

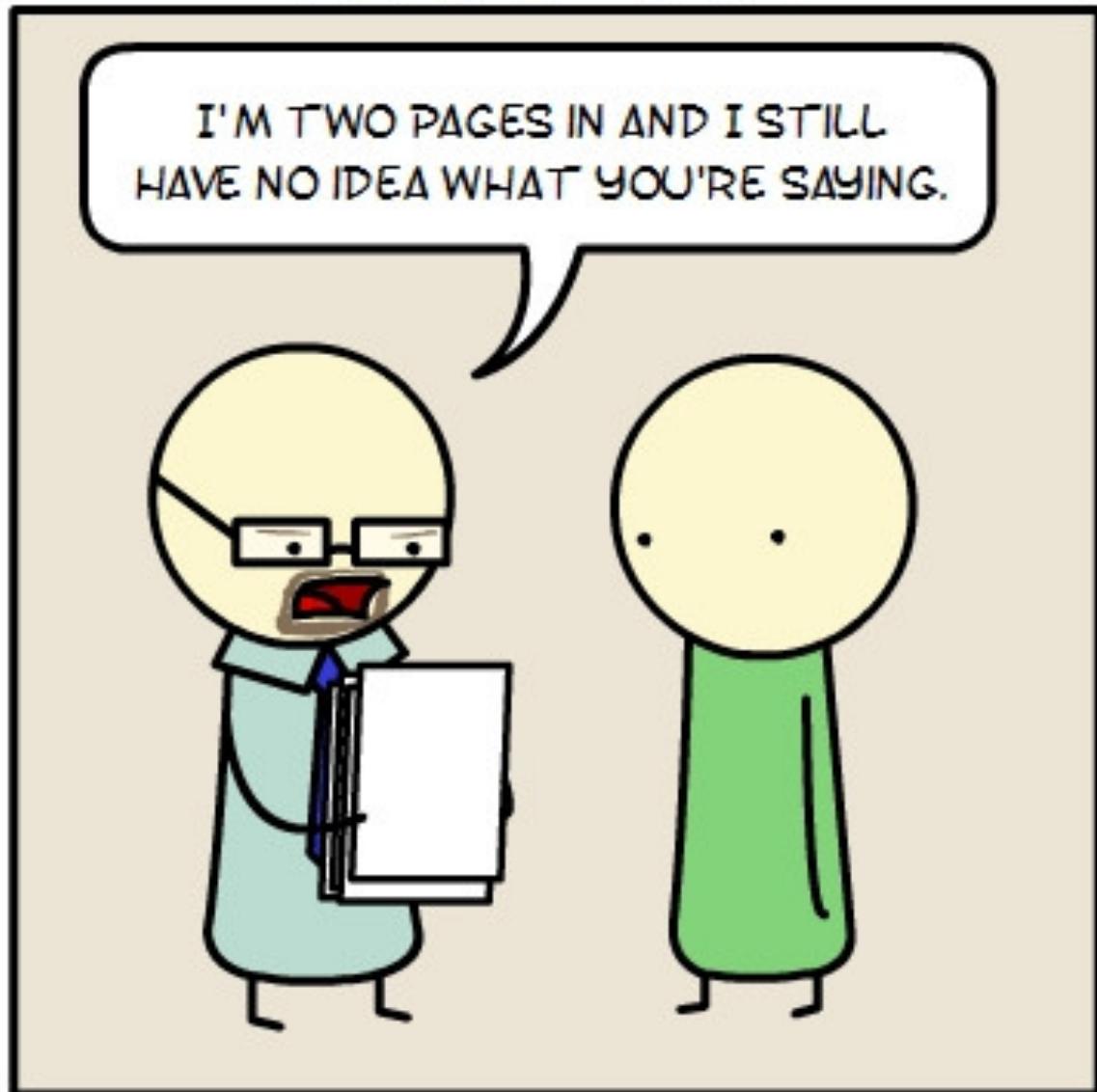
# **Python tools for computational physics/chemistry**

