

NOMAD: a federated data infrastructure transforming materials-science laboratories

Ahmed Mansour

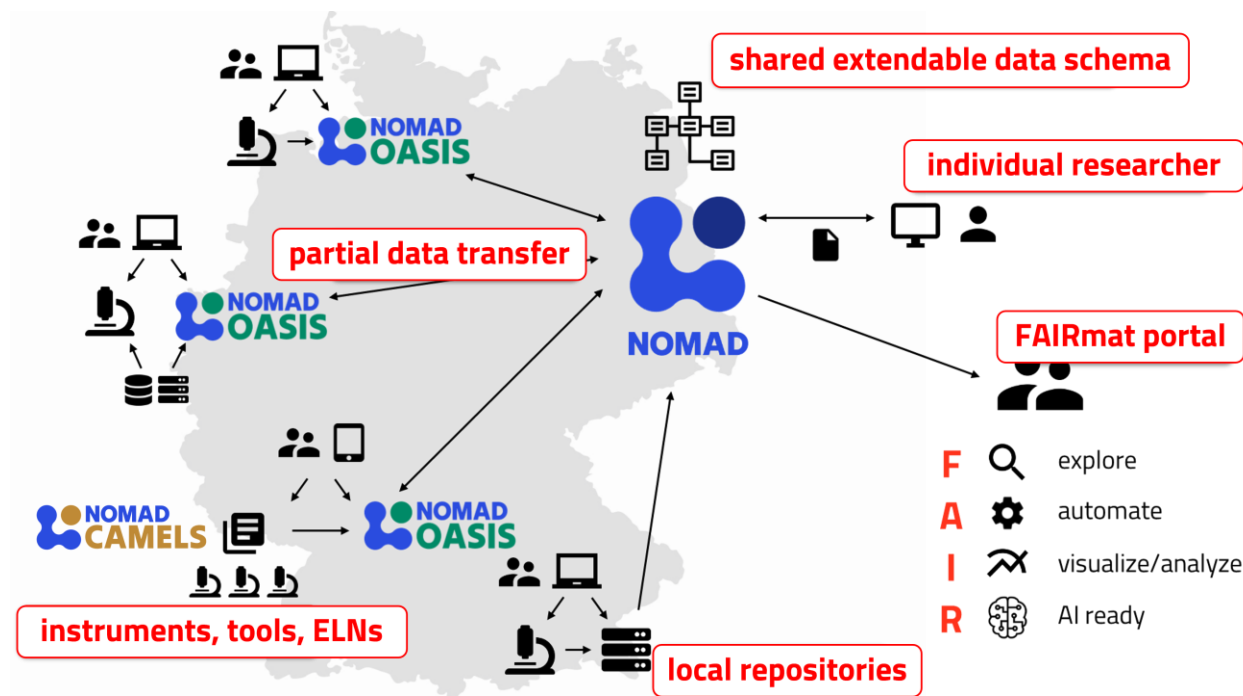
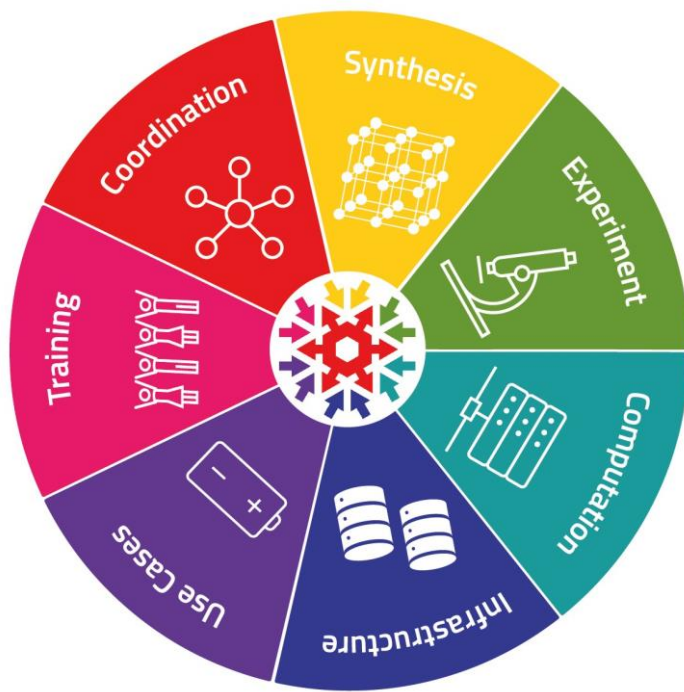
HU Berlin | FAIRmat | NOMAD



FORSCHUNGSDATEN@RMU
October 30, 2025

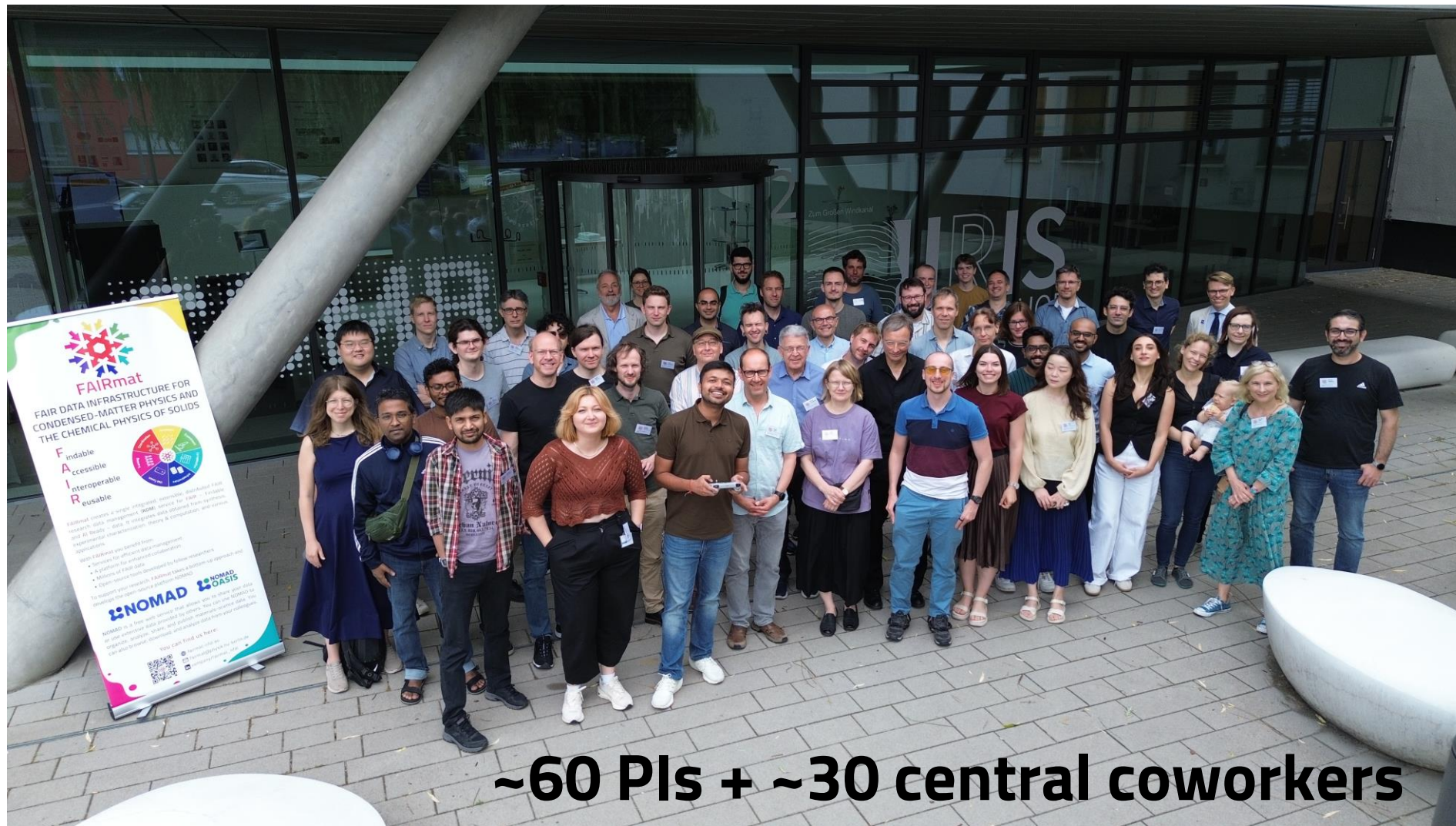
What is FAIRmat

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



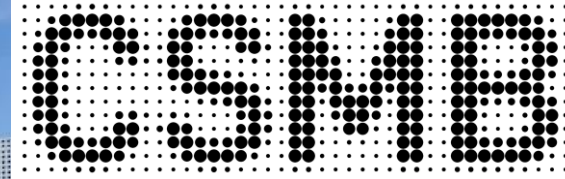
NFDI: National (German) Research Data Infrastructure

The FAIRmat team



The FAIRmat Hub in Berlin

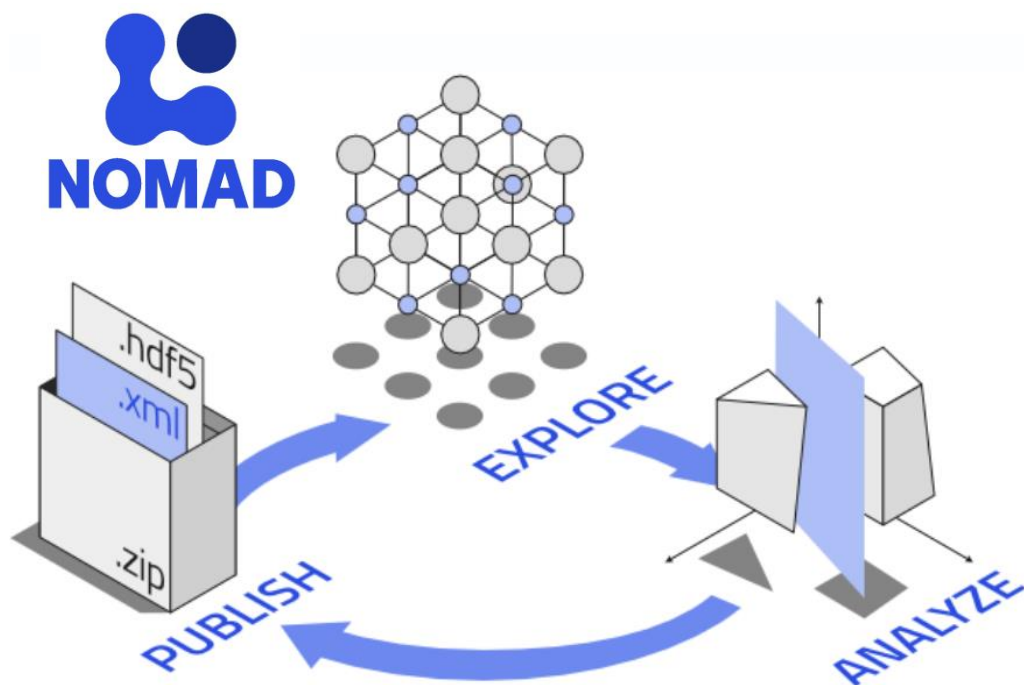
**Office space for ~40 people,
seminar rooms, etc.**



