub in Berlin

NOMAD comes in two flavours

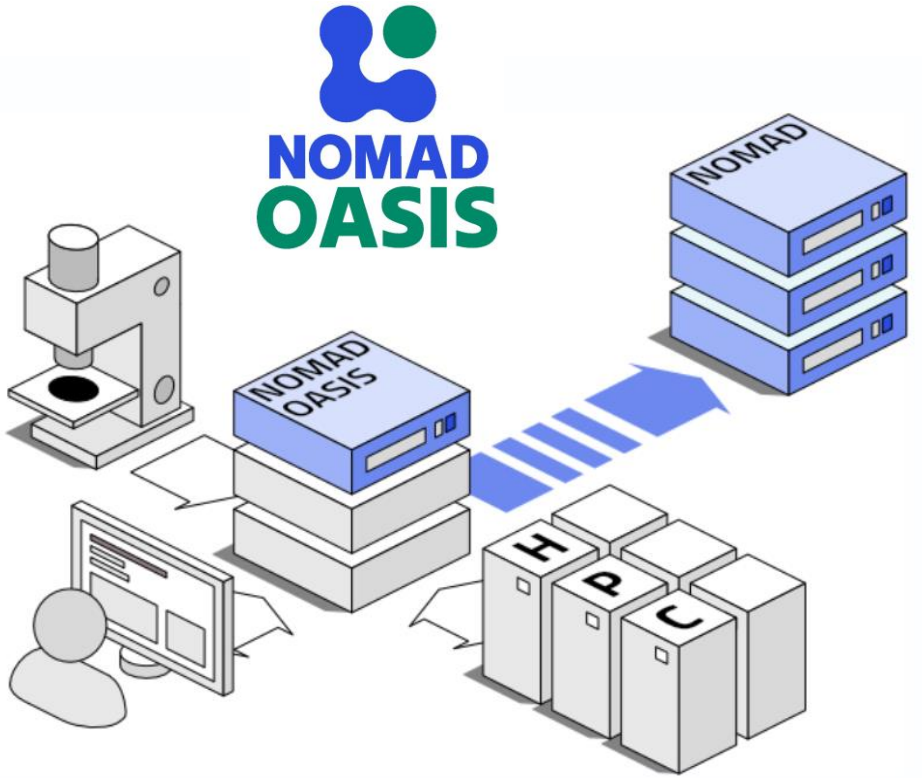
Publish & explore data

Central RDM platform



Manage your lab

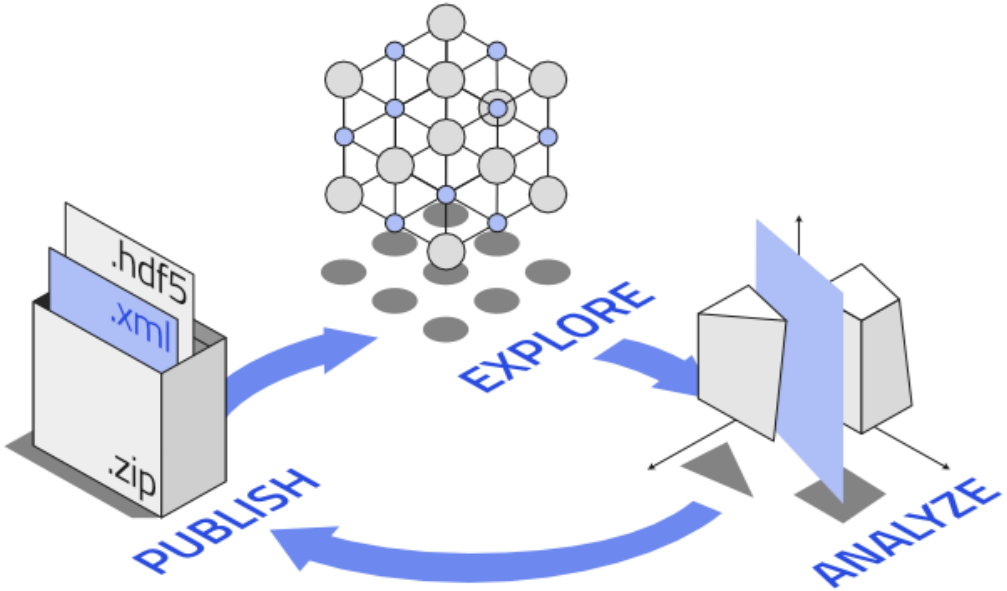
Local RDM tool | ELN



NOMAD

Web-based software for FAIR research data management in materials science.

- Processes files to extract structured data and rich metadata.
- Explore and reuse millions of FAIR data from different sources.



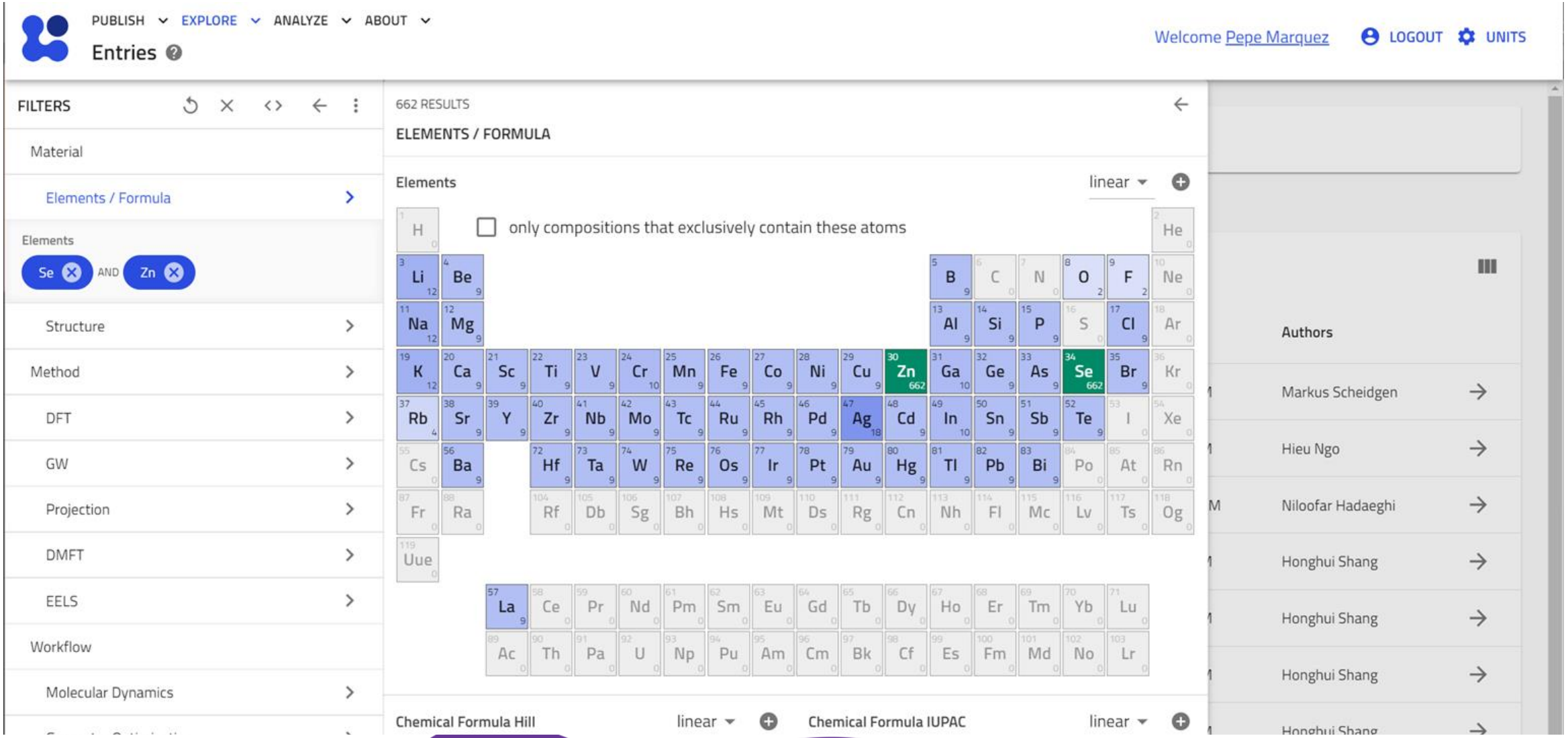
UPLOADED ENTRIES	UPLOADED FILES	REGISTERED USERS
19,221,889	**113.4 TB**	**> 4000**

https://nomad-lab.eu/

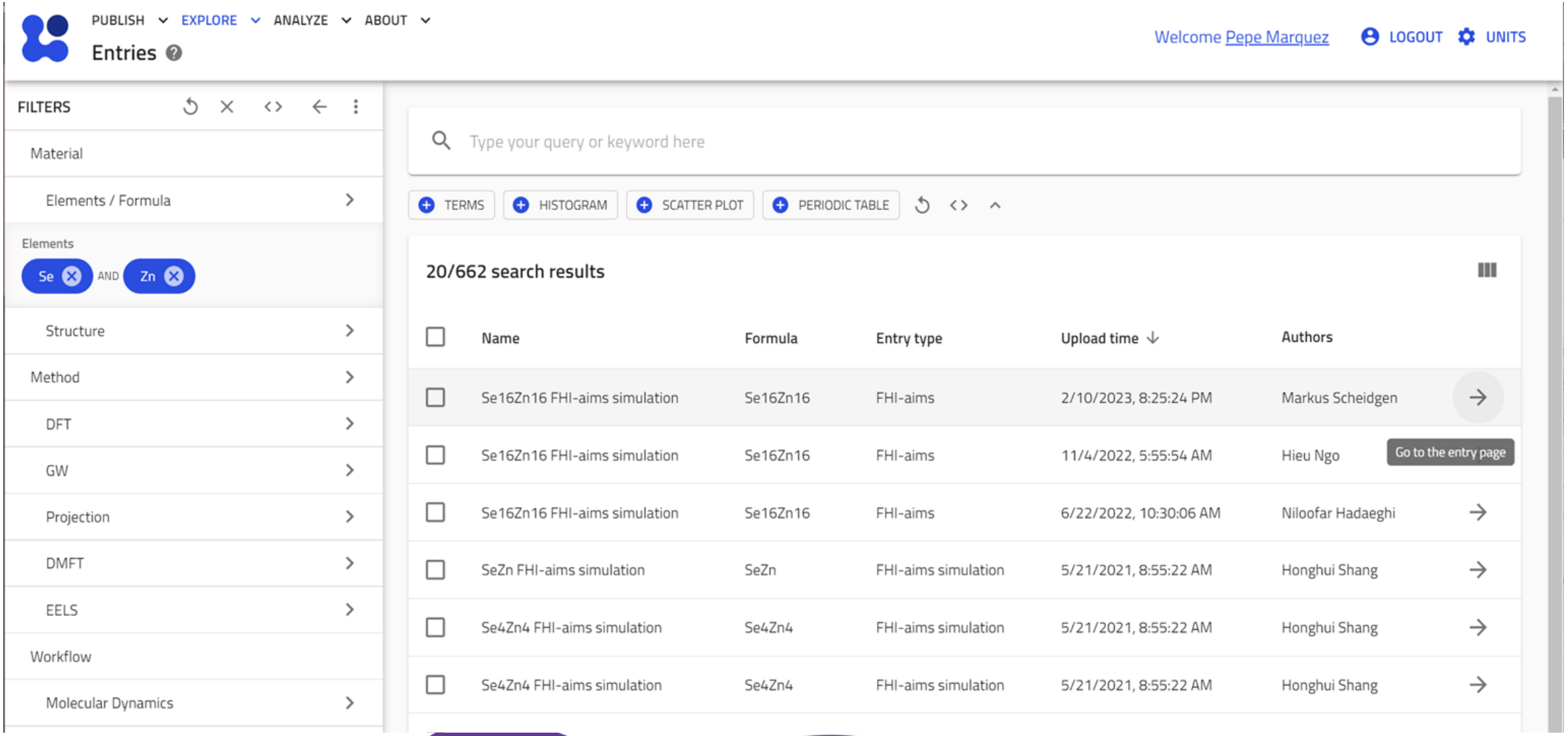
NOMAD core functionalities

Query the repository by element, material, or method, using *NOMAD's customized GUI* dashboard or programmatically.