**Adam Fekete @ Namur 25/05/2022**

<https://github.com/fekad/python-tutorial-unamur>

# „Best” programming language

**JAVA**



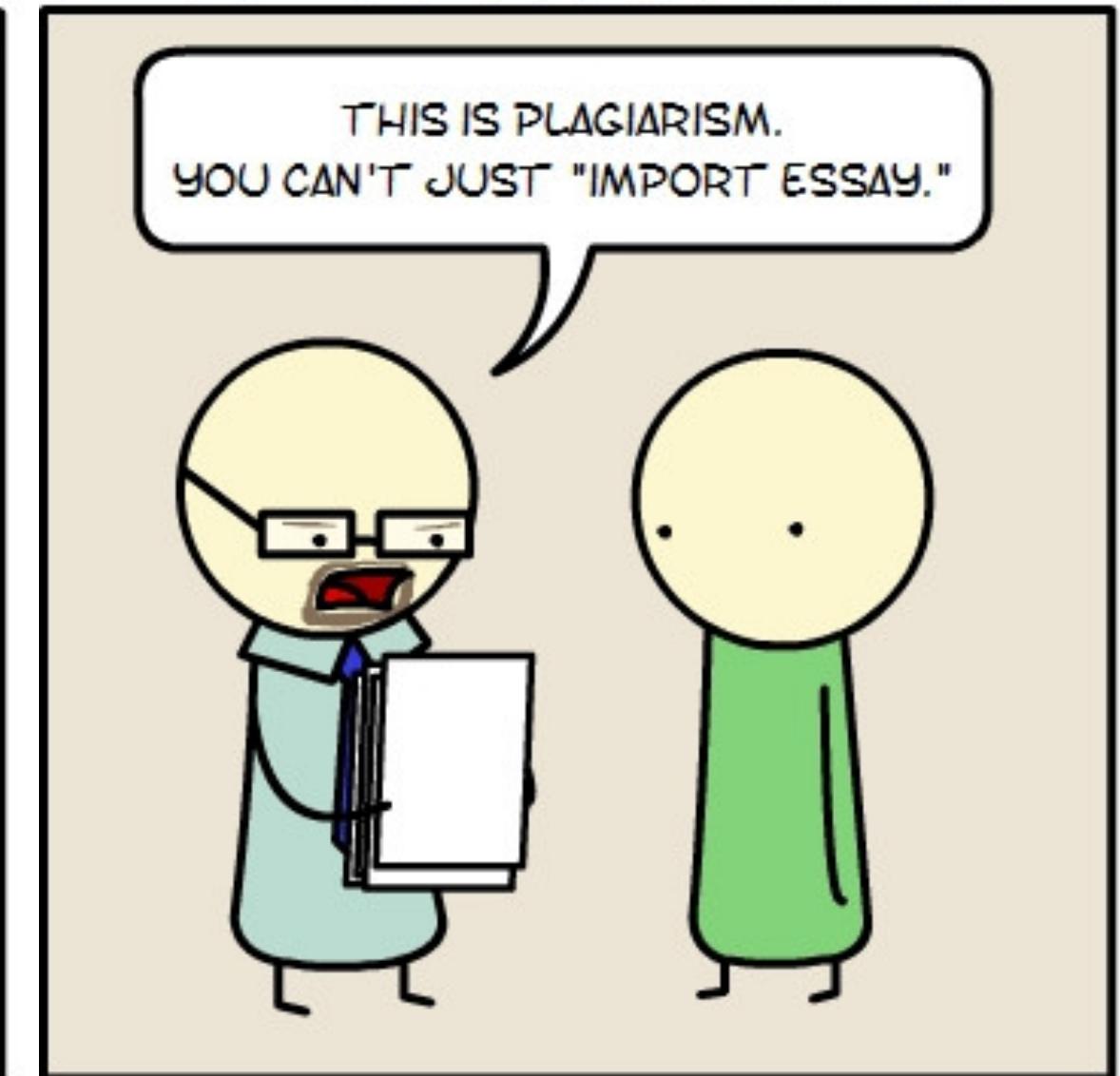
**C**



**LATEX**



**PYTHON**



julia

# Useful tools

- [github/gitlab](#)
- [gitkraken](#)
- [vscode](#)
- [copilot](#)
- [jupyter notebook/lab](#)
- [mybinder.org](#)



Your AI neighbor programmer

Build and launch a repository

Gist ID (username/gistId) or URL  
Gist ▾ diehl/0741a174558a60a1fc5e772554bbe755

Git commit SHA  
HEAD

Path to a notebook file (optional)  
voila/render/pydeck\_demo.ipynb File ▾ launch

Copy the URL below and share your Binder with others:  
<https://mybinder.org/v2/gist/diehl/0741a174558a60a1fc5e772554bbe755/HEAD?labpath=voila%2Frenderer%2Fpyde>

Expand to see the text below, paste it into your README to show a binder badge: [launch](#) [binder](#)

The image shows a composite screenshot of a desktop interface. In the top left, the GitKraken application window is visible, displaying a GitHub repository named 'electron' with the 'master' branch selected. The repository details show 1181 commits. In the center, a web browser window displays the 'vscode.dev' website, specifically a page titled 'In Depth: Linear Regression'. The page content includes code snippets for Python 3, a Jupyter Notebook interface, and a scatter plot titled 'Seattle Weather: 2012-2015'. In the bottom right corner, there is a separate window for the Jupyter Notebook, showing a Python 3 kernel and a 'Simple' notebook cell containing code. The overall theme is a developer's workspace.

# ASE

## Atomic Simulation Environment

- setting up, manipulating,
- running (see below),
- visualizing and
- analyzing atomistic simulations

# pymatgen

## Python Materials Genomics

- materials analysis
- mostly VASP, ABINIT, Gaussian
- CIF, XYZ and many other file format
- Electronic structure analyses



molecular structures



material/crystal structures

The Materials Project:

