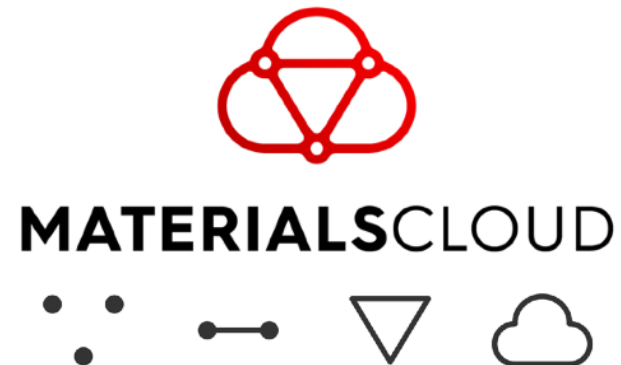
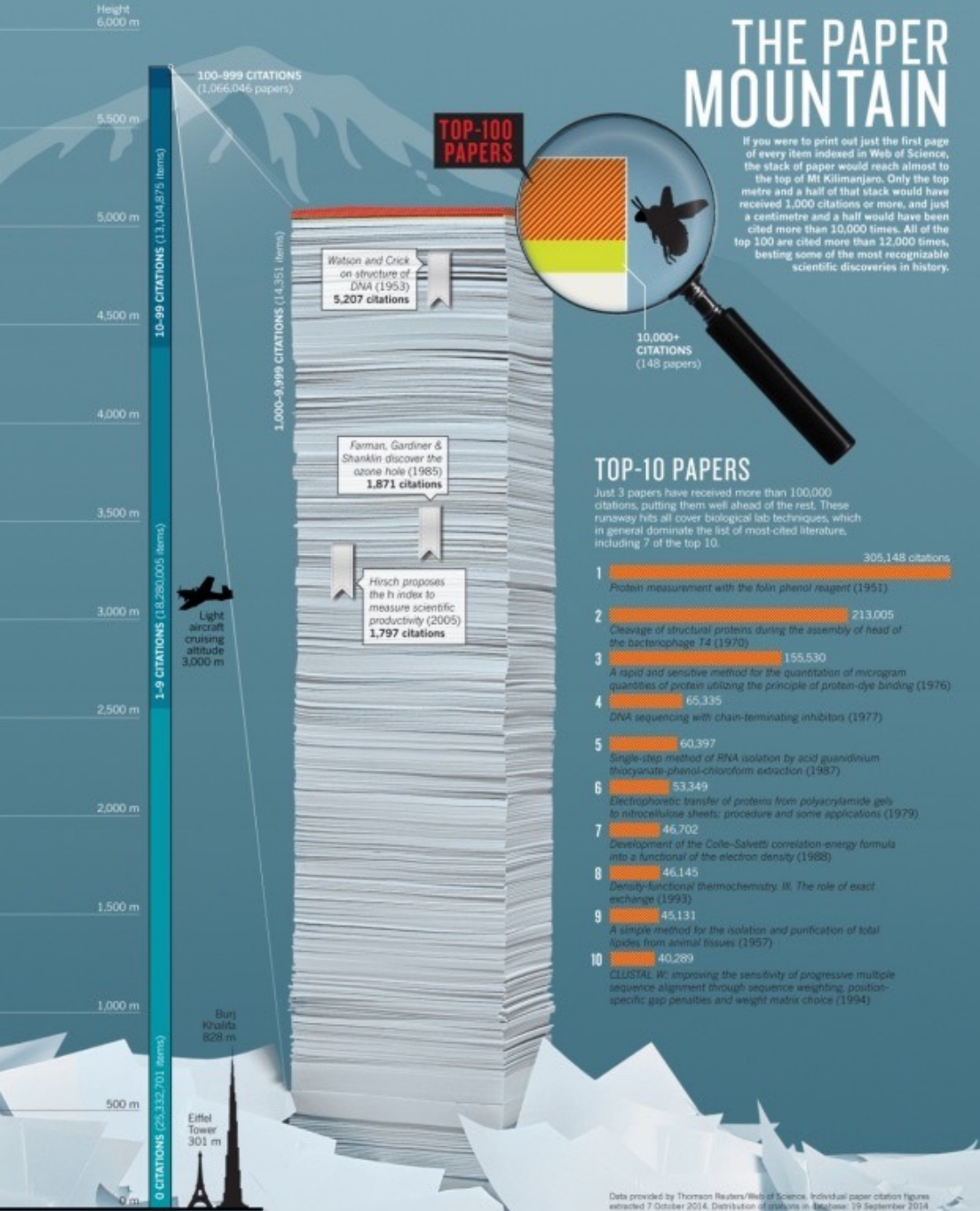


Open Science Platform for Materials Science: AiiDA and the Materials Cloud

Giovanni Pizzi (EPFL)



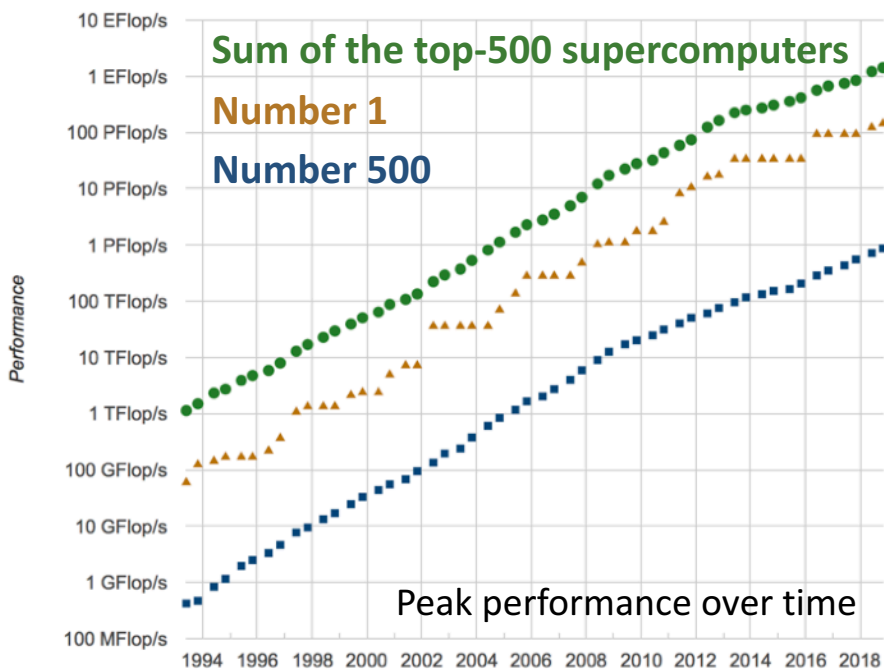


Our research: Materials simulations

Nature (2014): 12 papers on **Density Functional Theory** among the top-100 most cited papers in the *entire scientific literature*



Accuracy and predictive power of quantum engines



150,000x increase in the past 20 years

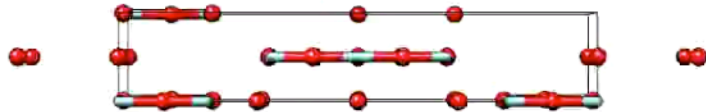
1 month (1998)



10 seconds (2018)

Result: materials design and discovery via high-throughput computations

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**



Open Science Platform: definition

- Our definition of an Open Science Platform [1]:
 - **Open simulation codes**
 - **Open architecture** to manage simulations and **open workflows**
 - Support for **Open Data, Data Management Plans** and FAIR-compliant sharing
 - **Straightforward availability** of the tools, with **curated open-data services** enabling turn-key workflows (pseudopotential libraries, ...)

[1] Pizzi G. (2018) *Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud*. In: Andreoni W., Yip S. (eds), *Handbook of Materials Modeling* (Springer, Cham).