NOMAD core functionalities



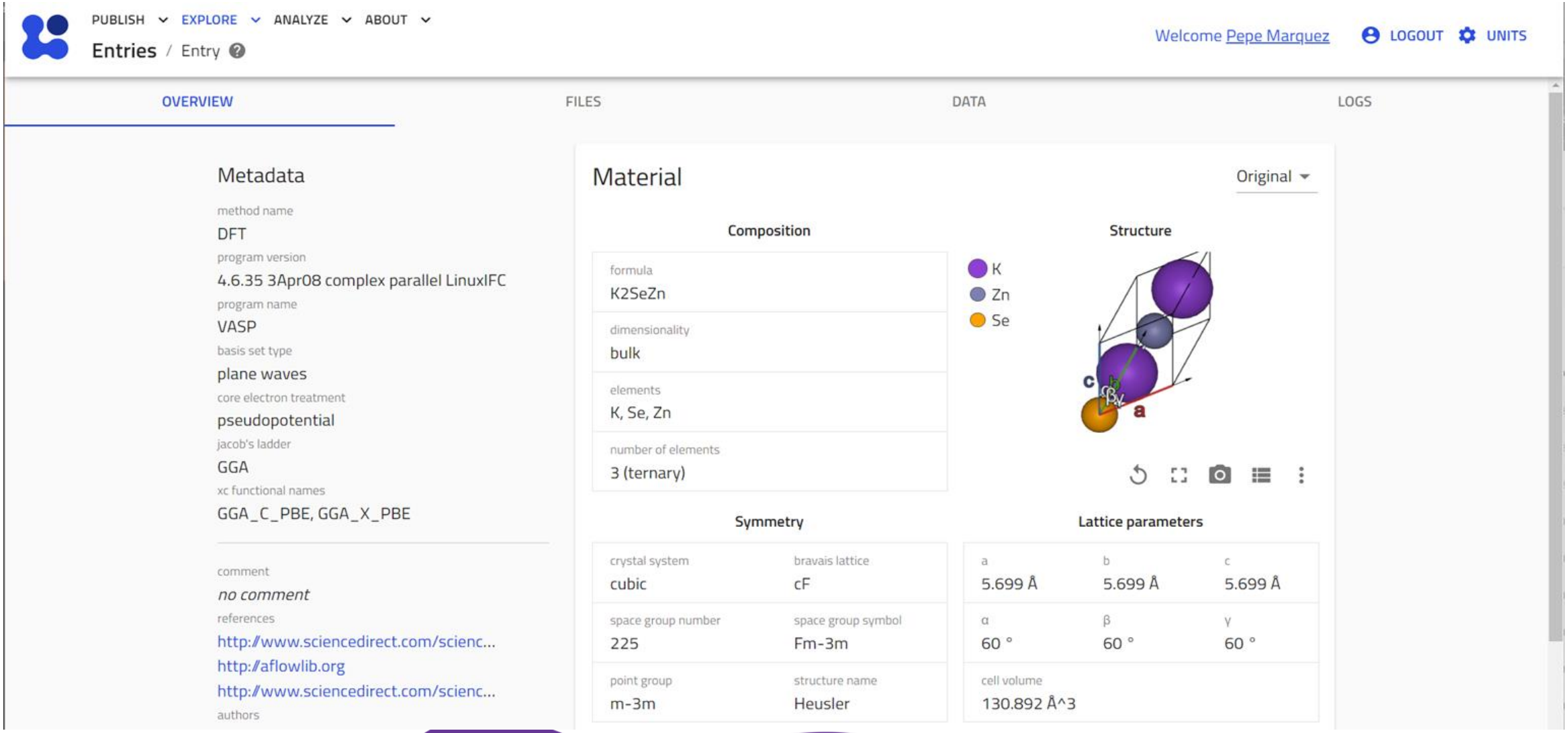
NOMAD core functionalities



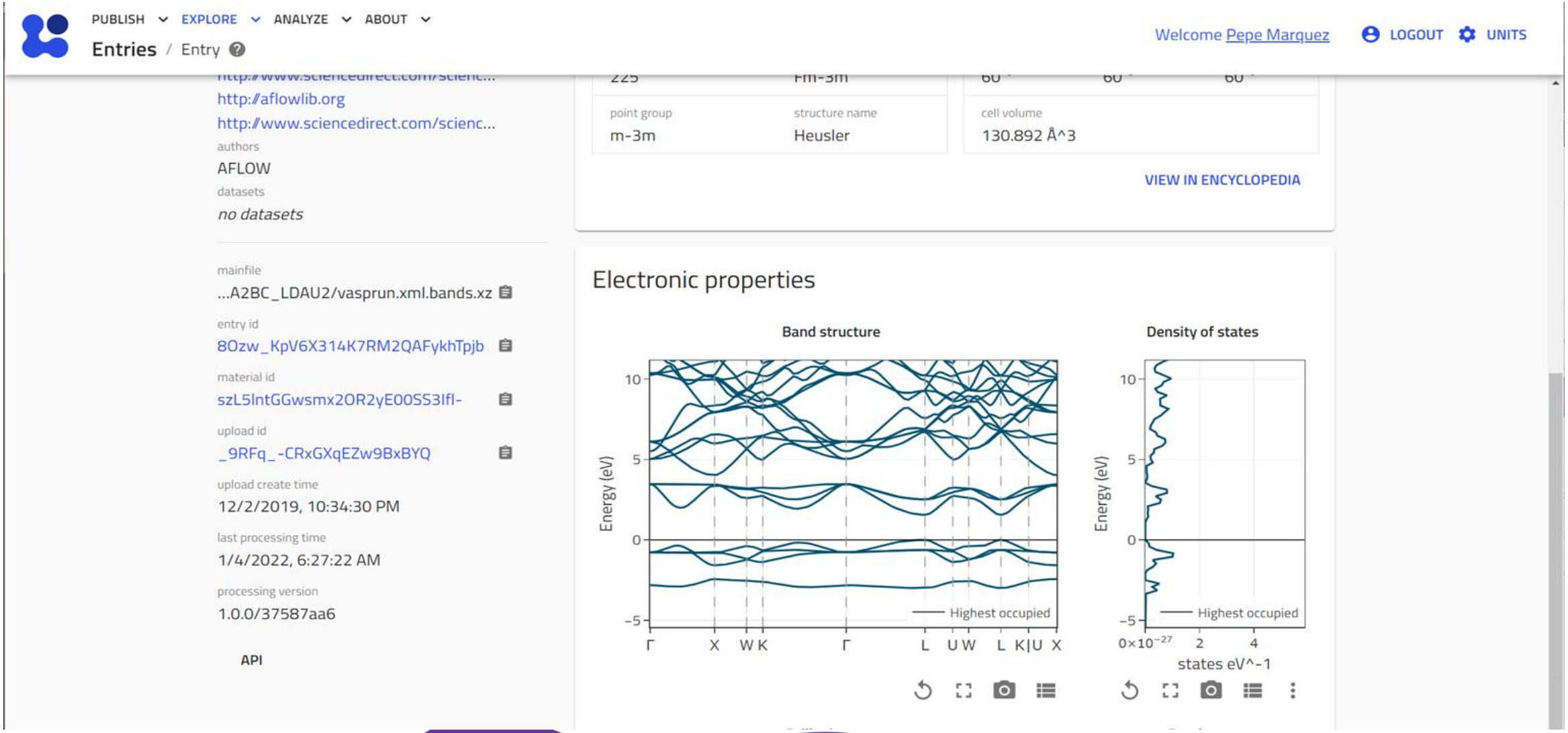
NOMAD core functionalities

Access effortlessly *essential (meta)data* visualized in the overview page of each entry.

NOMAD core functionalities



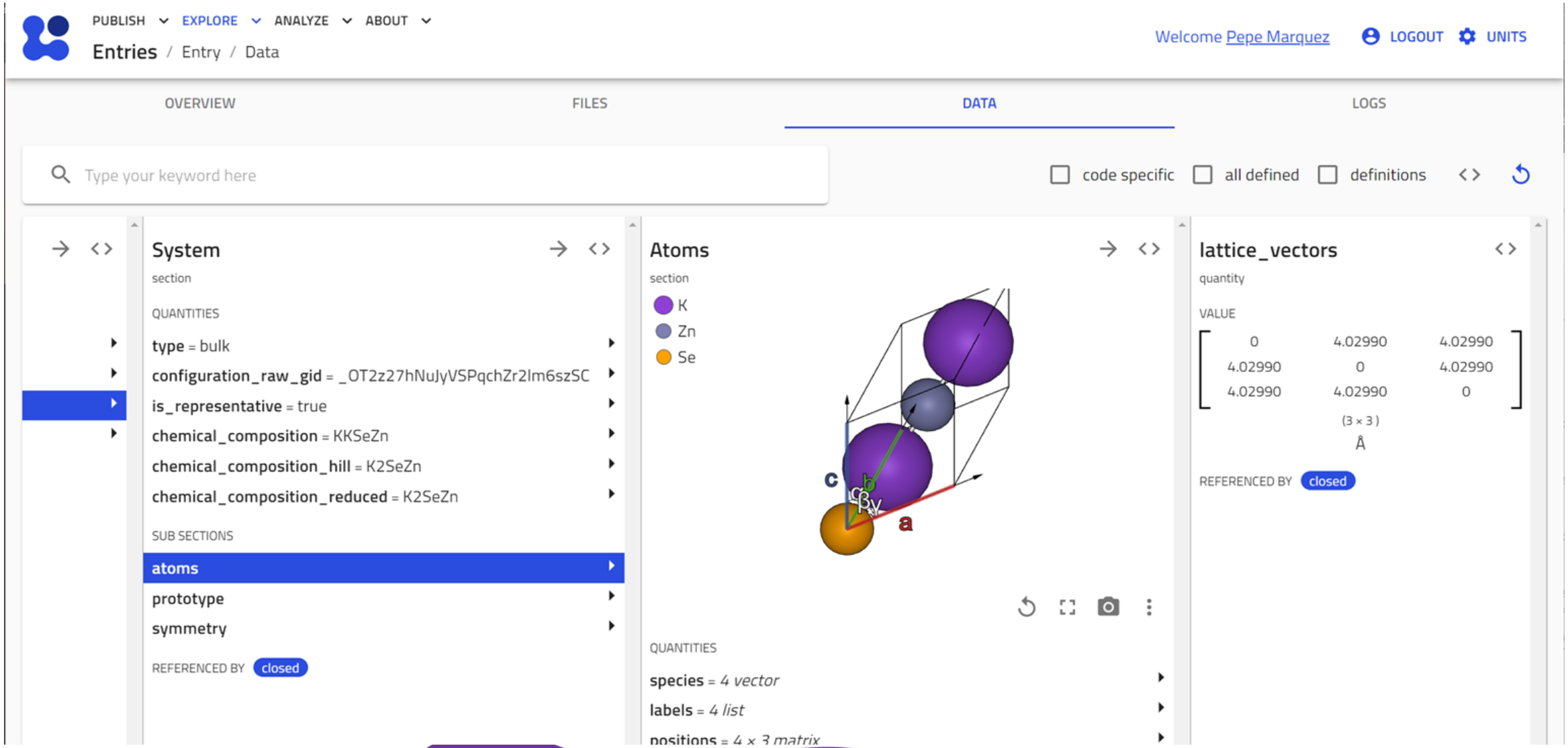
NOMAD core functionalities



NOMAD core functionalities

Browse the *detailed (meta)data* of each entry within a standardized structured schema.