<https://materialsproject.org/>

# materialsproject.org

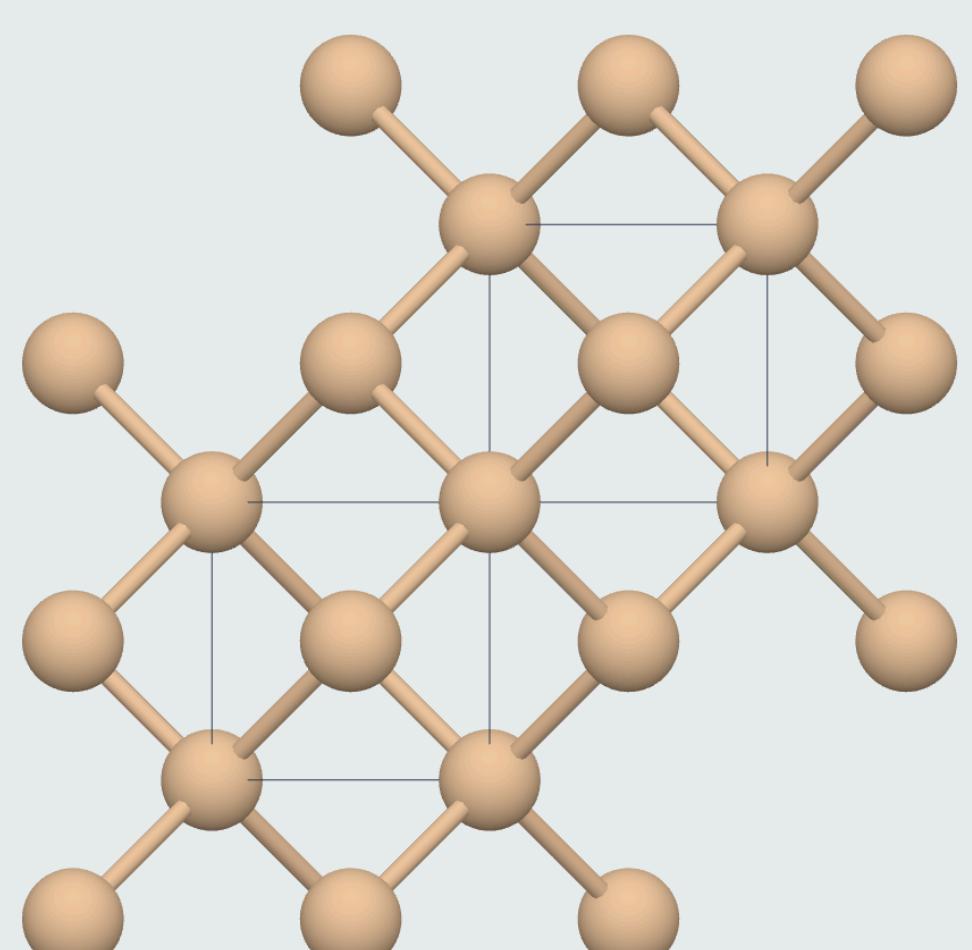
## pymatgen

Home About Apps Documentation Forum API Tutorials Dashboard

MATERIAL ID: DOI:  
Si mp-149 10.17188/1190959

Show Help Guides

Electronic Structure Phonon Dispersion X-Ray Diffraction X-Ray Absorption Substrates Surfaces Elasticity  
Dielectric Properties Equations of State Similar Structures Calculation Summary User Contributions Provenance/Citation