NOMAD comes in two flavours

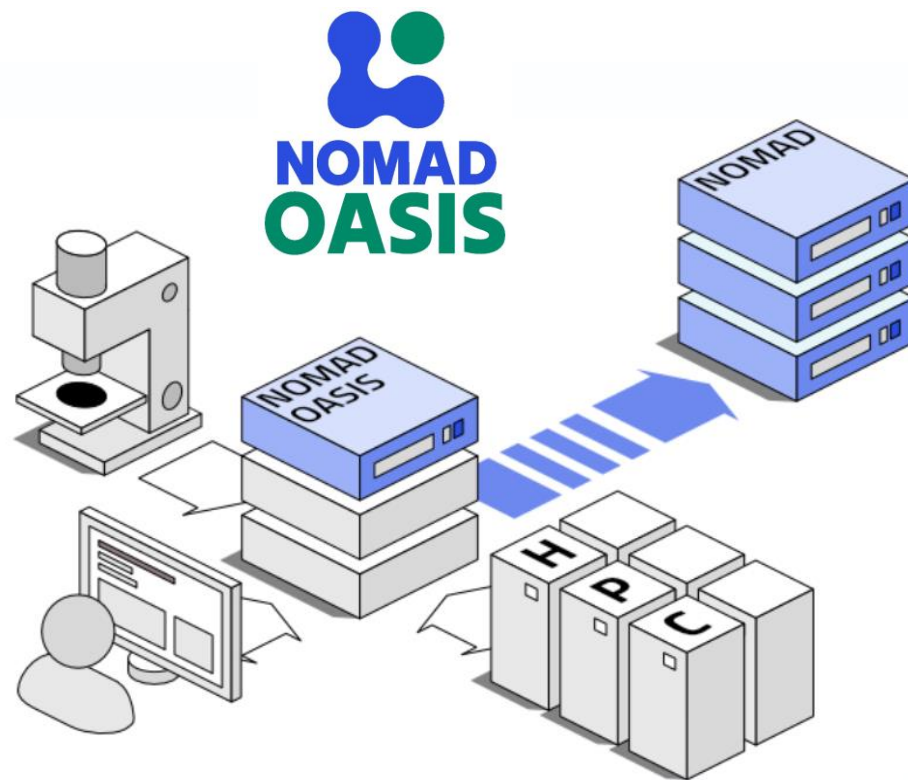
Publish & explore data

Central RDM platform



Manage your lab

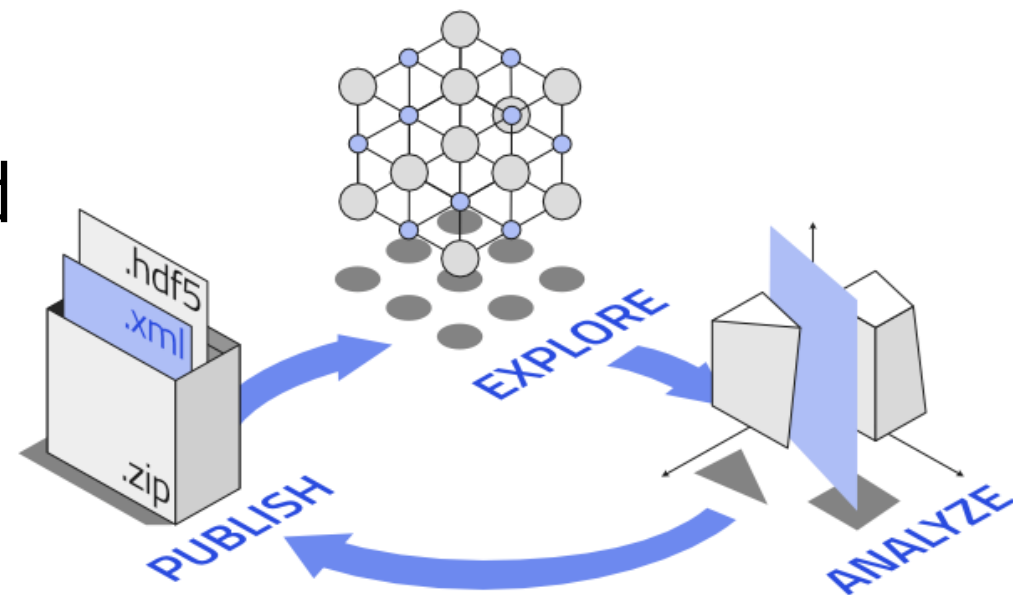
Local RDM tool | ELN



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

19,221,889

UPLOADED FILES

113.4 TB


REGISTERED USERS

> 4000



NOMAD core functionalities

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

NOMAD core functionalities

 PUBLISH ▾ EXPLORE ▾ ANALYZE ▾ ABOUT ▾

Entries ?

Welcome [Pepe Marquez](#)  LOGOUT  UNITS

FILTERS

Material

Elements / Formula

Elements

Se X AND Zn X

Structure

Method

DFT

GW

Projection

DMFT

EELS

Workflow

Molecular Dynamics

662 RESULTS

ELEMENTS / FORMULA

linear ▾ +

☐ only compositions that exclusively contain these atoms

1	H	2	He
3	Li	4	Be
5	B	6	C
7	N	8	O
9	F	10	Ne
11	Na	12	Mg
13	Al	14	Si
15	P	16	S
17	Cl	18	Ar
19	K	20	Ca
21	Sc	22	Ti
23	V	24	Cr
25	Mn	26	Fe
27	Co	28	Ni
29	Cu	30	Zn
31	Ga	32	Ge
33	As	34	Se
35	Br	36	Kr
37	Rb	38	Sr
39	Y	40	Zr
41	Nb	42	Mo
43	Tc	44	Ru
45	Rh	46	Pd
47	Ag	48	Cd
49	In	50	Sn
51	Sb	52	Te
53	I	54	Xe
55	Cs	56	Ba
57	La	58	Ce
59	Pr	60	Nd
61	Pm	62	Sm
63	Eu	64	Gd
65	Tb	66	Dy
67	Ho	68	Er
69	Tm	70	Yb
71	Lu	72	Hf
73	Ta	74	W
75	Re	76	Os
77	Ir	78	Pt
79	Au	80	Hg
81	Tl	82	Pb
83	Bi	84	Po
85	At	86	Rn
87	Fr	88	Ra
89	Ac	90	Th
91	Pa	92	U
93	Np	94	Pu
95	Am	96	Cm
97	Bk	98	Cf
99	Es	100	Fm
101	Md	102	No
103	Lr	104	Rf
105	Db	106	Sg
107	Bh	108	Hs
109	Mt	110	Ds
111	Rg	112	Cn
113	Nh	114	Fl
115	Mc	116	Lv
117	Ts	118	Og
119	Uue		

Chemical Formula Hill linear +

Chemical Formula IUPAC linear +

Authors

Markus Scheidgen →

Hieu Ngo →

Niloofer Hadaeghi →


Honghui Shang →



Honghui Shang →

Honghui Shang →

Honghui Shang →

NOMAD core functionalities

 PUBLISH ▾ EXPLORE ▾ ANALYZE ▾ ABOUT ▾

Welcome [Pepe Marquez](#)  LOGOUT  UNITS



Entries ?

FILTERS

Material

Elements / Formula >

Elements

Se  AND Zn 

Structure >

Method >

DFT >

GW >


Projection >

DMFT >

EELS >

Workflow

Molecular Dynamics >


 Type your query or keyword here

+ TERMS






+ HISTOGRAM

+ SCATTER PLOT

+ PERIODIC TABLE

 <> ^


20/662 search results



<input type="checkbox"/>	Name	Formula	Entry type	Upload time ↓	Authors	
<input type="checkbox"/>	Se16Zn16 FHI-aims simulation	Se16Zn16	FHI-aims	2/10/2023, 8:25:24 PM	Markus Scheidgen	
<input type="checkbox"/>	Se16Zn16 FHI-aims simulation	Se16Zn16	FHI-aims	11/4/2022, 5:55:54 AM	Hieu Ngo	<div>Go to the entry page</div>
<input type="checkbox"/>	Se16Zn16 FHI-aims simulation	Se16Zn16	FHI-aims	6/22/2022, 10:30:06 AM	Niloofer Hadaeghi	
<input type="checkbox"/>	SeZn FHI-aims simulation	SeZn	FHI-aims simulation	5/21/2021, 8:55:22 AM	Honghui Shang	
<input type="checkbox"/>	Se4Zn4 FHI-aims simulation	Se4Zn4	FHI-aims simulation	5/21/2021, 8:55:22 AM	Honghui Shang	
<input type="checkbox"/>	Se4Zn4 FHI-aims simulation	Se4Zn4	FHI-aims simulation	5/21/2021, 8:55:22 AM	Honghui Shang	


NOMAD core functionalities

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

NOMAD core functionalities

 PUBLISH ▾ EXPLORE ▾ ANALYZE ▾ ABOUT ▾

Welcome [Pepe Marquez](#)  LOGOUT  UNITS

Entries / Entry 

OVERVIEW FILES DATA LOGS

Metadata

method name
DFT

program version
4.6.35 3Apr08 complex parallel LinuxIFC

program name
VASP

basis set type
plane waves

core electron treatment
pseudopotential

jacob's ladder
GGA

xc functional names
GGA_C_PBE, GGA_X_PBE

comment
no comment

references
<http://www.sciencedirect.com/scienc...>
<http://aflowlib.org>
<http://www.sciencedirect.com/scienc...>

authors

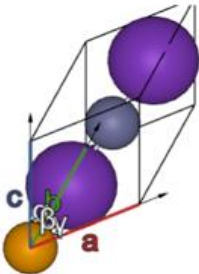
Material

Original ▾

Composition

formula	K2SeZn
dimensionality	bulk
elements	K, Se, Zn
number of elements	3 (ternary)