Our goal

Build an open-science infrastructure
with computational services offered
to scientific, industrial community and beyond

Like a synchrotron, but for
open and reproducible simulations



Our two core infrastructures

AiiDA as the “operating system” to manage, automate and store simulations and their results

and

Materials Cloud as the open-science dissemination portal and cloud simulation platform




OPEN SCIENCE PLATFORM:



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



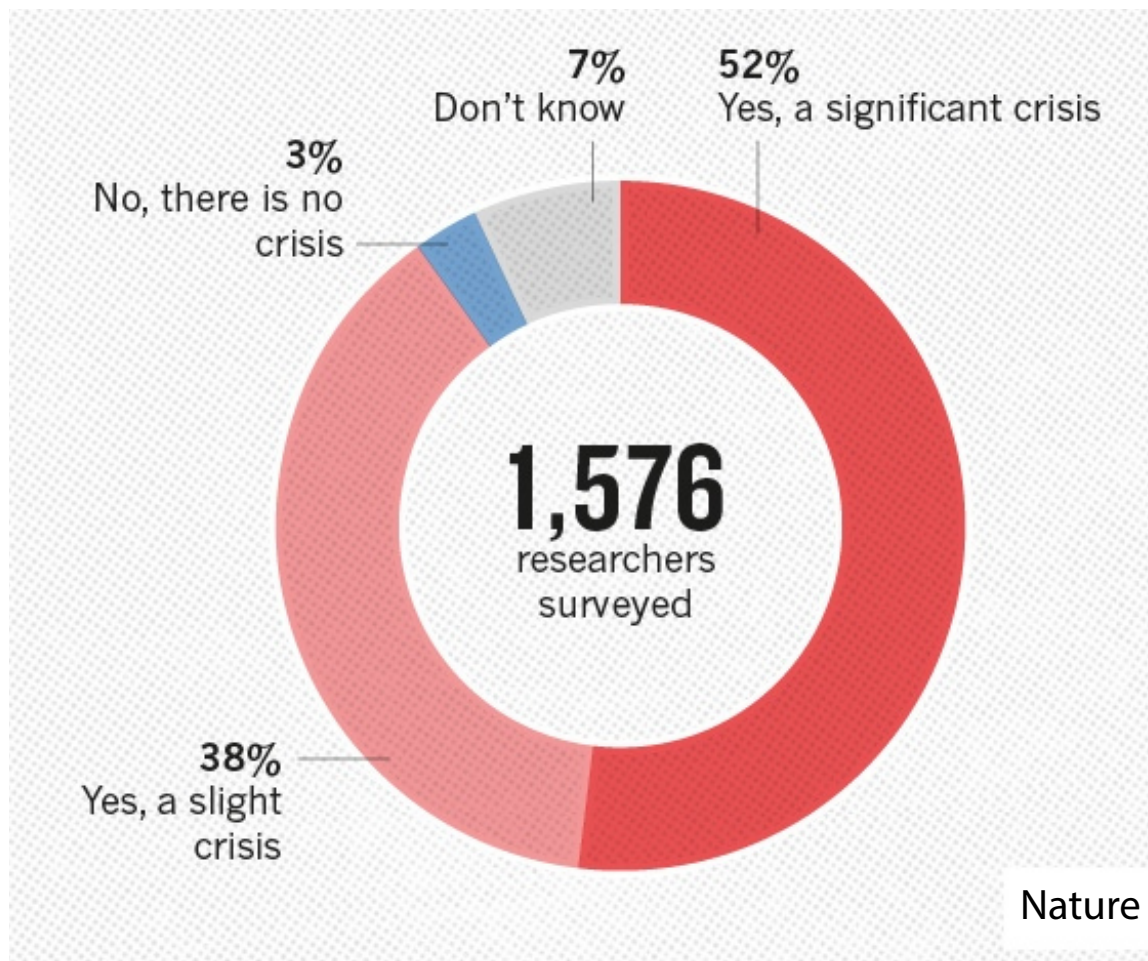
How to manage simulations and their provenance?



We need a **tool** to help us
organise research and store provenance

Reproducibility: a cornerstone of the scientific method

IS THERE A REPRODUCIBILITY CRISIS?



Reproducibility: a cornerstone of the scientific method

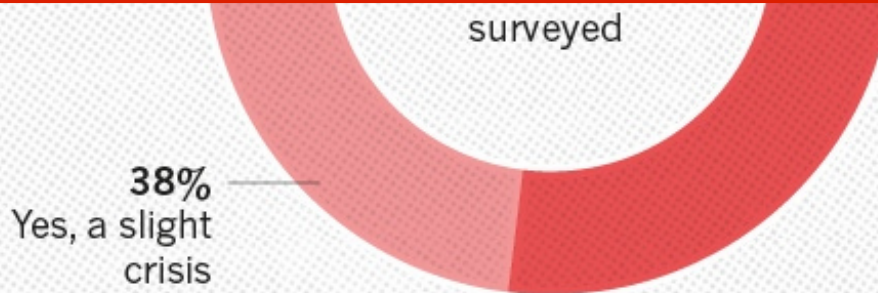
IS THERE A REPRODUCIBILITY CRISIS?

30%
7% Don't know
52% Yes, a significant crisis

No excuses in **computational** science

We can and **must** be fully reproducible

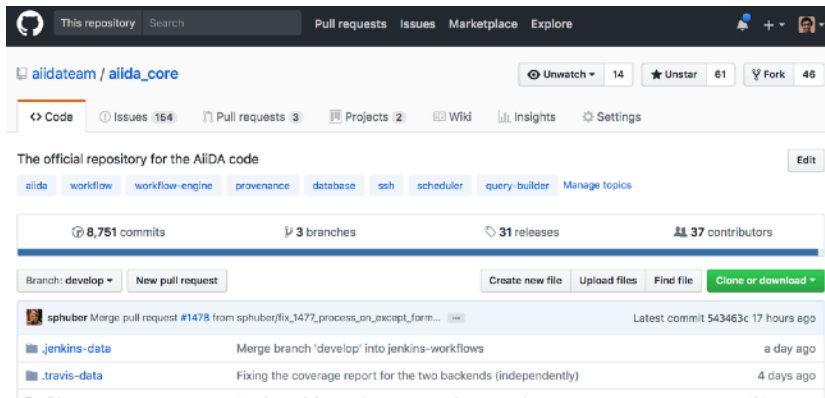
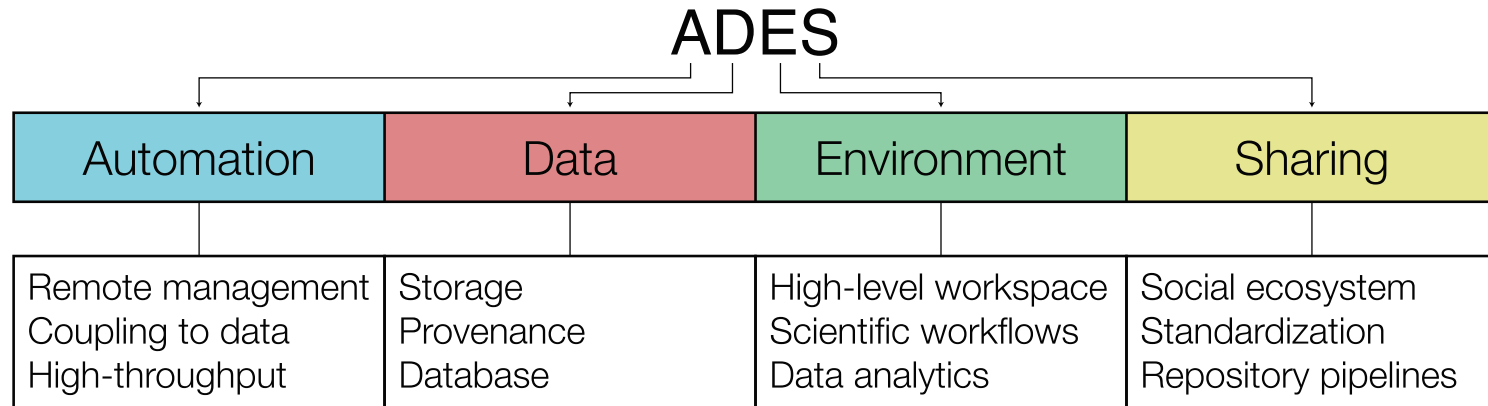
CHALLENGE #2: make open-science **easier**