**Material Details**

- Final Magnetic Moment: 0.000  $\mu_B$
- Magnetic Ordering: NM
- Formation Energy / Atom: 0.000 eV
- Energy Above Hull / Atom: 0.000 eV
- Density: 2.28 g/cm<sup>3</sup>
- Decomposes To: Stable
- Band Gap: 0.853 eV

**Lattice Parameters**

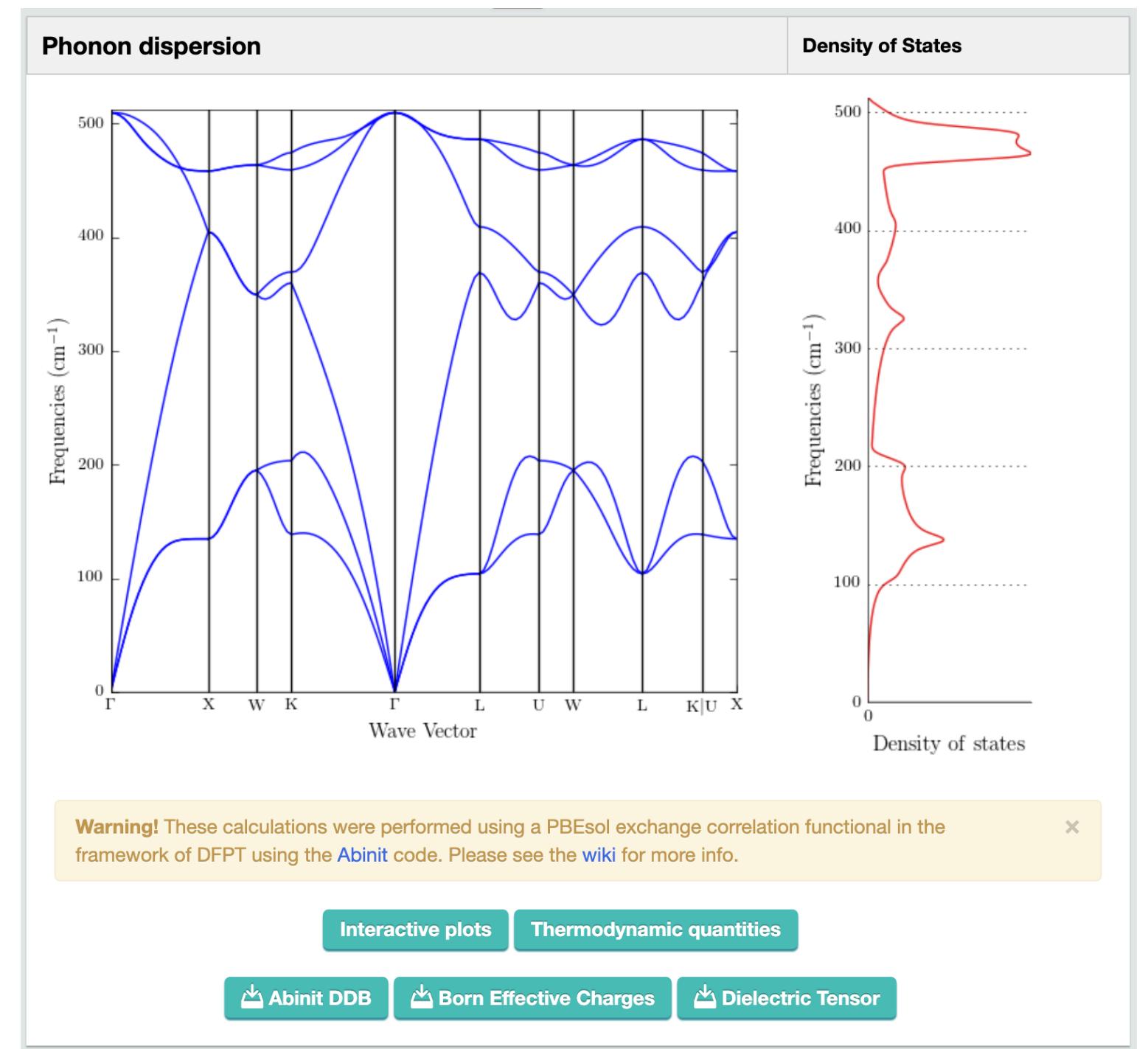
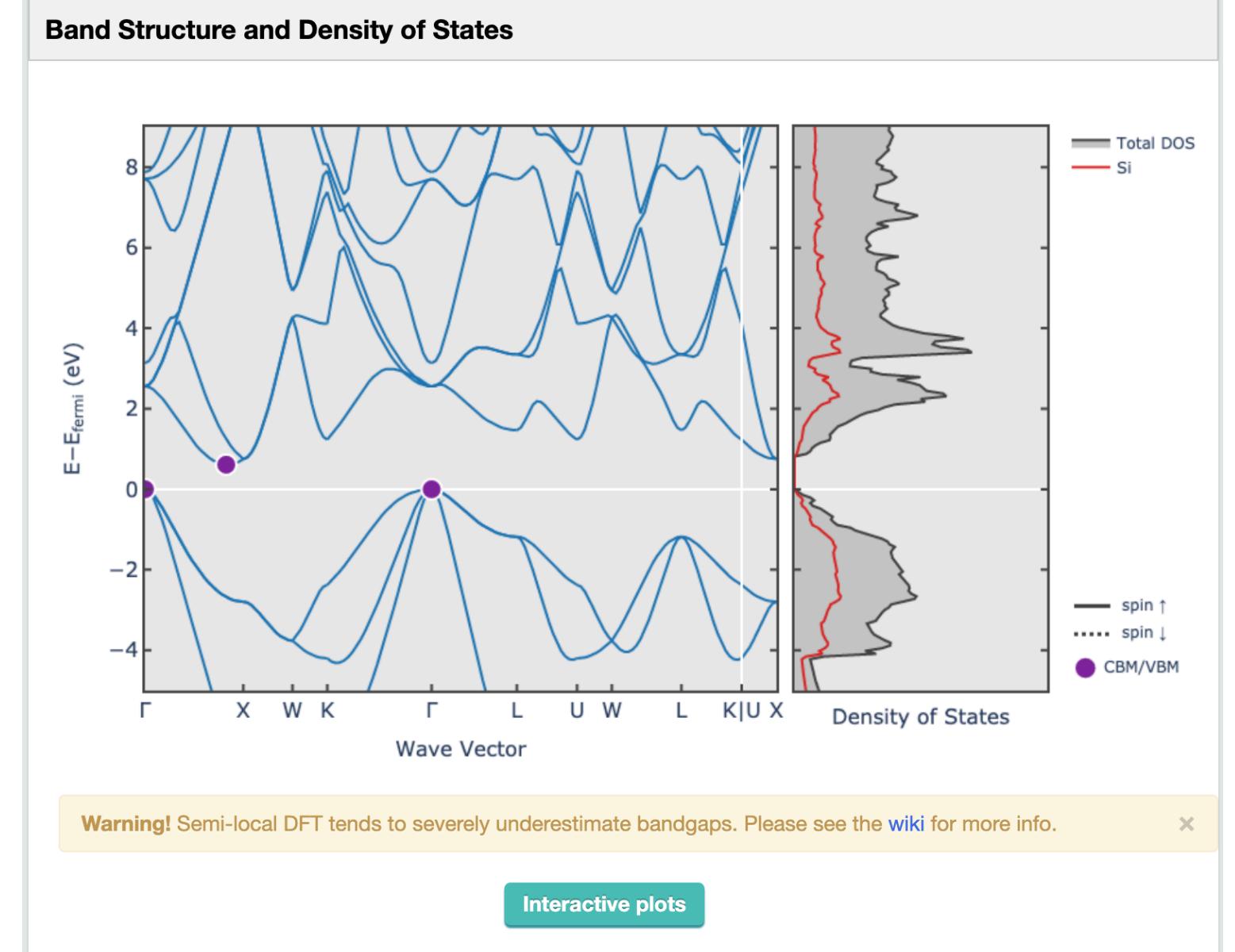
a	3.867 Å	a	60.000°
b	3.867 Å	β	60.000°
c	3.867 Å	γ	60.000°
Volume	40.888 Å <sup>3</sup>		