NOMAD core functionalities



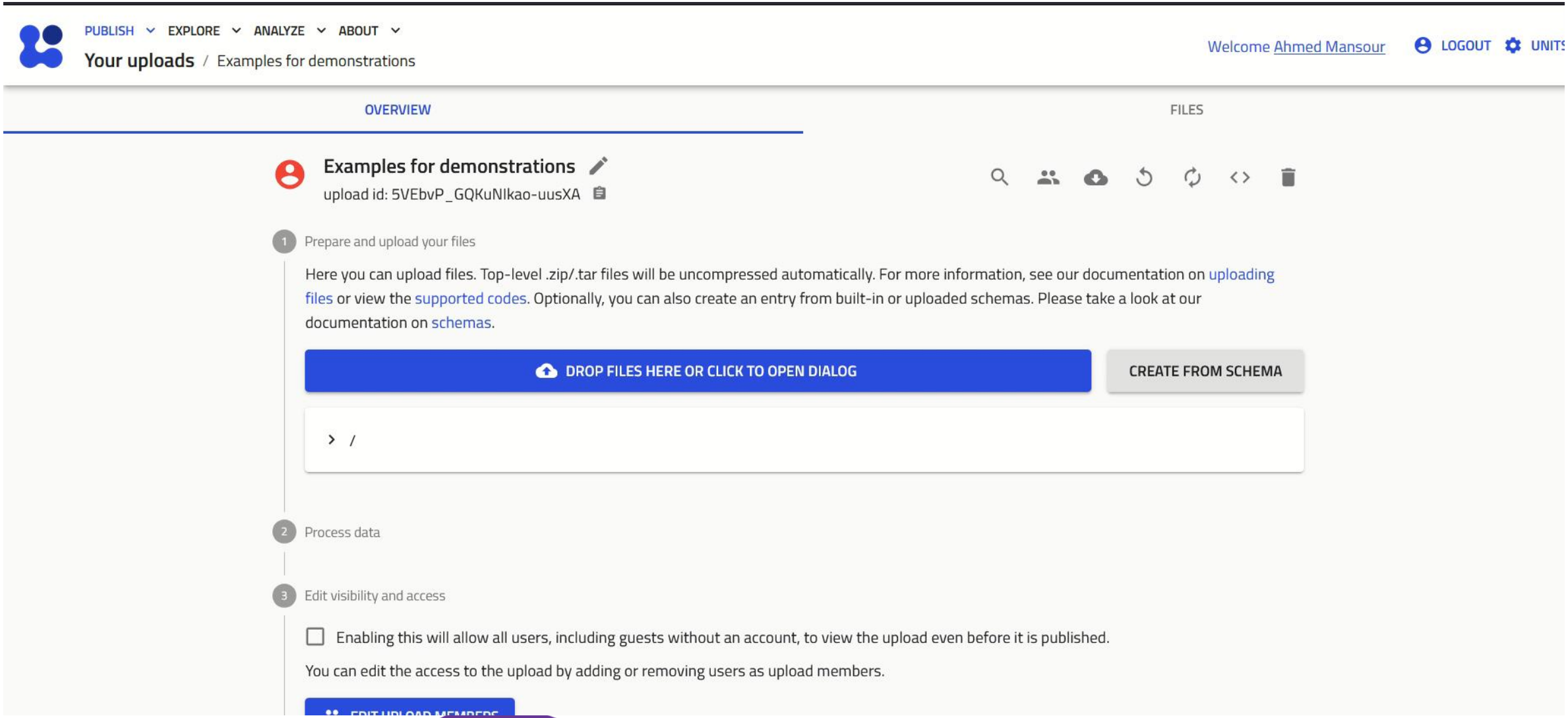
NOMAD core functionalities

Upload your research data into NOMAD, share them with collaborators, and publish datasets with DOI.

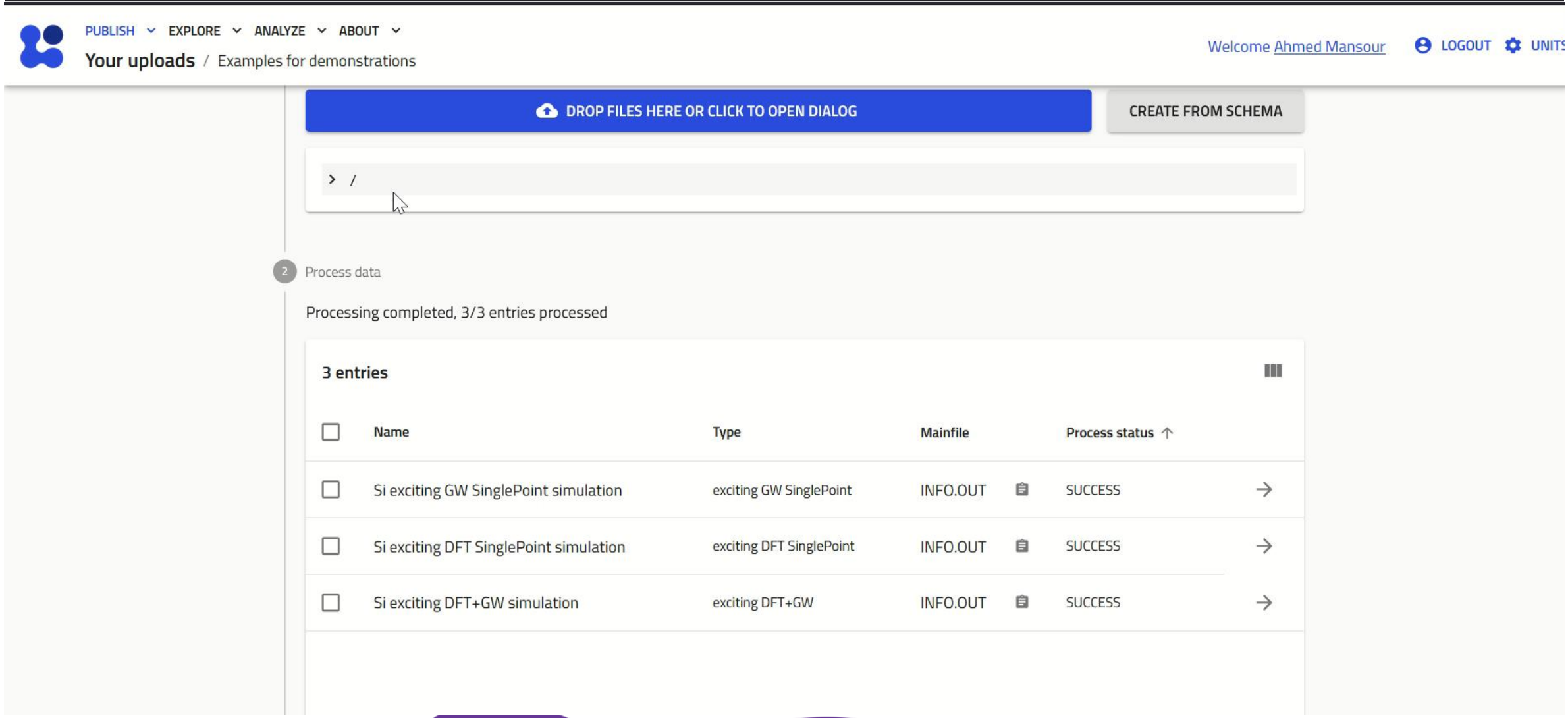
NOMAD core functionalities

Name	Type
BAND.OUT	OUT File
BAND-QP.OUT	OUT File
bandstructure	DAT File
bandstructure	XML Document
bandstructure-qp	DAT File
dos	XML Document
EIGVAL.OUT	OUT File
EIGVAL_GW.OUT	OUT File
EVALQP	DAT File
GW_INFO.OUT	OUT File
info	XML Document
INFO.OUT	OUT File
input	XML Document
TDOS.OUT	OUT File
TDOS-QP.OUT	OUT File

NOMAD core functionalities



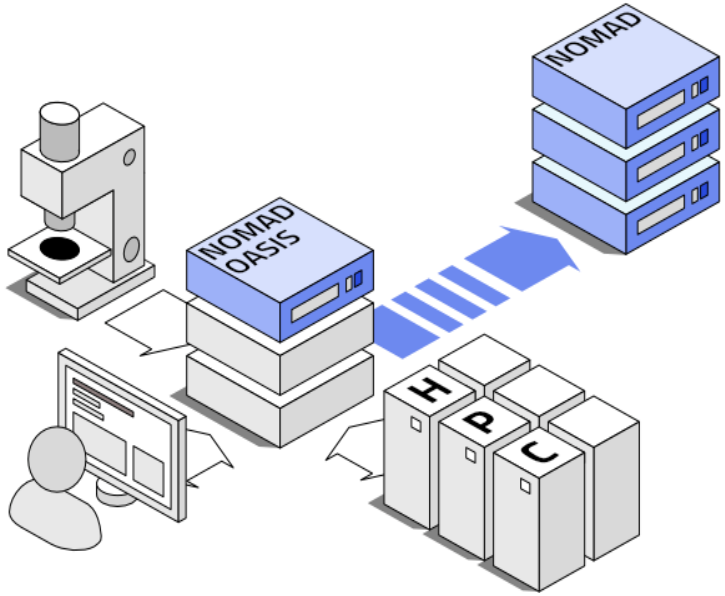
NOMAD core functionalities



NOMAD Oasis

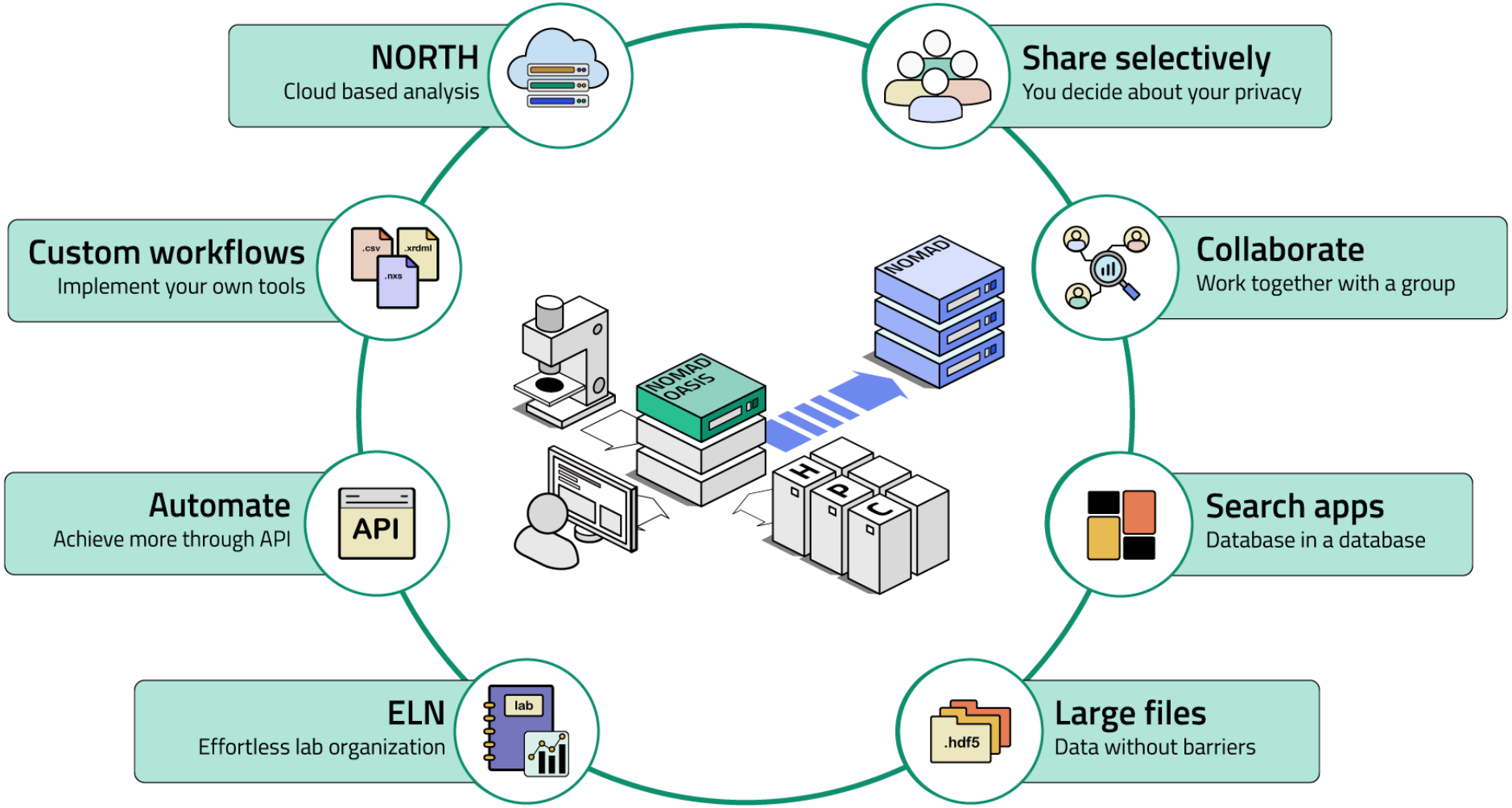
Local management tool for your lab, adapted to your data-management needs and lab policies.