Nature **533**, 452–454 (2016)



AiiDA development timeline

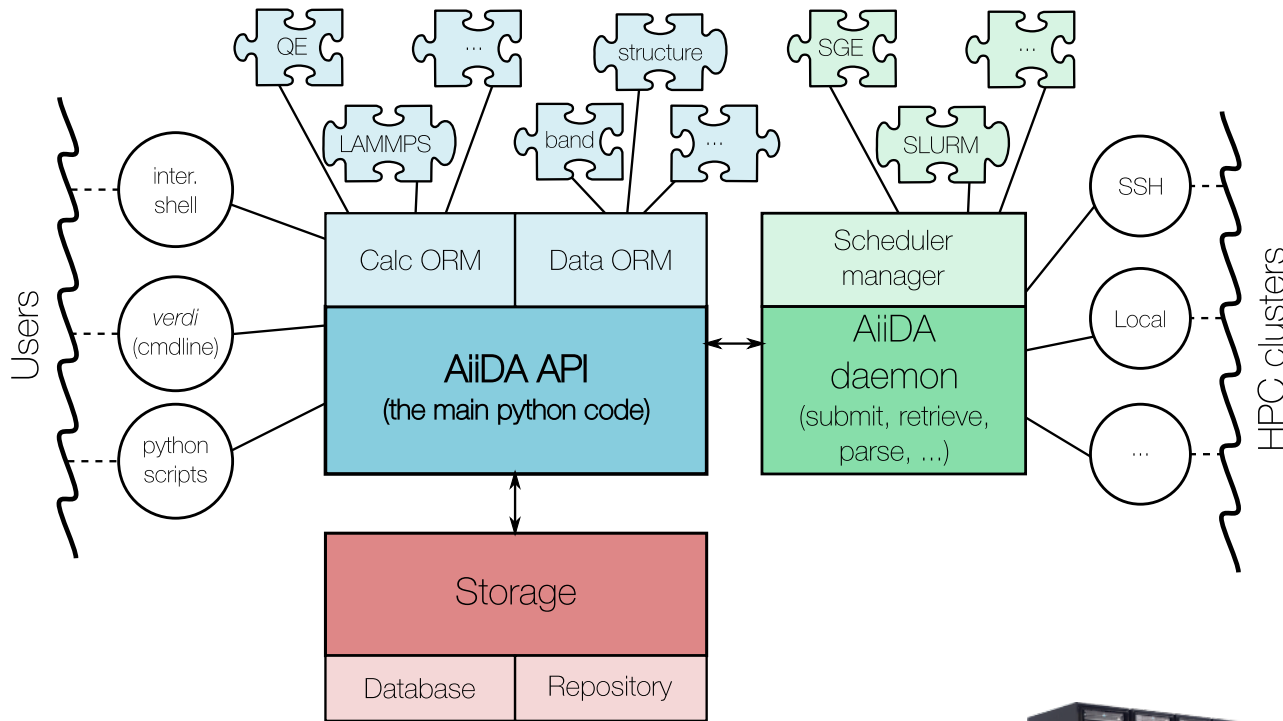


G. Pizzi et al., *Comp. Mat. Sci.* 111, 218-230 (2016)

<http://www.aiida.net>



AiiDA



Main features

- Python (2.7 & 3.6) infrastructure
- SQL database backend, access via a Python ORM
- Local connection to clusters, or via ssh using a python API
- Interface to various job schedulers (SGE, Torque, LSF, PBS Pro, SLURM, ...)
- Event-based daemon with remote management and workflow execution manager
- REST APIs using Flask to expose one own's data
- Plugin management system and extended code support
- Easy sharing of the results with other users in the community



AiiDA submission

```
code = Code.get('pw-6.3@daint-mr25')
builder = code.new_builder()

builder.metadata.options = {
    'max_wallclock_seconds': 600,
    'max_wallclock_seconds': {"num_machines": 2}}

Structure = DataFactory('structure')
structure = Structure(ase = read('TiO2.cif'))

Dict = DataFactory('dict')
parameters = Dict(dict={
    'CONTROL': {
        'calculation': 'scf',
        'restart_mode': 'from_scratch'},
    'SYSTEM': {'ecutwfc': 40.}})

Kpoints = DataFactory('array.kpoints')
kpoints = Kpoints(kpoints_mesh = [4,4,4])

builder.structure = structure
builder.parameters = parameters
builder.kpoints = kpoints
builder.pseudos = get_pseudos_from_family(structure,
    'SSSP_efficiency_v1.0')

aiida.engine.submit(builder)
```



AiiDA submission

```
code = Code.get('pw-6.3@daint-mr25')
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    'max_wallclock_seconds': 600,
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builder.pseudos = get_pseudos_from_family(structure,
    'SSSP_efficiency_v1.0')
```

```
aida.engine.submit(builder)
```

Switch computers in one line
supports different schedulers,
version of codes, ...

