# Open Science Platform: AiiDA and Materials Cloud

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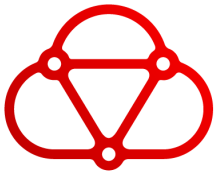
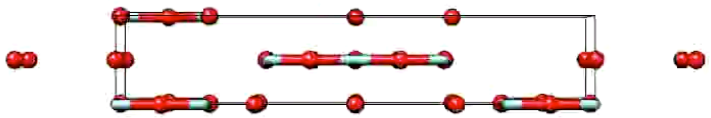


MATERIALSCLOUD

FNSNF
MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH
MAX DRIVING THE EXASCALE TRANSITION
swissuniversities
EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

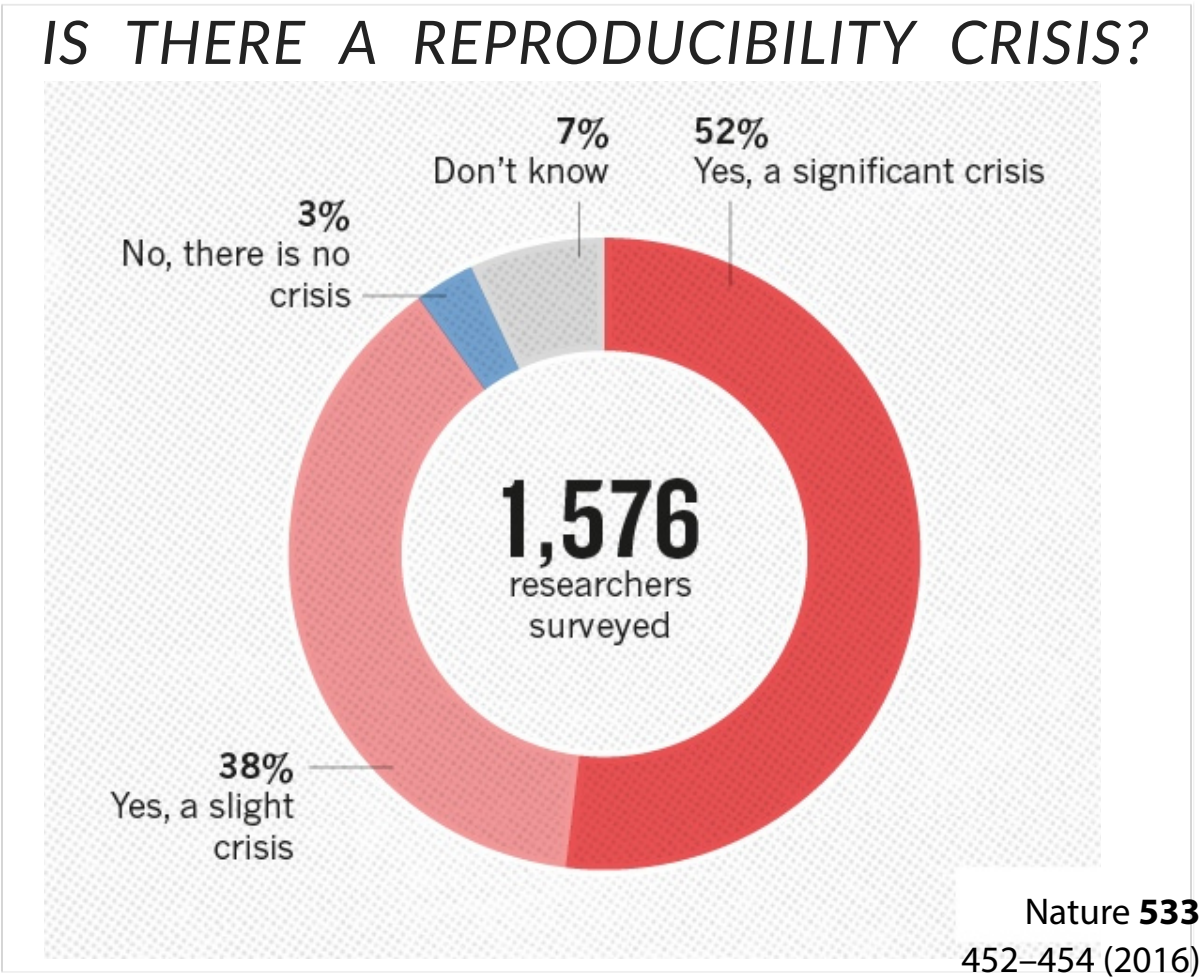
# Leverage supercomputers to compute and predict materials' properties





