NOMAD / FAIRmat

Enabling material scientists to define, share, and use data

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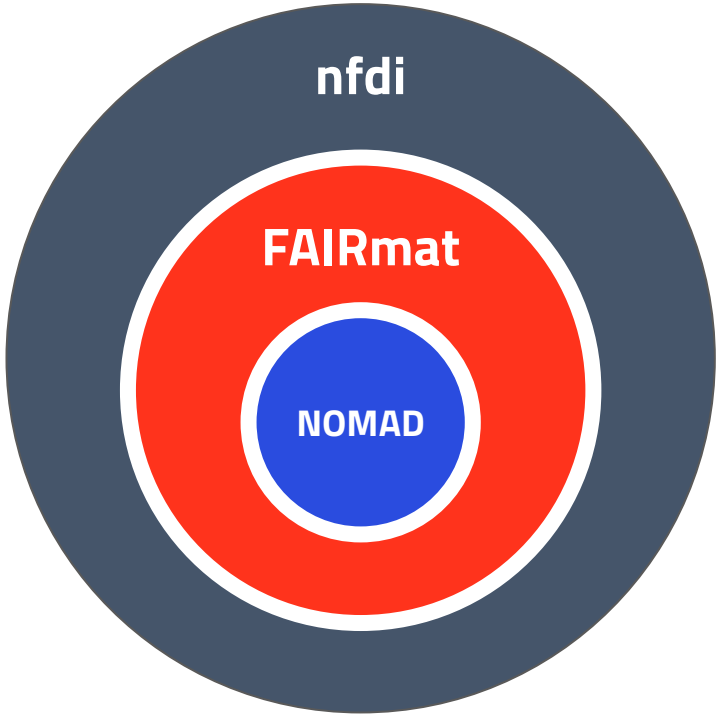
NOMAD, FAIRmat, IRIS, Physik, HU Berlin

Agenda

- What is NFDI, FAIRmat, and NOMAD
- How does NOMAD work?
- Demo
- Comparison to other systems

What are NFDI / FAIRmat / NOMAD



nfdi: Nationale Forschungsdaten Infrastructure, link
(national research data infrastructure)

FAIRmat: NFDI consortium for FAIR materials science data, link
(FAIR: findable, accessible, interoperable, re-usable)

NOMAD: A web-based service and software for managing FAIR materials science data, link
FAIRmat uses NOMAD to build a federated infrastructure of connected NOMAD installations

FAIRmat values

FAIR

Findable, Accessible, Interoperable, Re-usable

FAIR principles can transform the field of condensed-matter physics and the chemical physics of solids.

Open access

Use open processes to support a wide community

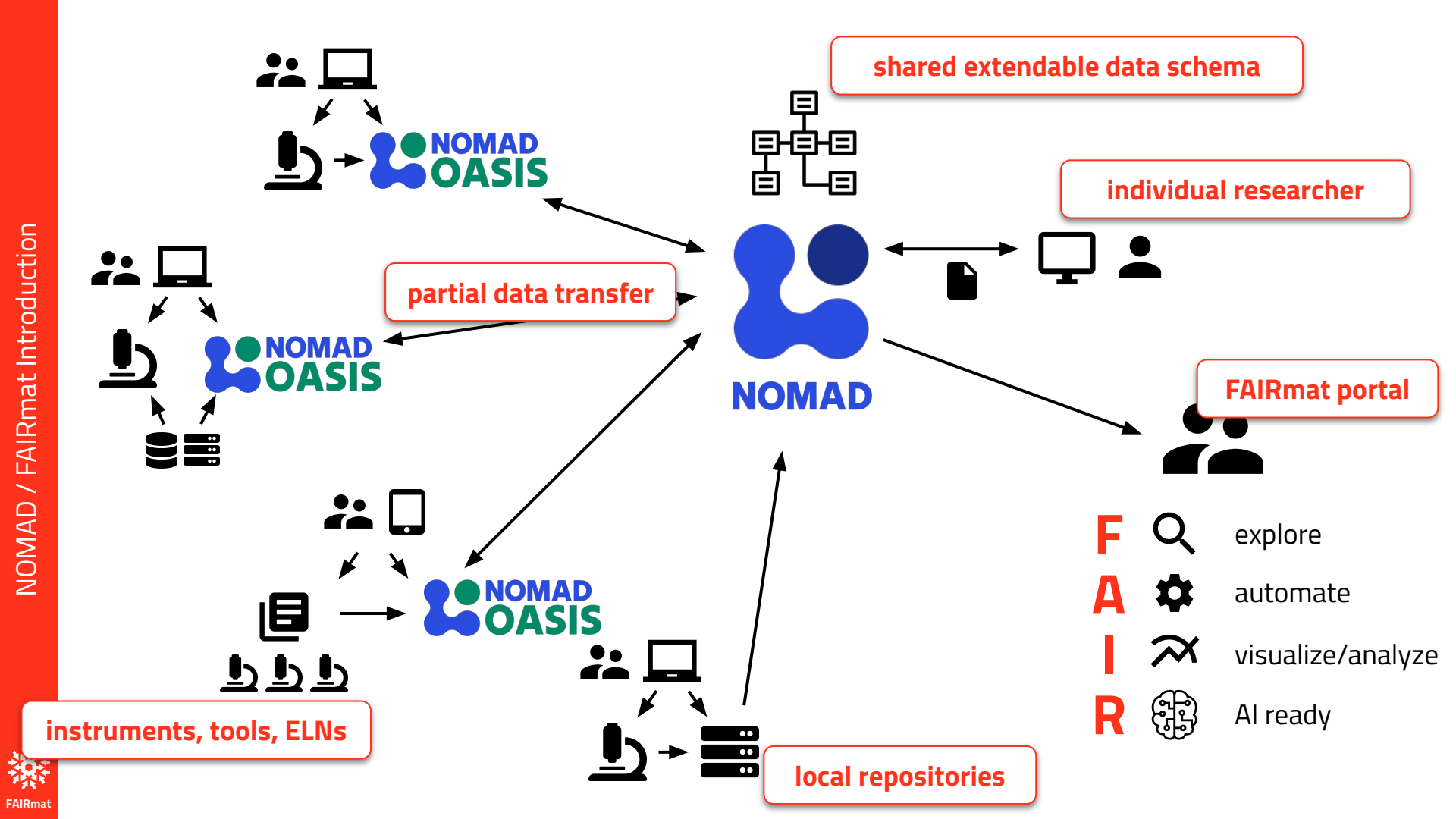
FAIRmat advocates for an urgently needed culture shift towards data sharing, and stands for open access to scientific materials data and tools.