REGISTERED INSTALLATIONS
> 80

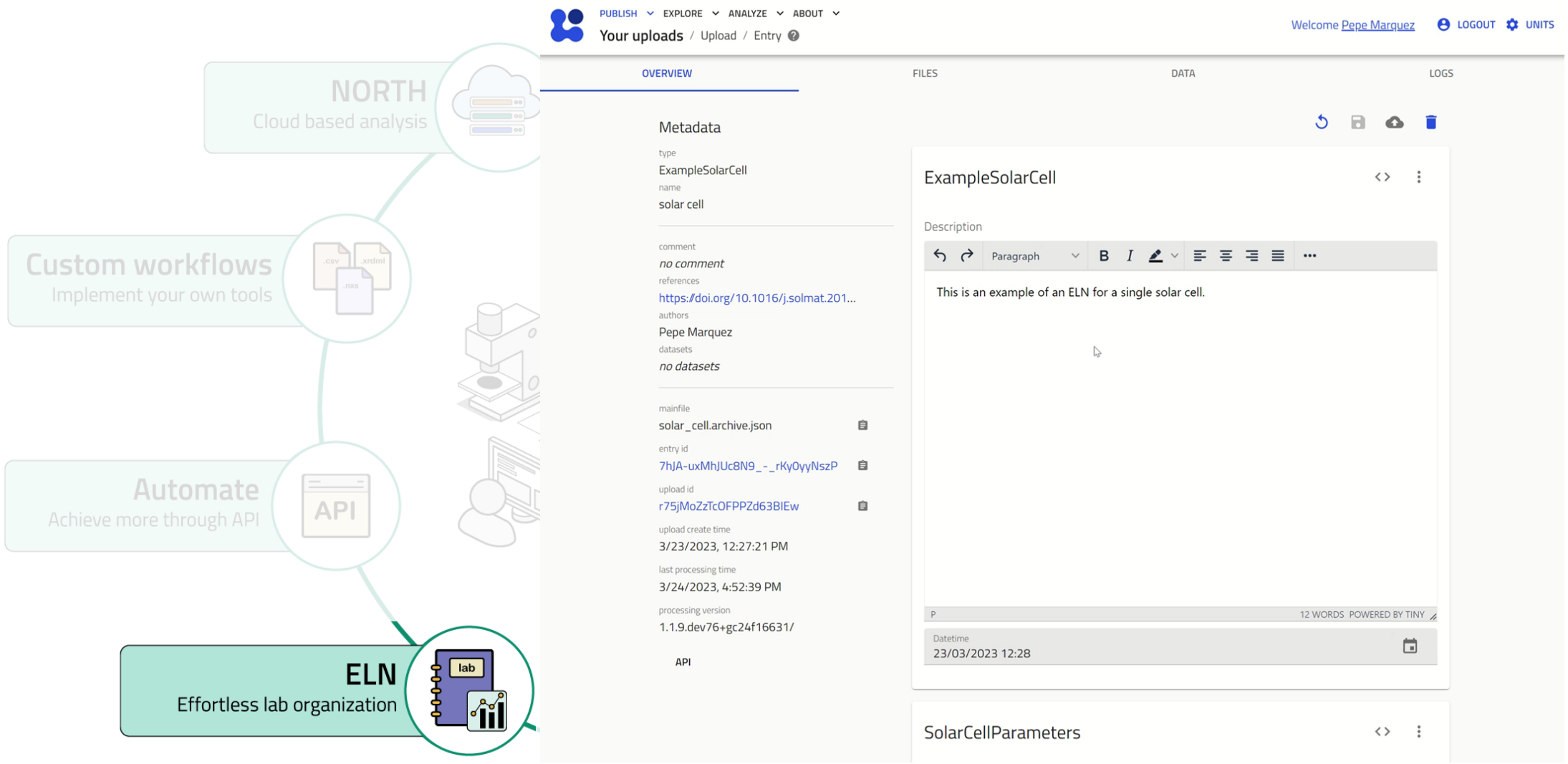


https://nomad-lab.eu/

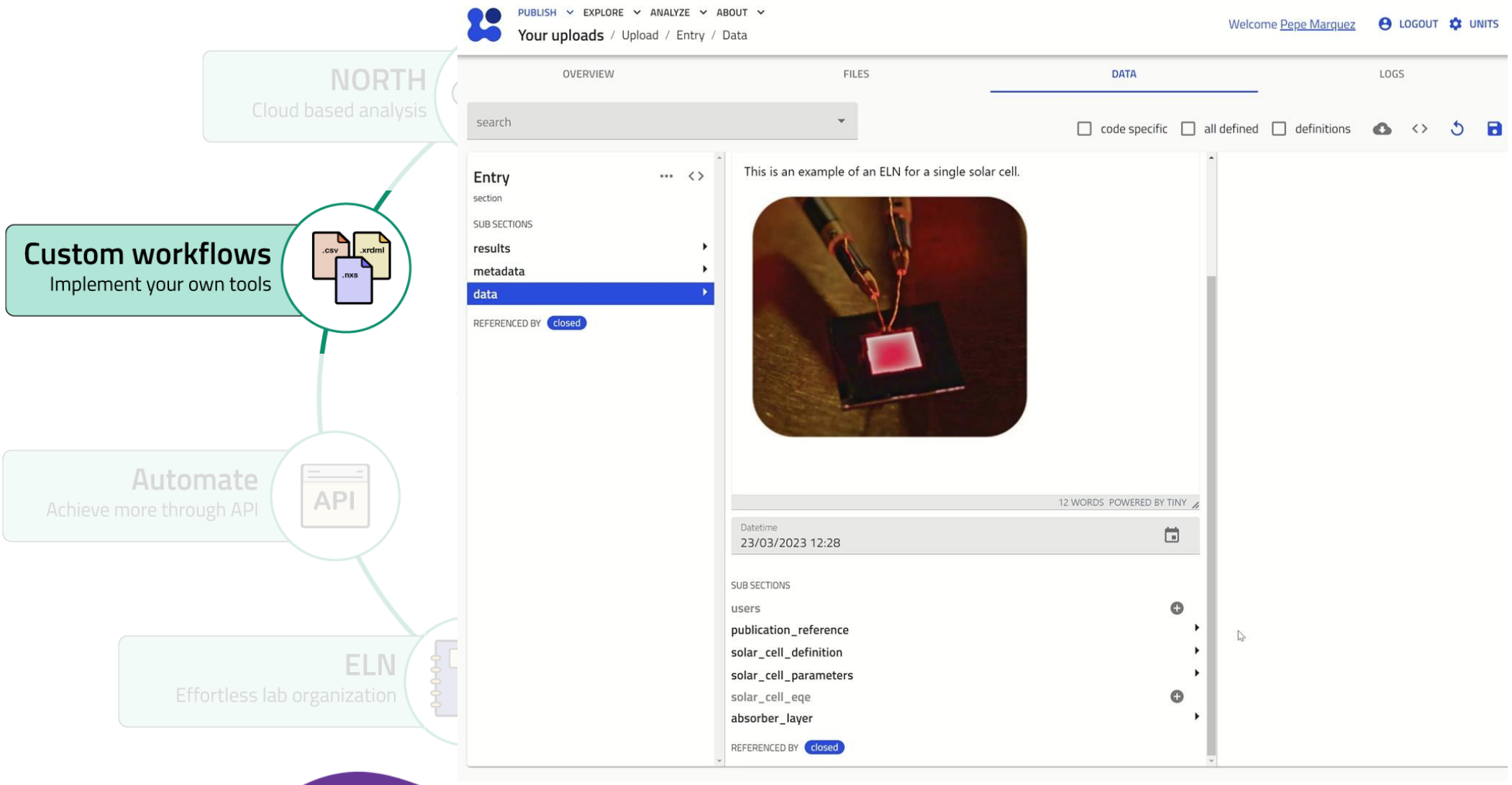
NOMAD Oasis


NORTH
Cloud based analysis
Share selectively
You decide about your privacy
Custom workflows
Implement your own tools
.csv
.xrdml
.nxs
Collaborate
Work together with a group
NOMAD
NOMAD OASIS
H
P
C
Automate
Achieve more through API
API
Search apps
Database in a database
ELN
Effortless lab organization
lab
Large files
Data without barriers
.hdf5

NOMAD Oasis


NORTH
Cloud based analysis
Custom workflows
Implement your own tools
.csv
.xrdml
.nxs
Automate
Achieve more through API
API
ELN
Effortless lab organization
lab
PUBLISH
EXPLORE
ANALYZE
ABOUT
Your uploads / Upload / Entry
Welcome Pepe Marquez
LOGOUT
UNITS
OVERVIEW
FILES
DATA
LOGS
Metadata
type
ExampleSolarCell
name
solar cell
comment
no comment
references
https://doi.org/10.1016/j.solmat.201...
authors
Pepe Marquez
datasets
no datasets
mainfile
solar_cell.archive.json
entry id
7hJA-uxMhJUc8N9_-_rKy0yyNszP
upload id
r75jMoZzTcOFPPZd63BIEw
upload create time
3/23/2023, 12:27:21 PM
last processing time
3/24/2023, 4:52:39 PM
processing version
1.1.9.dev76+gc24f16631/
API
ExampleSolarCell
Description
Paragraph
This is an example of an ELN for a single solar cell.
P
12 WORDS POWERED BY TINY
Datetime
23/03/2023 12:28
SolarCellParameters

NOMAD Oasis


NORTH
Cloud based analysis
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.csv
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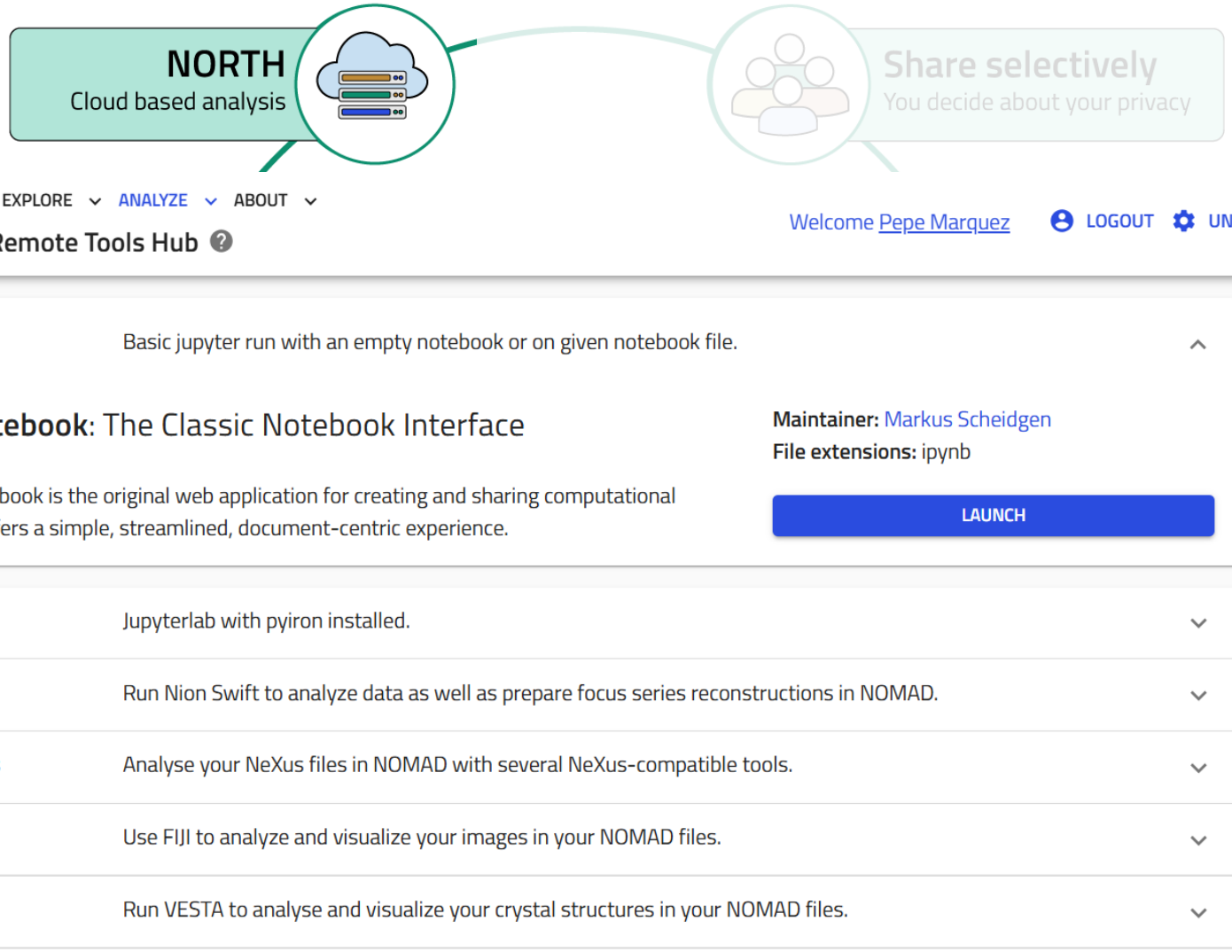
.nxs
Automate
Achieve more through API
API
ELN
Effortless lab organization
PUBLISH
EXPLORE
ANALYZE
ABOUT
Welcome Pepe Marquez
LOGOUT
UNITS
Your uploads / Upload / Entry / Data
OVERVIEW
FILES
DATA
LOGS
search
code specific
all defined
definitions
Entry
section
SUB SECTIONS
results
metadata
data
REFERENCED BY
closed
This is an example of an ELN for a single solar cell.
12 WORDS POWERED BY TINY
Datetime
23/03/2023 12:28
SUB SECTIONS
users
publication_reference
solar_cell_definition
solar_cell_parameters
solar_cell_eqe
absorber_layer
REFERENCED BY
closed