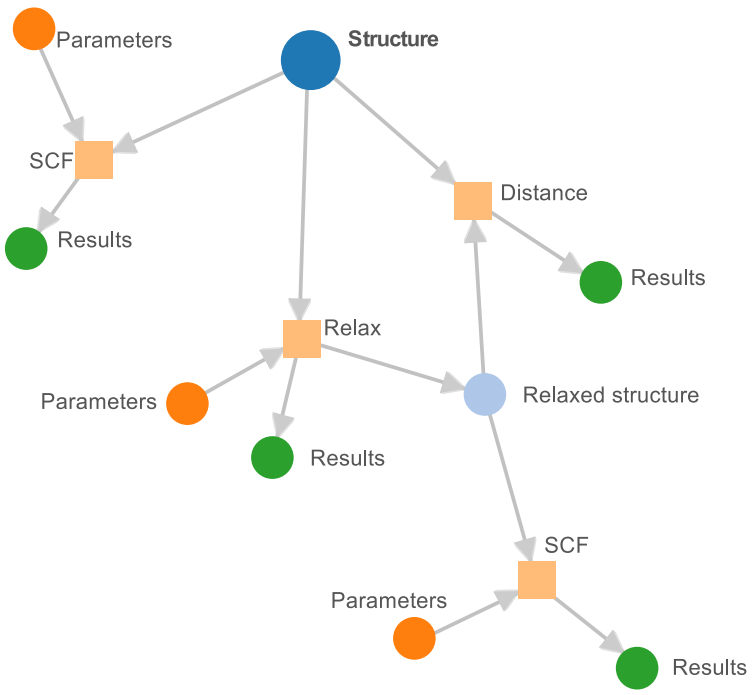

Aim: Compute properties for all of them
(and even new, invented ones)
and **discover novel functional materials**

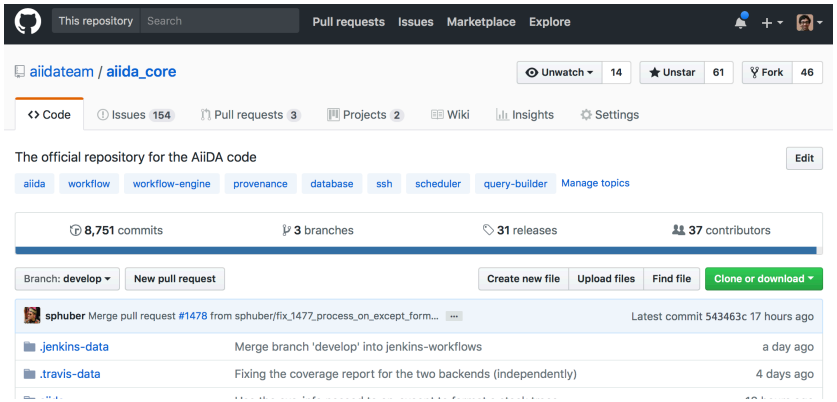
# How to manage simulations and their provenance?



# Data provenance: Directed Acyclic Graphs

AiiDA



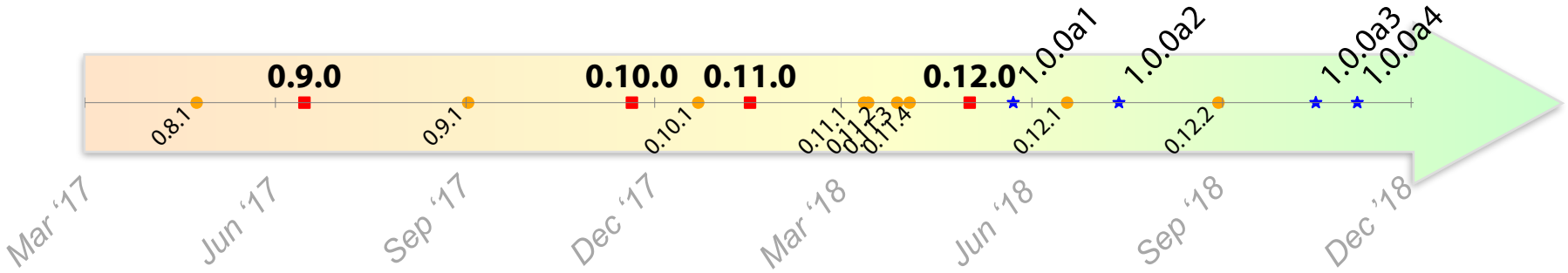

MIT license (open source)