Structure



● K
● Zn
● Se


Symmetry

crystal system	bravais lattice
cubic	cF
space group number	space group symbol
225	Fm-3m
point group	structure name
m-3m	Heusler


Lattice parameters

a	b	c
5.699 Å	5.699 Å	5.699 Å
α	β	γ
60 °	60 °	60 °
cell volume 130.892 Å ³		


NOMAD core functionalities


 [PUBLISH](#) [EXPLORE](#) [ANALYZE](#) [ABOUT](#)


Welcome [Pepe Marquez](#) [LOGOUT](#) [UNITS](#)


Entries / Entry 

[http://www.sciencedirect.com/science...](http://www.sciencedirect.com/science)
<http://aflowlib.org>
[http://www.sciencedirect.com/science...](http://www.sciencedirect.com/science)
authors
AFLOW
datasets
no datasets

mainfile
...A2BC_LDAU2/vasprun.xml.bands.xz 

entry id
[80zw_KpV6X314K7RM2QAFykhTpjb](#) 

material id
[szL5IntGGwsmx2OR2yE00SS3IfI-](#) 

upload id
[_9RFq_-CRxGXqEZw9BxBYQ](#) 

upload create time
12/2/2019, 10:34:30 PM

last processing time
1/4/2022, 6:27:22 AM

processing version
1.0.0/37587aa6

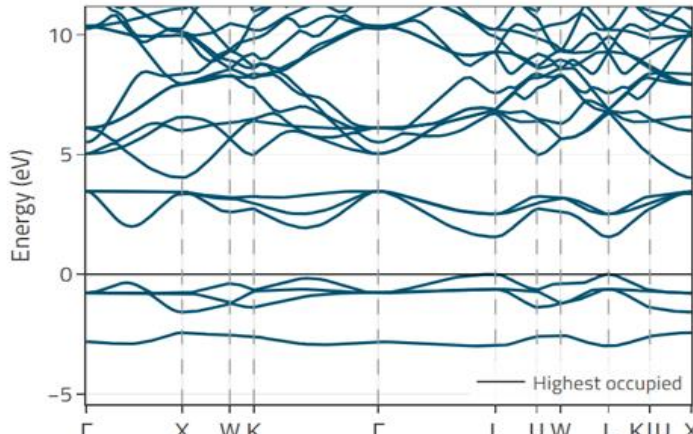
API

225	Fm-3m	60	60	60
point group	structure name	cell volume		
m-3m	Heusler	130.892 Å ³		

[VIEW IN ENCYCLOPEDIA](#)

Electronic properties

Band structure

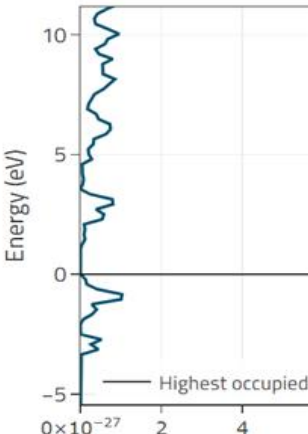


Energy (eV)

Gamma X W K Gamma L U W L K U X

— Highest occupied

Density of states



Energy (eV)

0 × 10⁻²⁷ 2 4


states eV⁻¹

— Highest occupied



NOMAD core functionalities

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

NOMAD core functionalities

 PUBLISH ▾ EXPLORE ▾ ANALYZE ▾ ABOUT ▾

Entries / Entry / Data

Welcome [Pepe Marquez](#)  LOGOUT  UNITS

OVERVIEW FILES DATA LOGS

☐ code specific ☐ all defined ☐ definitions <> ↺

→ <>

System

section

QUANTITIES

▶ type = bulk

▶ configuration_raw_gid = _OT2z27hNuJyVSPqchZr2Im6szSC

▶ is_representative = true

▶ chemical_composition = KKSeZn

chemical_composition_hill = K2SeZn

chemical_composition_reduced = K2SeZn

SUB SECTIONS

atoms

prototype


symmetry

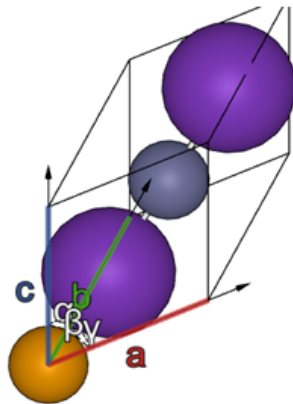
REFERENCED BY closed

→ <>

Atoms

section





QUANTITIES

species = 4 vector

labels = 4 list

positions = 4 × 3 matrix

→ <>

lattice_vectors

quantity

VALUE

$$\begin{bmatrix} 0 & 4.02990 & 4.02990 \\ 4.02990 & 0 & 4.02990 \\ 4.02990 & 4.02990 & 0 \end{bmatrix}$$

(3 × 3)
Å
















REFERENCED BY closed

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




[PUBLISH](#)  [EXPLORE](#)  [ANALYZE](#)  [ABOUT](#) 


Your uploads / Examples for demonstrations


Welcome [Ahmed Mansour](#)  [LOGOUT](#)  [UNITS](#)








OVERVIEW

FILES




Examples for demonstrations 

upload id: 5VEbvP_GQKuNlkao-uusXA 

1 Prepare and upload your files

Here you can upload files. Top-level .zip/.tar files will be uncompressed automatically. For more information, see our documentation on [uploading files](#) or view the [supported codes](#). Optionally, you can also create an entry from built-in or uploaded schemas. Please take a look at our documentation on [schemas](#).

 DROP FILES HERE OR CLICK TO OPEN DIALOG

CREATE FROM SCHEMA


> /

2 Process data

3 Edit visibility and access

☐ Enabling this will allow all users, including guests without an account, to view the upload even before it is published.

You can edit the access to the upload by adding or removing users as upload members.

 EDIT UPLOAD MEMBERS

NOMAD core functionalities



[PUBLISH](#) ▾ [EXPLORE](#) ▾ [ANALYZE](#) ▾ [ABOUT](#) ▾

Your uploads / Examples for demonstrations

Welcome [Ahmed Mansour](#)

LOGOUT UNITS

DROP FILES HERE OR CLICK TO OPEN DIALOG

CREATE FROM SCHEMA

> /

2 Process data

Processing completed, 3/3 entries processed

3 entries



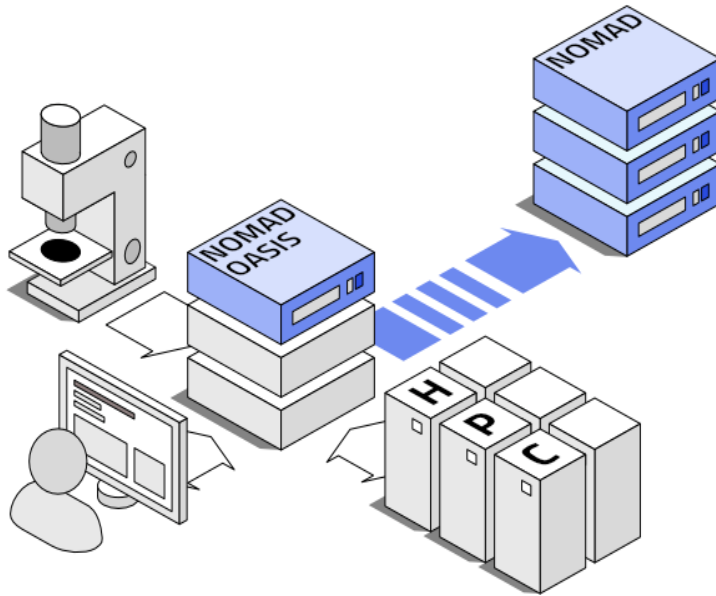
<input type="checkbox"/>	Name	Type	Mainfile	Process status ↑
<input type="checkbox"/>	Si exciting GW SinglePoint simulation	exciting GW SinglePoint	INFO.OUT	SUCCESS →
<input type="checkbox"/>	Si exciting DFT SinglePoint simulation	exciting DFT SinglePoint	INFO.OUT	SUCCESS →
<input type="checkbox"/>	Si exciting DFT+GW simulation	exciting DFT+GW	INFO.OUT	SUCCESS →