Bottom-up approach

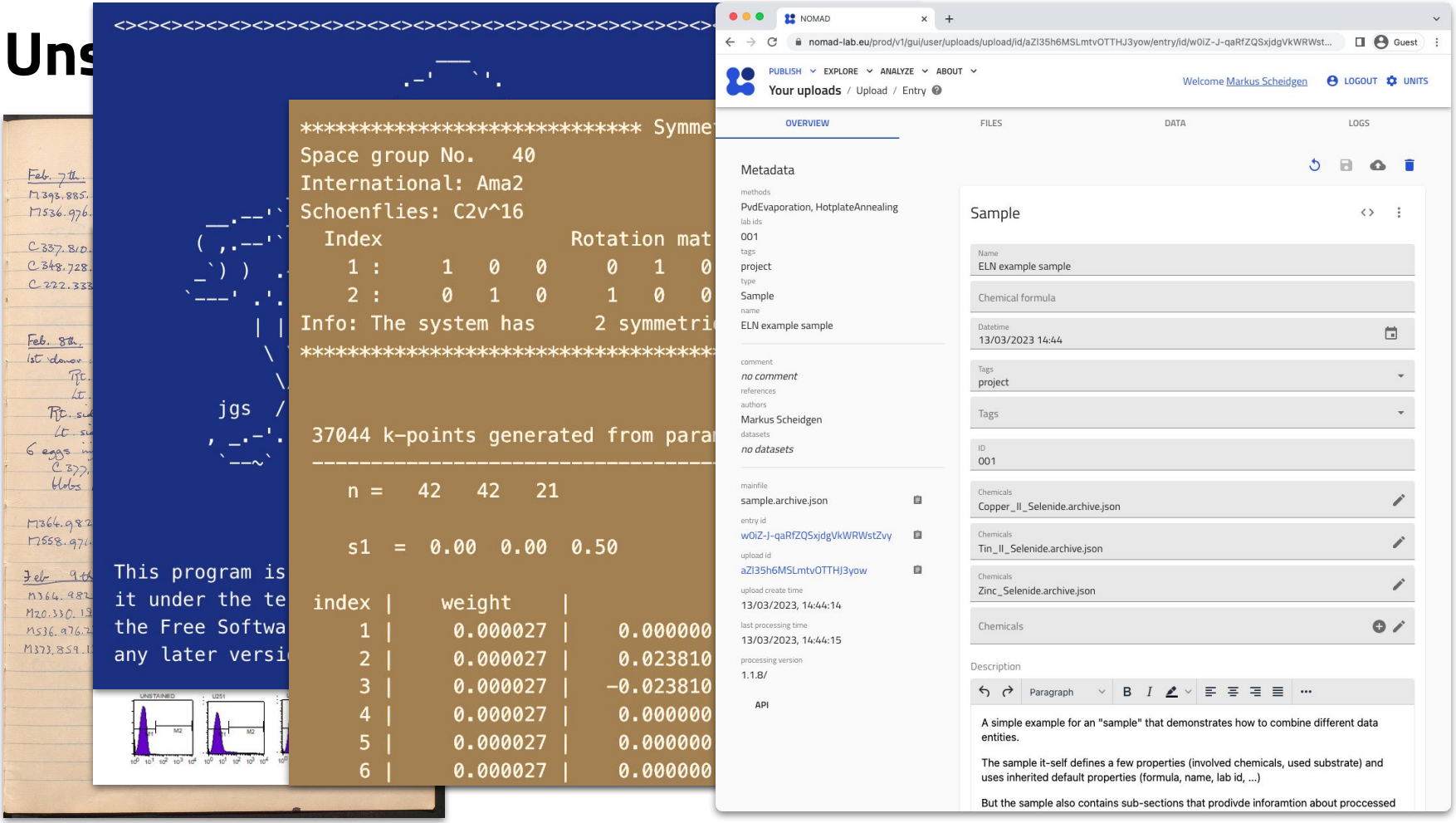
Embracing the community

FAIRmat follows an approach that is driven by the needs of scientists and already enjoys strong support from the community.

FAIRmat structure


shared extendable data schema
individual researcher
partial data transfer
NOMAD OASIS
NOMAD OASIS
NOMAD OASIS
NOMAD
FAIRmat portal
F explore
A automate
I visualize/analyze
R AI ready
instruments, tools, ELNs
local repositories