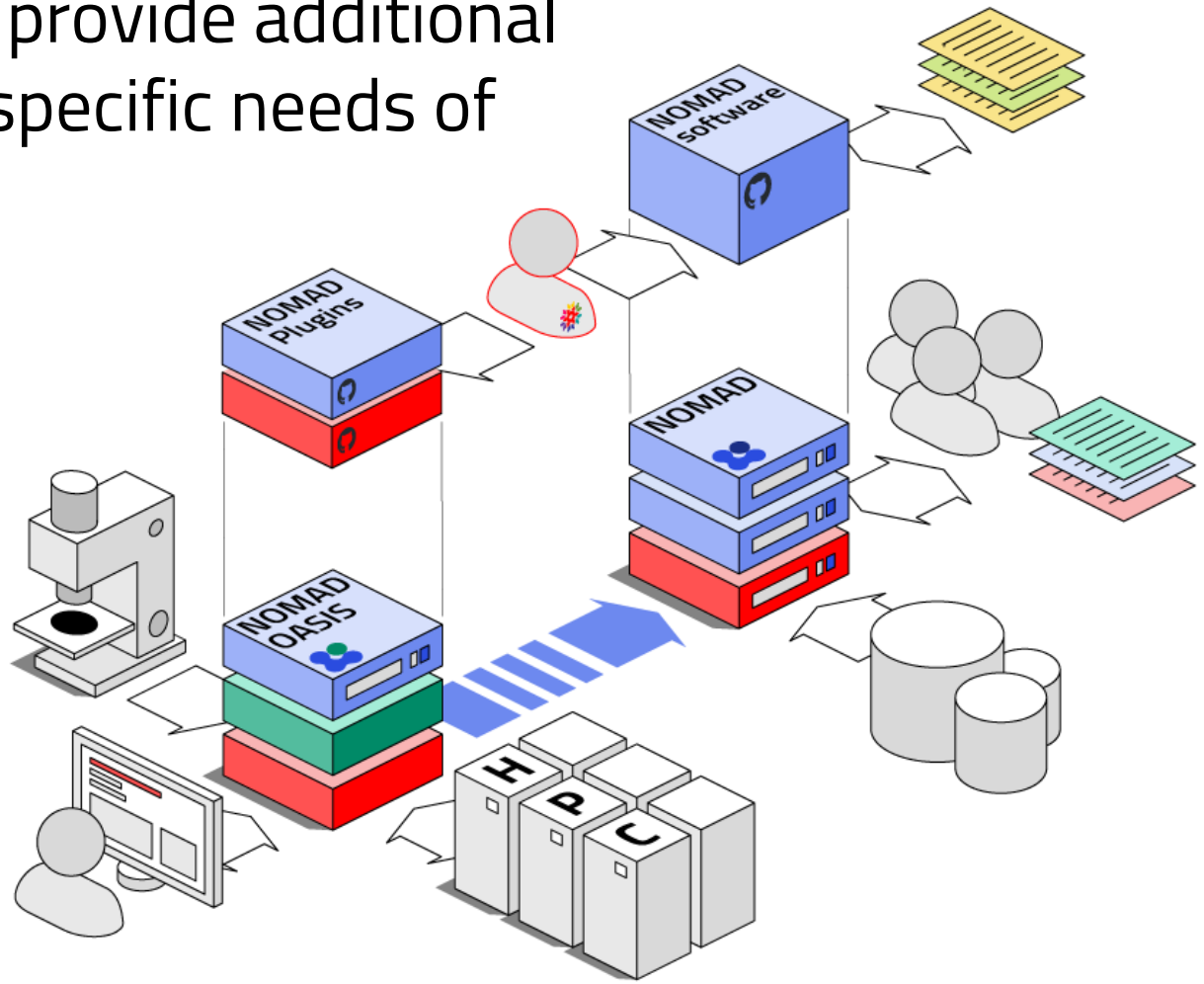
NOMAD Oasis


NORTH
Cloud based analysis
Share selectively
You decide about your privacy
PUBLISH
EXPLORE
ANALYZE
ABOUT
NOMAD Remote Tools Hub
Welcome Pepe Marquez
LOGOUT
UNITS
jupyter
Basic jupyter run with an empty notebook or on given notebook file.
Jupyter Notebook: The Classic Notebook Interface
Maintainer: Markus Scheidgen
File extensions: ipynb
The Jupyter Notebook is the original web application for creating and sharing computational documents. It offers a simple, streamlined, document-centric experience.
LAUNCH
pyiron
Jupyterlab with pyiron installed.
nionswift
Run Nion Swift to analyze data as well as prepare focus series reconstructions in NOMAD.
nexustools
Analyse your NeXus files in NOMAD with several NeXus-compatible tools.
fiji
Use FIJI to analyze and visualize your images in your NOMAD files.
vesta
Run VESTA to analyse and visualize your crystal structures in your NOMAD files.

Customize your NOMAD using NOMAD PLUGIN

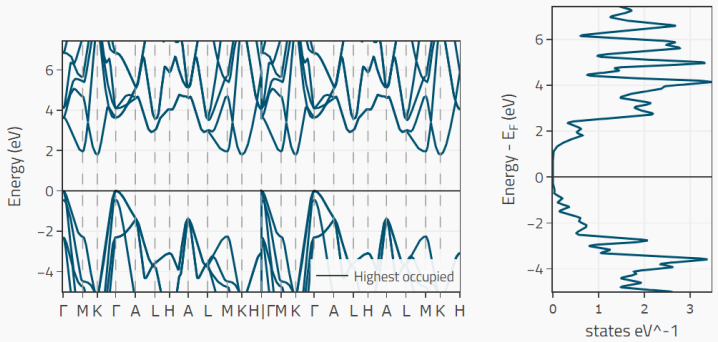
NOMAD plugins are “add-ons” that provide additional capabilities and adapt NOMAD the specific needs of your research group.

- **Schema packages**
- **Parsers**
- **Apps**
- **Example uploads**
- **Normalizers**