NOMAD Oasis

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

REGISTERED INSTALLATIONS

> 80



HZB Helmholtz
Zentrum Berlin



**universität
innsbruck**

I ILLINOIS



**TECHNISCHE UNIVERSITÄT
KAISERSLAUTERN**

li.u LINKÖPING
UNIVERSITY



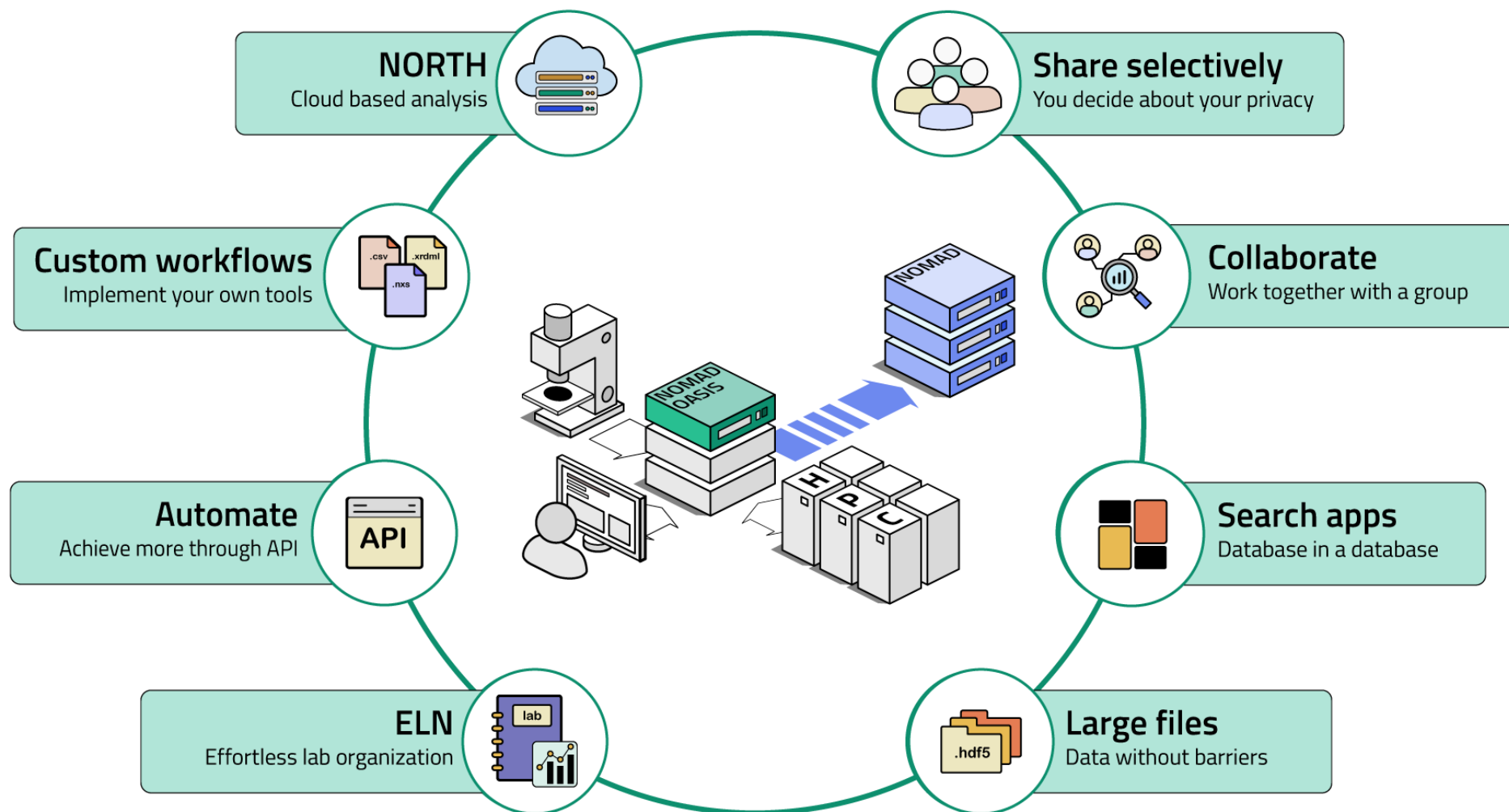
ikz

Technische
Universität
Berlin

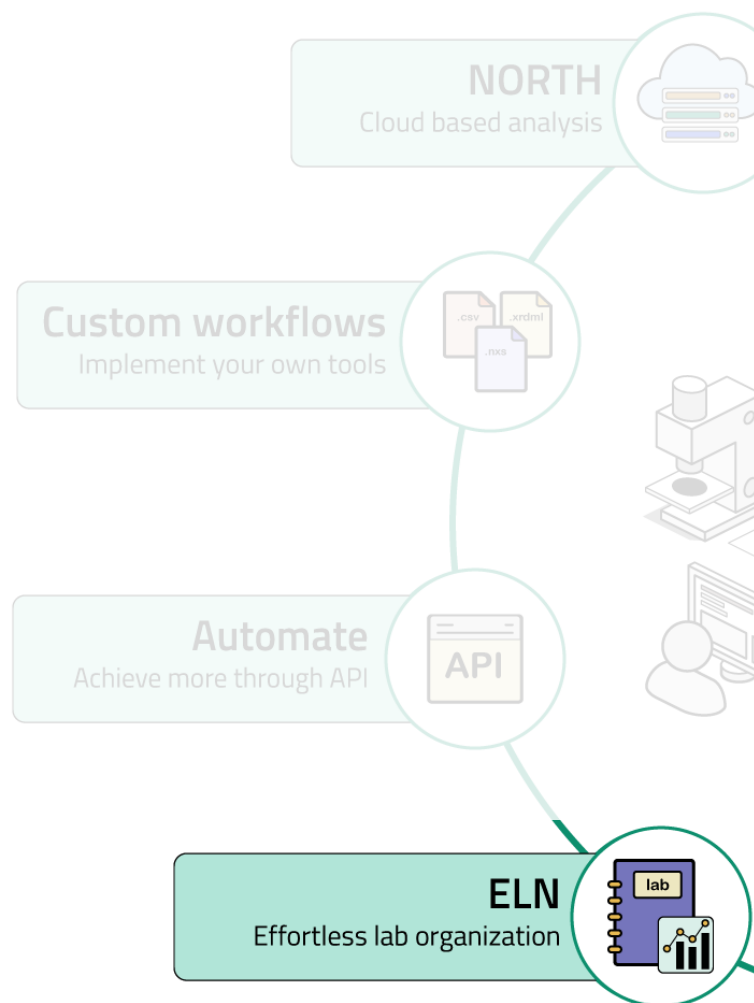
WARWICK
THE UNIVERSITY OF WARWICK



NOMAD Oasis



NOMAD Oasis



PUBLISH ▾ **EXPLORE** ▾ **ANALYZE** ▾ **ABOUT** ▾

Welcome [Pepe Marquez](#) **LOGOUT** **UNITS**

Your uploads / Upload / Entry ?

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_-rKyOyyNsZP](#)

upload id
[r75jMoZzTcOFFPZd63BIEw](#)

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.

12 WORDS POWERED BY TINY

Datetime
23/03/2023 12:28

SolarCellParameters

NOMAD Oasis

Custom workflows
Implement your own tools



Automate
Achieve more through API



ELN
Effortless lab organization

NORTH
Cloud based analysis

Entry

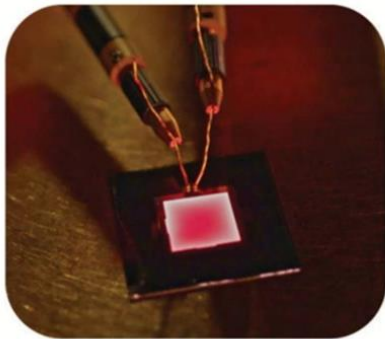
section

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**

PUBLISH EXPLORE ANALYZE ABOUT

Your uploads / Upload / Entry / Data

Welcome [Pepe Marquez](#) LOGOUT UNITS

OVERVIEW FILES DATA LOGS

search


☐ code specific ☐ all defined ☐ definitions

<> ↺ ↻


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

The Jupyter Notebook is the original web application for creating and sharing computational documents. It offers a simple, streamlined, document-centric experience.


Maintainer: [Markus Scheidgen](#)


File extensions: ipynb

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.