Uns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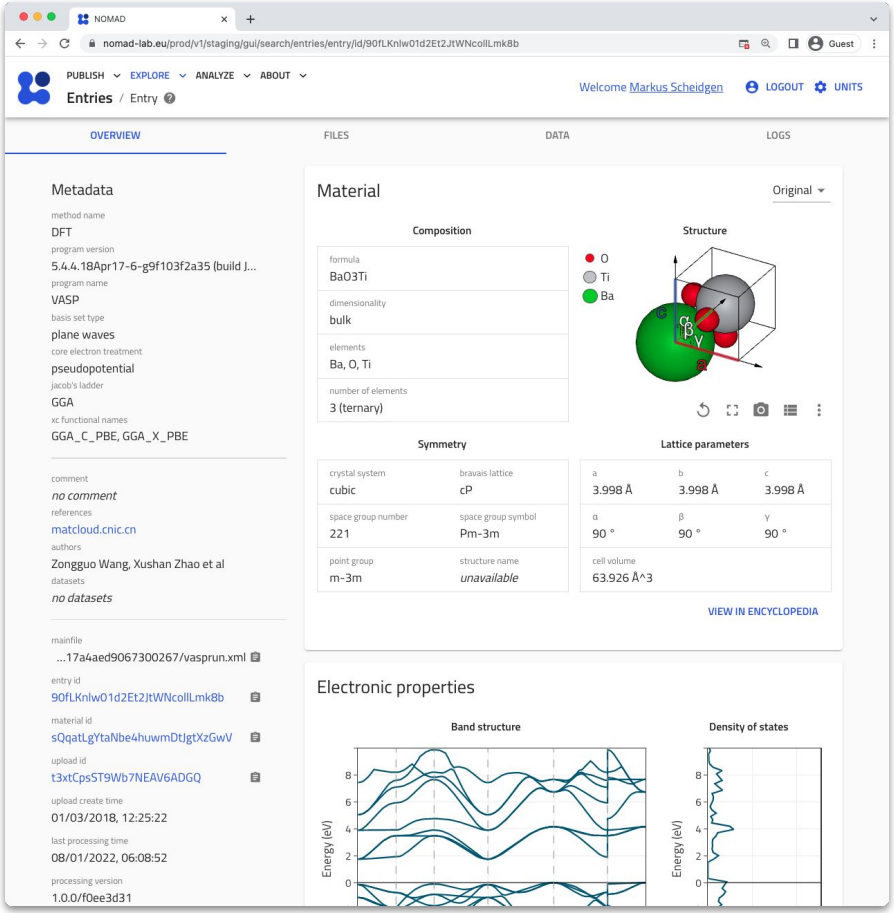
Chemicals
Description
Paragraph
A simple example for an "sample" that demonstrates how to combine different data entities.
The sample it-self defines a few properties (involved chemicals, used substrate) and uses inherited default properties (formula, name, lab id, ...)
But the sample also contains sub-sections that prodivde inforamtion about proccessed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authors
Zongguo Wang, Xushan Zhao et al
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processing version
1.0.0/f0ee3d31
Material
Original
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elements
Ba, O, Ti
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3 (ternary)
Structure
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221