Developed since 2013
Used in production from many scientific research projects

**G. Pizzi et al.,**
**Comp. Mat. Sci. 111, 218-230 (2016)**

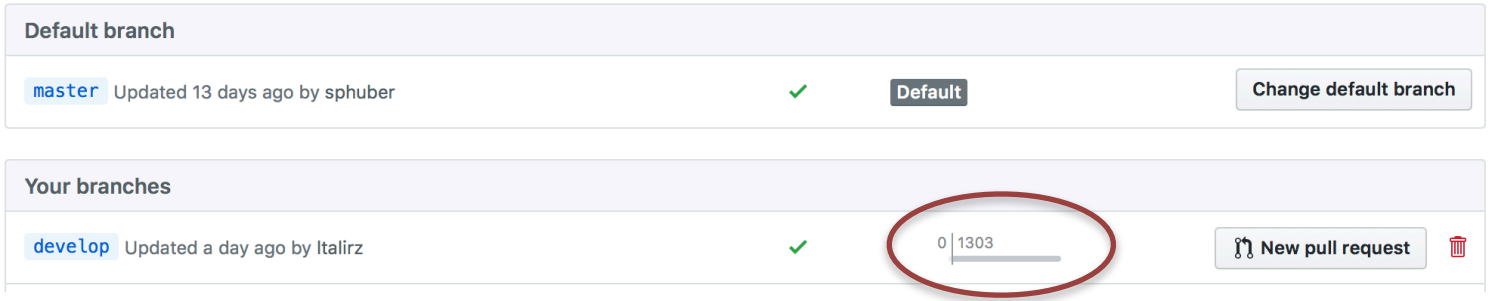
**http://www.aiida.net**

# The workflow and automation engine: AiiDA

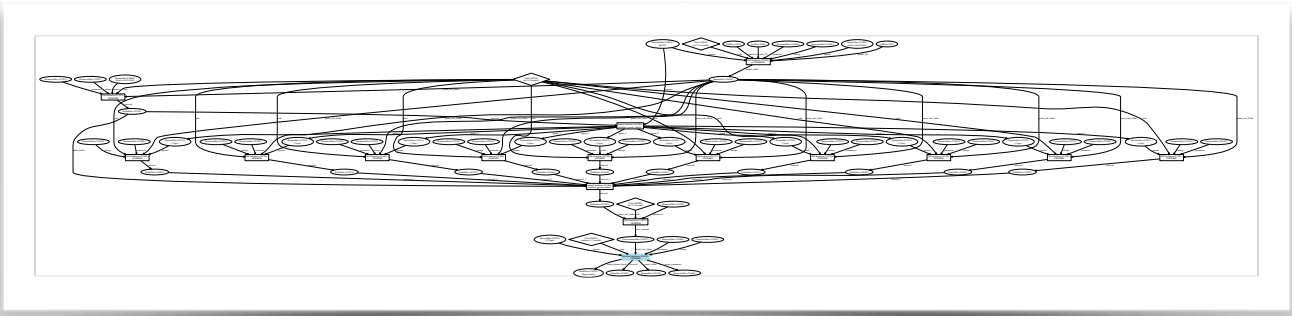



- **AiiDA has been used in production mode for the past 3 years**

- Many development efforts ready to go in 1.0.0
  (four alpha releases already out, **with 1300+ commits** w.r.t. stable 0.12.x)