Define (only) necessary inputs
Interface designed by plugin

**Inputs stored in the DB, and
handing over to the daemon**

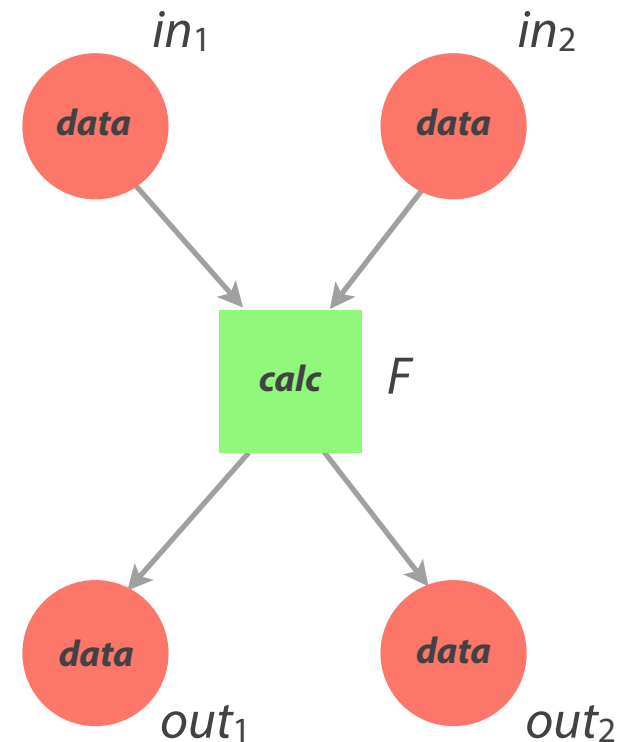


Storage and provenance

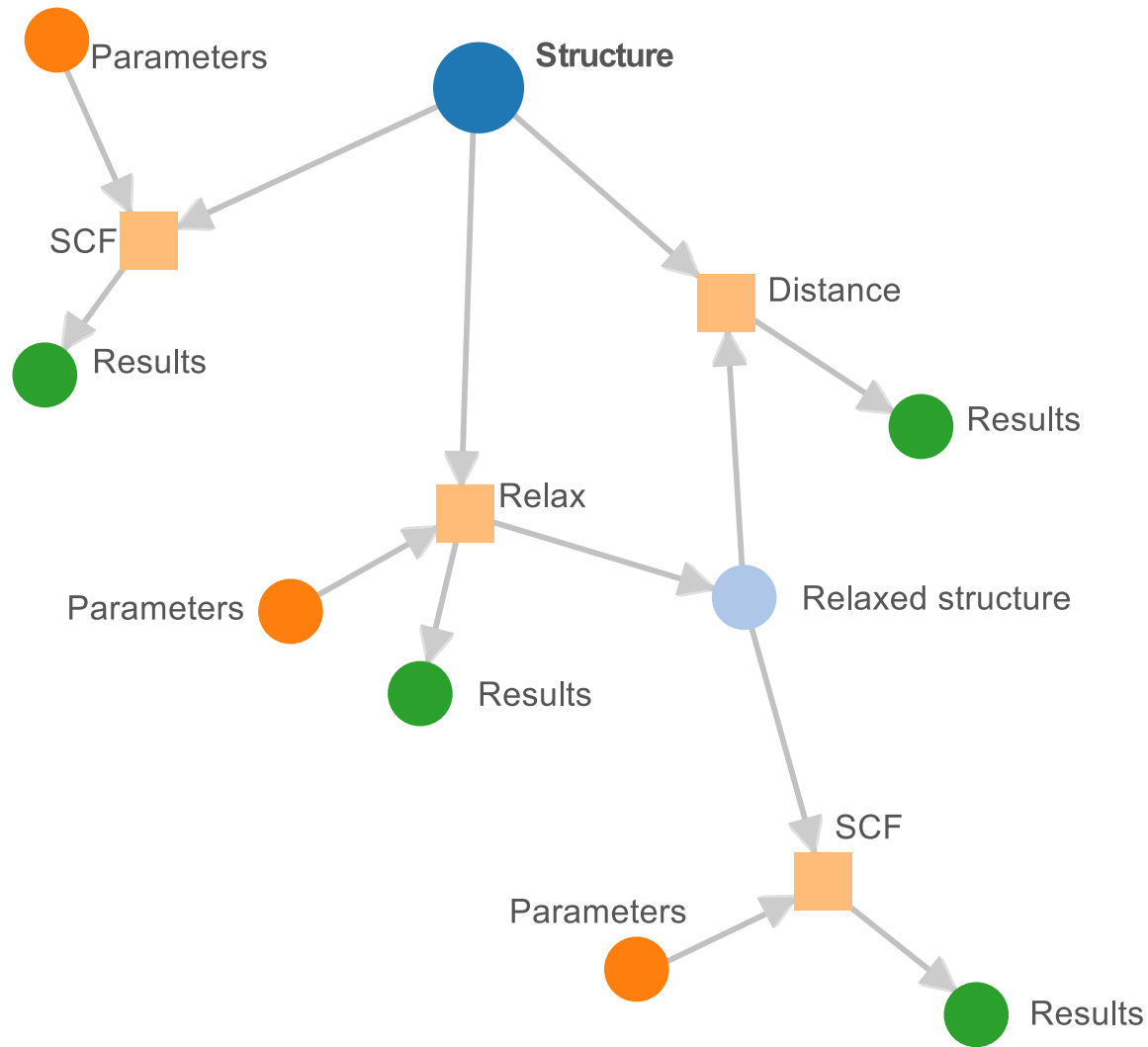
- *Calculated properties*: result of complex, connected calculations
- How do we store simulations **preserving the connected structure?**
- Inspiration from the *open provenance model*
- **Any calculation: a function**, converting inputs to outputs:

$$out_1, out_2 = F(in_1, in_2)$$

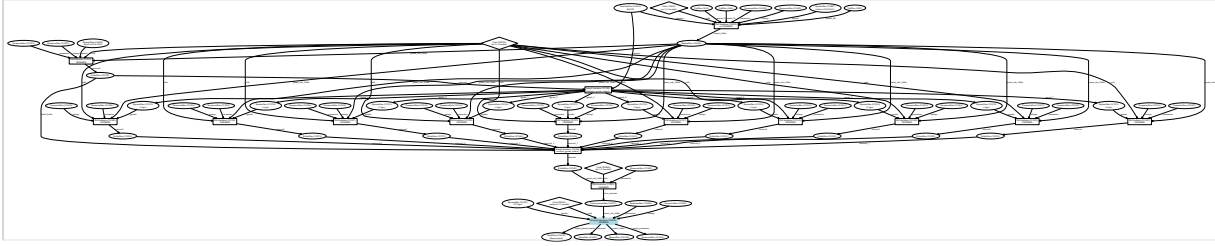
- **Each object is a node in a graph**, connected by directional labeled links
- Output nodes can be used as inputs