1 a group

5 abase

Customize your NOMAD using



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

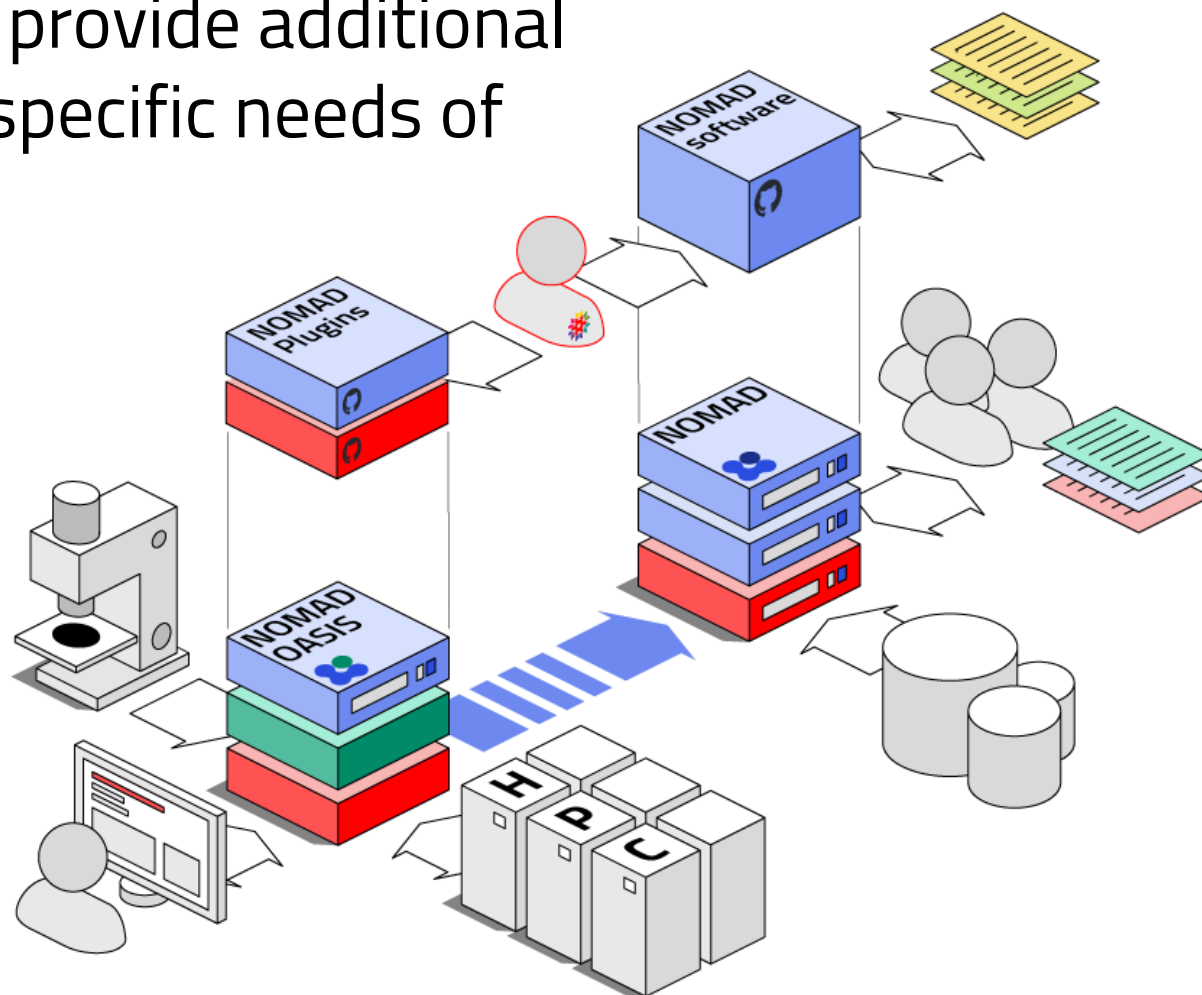
Schema packages

Parsers

Apps

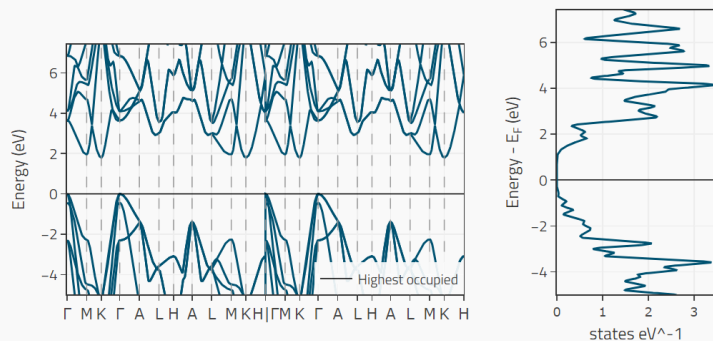
Example uploads

Normalizers

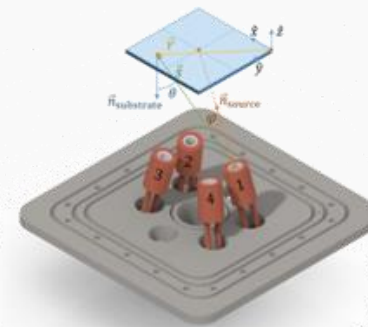


Working areas in FAIRmat

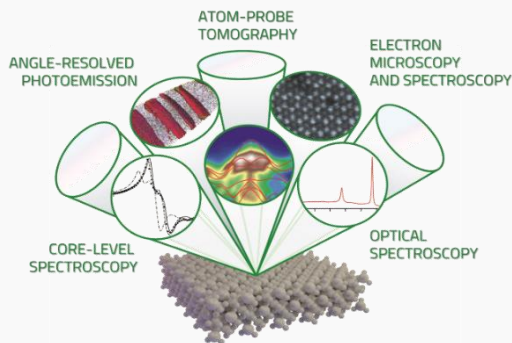
Theory and Computations



Synthesis



Experiment | Characterization

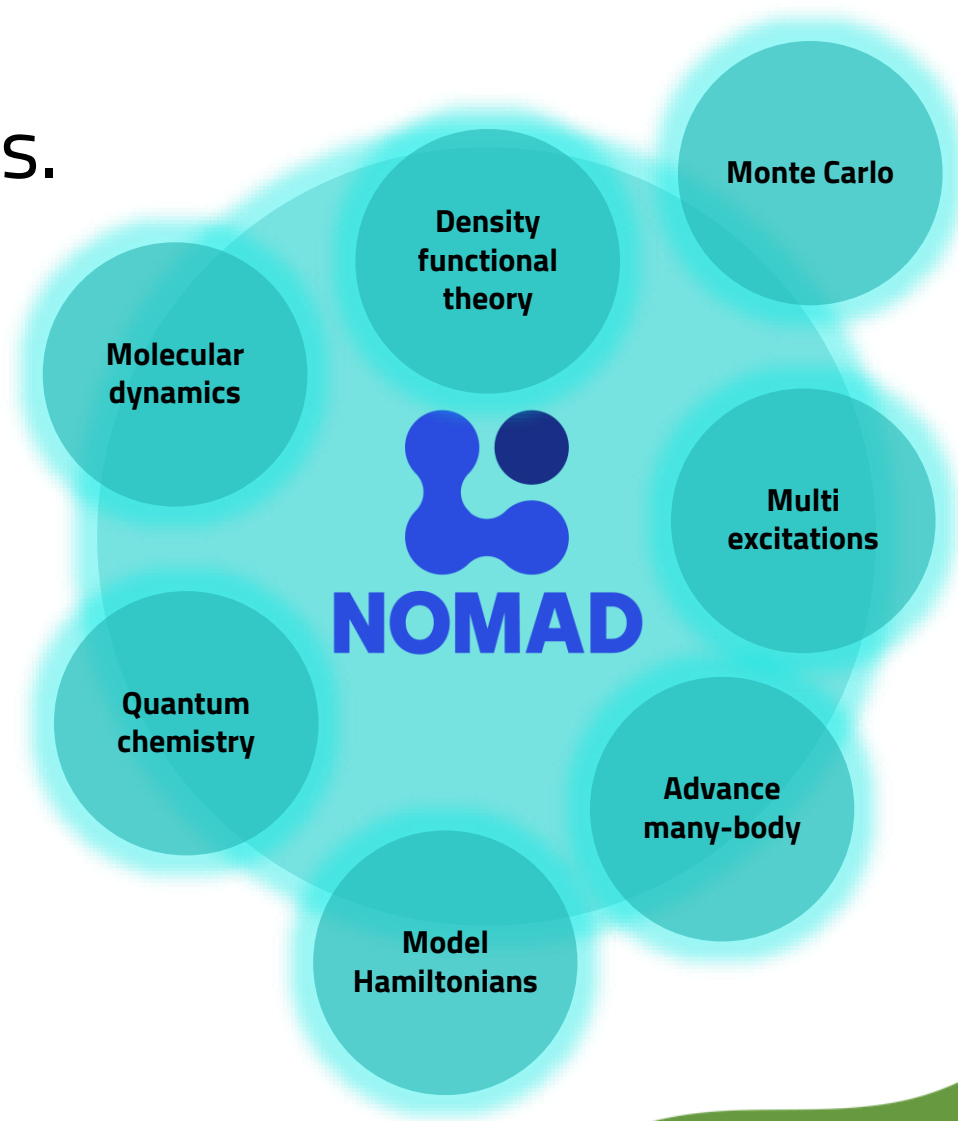


Use cases



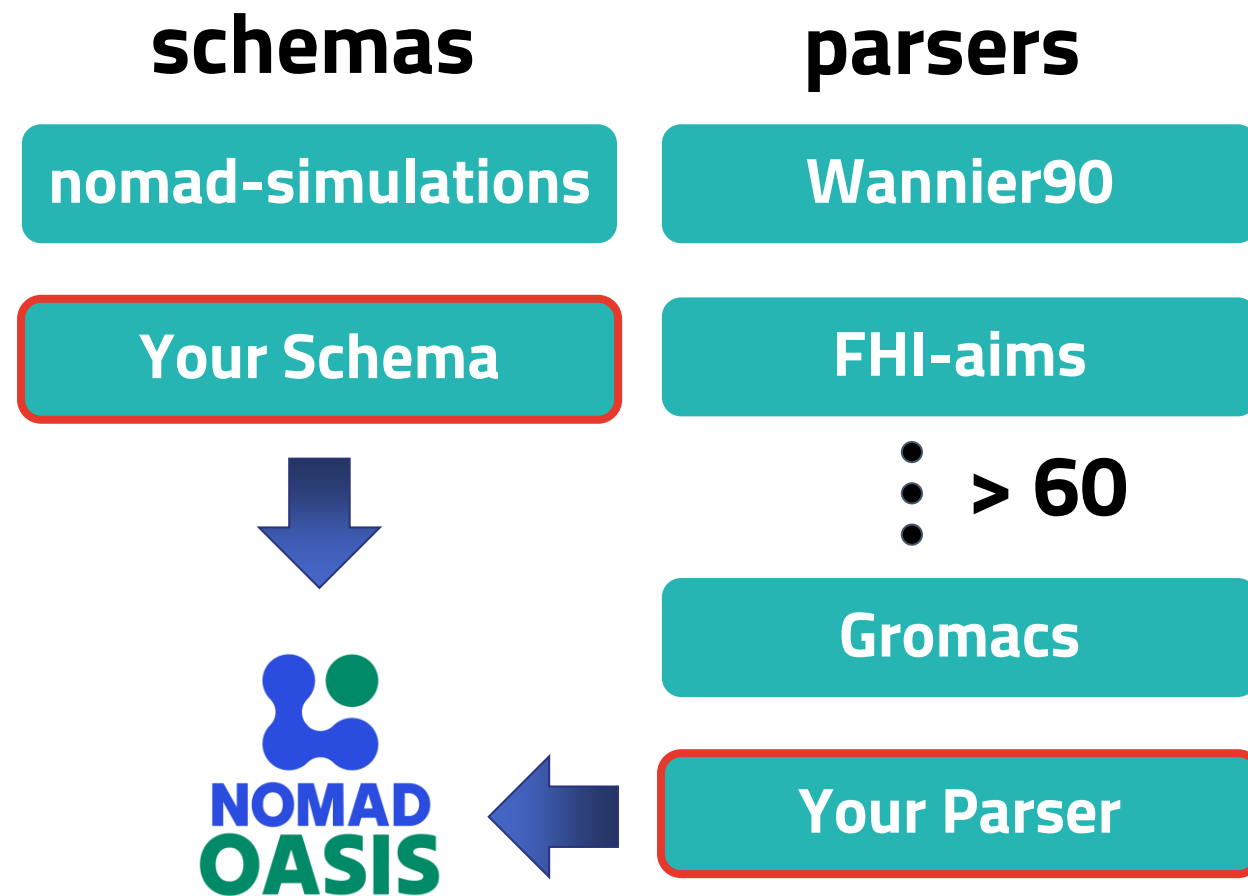
Theory and computation

- 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.