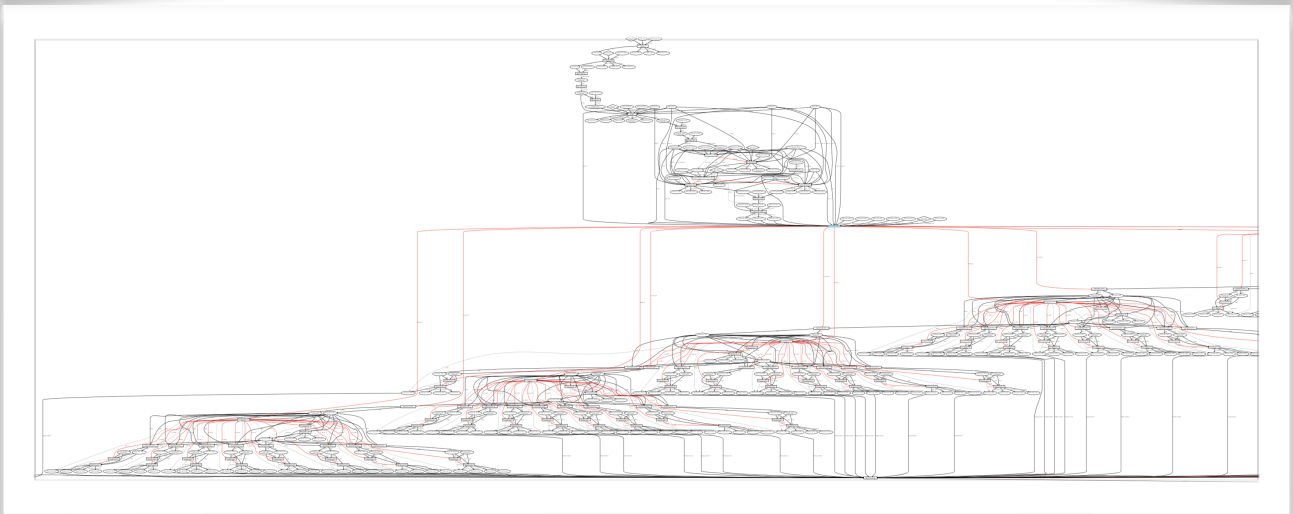


# “Simple” graphs of workflows for a single material



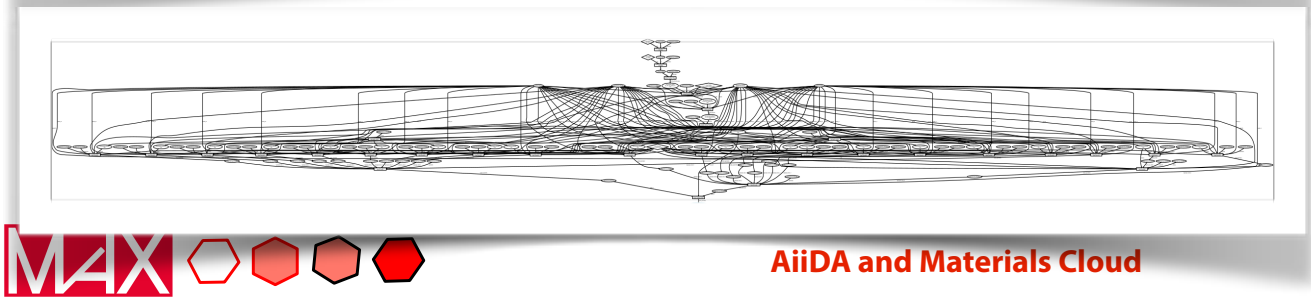
## Phonon dispersion

(atom oscillations around equilibrium positions: thermal transport, electronic mobility, …)



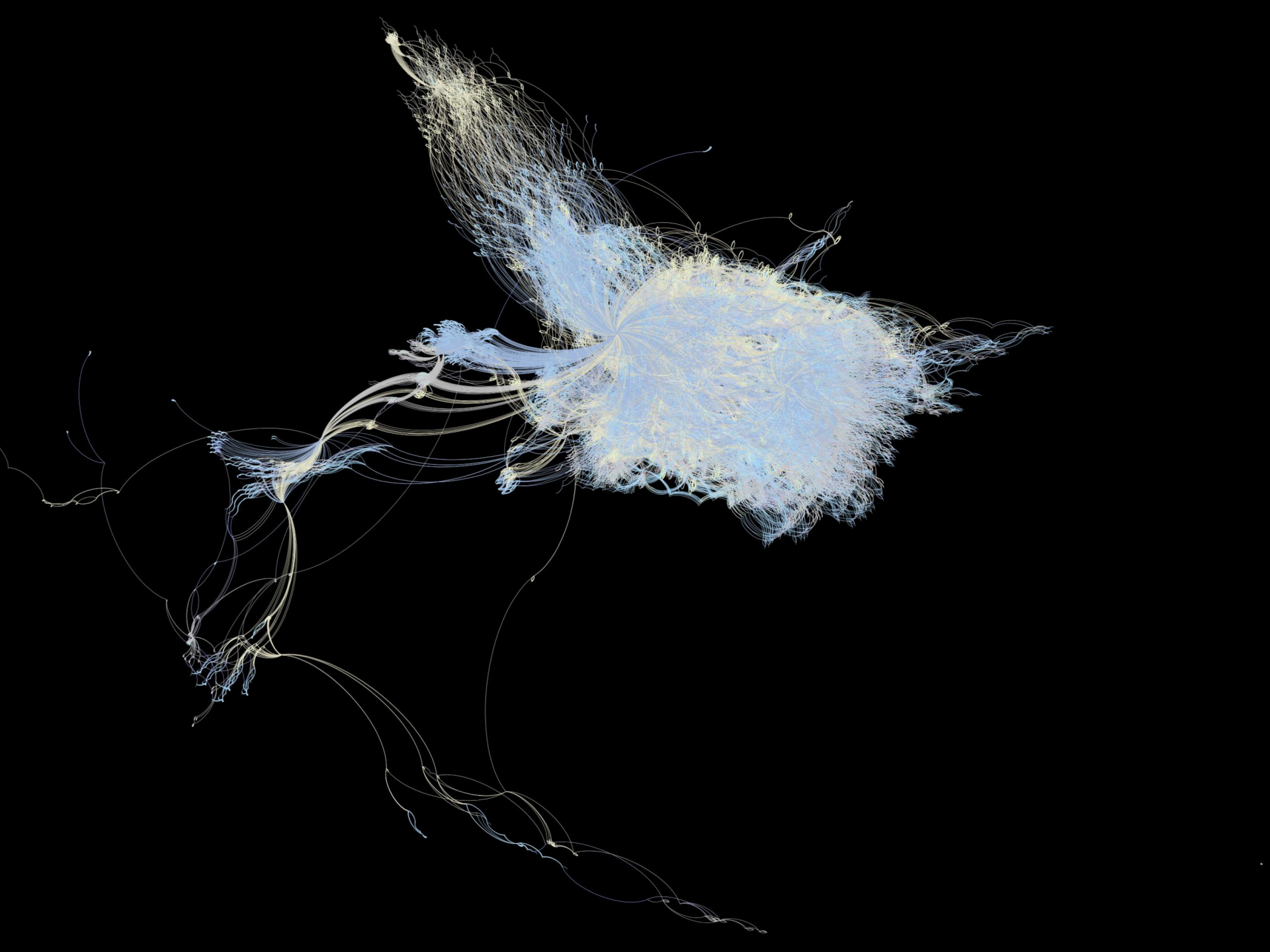
## Molecular dynamics of Lithium in a solid electrolyte