Data provenance: Directed Acyclic Graphs

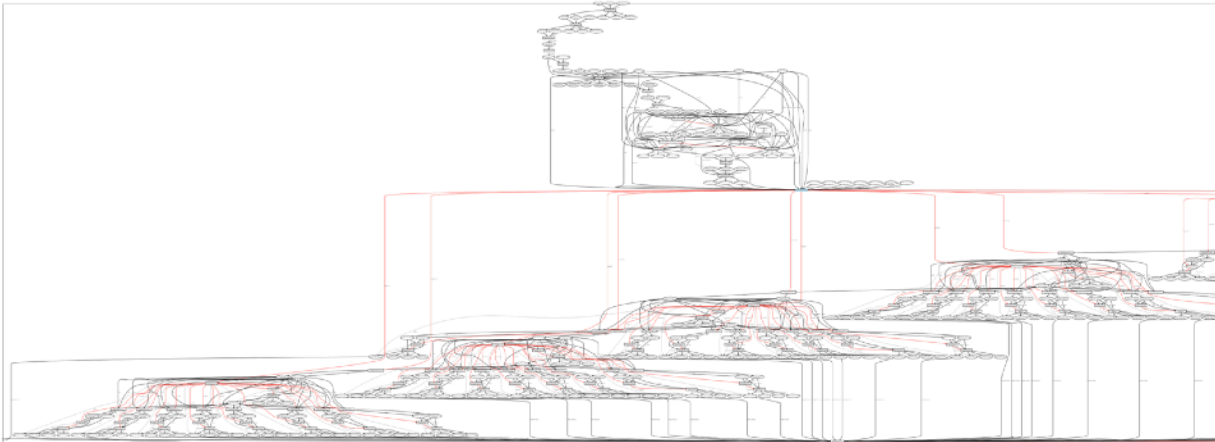


“Simple” graphs of workflows for a single material



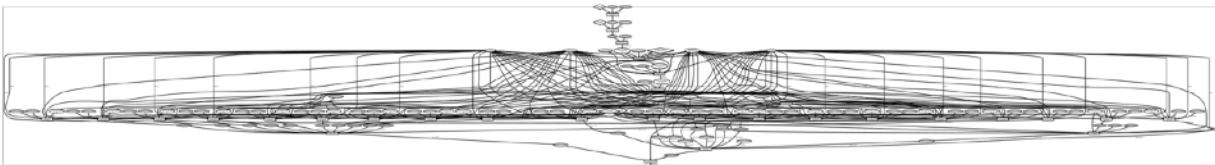
Phonon dispersion

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



Molecular dynamics of Lithium in a solid electrolyte

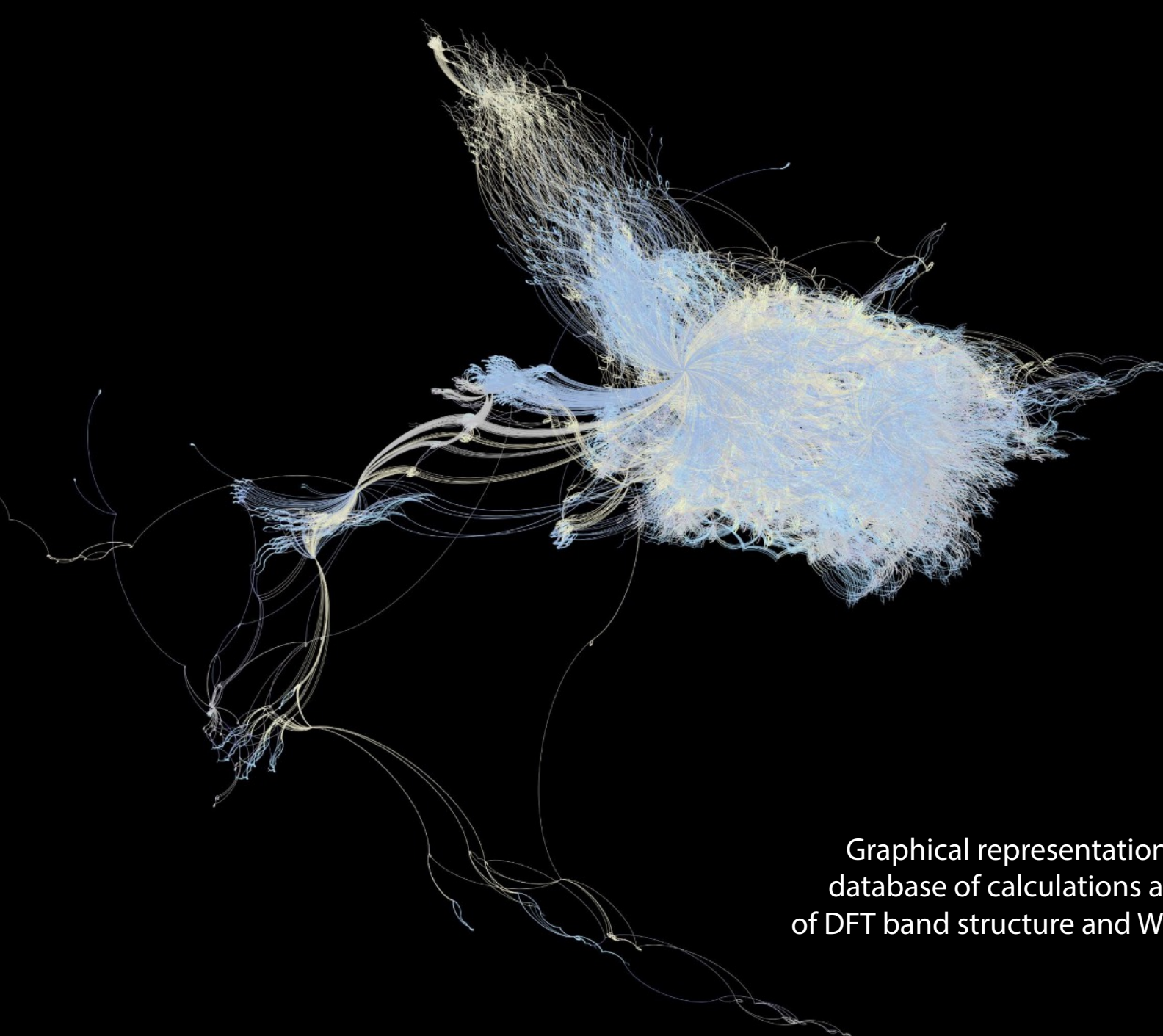
(Discover novel, safe and efficient electrolytes for Li-batteries)



Elastic constants

(response of materials to stresses and deformations)

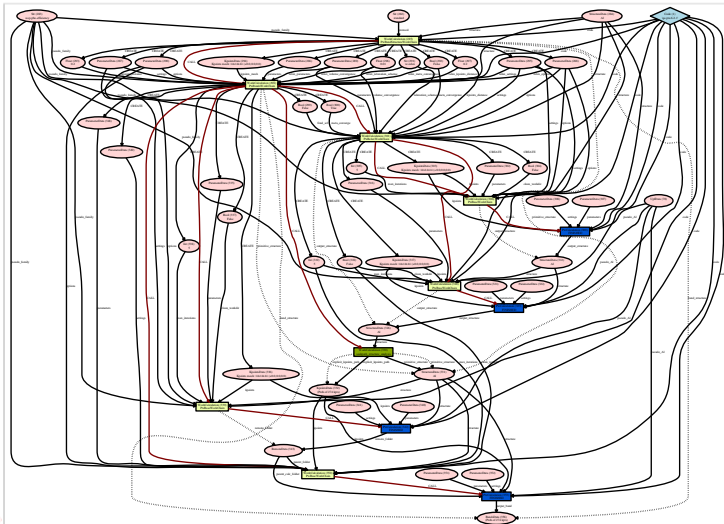
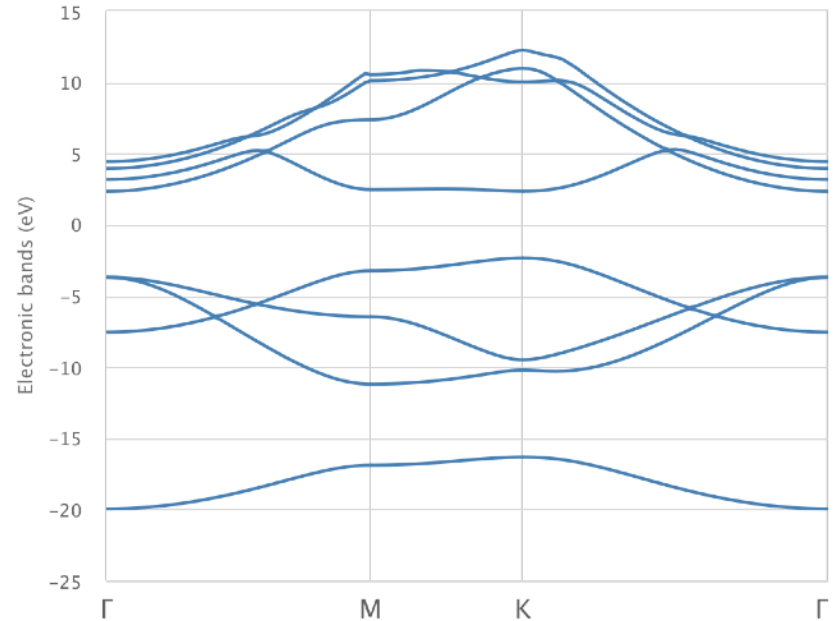
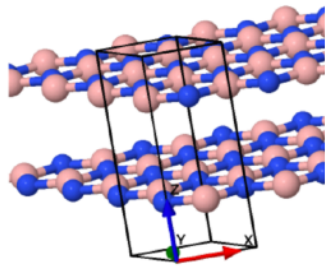




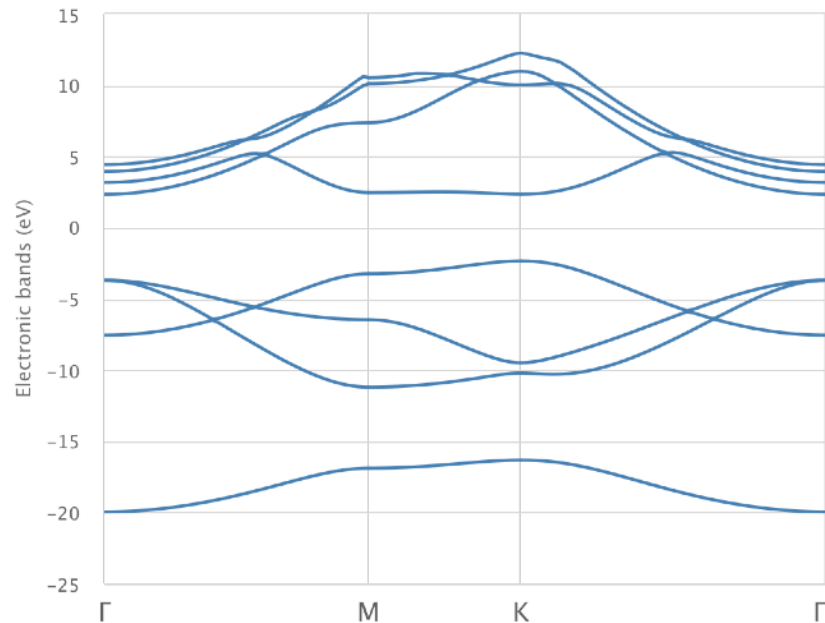
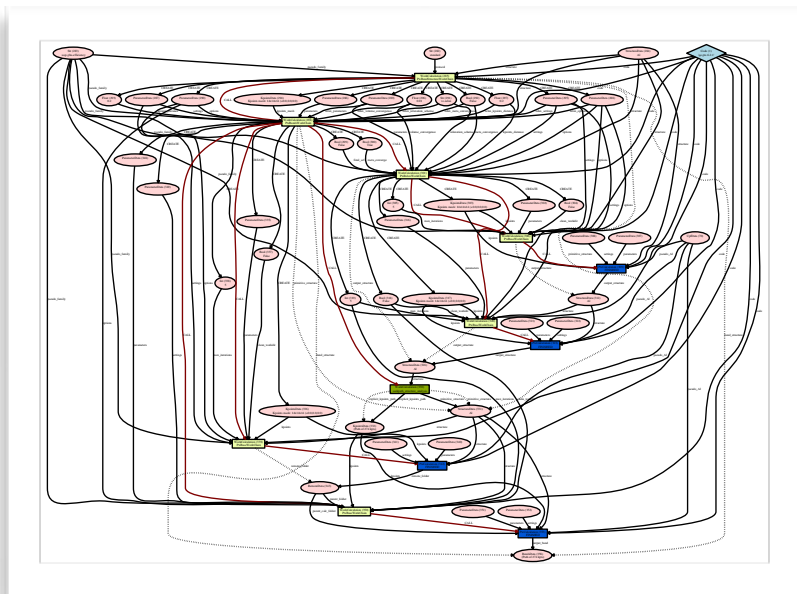
Graphical representation of an AiiDA
database of calculations and workflows
of DFT band structure and Wannier functions