space group symbol
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m-3m
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b
3.998 Å
c
3.998 Å
α
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β
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γ
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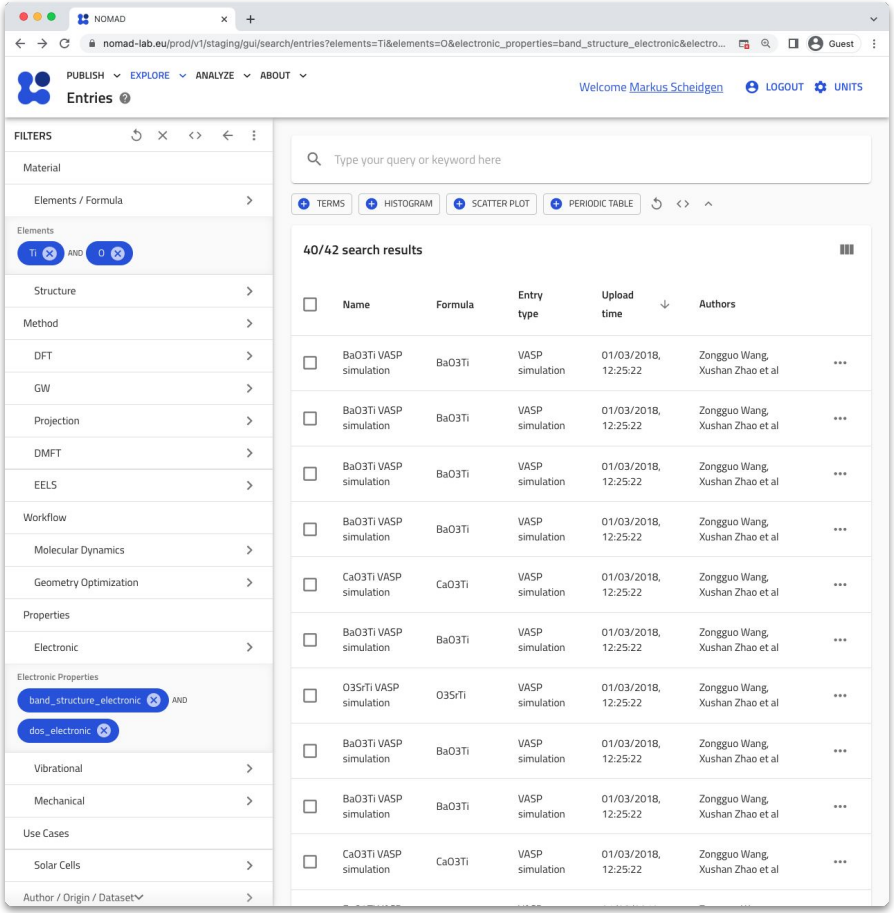
63.926 Å^3
VIEW IN ENCYCLOPEDIA
Electronic properties
Band structure
Density of states
Energy (eV)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40/42 search results
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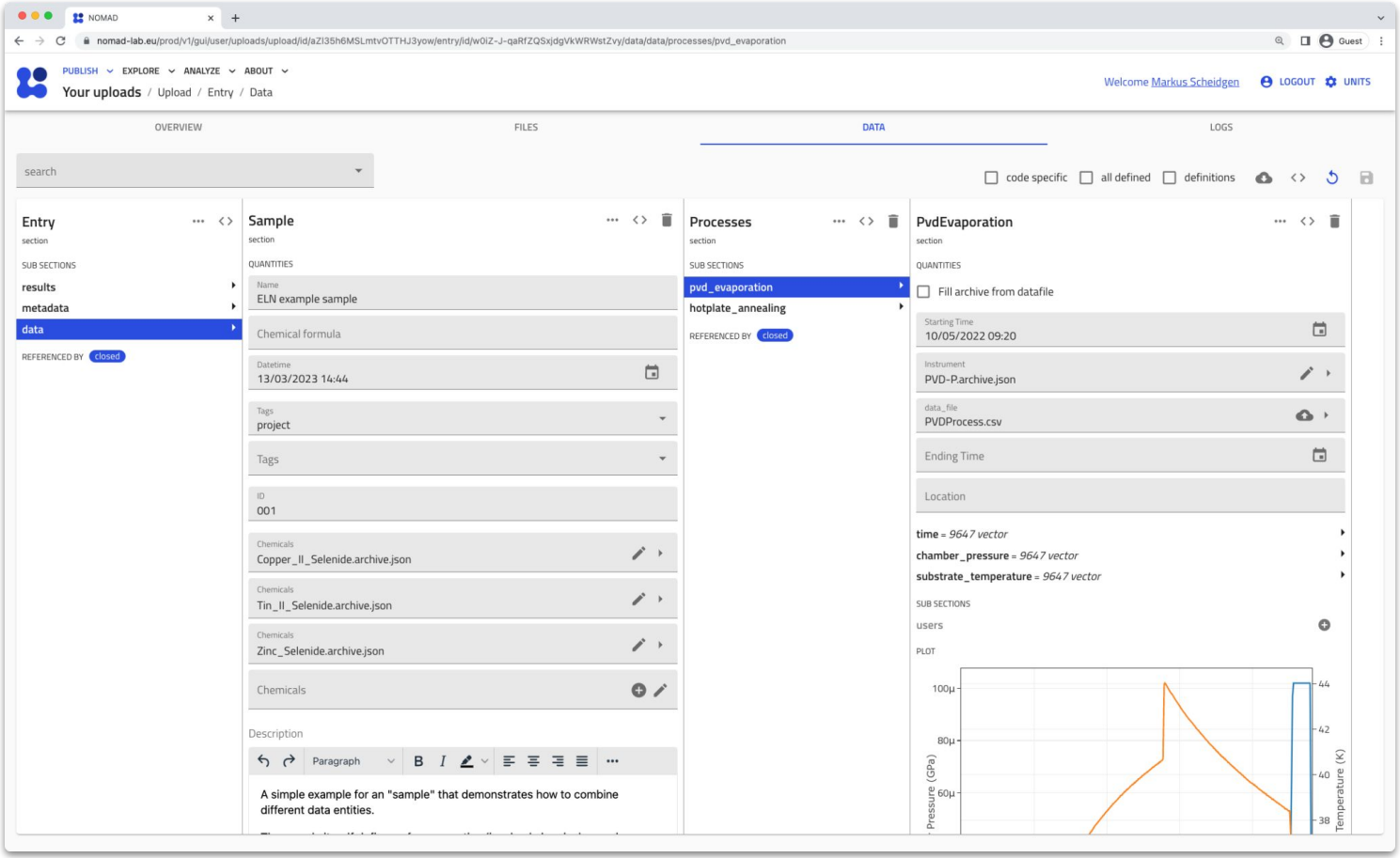
Entry type
Upload time
Authors
BaO3Ti VASP simulation
BaO3Ti
VASP simulation
01/03/2018, 12:25:22
Zongguo Wang, Xushan Zhao et al
CaO3Ti VASP simulation
CaO3Ti
O3SrTi VASP simulation
O3SrTi