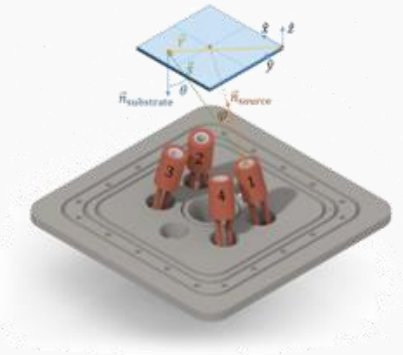


Working areas in FAIRmat

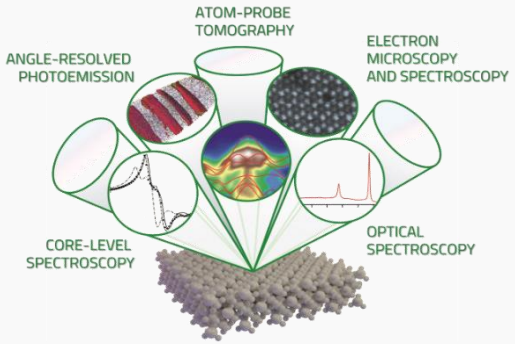
Theory and Computations



Synthesis



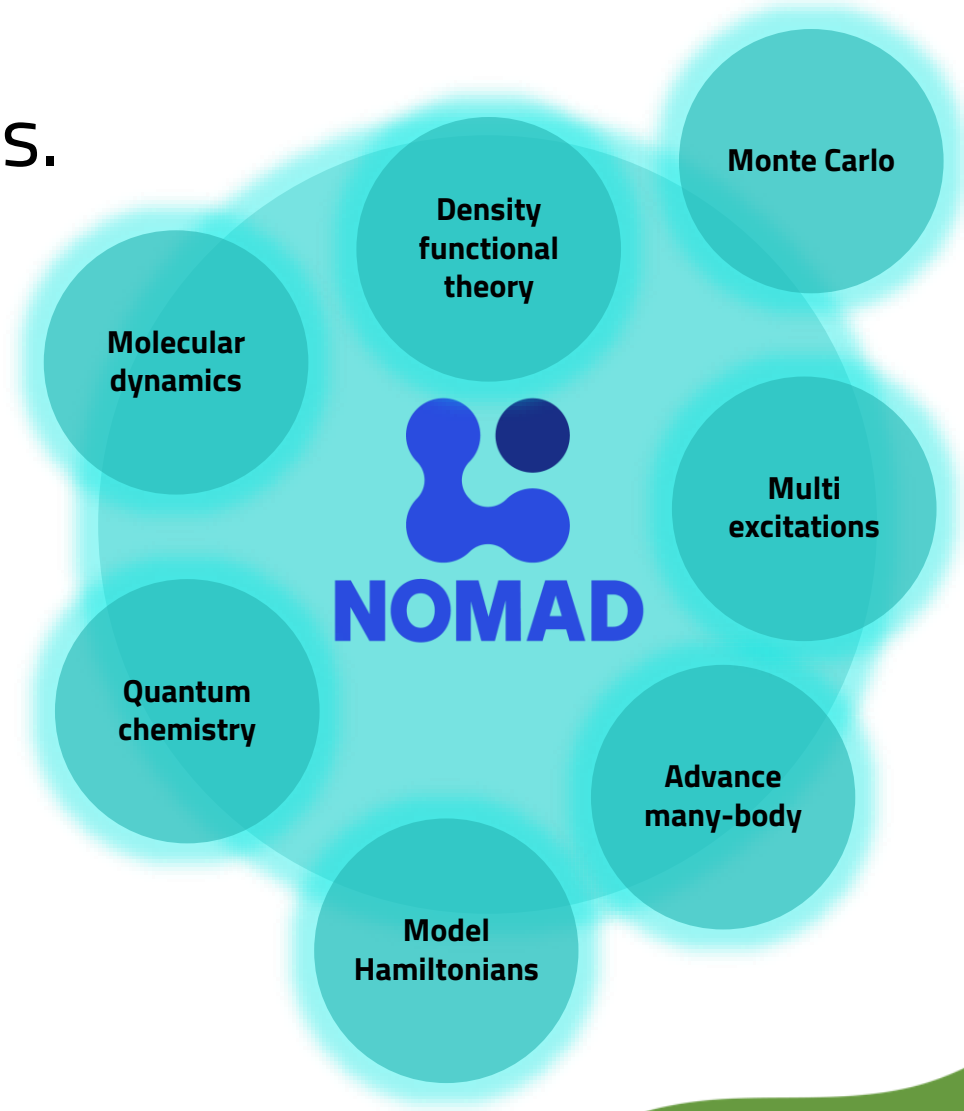
Experiment | Characterization



Use cases

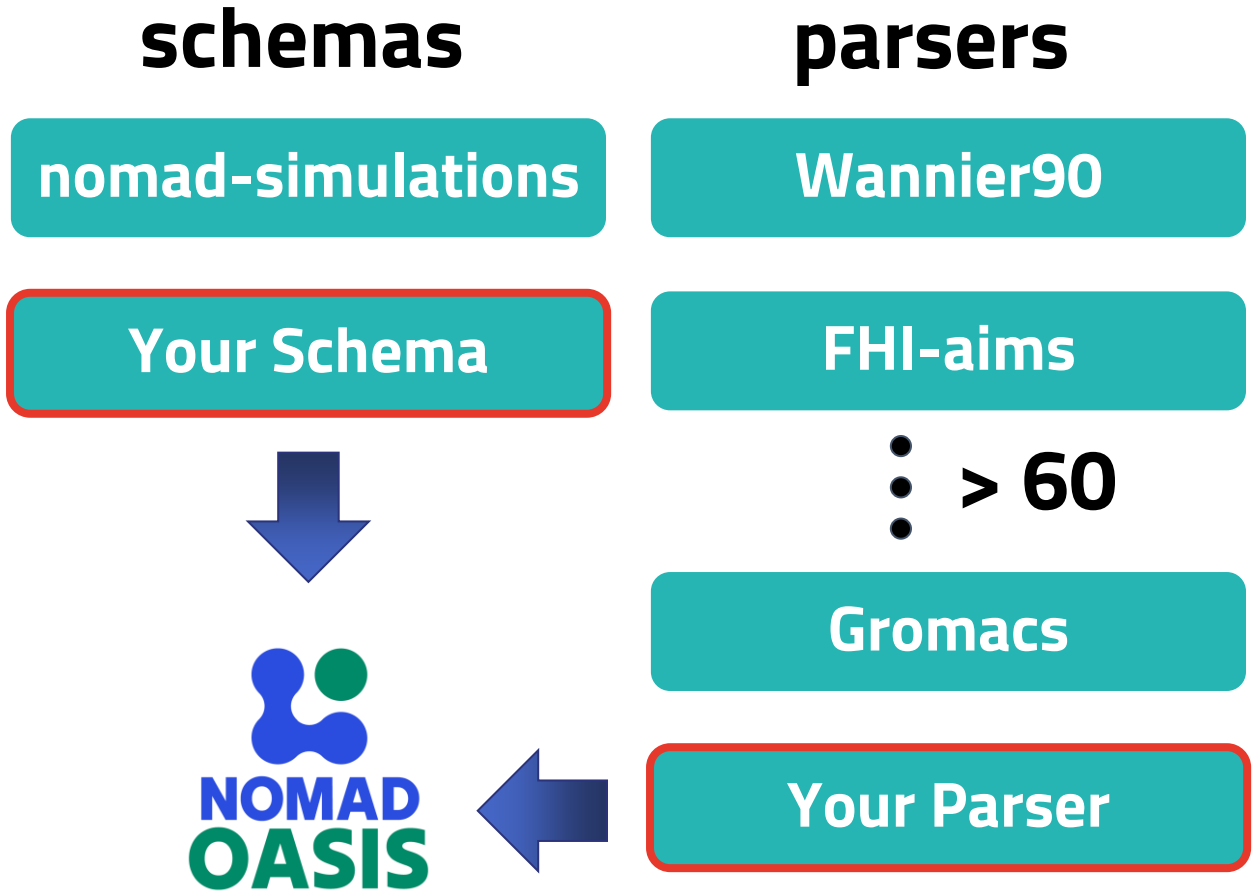
Theory and computation

- Unified schema for all targeted methods.
- Parsing tools that simplify metadata extraction from method-specific files.
- Modular functions enabling standardized metadata processing.
- Robust and flexible workflow support.



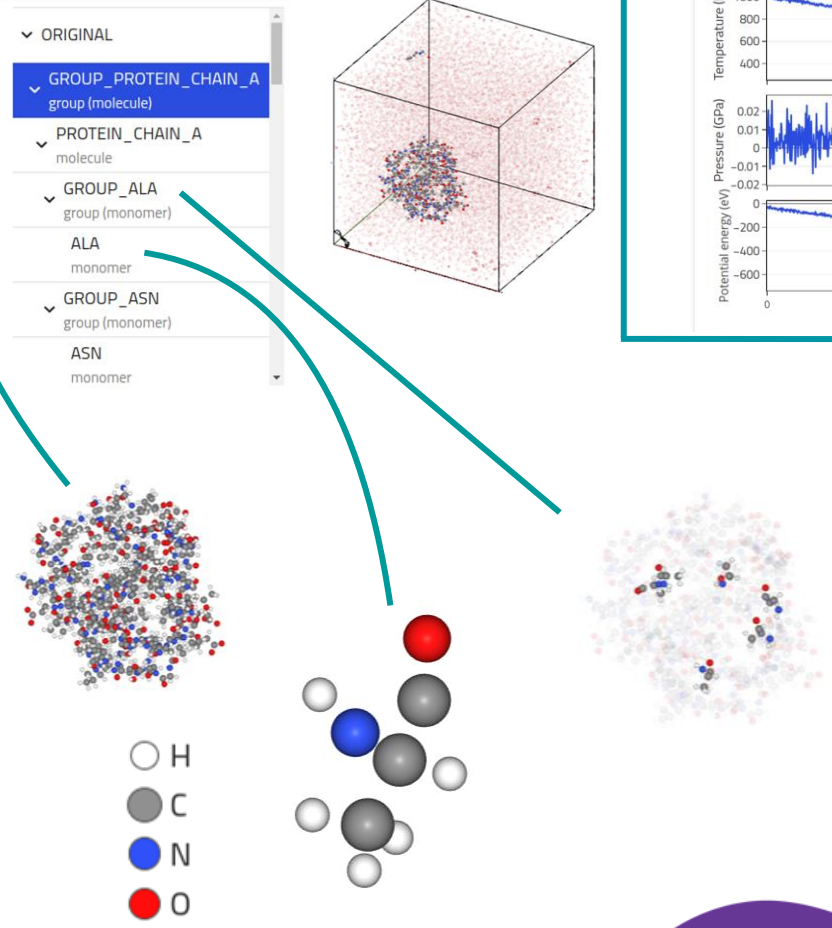
Extensible support for computational data

- Native support for 60+ codes and software packages.
- Create your own plugins and leverage NOMAD's built-in tools for specialized use cases

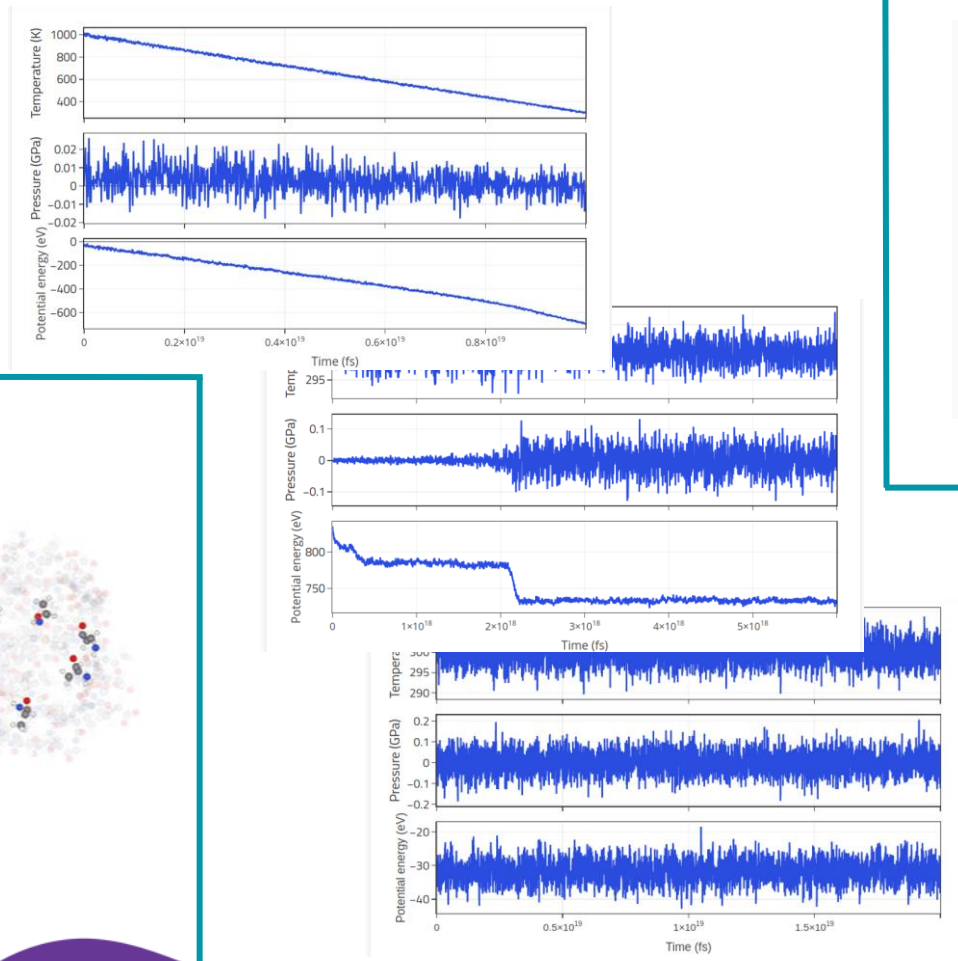


Support for Molecular Dynamics Simulations

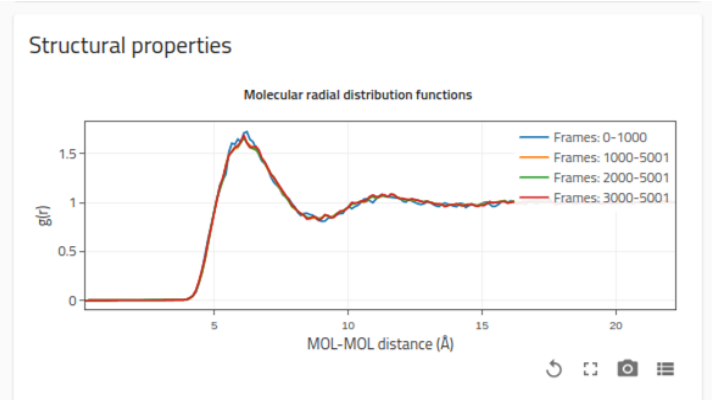
Visualization of system hierarchies

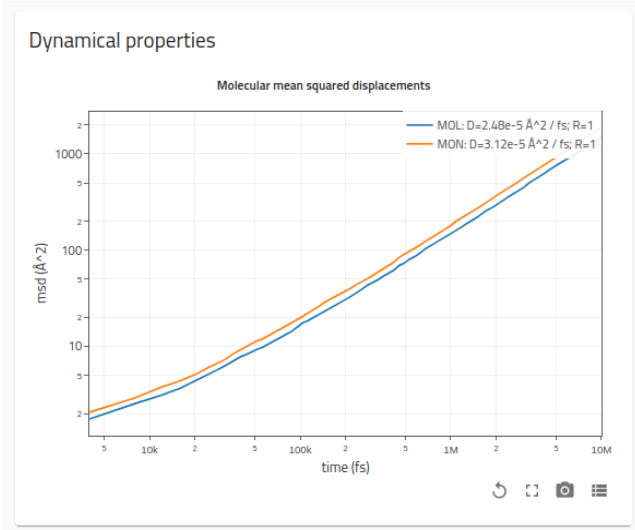


Storage and **display** of trajectory properties



Automated calculation of basic molecular properties

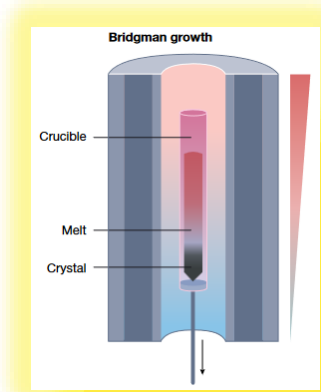


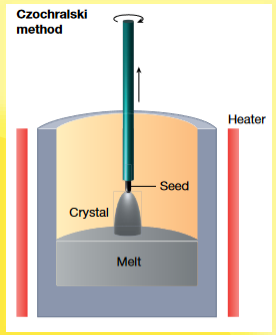


Synthesis

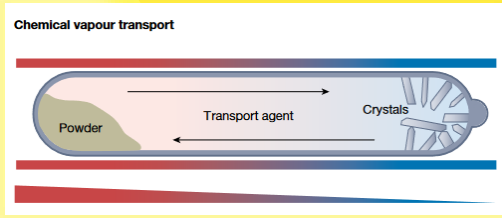
Formalized data models for key synthesis routes.