Turn-key workflows in AiiDA

- Given a material, we often need to compute advanced quantities
- These are often non-trivial and result from a complex workflow



Turn-key workflows in AiiDA



- The AiiDA provenance graph allows to know how the structure was computed and to **reproduce that single specific calculation**: *log of "what happened in the past"*
- We need also an **easy way to re-run the same calculation again** with different parameters or for a different material: **turn-key workflows**



Turn-key workflows in AiiDA

```
class PwBandsWorkChain(WorkChain):
    @classmethod
    def define(cls, spec):

        spec.input('code',
                   valid_type=Code)
        spec.input('structure',
                   valid_type=StructureData)
        spec.input('pseudo_family',
                   valid_type=Str)

        spec.outline(
            cls.setup,
            cls.validate_inputs,
            if_(cls.should_do_relax)(
                cls.run_relax,
            ),
            cls.run_seekpath,
            cls.run_scf,
            cls.run_bands,
            cls.results,
        )
```

- **“Operating system” for all calculations**
- Automatic provenance tracking in the DB
- Control provenance granularity
store level of detail relevant to the workflows
- Progress checkpointing
restart from arbitrary step, retry on failure, allows to shut down daemon and continue later
- Easy debugging, self-documenting



Turn-key workflows in AiiDA

```
class PwBandsWorkChain(WorkChain):
    @classmethod
    def define(cls, spec):

        spec.input('code',
                   valid_type=Code)
        spec.input('structure',
                   valid_type=StructureData)
        spec.input('pseudo_family',
                   valid_type=Str)

        spec.outline(
            cls.setup,
            cls.validate_inputs,
            if_(cls.should_do_relax)(
                cls.run_relax,
            ),
            cls.run_seekpath,
            cls.run_scf,
            cls.run_bands,
            cls.results
        )
```

- **“Operating system” for all calculations**
- Automatic provenance tracking in the DB
- Control provenance granularity
store level of detail relevant to the workflows
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restart from arbitrary step, retry on failure, allows to shut down daemon and continue later
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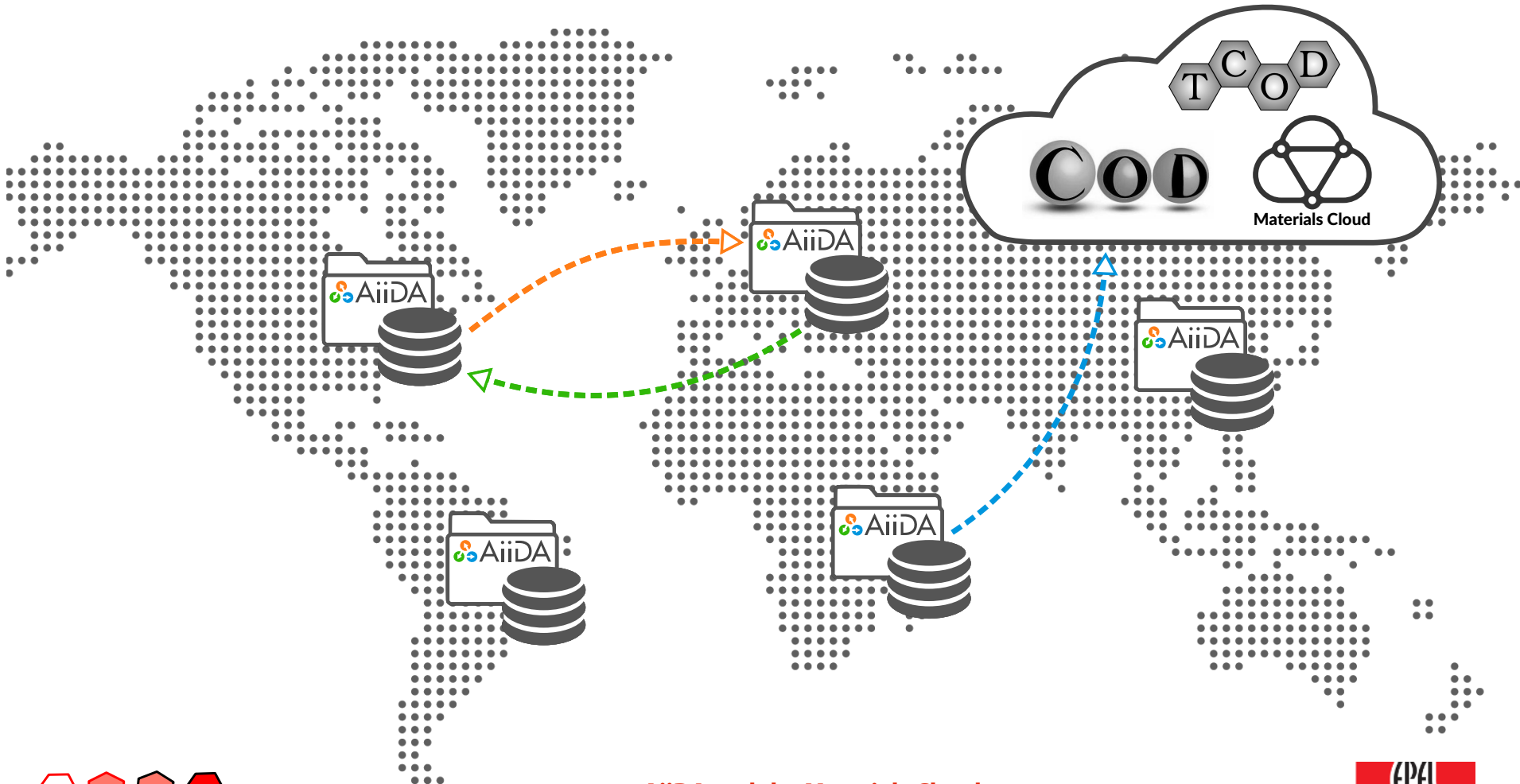
- Turn-key solution:

```
PwBandStructureWorkChain.run(
    code=Code.get_from_string(
        'qe-pw-6.2.1@localhost'),
    structure=StructureData(
        ase=ase.build.bulk('Al')),
    pseudo_family=Str('sssp-pbe-efficiency'))
```



Sharing in AiiDA: data and graphs

- *Private* AiiDA instances
- UUIDs to uniquely identify nodes
- Data can be shared to other AiiDA repositories **or to online repositories**



Sharing in AiiDA: codes, plugins and workflows



Calculation



Data



Parsers



Transport and
scheduler



Workflows



Importers &
exporters

AiiDA plugin registry

Calculations 71 plugins in 30 entries

Parsers 64 plugins in 30 entries

Data 35 plugins in 18 entries

Workflows 72 plugins in 13 entries

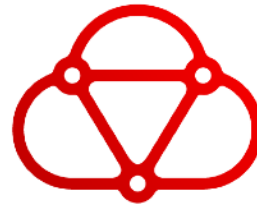
Other 61 plugins in 17 entries

- Plugins are collected in the AiiDA plugin registry
- Over **70 different code executables currently supported from over 30 different codes**, with almost 50 workflows
- Many are **community-contributed**