**Final Structure** Fractional Coordinates

Si		
a	b	c
0	0	0
0.25	0.25	0.25

Atoms Unit Cell Bonds Polyhedra CIF

Space Group



# ASE

- DTU
- **Atoms** object
- Cell object
- info attribute  
(properties for the whole system)
- array attribute  
(properties per elements)
- Calculators

# pymatgen

- Berkeley, UCLouvain, etc
- **Structure** and **Molecule** objects
- Lattice object
- site\_properties attribute
- sites attribute: List of Sites
- „Pythonic” way



structure of arrays (SoA) VS array of structures (AoS)

**Live demo** 🤞

<https://github.com/fekad/python-tutorial-unamur>

# In conclusion

## Doing calculations in a slightly more programmatic way

Advantages:

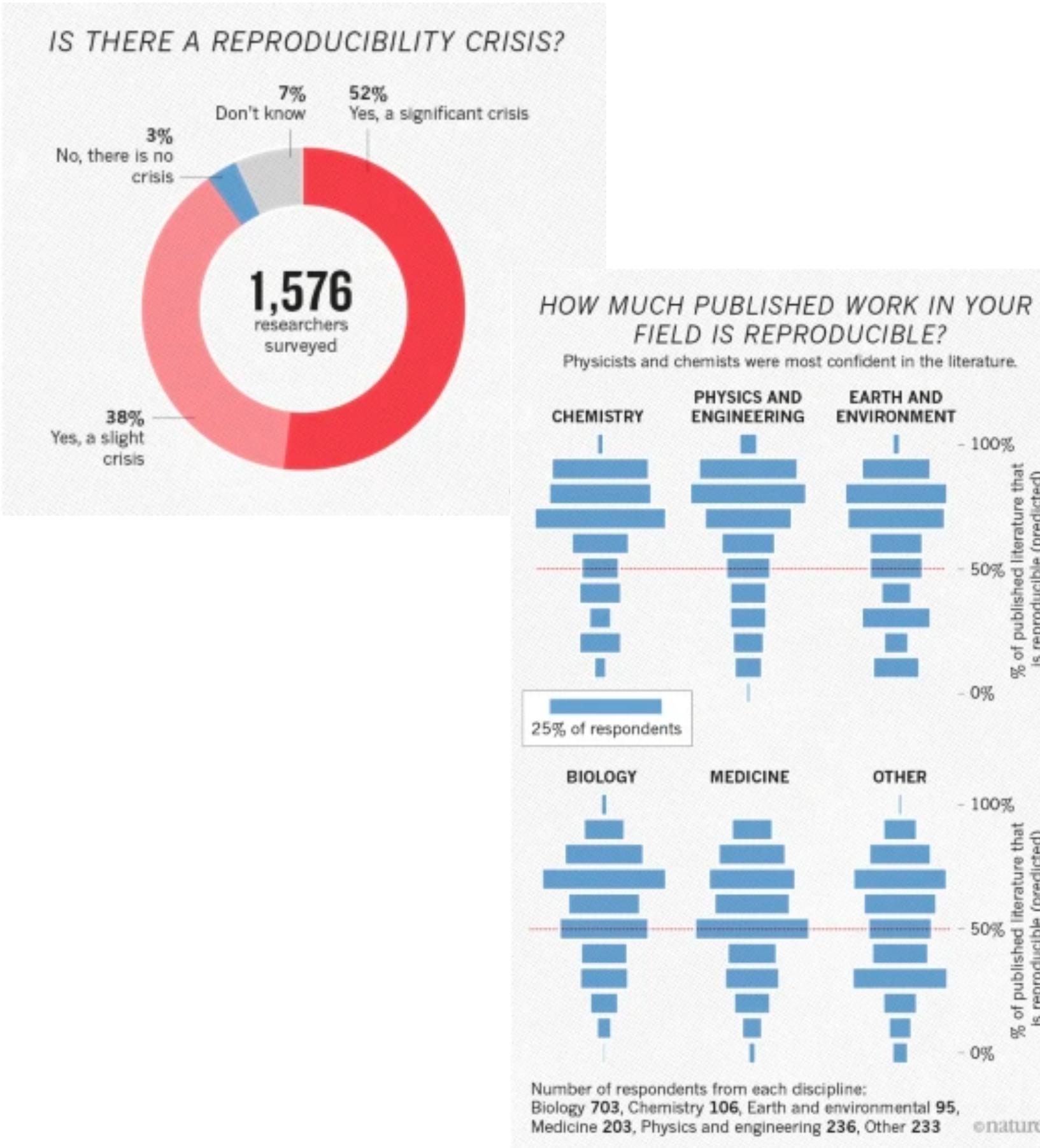
- quick/easy way to produce structures
- reusability
- parameter optimisation / sweep
- generate high throughput calculations
- tools for analysing the results