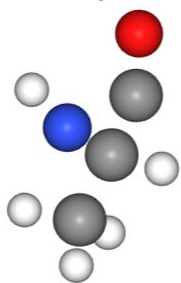
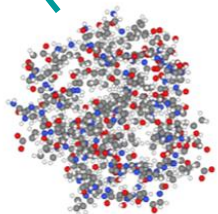
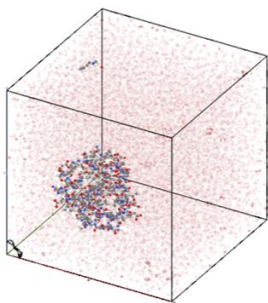
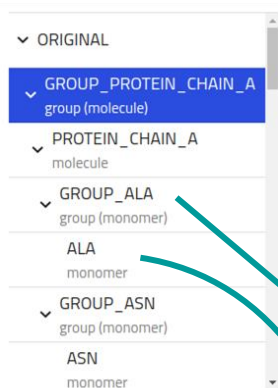
Extensible support for computational data

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

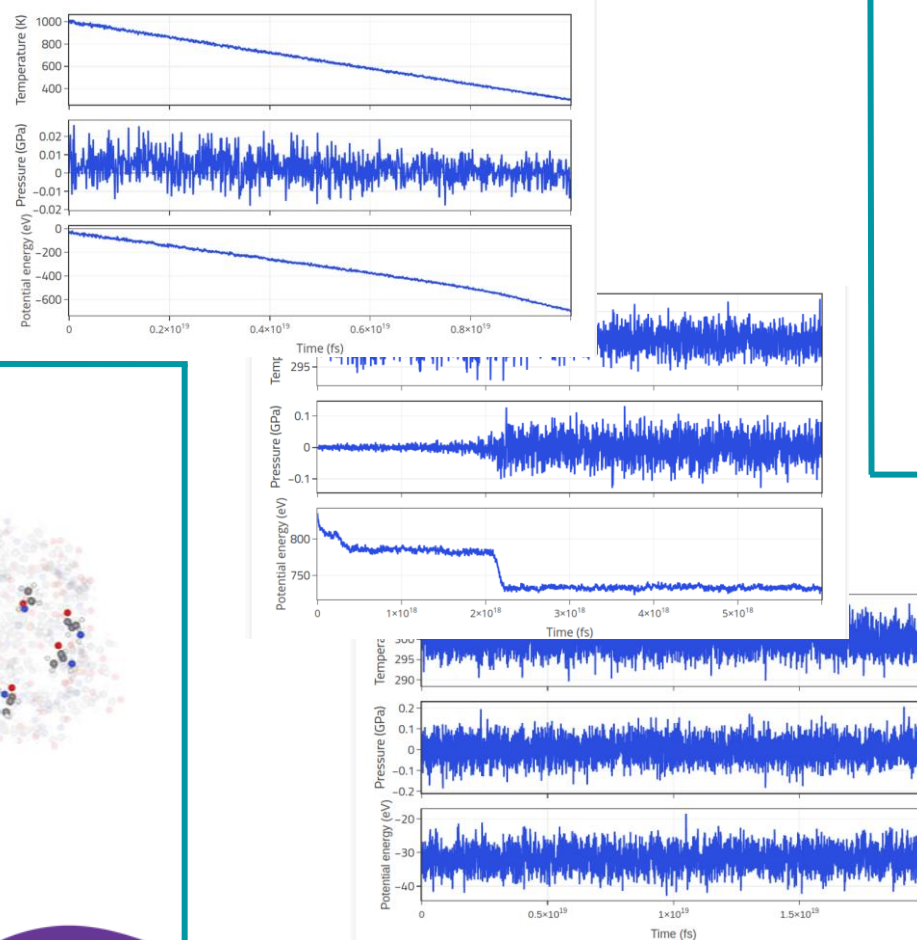


Support for Molecular Dynamics Simulations

Visualization of system hierarchies

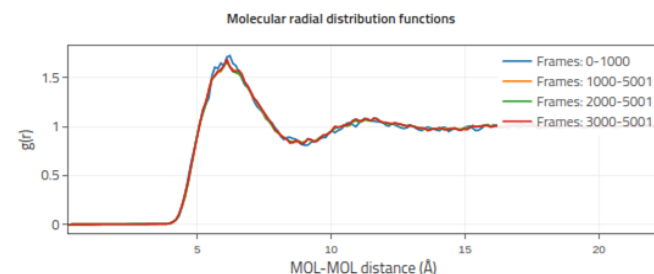


Storage and display of trajectory properties

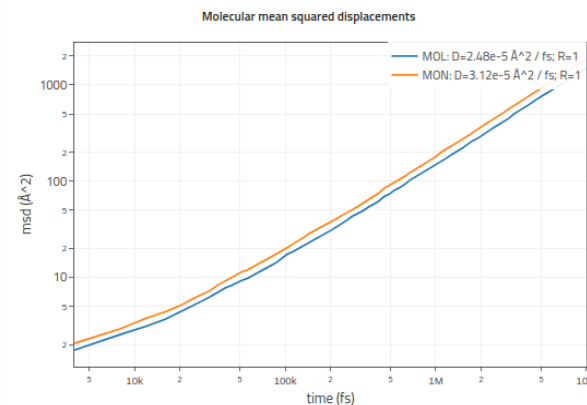


Automated calculation of basic molecular properties

Structural properties



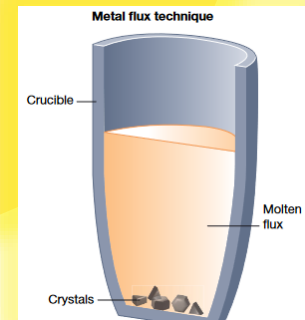
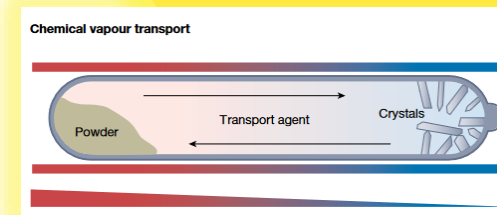
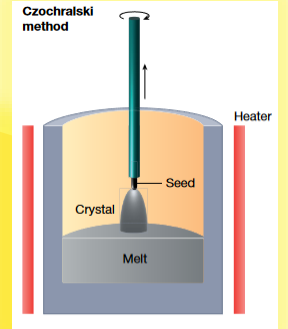
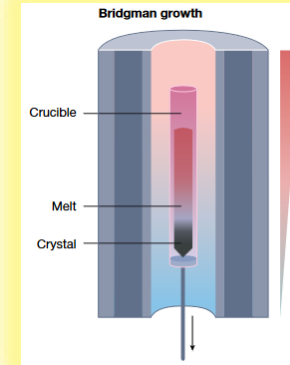
Dynamical properties



Synthesis

Formalized data models for key synthesis routes.

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



Modular classes for schema development

Base sections

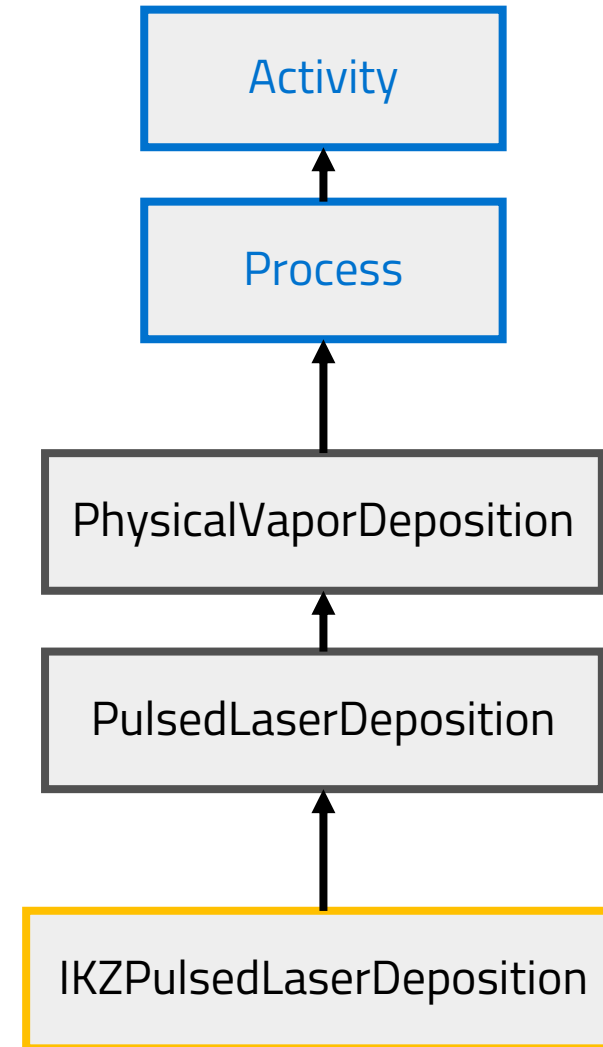
General definitions, not for specific field