<https://aiidateam.github.io/aiida-registry/>



OPEN SCIENCE PLATFORM:



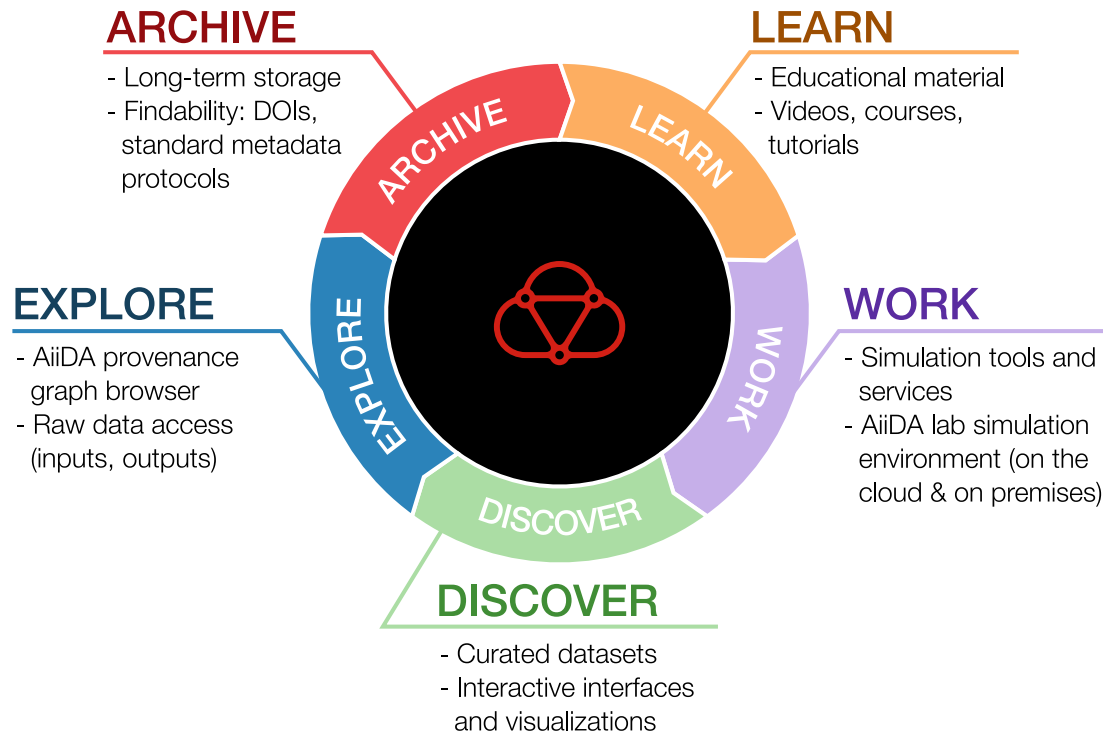
MATERIALSCLOUD

<https://www.materialscloud.org>



Materials Cloud

- **AiiDA** is the 'engine', like **Git** - used in production *since 2015*
- **Materials Cloud** is the dissemination platform (like **GitHub**) **and more** (cloud computing and data generation platform) - online since *Dec 2017*



Data generation: Materials Cloud **Work**



LEARN **WORK** DISCOVER EXPLORE ARCHIVE

More >



Tools

Online web tools to work with your data



AiiDA Lab

Run your own simulations using AiiDA on the cloud via Jupyter apps



Quantum Mobile

A virtual machine with quantum codes ready to be used via AiiDA



AiiDA registry

The official registry of AiiDA plugins

AiiDA Lab

- Comes with a preconfigured AiiDA setup, **ideal interface for turn-key workflows**
- Custom **AppMode** extension to make notebooks look&feel like real web apps **knowing only python**
- Using JupyterHub + DockerSpawner

Quantum Mobile

- **Downloadable VM** with preinstalled **AiiDA and codes** like QE, Yambo, Fleur, Siesta, CP2K, ...
- Includes **same AiiDA Lab apps environment** as on Materials Cloud
- Ideal for **education**



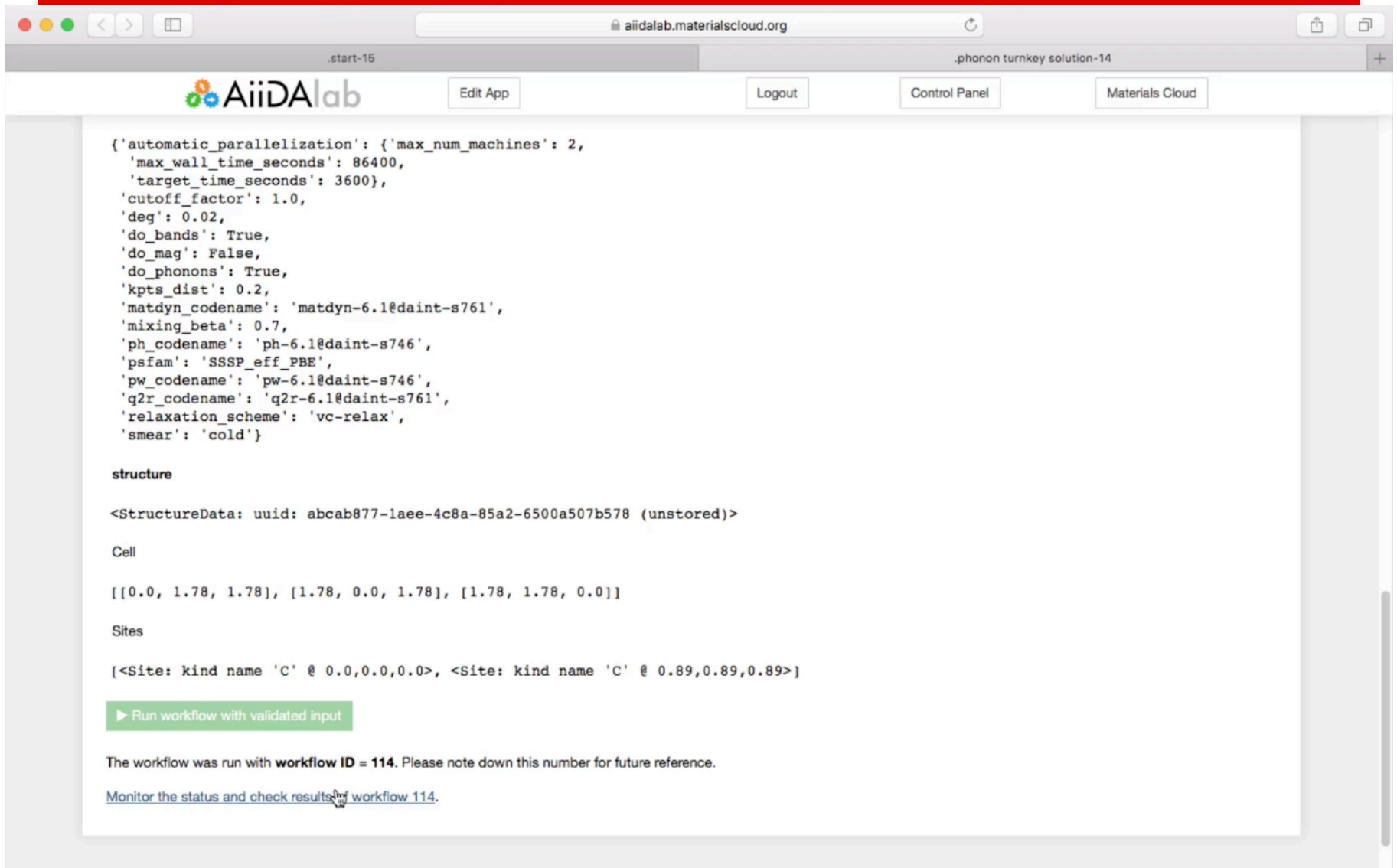
AiiDA Lab: submitting a turn-key solution (phonons)