FAIRmat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OVERVIEW FILES DATA LOGS
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SUB SECTIONS
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data
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Sample
section
QUANTITIES
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ELN example sample
Chemical formula
Datetime
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Tags
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001
Chemicals
Copper_II_Selenide.archive.json
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Chemicals
Zinc_Selenide.archive.json
Chemicals
Description
Paragraph
A simple example for an "sample" that demonstrates how to combine different data entities.
Processes
section
SUB SECTIONS
pvd_evaporation
hotplate_annealing
REFERENCED BY closed
PvdEvaporation
section
QUANTITIES
Fill archive from datafile
Starting Time
10/05/2022 09:20
Instrument
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data_file
PVDProcess.csv
Ending Time
Location
time = 9647 vector
chamber_pressure = 9647 vector
substrate_temperature = 9647 vector
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Pressure (GPa)
44
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40
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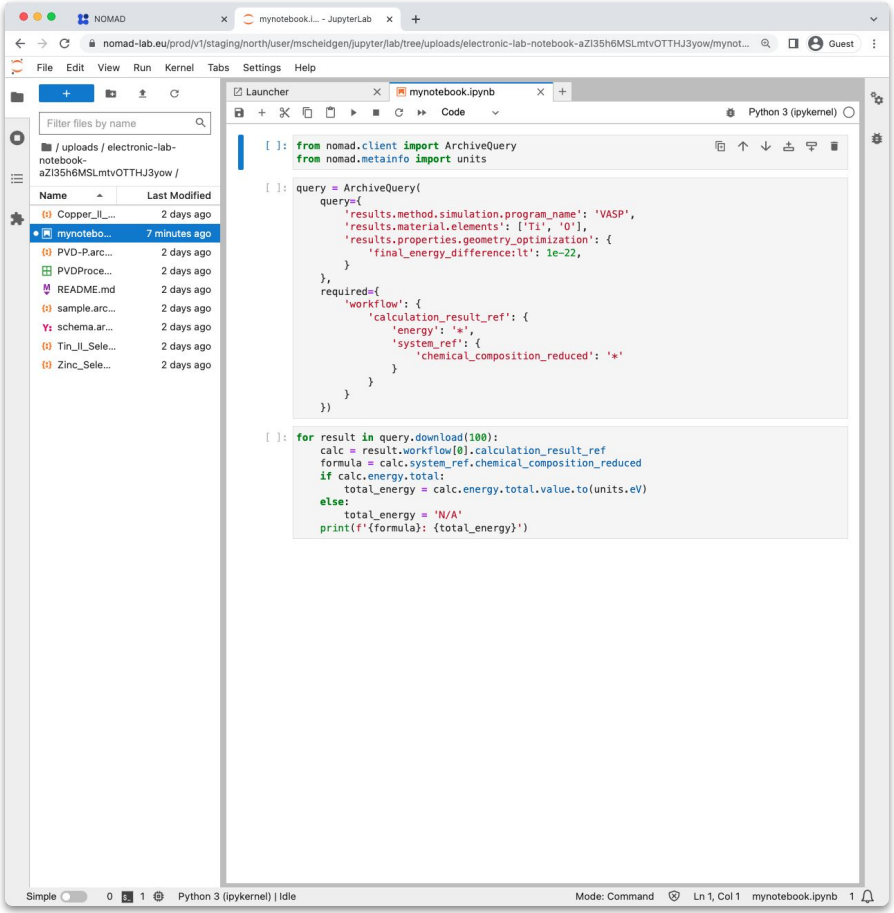
Temperature (K)