The code is the input and the output, ergo the result

article + code + data = results

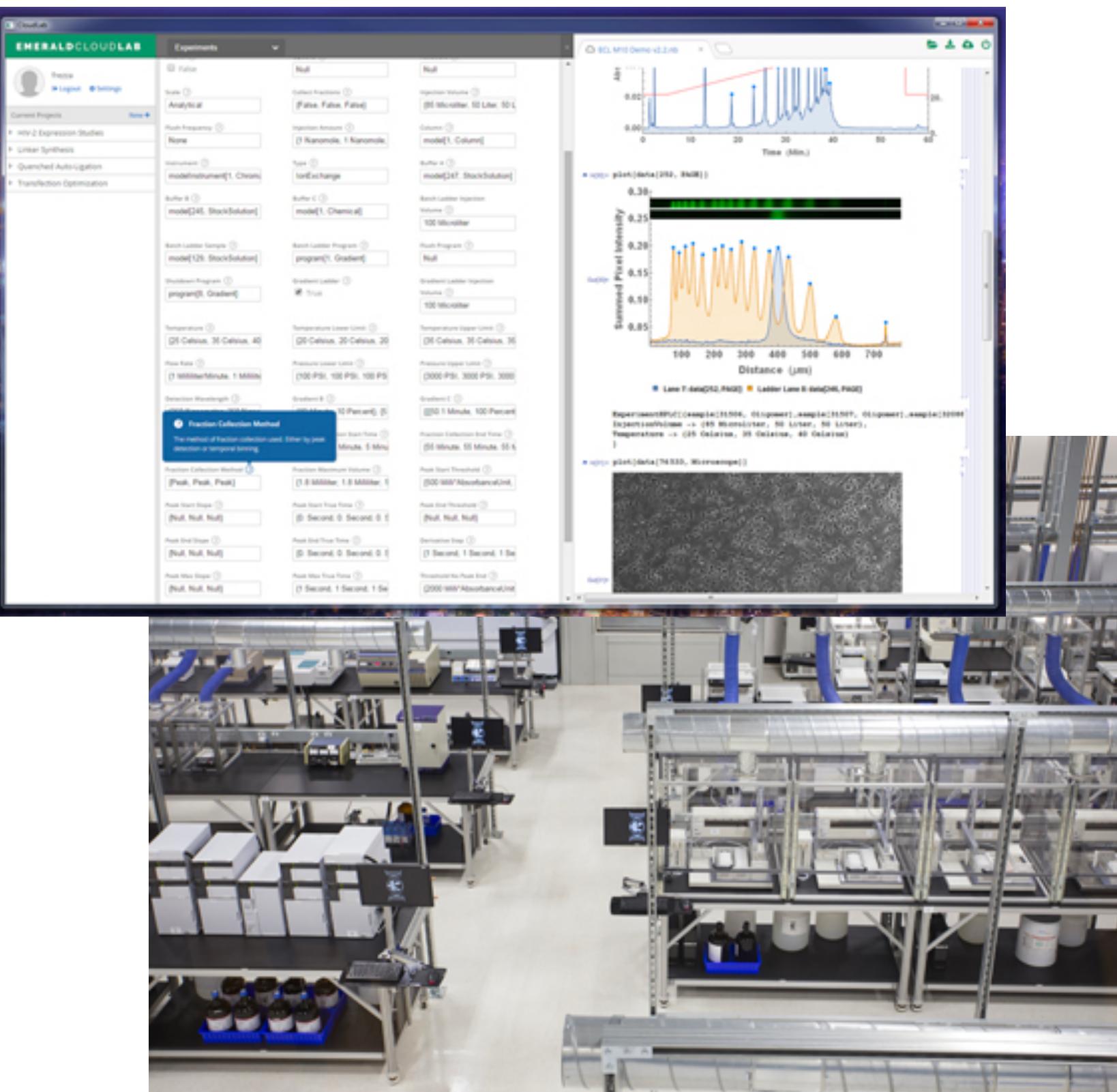
# Doing research

## The reproducibility problem



Nature 533, 452–454 (2016). <https://doi.org/10.1038/533452a>

## Emerald Cloud Lab



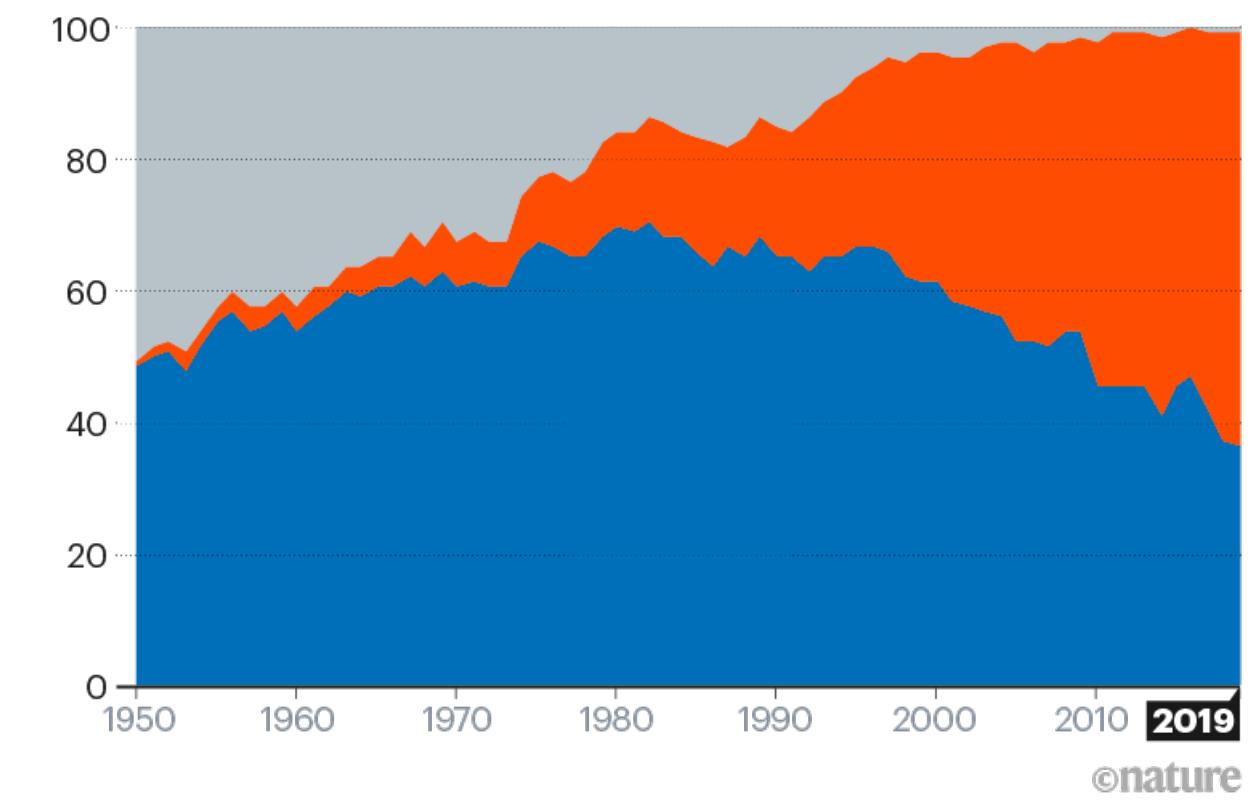
## Collaboration

### INTERNATIONAL COLLABORATIONS

Author lists on research publications show a shift towards multinational teams; fewer teams are composed entirely of researchers from one country.

#### Proportion of papers

■ Multinational ■ Domestic ■ Single author



Nature 575, 22–23 (2019).