Standard plugins

For a specific field/method
Developed by FAIRmat

User-defined schema

User-developed schema specific to lab/instrument

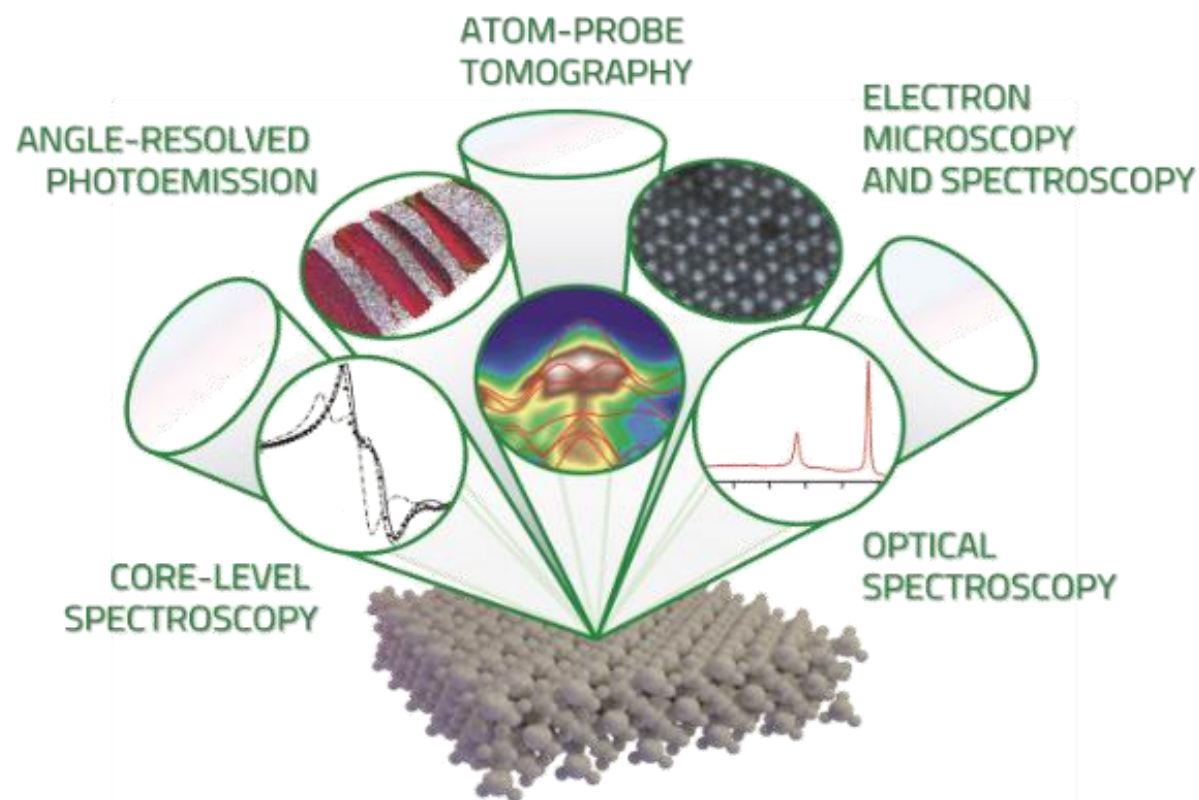


Experiments: NeXus standardization

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



pynxtools
pynxtools-apm
pynxtools-em

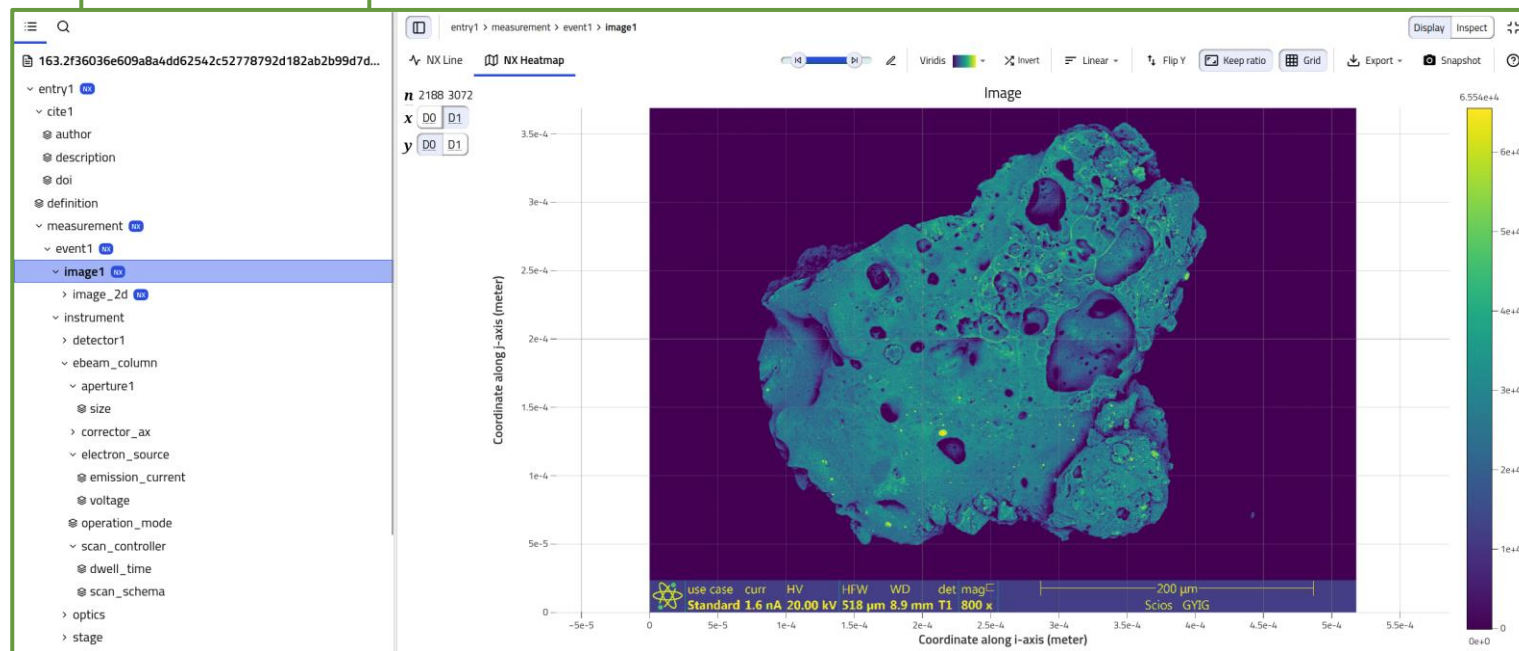


Electron microscopy: Nxem and pynxtools-em

Imaging

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

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



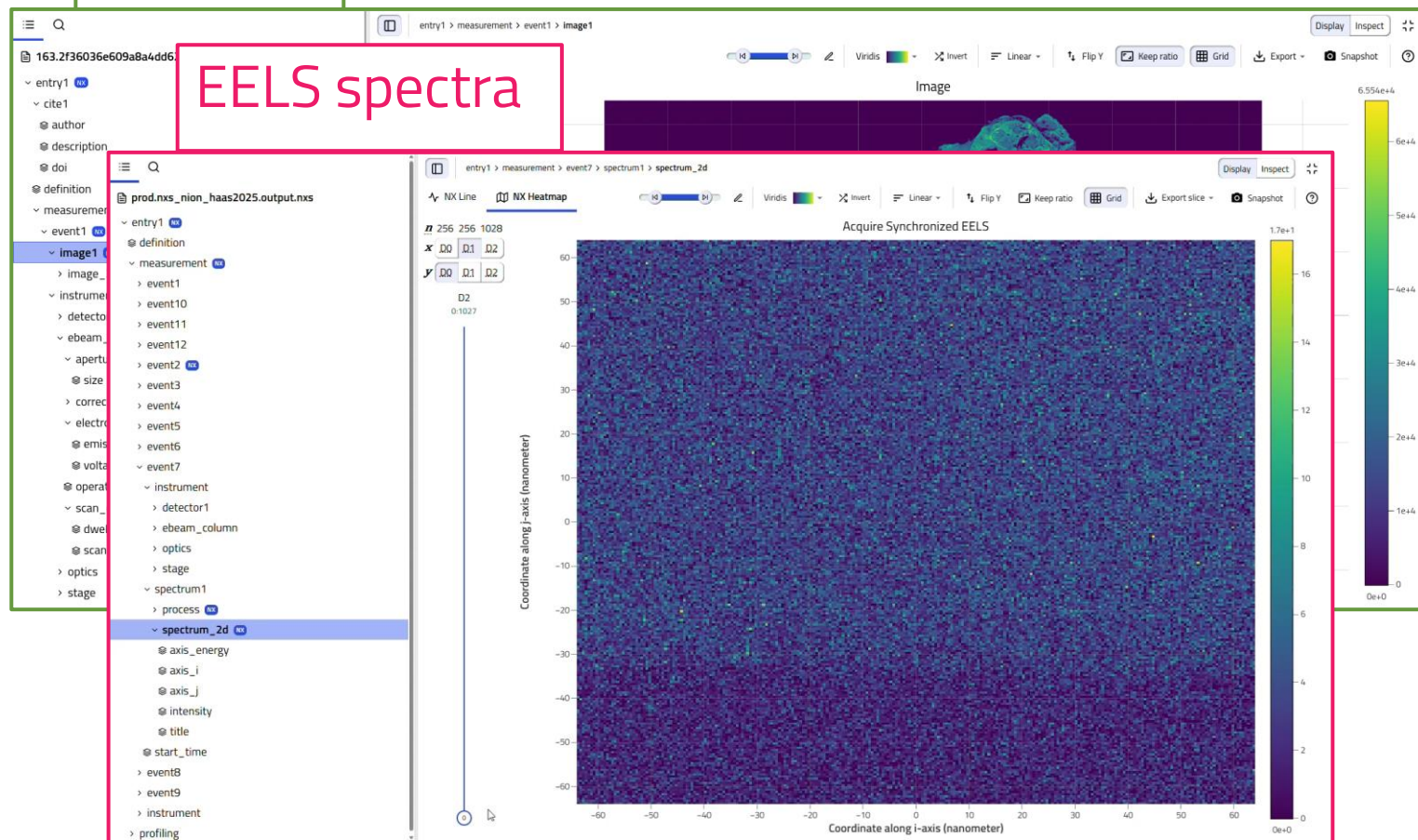
Electron microscopy: Nxem and pynxtools-em