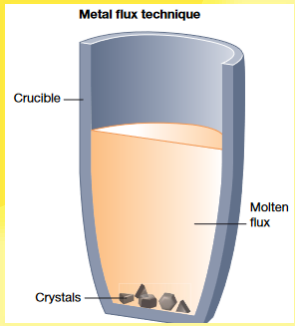
- From melt
- From gas phase
- Solid phase and solution
- By assembly





NOMAD





Modular classes for schema development

Base sections

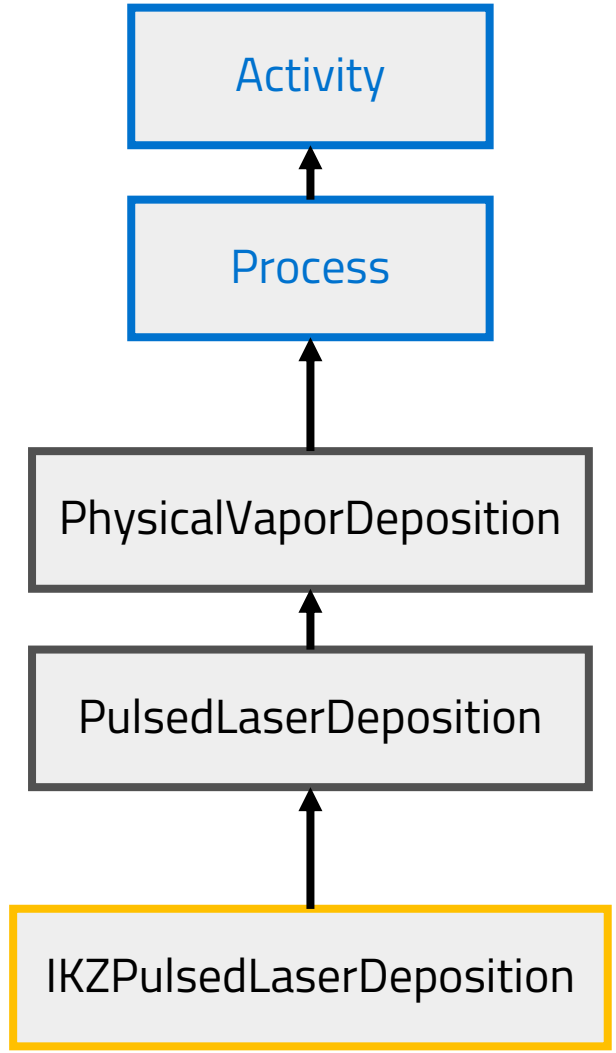
General definitions, not for specific field

Standard plugins

For a specific field/method
Developed by FAIRmat

User-defined schema

User-developed schema specific to lab/instrument



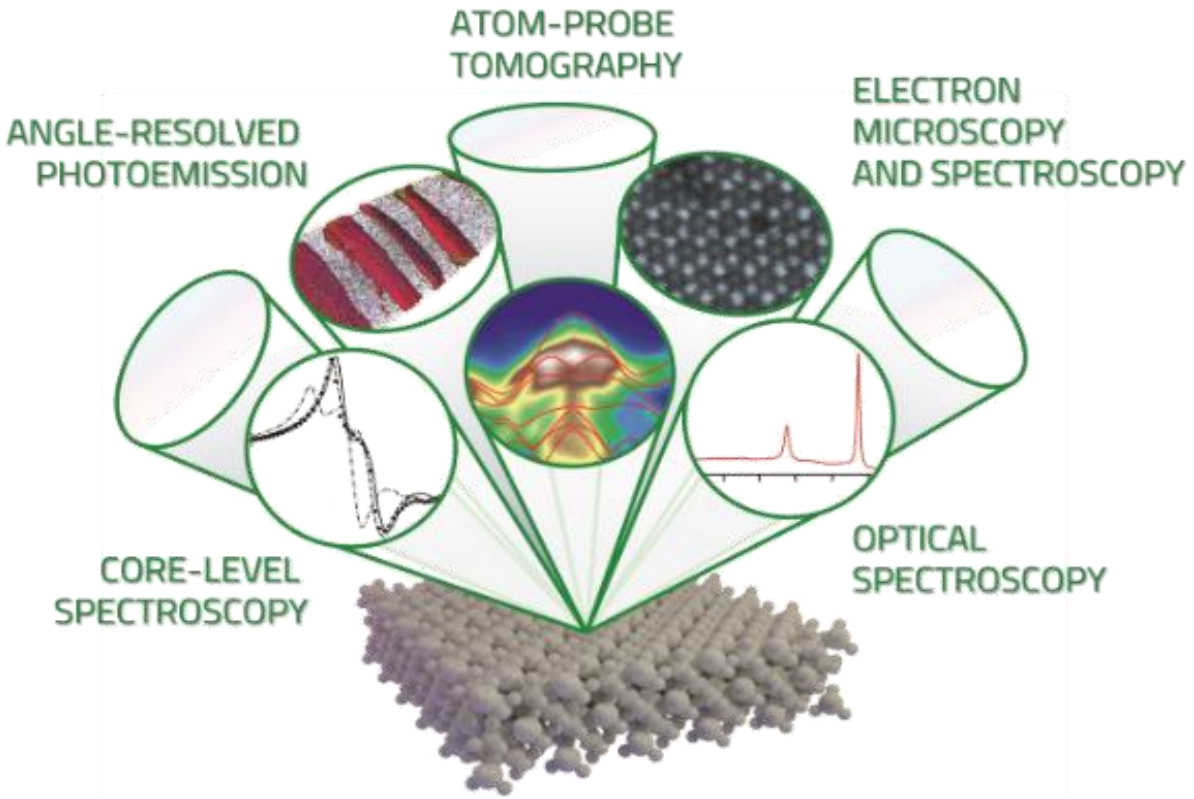
NOMAD

NOMAD PLUGIN

NOMAD OASIS

Experiments: NeXus standardization

Standardized (meta)data schema for a subset of methods from materials science based on the **NeXus** format