<https://doi.org/10.1038/d41586-019-03305-w>

# FAIR data

## NOMAD makes materials science data FAIR

Findable, Accessible, Interoperable, and Re-purposable

*More than 12 million of simulations from over 400 authors world-wide*

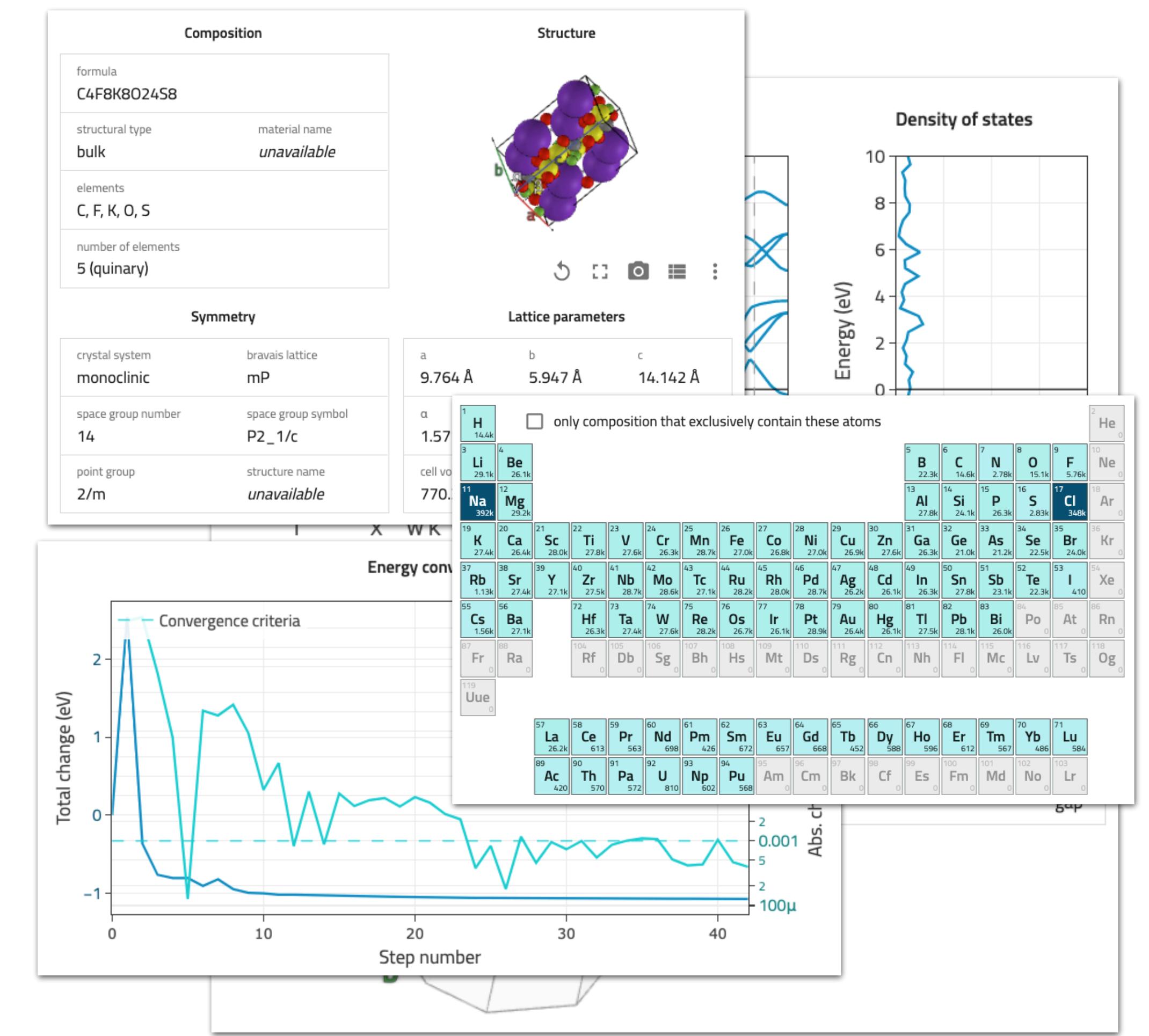
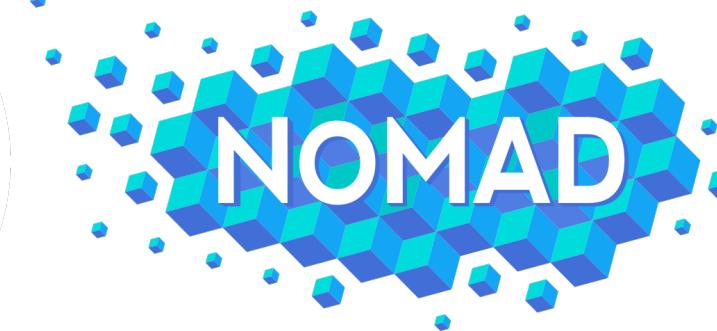
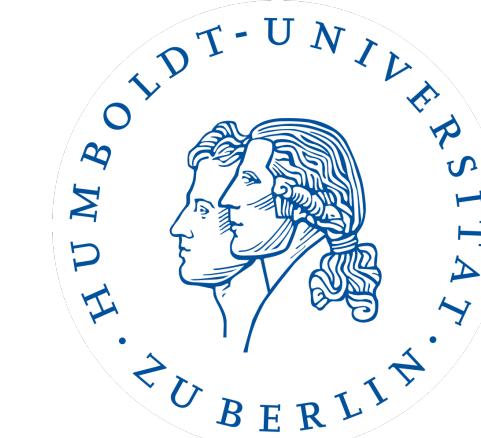
- Free publication and **sharing** data of data
- Extracts **rich metadata** for more than **40 codes**
- All data in a **raw** and a common **machine readable** form
- Use integrated tools to **explore**, **visualize**, and **analyze**