FAIRmat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from nomad.metainfo import units
[ ]:
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'results.material.elements': ['Ti', 'O'],
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},
required={
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'system_ref': {
'chemical_composition_reduced': '*'
}
}
}
})
[ ]:
for result in query.download(100):
calc = result.workflow[0].calculation_result_ref
formula = calc.system_ref.chemical_composition_reduced
if calc.energy.total:
total_energy = calc.energy.total.value.to(units.eV)
else:
total_energy = 'N/A'
print(f'{formula}: {total_energy}')
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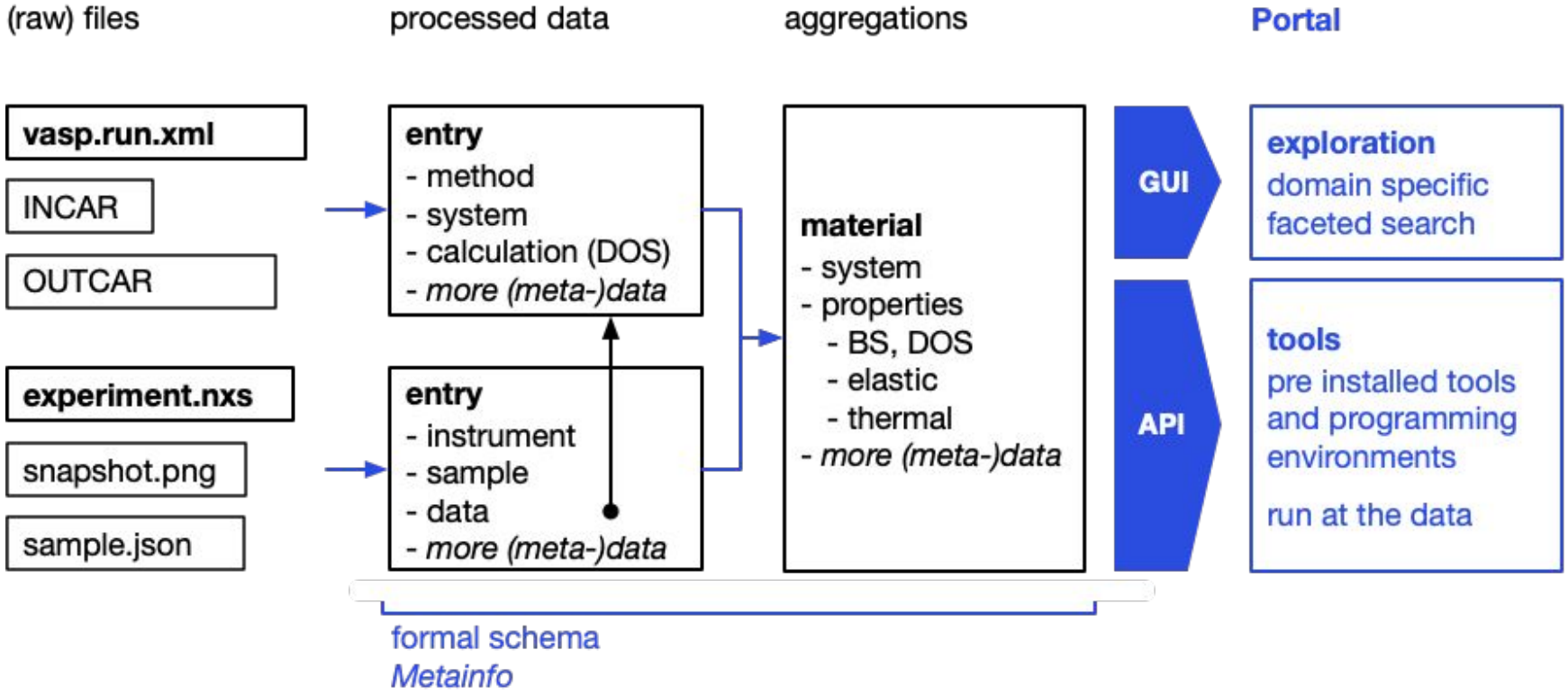
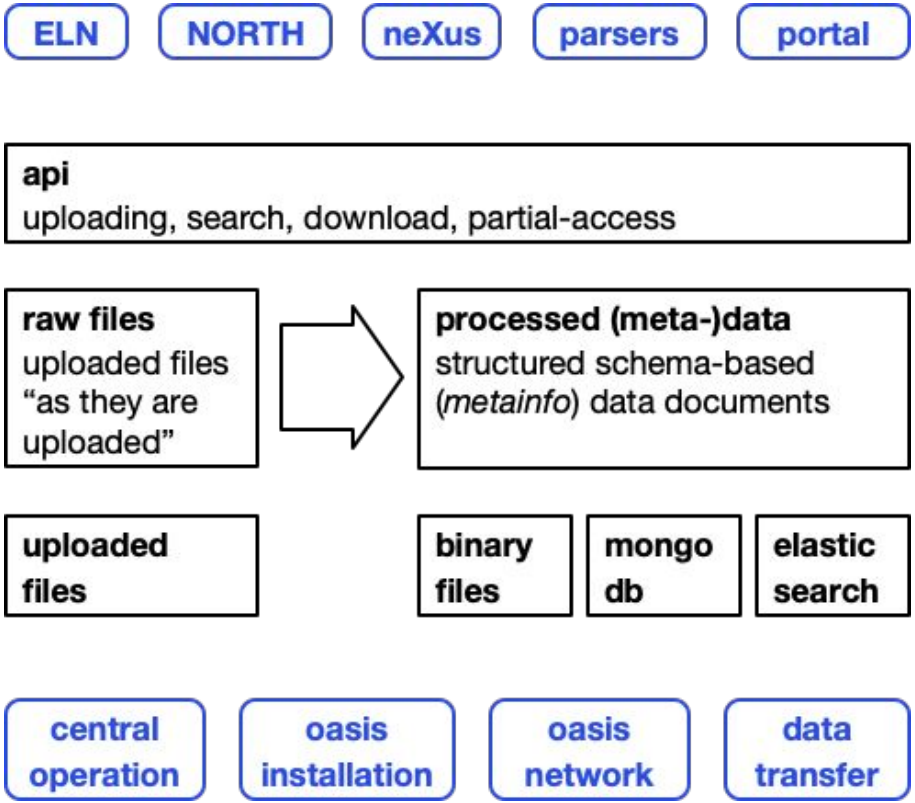
Extracting structured (meta-)data from files