(Discover novel, safe and efficient electrolytes for Li-batteries)



## Elastic constants

(response of materials to stresses and deformations)



# Open Science Platform: AiiDA + Materials Cloud

MATERIALSCLOUD

https://www.materialscloud.org

*Online since February 2018*

**Cloud dissemination platform for FAIR data sharing**
and **more (cloud simulation and data generation platform)**

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# Open and FAIR data sharing: **Archive, Discover, Explore**

materialscloud:2017.0008

SCIENTIFIC DATA

re3data.org

FAIRsharing.org

## Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

Authors: Nicolas Mounet[1*], Marco Gibertini[1], Philippe Schwaller[1], Davide Campi[1], Andrius Merkys[1,2], Antimo Marrazzo[1], Thibault Sohier[1], Ivano E. Castelli[1], Andrea Cepellotti[1], Giovanni Pizzi[1], Nicola Marzari[1*]

1 Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

2 Vilnius University Institute of Biotechnology, Sauletekio al. 7, LT-10257 Vilnius, Lithuania

* Corresponding authors emails: nicolas.mounet@epfl.ch, nicola.marzari@epfl.ch

DOI 10.24435/materialscloud:2017.0008/v2 (version v2, submitted on 21 March 2018)

### How to cite this entry

Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Davide Campi, Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano E. Castelli, Andrea Cepellotti, Giovanni Pizzi, Nicola Marzari, *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, Materials Cloud Archive (2018), doi: 10.24435/materialscloud:2017.0008/v2.

### Description

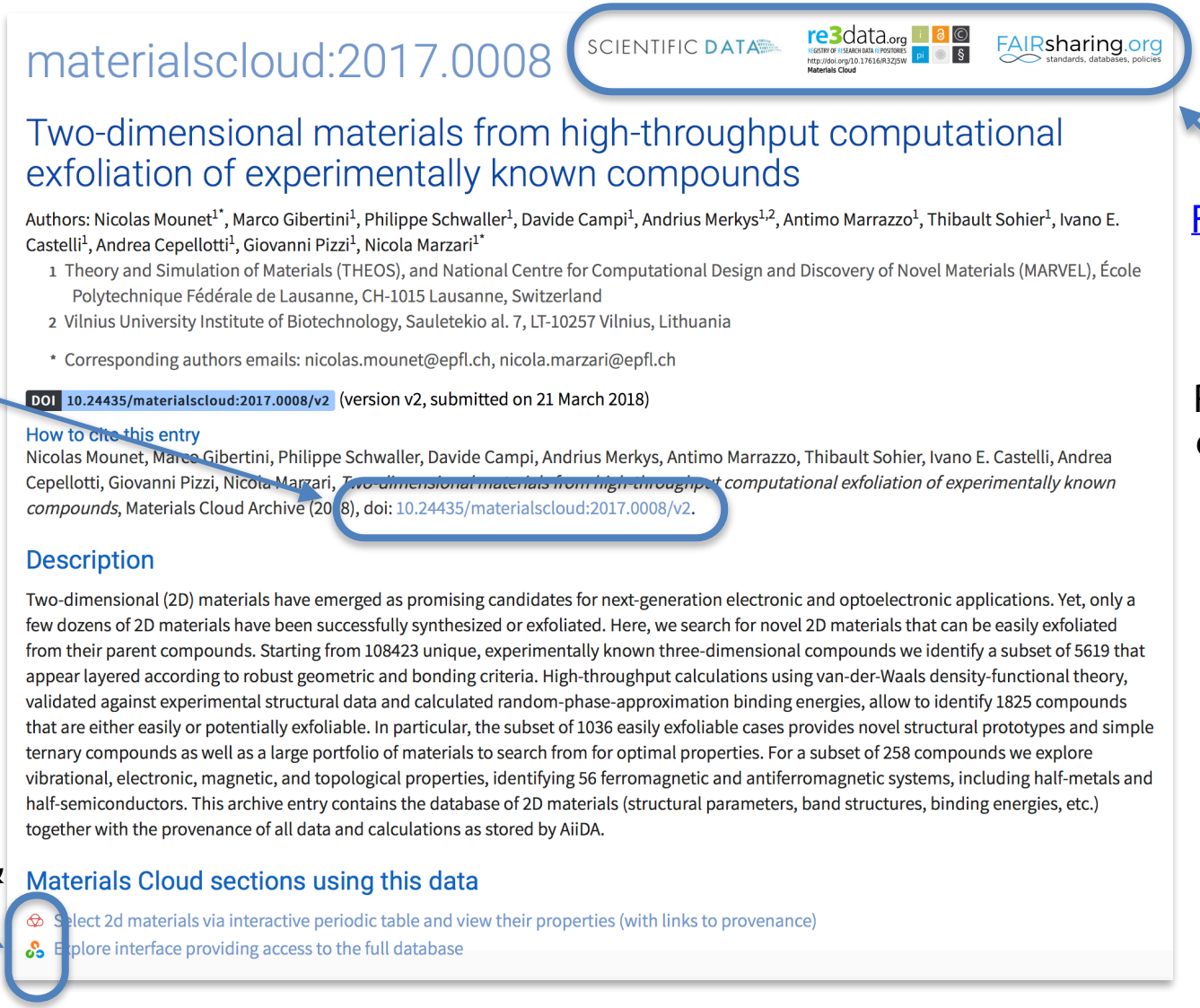
Two-dimensional (2D) materials have emerged as promising candidates for next-generation electronic and optoelectronic applications. Yet, only a few dozens of 2D materials have been successfully synthesized or exfoliated. Here, we search for novel 2D materials that can be easily exfoliated from their parent compounds. Starting from 108423 unique, experimentally known three-dimensional compounds we identify a subset of 5619 that appear layered according to robust geometric and bonding criteria. High-throughput calculations using van-der-Waals density-functional theory, validated against experimental structural data and calculated random-phase-approximation binding energies, allow to identify 1825 compounds that are either easily or potentially exfoliable. In particular, the subset of 1036 easily exfoliable cases provides novel structural prototypes and simple ternary compounds as well as a large portfolio of materials to search from for optimal properties. For a subset of 258 compounds we explore vibrational, electronic, magnetic, and topological properties, identifying 56 ferromagnetic and antiferromagnetic systems, including half-metals and half-semiconductors. This archive entry contains the database of 2D materials (structural parameters, band structures, binding energies, etc.) together with the provenance of all data and calculations as stored by AiiDA.