Publish

Explore

Analyse

<https://nomad-lab.eu/>

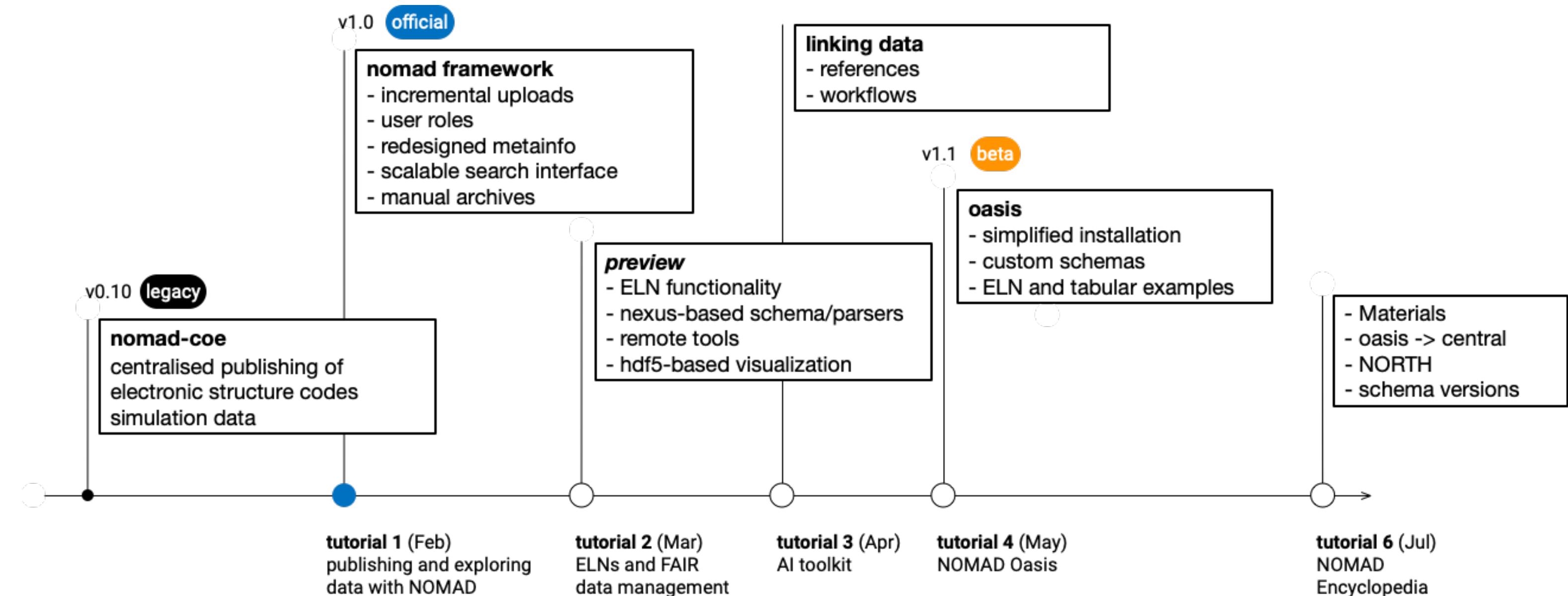
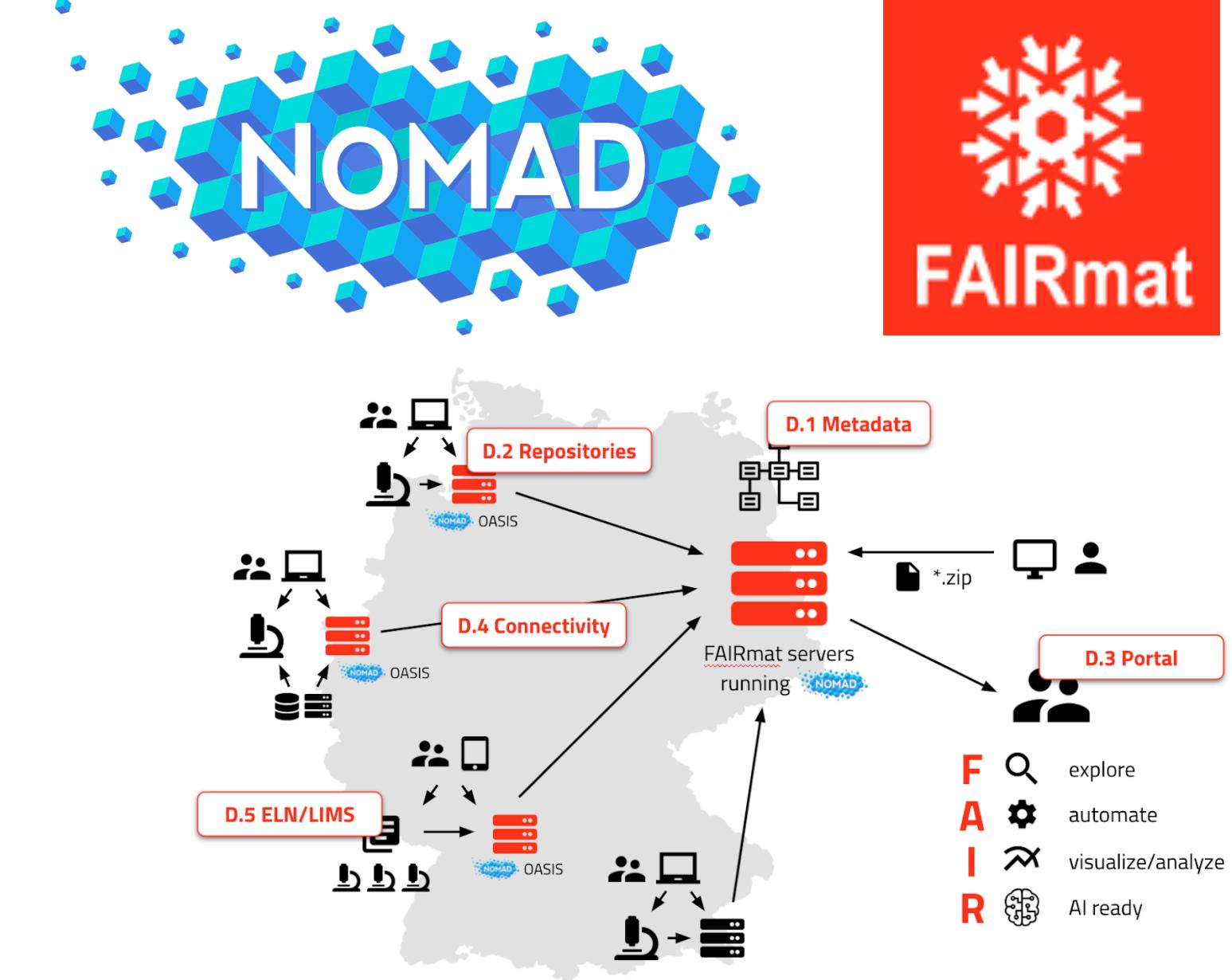


# NOMAD Oasis

## Manage materials science research data

FAIRmat builds on a federated infrastructure of local repositories

- › Organise research data though its whole life-cycle
- › Adaptable to your workflows and data-types
- › A first step to connect with in the FAIRmat network



# The end

Thank you for your attention!