Extracting structured (meta-)data from files



demo

Pros

- **schema-focused**, produces consistent FAIR data
- supports growing number of file-types, e.g. **neXus**
- **file-based**, easy to import and export
- **API** covers all functionality
- integrated **JupyterHUB** to work with and analyse managed data
- data can be **shared** and **published** through a central NOMAD

Cons

- **schema-focused**, requires you to structure data first
- designed to be **extendable**, adapt NOMAD to your needs
- integration with others ELNs has just begun
- young constantly **evolving project**, not all features are there yet

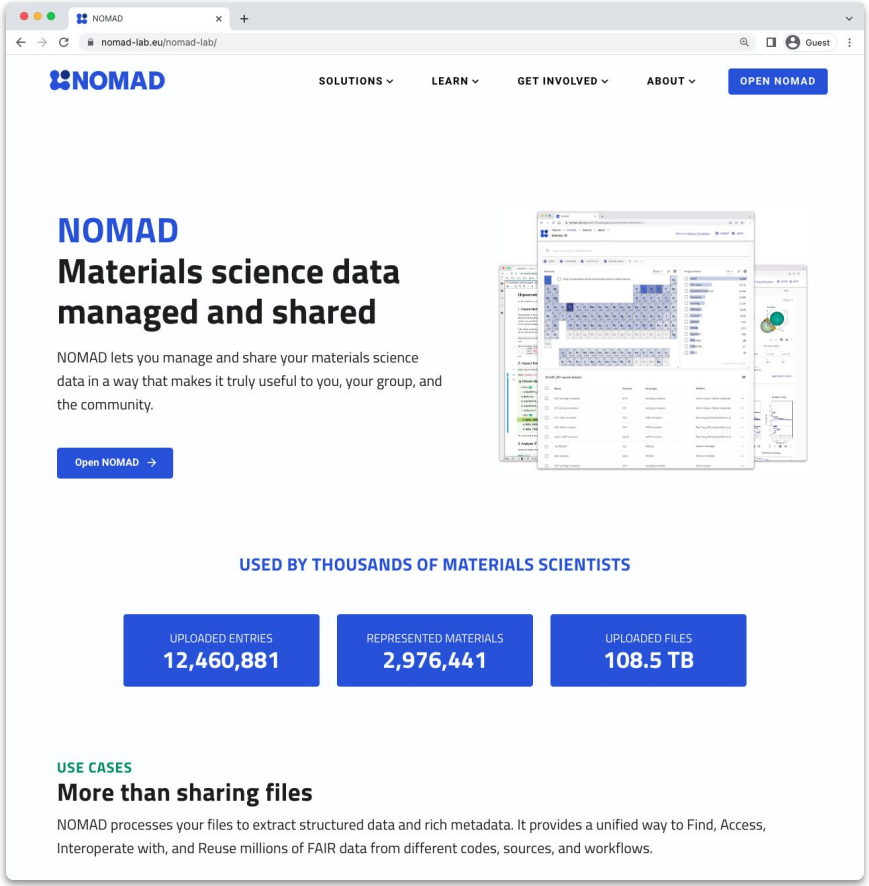
FAIR, extendable, scalable: 