### Materials Cloud sections using this data

Select 2d materials via interactive periodic table and view their properties (with links to provenance)

Explore interface providing access to the full database

# Open and FAIR data sharing: **Archive, Discover, Explore**



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SCIENTIFIC DATA · re3data.org · FAIRsharing.org standards, databases, policies

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DOIs assigned

Direct links to Discover & Explore

FAIRsharing.org
re3data.org

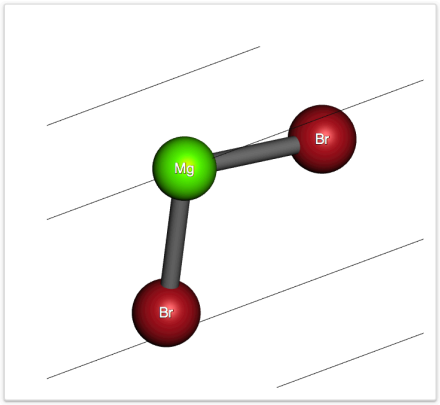
+

Recommended data repository by Nature's journal *Scientific Data*

# DISCOVER (CURATED DATA) & EXPLORE (RAW DATA)

**DISCOVER**

## Compound: $MgBr_2$




Info and properties

See definitions...

Formula: $MgBr_2$
Spacegroup: P-3m1
Pointgroup: -3m
Prototype: CdI2
Band gap [eV]: 4.8

Magnetic properties:

- Magnetic State: non-magnetic
- Tot. Magnetization [$\mu$B/cell]: -
- Abs. Magnetization [$\mu$B/cell]: -

Binding Energies:

- DF2-C09 Binding energy [meV/Å$^2$]: 10.2 (From parent COD 9009107)
- rVV10 Binding energy [meV/Å$^2$]: 15.3 (From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):

- $\Delta_{DF2}$ [%]: 17.1 (From parent COD 9009107)
- $\Delta_{rVV10}$ [%]: 18.3 (From parent COD 9009107)

Band structure

UUID links to jump to the provenance graph in the EXPLORE section

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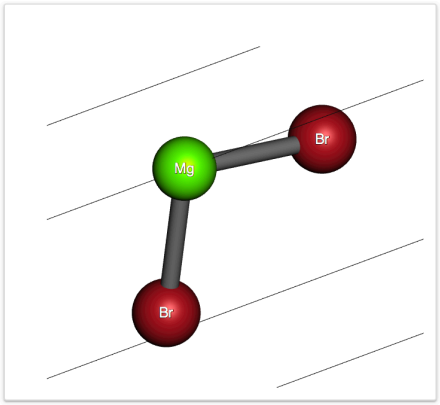