Imaging

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

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

EELS spectra



Electron microscopy: Nxem and pynxtools-em

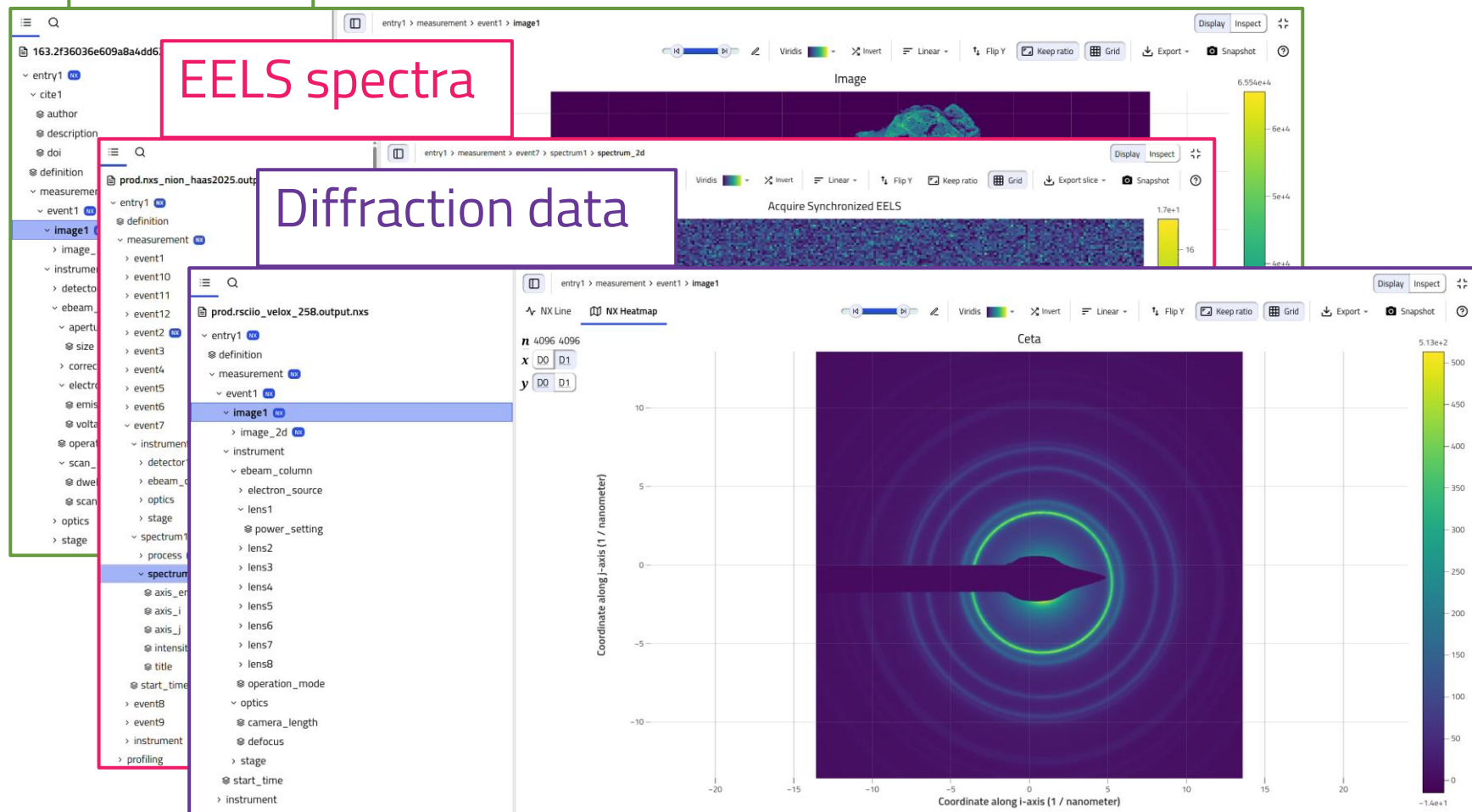
Imaging

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

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

EELS spectra

Diffraction data



Use Cases

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

Solar cells

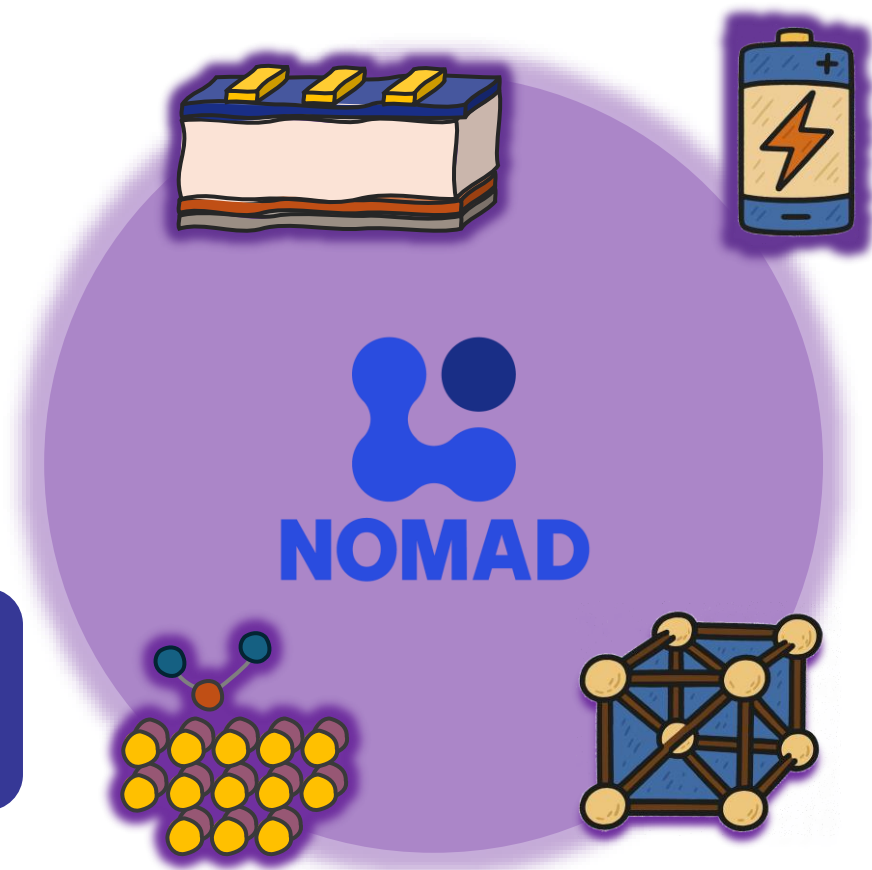
> 40k devices

**Heterogeneous
catalysis**

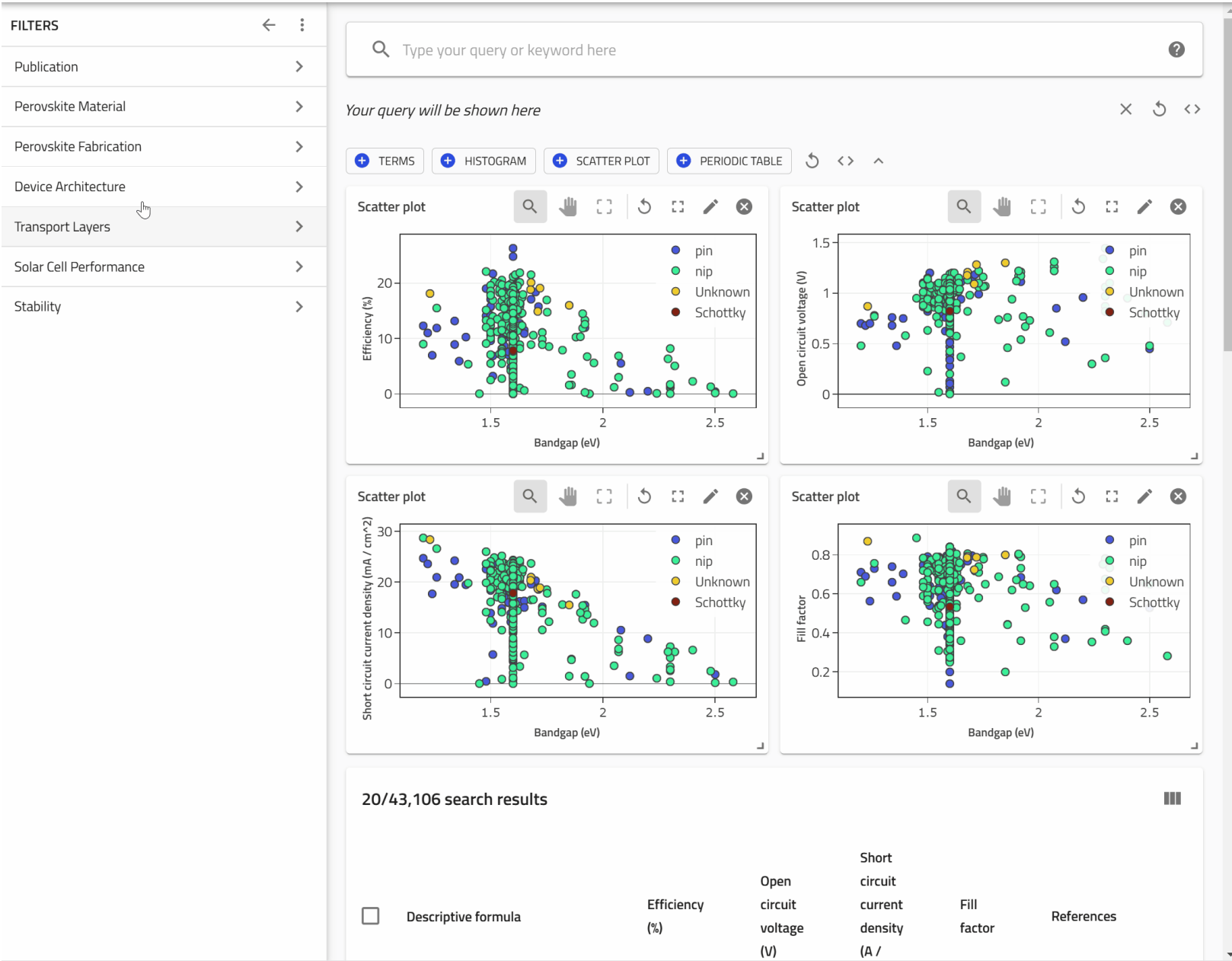
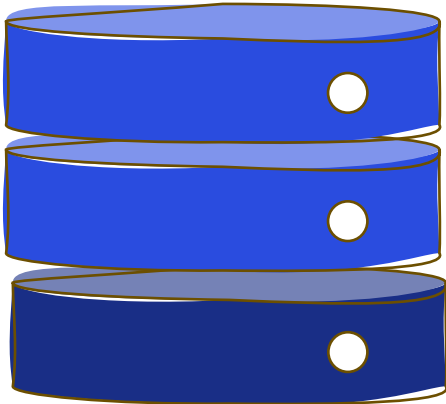
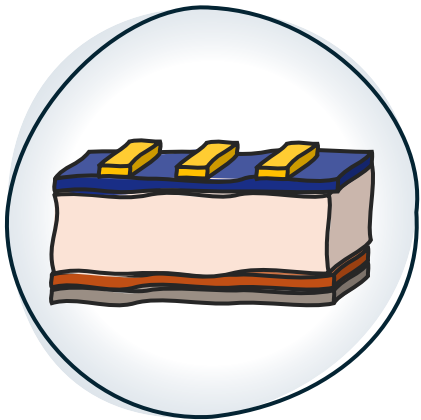
> 2.4k entries

**Metal-organic
frameworks**

> 17k calculations



Solar cells



7th FAIRmat Users Meeting





When? November 20, 2025

Where? Center for the Science of Materials Berlin

Who's invited? All interested scientists

Learn more:



-  [linkedin.com/company/fairmat-nfdi/](https://www.linkedin.com/company/fairmat-nfdi/)
-  fairmat-nfdi.eu
-  discord.gg/R3SuWTBvkk
-  [@fairmat.bsky.social](https://bsky.social/@fairmat)



<https://events.fairmat-nfdi.eu/event/46/>



www.fairmat-nfdi.eu



[@fairmat.bsky.social](https://bsky.app/@fairmat)



fairmat@physik.hu-berlin.de



[company/fairmat-nfdi](https://www.linkedin.com/company/fairmat-nfdi)



www.nomad-lab.eu



[**FAIRmat Digital Flyer**](#)