simple, low maintenance: 

NOMAD Links

- homepage – nomad-lab.eu
- central NOMAD service – https://nomad-lab.eu/prod/v1
- NOMAD Dokumentation
  - installing Oasis
  - schemas and ELNs
- Tutorials and videos
  - NOMAD Oasis tutorial video playlist
  - Publishing, Exploring, API video playlist
  - All FAIRmat tutorials
- NOMAD forum
- NOMAD's main gitlab (and github)

Questions?


NOMAD
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NOMAD
SOLUTIONS
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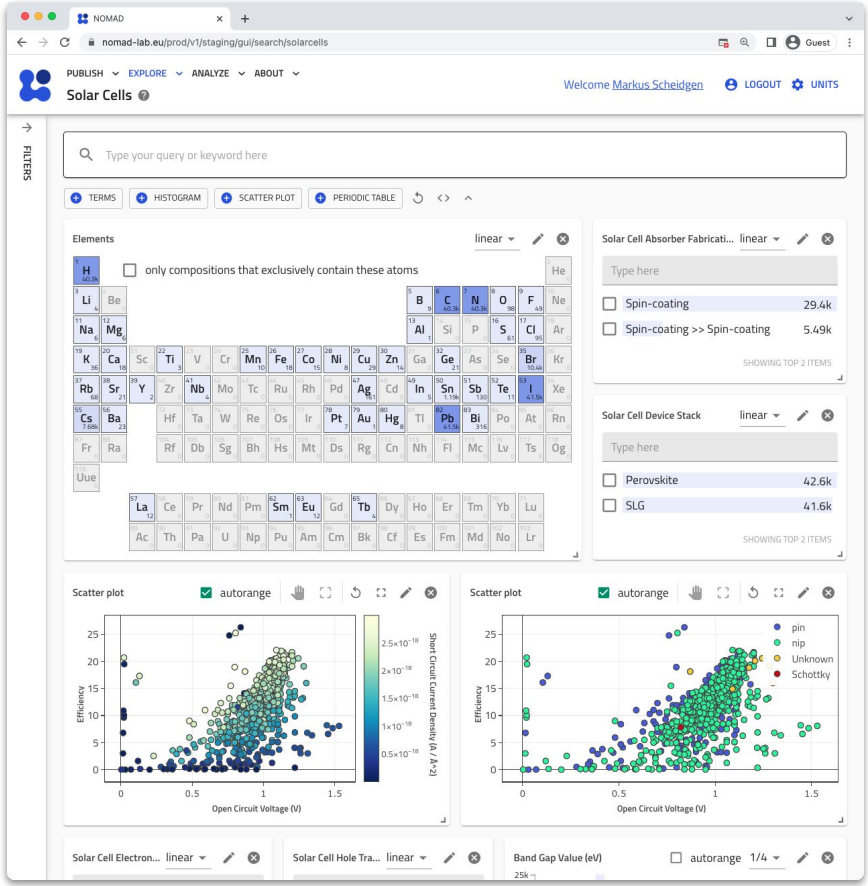
ABOUT
OPEN NOMAD
NOMAD
Materials science data managed and shared
NOMAD lets you manage and share your materials science data in a way that makes it truly useful to you, your group, and the community.
Open NOMAD
USED BY THOUSANDS OF MATERIALS SCIENTISTS
UPLOADED ENTRIES
12,460,881
REPRESENTED MATERIALS
2,976,441
UPLOADED FILES
108.5 TB
USE CASES
More than sharing files
NOMAD processes your files to extract structured data and rich metadata. It provides a unified way to Find, Access, Interoperate with, and Reuse millions of FAIR data from different codes, sources, and workflows.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Elements
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SHOWING TOP 2 ITEMS
Solar Cell Device Stack
Perovskite 42.6k
SLG 41.6k
Scatter plot
autorange
Efficiency
Open Circuit Voltage (V)
Short Circuit Current Density (A / m^2)
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nip
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Schottky
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Solar Cell Hole Tra...
Band Gap Value (eV)
1/4