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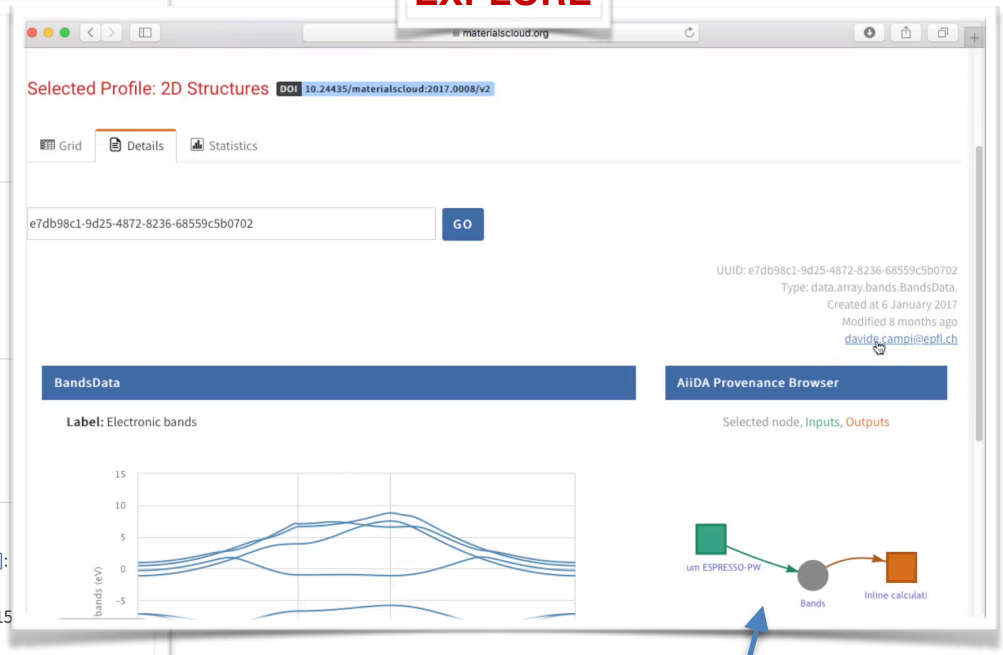
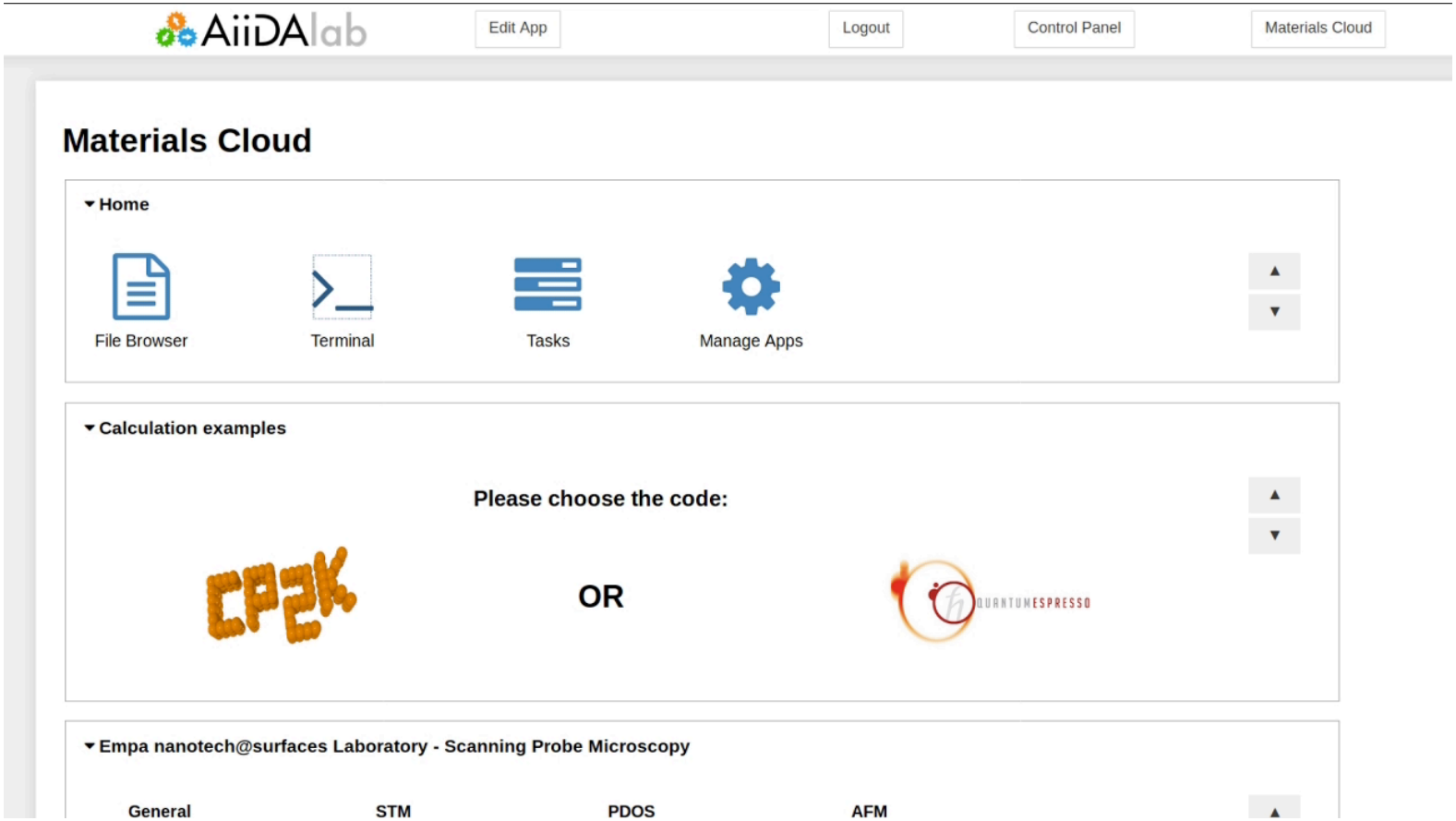