pynxtools
pynxtools-apm
pynxtools-em

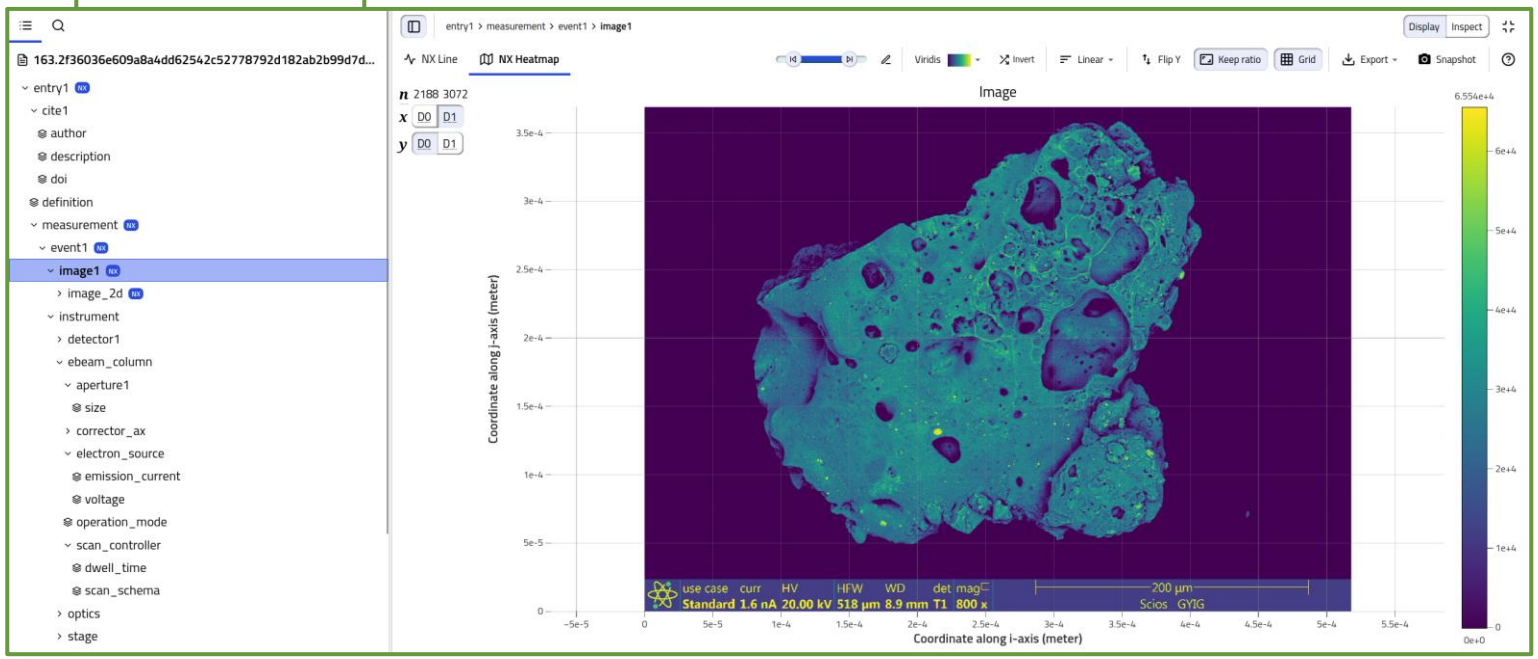
NOMAD PLUGIN

Electron microscopy: Nxem and pynxtools-em

NXem: Standardized NeXus schema for all data acquired with electron microscopes

pynxtools-em: parser for most instruments used in the community

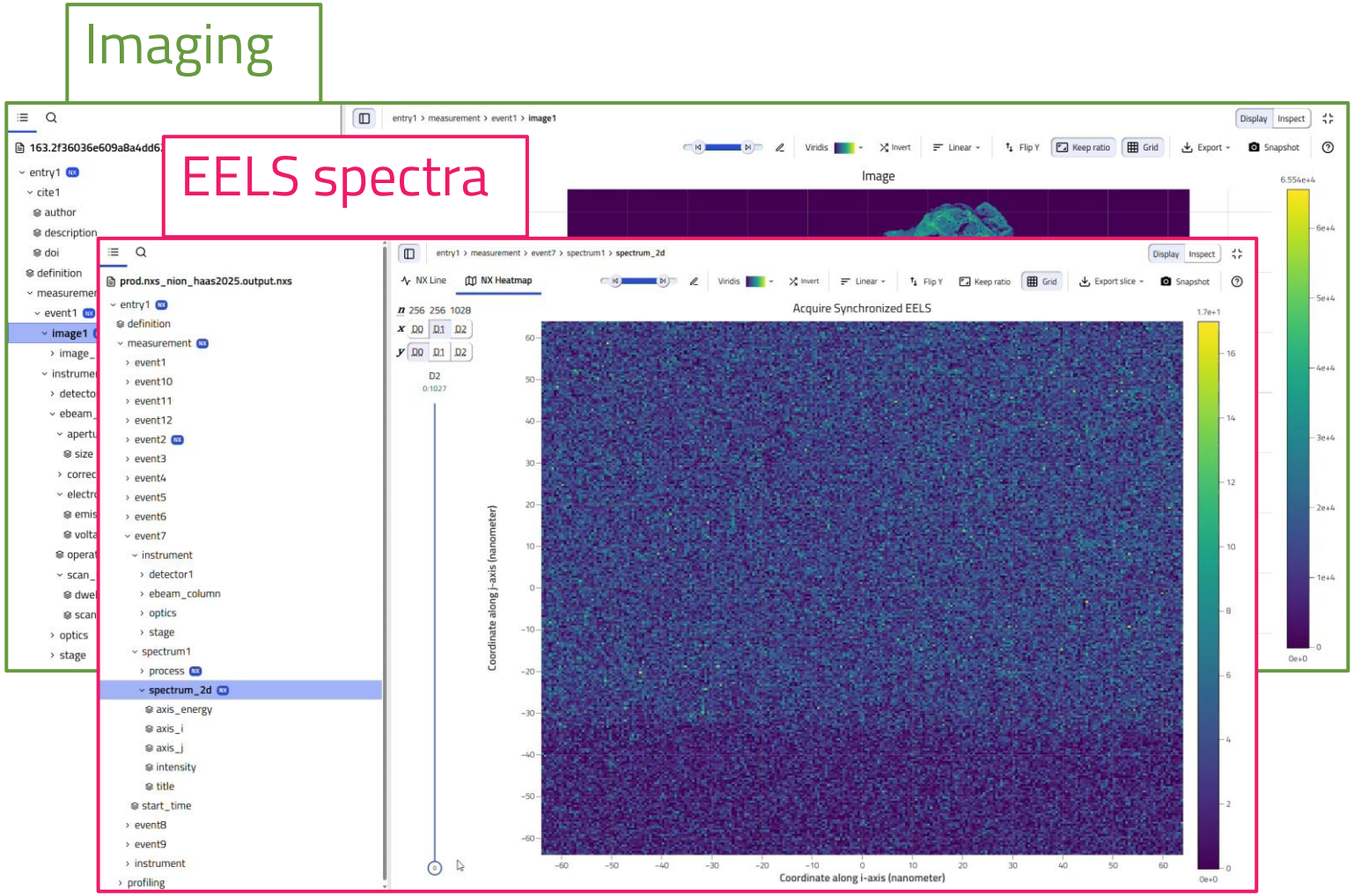
Imaging



Electron microscopy: Nxem and pynxtools-em

NXem: Standardized NeXus schema for all data acquired with electron microscopes

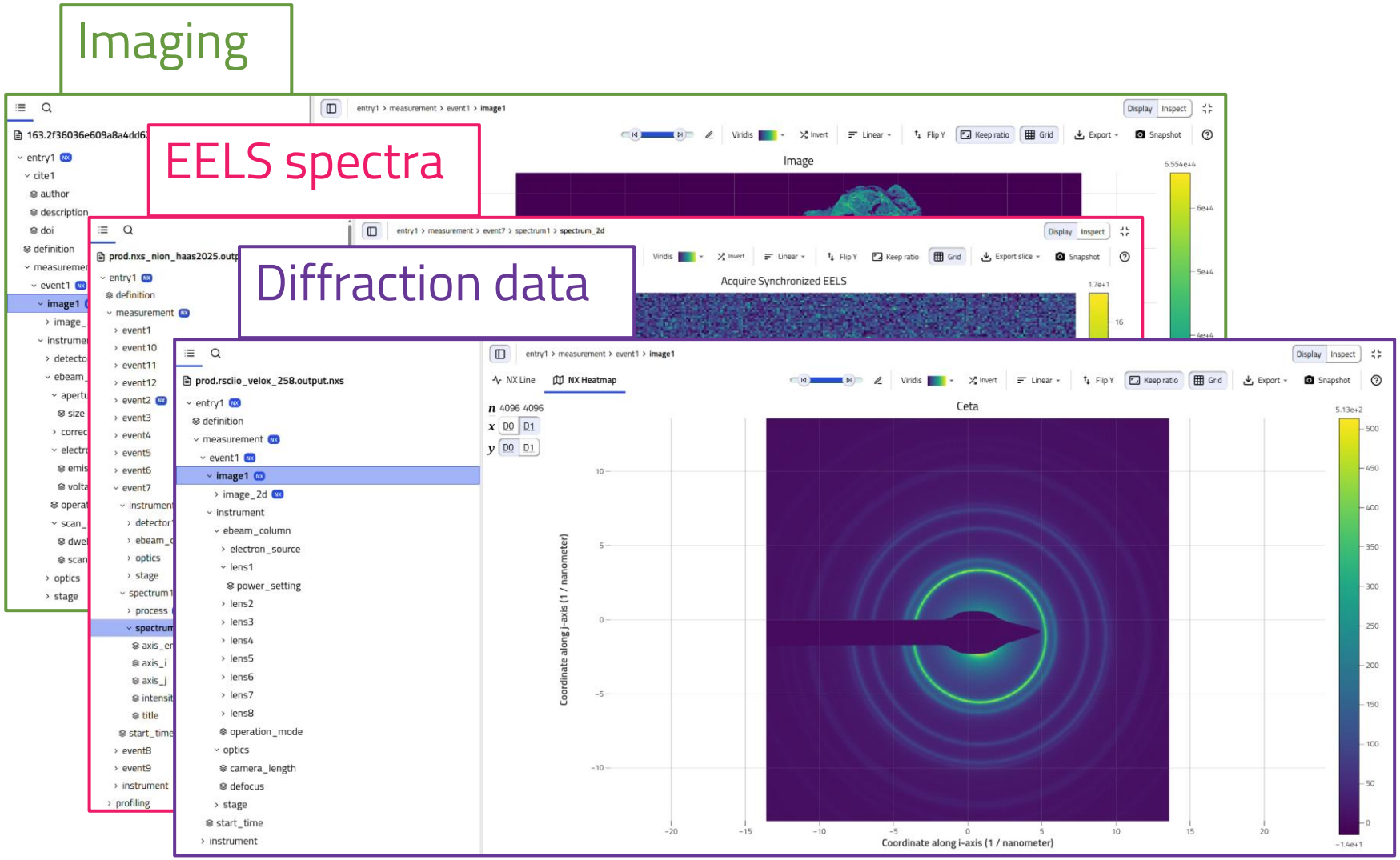
pynxtools-em: parser for most instruments used in the community



Electron microscopy: Nxem and pynxtools-em

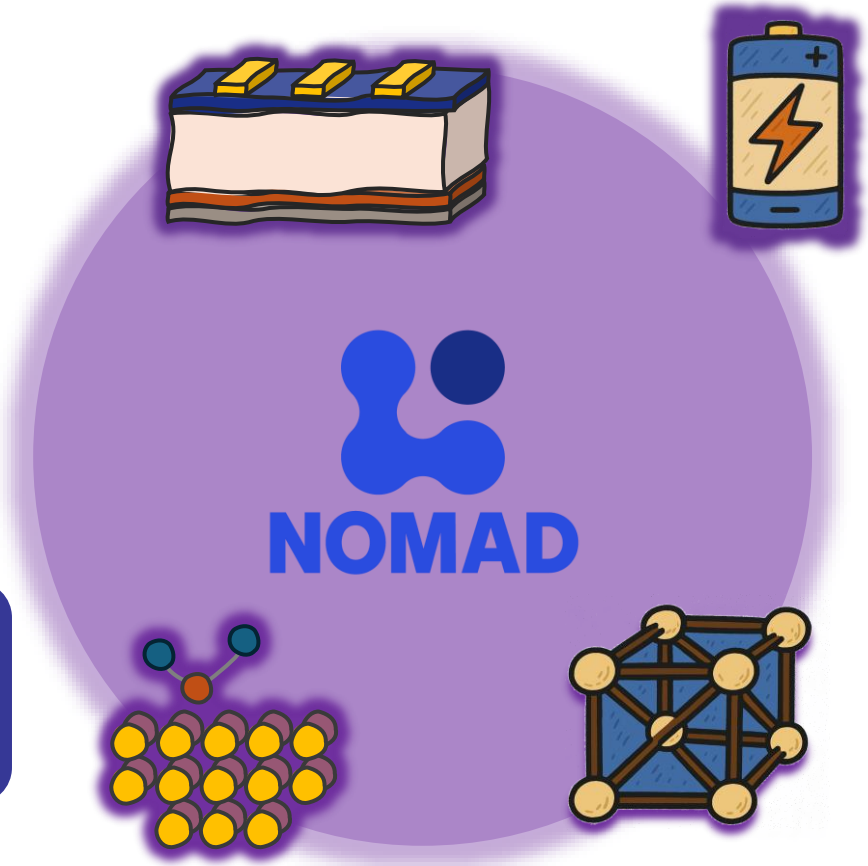
NXem: Standardized NeXus schema for all data acquired with electron microscopes

pynxtools-em: parser for most instruments used in the community



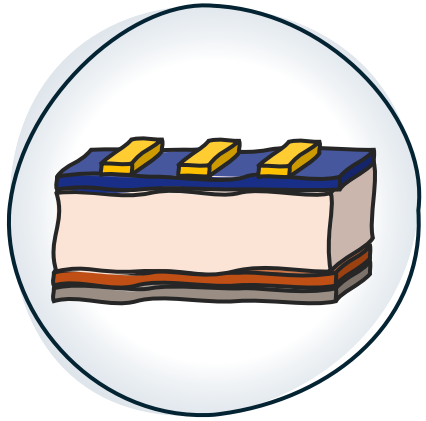
Use Cases

- Domain-specific curated and structured datasets.
- Search dashboards offer visualization, comparison, and filtering.

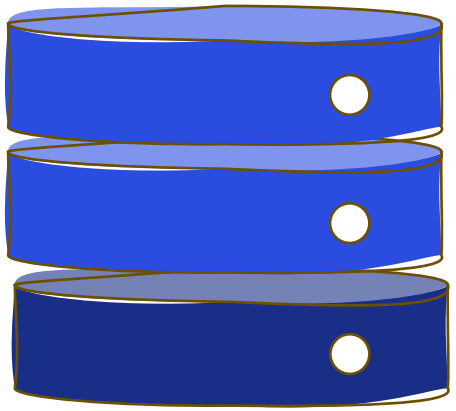


Solar cells	Heterogeneous catalysis	Metal-organic frameworks
> 40k devices	> 2.4k entries	> 17k calculations

Solar cells



NOMAD



PUBLISH EXPLORE ANALYZE ABOUT

The Perovskite Solar Cell Database

LOGIN / REGISTER UNITS

FILTERS

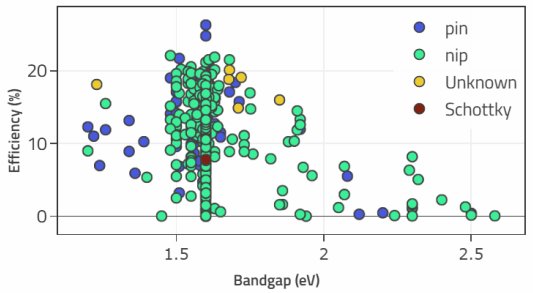
- Publication
- Perovskite Material
- Perovskite Fabrication
- Device Architecture
- Transport Layers
- Solar Cell Performance
- Stability

Type your query or keyword here

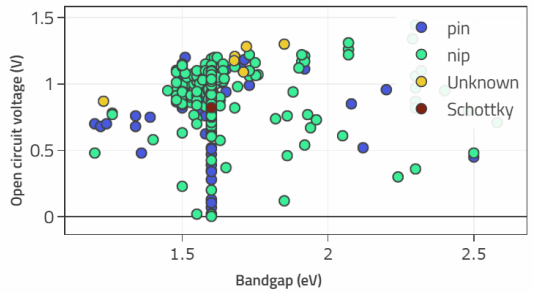
Your query will be shown here

TERMS HISTOGRAM SCATTER PLOT PERIODIC TABLE

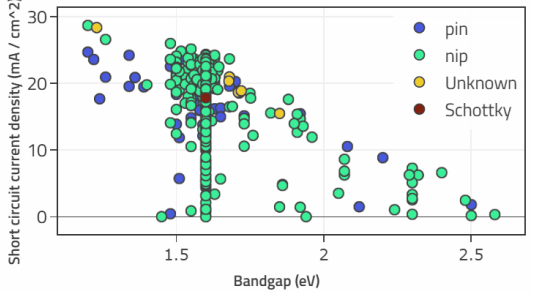
Scatter plot



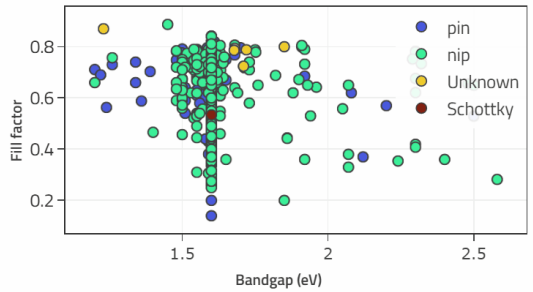
Scatter plot



Scatter plot



Scatter plot



20/43,106 search results

Descriptive formula	Efficiency (%)	Open circuit voltage (V)	Short circuit current density (A /	Fill factor	References

7th FAIRmat Users Meeting

When? November 20, 2025

Where? Center for the Science of Materials Berlin

Who's invited? All interested scientists

Learn more:

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