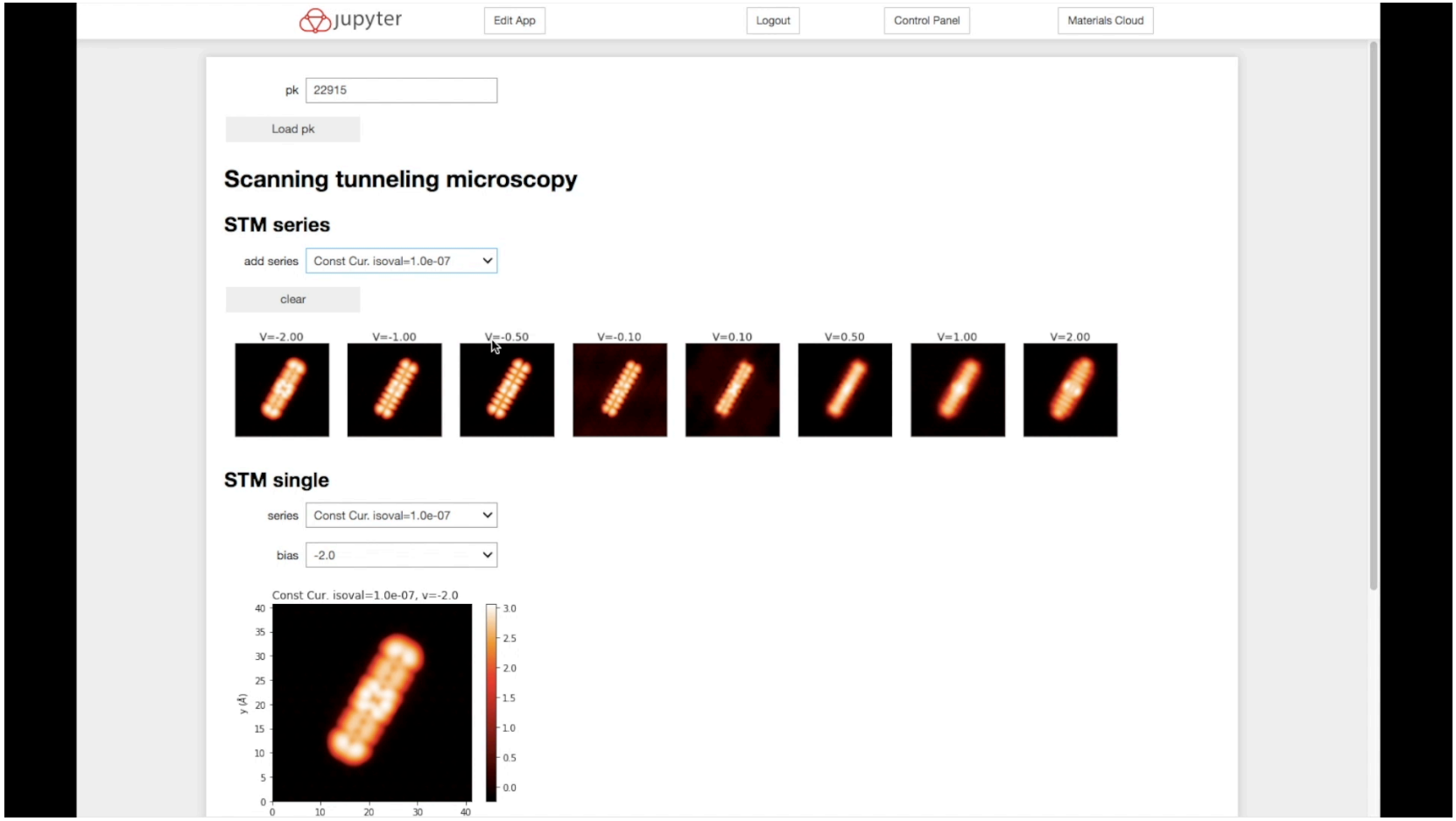

Browse the full AiiDA provenance graph (inputs, outputs, …) at any level

# WORK: AiiDA Lab (submission)

- Our **cloud data generation platform** and **data analysis platform**
- Strongly based on AiiDA + Jupyter + App Mode



# WORK: AiiDA Lab



# Possible integration/collaboration points

- **Development and integration plans**:
  - **AiiDA Lab**
    - Deployment with kubernetes for autoscaling
    - Integration fo Authentication and Authorization with B2ACCESS
    - *Registration of AiiDA Lab as a service on EOSC?*
      - Development and deployment of "turn-key" workflows for the materials science community as the "services"
  - **Archive**
    - Migration of Archive to Invenio v3 or EUDAT's B2SHARE (based on Invenio) [deciding now, 2 developers participating in the Invenio Boot Camp in March; is B2SHARE still supported?]
    - Integration in EUDAT's B2FIND