The screenshot shows a web browser window with the URL `aiidalab.materialscloud.org`. The page header includes the AiiDA Lab logo and navigation buttons for "Edit App", "Logout", "Control Panel", and "Materials Cloud". The main content area is titled "AiiDA Lab" and is organized into several sections:

- Home**: Contains four main navigation icons: File Browser, Terminal, Tasks, and Manage Apps.
- AiiDA**: A list of links including Daemon Status, Graph Browser, Workflows, Delete nodes, and REST API.
- Quantum Mobile**: A list of links for Setup Connection to Quantum-Mobile and Setup Codes.
- LSMO apps**: A grid of application categories with sub-links:
 - Isotherm**: Compute one, Compute multiple
 - Charges**: Compute Charges
 - Pore analysis**: Compute Pores
 - Import your data to AiiDA**: Import database, Data imported data



AiiDA Lab: checking the workflow results (phonons)



The screenshot shows the AiiDA Lab web interface in a browser window. The address bar displays `aiidalab.materialscloud.org`. The page has a navigation bar with buttons for "Edit App", "Logout", "Control Panel", and "Materials Cloud". The main content area displays a JSON configuration for a workflow, followed by a "structure" section showing cell parameters and sites. A green button labeled "Run workflow with validated input" is visible. Below the button, a message states: "The workflow was run with **workflow ID = 114**. Please note down this number for future reference." A link is provided to "Monitor the status and check results of workflow 114."

```
{'automatic_parallelization': {'max_num_machines': 2,
  'max_wall_time_seconds': 86400,
  'target_time_seconds': 3600},
  'cutoff_factor': 1.0,
  'deg': 0.02,
  'do_bands': True,
  'do_mag': False,
  'do_phonons': True,
  'kpts_dist': 0.2,
  'matdyn_codename': 'matdyn-6.1@daint-s761',
  'mixing_beta': 0.7,
  'ph_codename': 'ph-6.1@daint-s746',
  'psfam': 'SSSP_eff_PBE',
  'pw_codename': 'pw-6.1@daint-s746',
  'q2r_codename': 'q2r-6.1@daint-s761',
  'relaxation_scheme': 'vc-relax',
  'smear': 'cold'}
```

structure

<StructureData: uuid: abcab877-1aee-4c8a-85a2-6500a507b578 (unstored)>

Cell

[[0.0, 1.78, 1.78], [1.78, 0.0, 1.78], [1.78, 1.78, 0.0]]

Sites

[<Site: kind name 'C' @ 0.0,0.0,0.0>, <Site: kind name 'C' @ 0.89,0.89,0.89>]

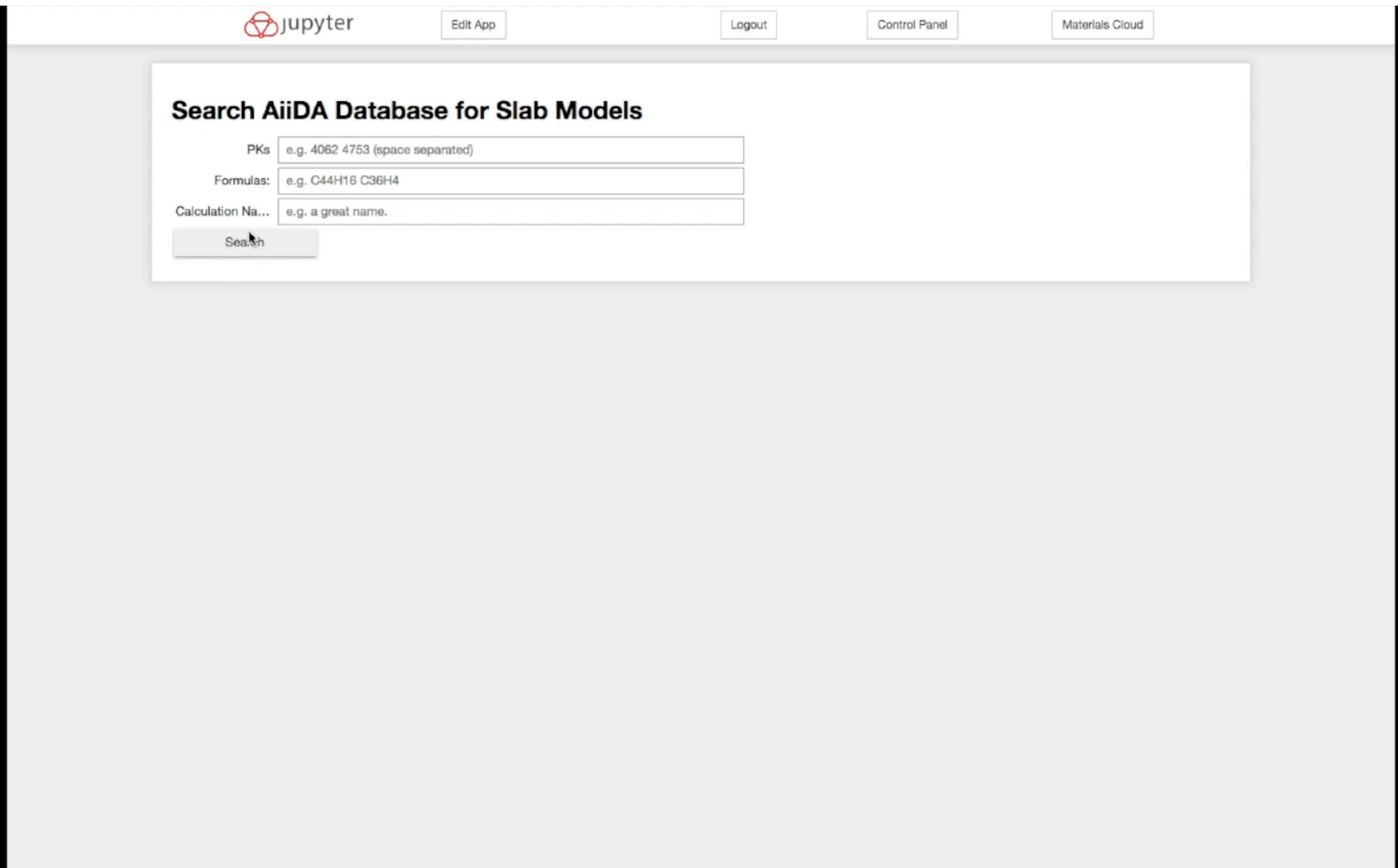
▶ Run workflow with validated input

The workflow was run with **workflow ID = 114**. Please note down this number for future reference.

[Monitor the status and check results of workflow 114.](#)



AiiDA Lab: checking the workflow results (STM)



The screenshot displays the Jupyter interface for AiiDA Lab. At the top, there is a navigation bar with the Jupyter logo and the text "jupyter". To the right of the logo are four buttons: "Edit App", "Logout", "Control Panel", and "Materials Cloud". Below the navigation bar is a search form titled "Search AiiDA Database for Slab Models". The form contains three input fields: "PKs" with the placeholder text "e.g. 4062 4753 (space separated)", "Formulas:" with the placeholder text "e.g. C44H16 C36H4", and "Calculation Na..." with the placeholder text "e.g. a great name.". Below the input fields is a "Search" button.



A solution tailored for every user

User	Skills	Goals	Solution
Computational Scientist	<i>Knows</i> Unix, bash, python	<ul style="list-style-type: none">• run high-throughput calculations• write complex workflows• develop AiiDA plugins	AiiDA on the laptop
Experimental Scientist	<i>Doesn't know</i> Unix, bash, python	<ul style="list-style-type: none">• run pre-defined workflows• analyze results	AiiDA Lab in the cloud
Student (tutorial/lecture)	<i>some familiarity with</i> Unix, bash, python	<ul style="list-style-type: none">• learn how to use AiiDA• learn how to use ab-initio codes• take materials home	Quantum Mobile on the laptop

Open data sharing: Archive, Discover, Explore

materialscloud:2017.0008

SCIENTIFIC DATA

re3data.org
REGISTERED RESEARCH DATA REPOSITORIES
In compliance with the FAIR Principles
Materials Cloud



FAIRsharing.org
standards, databases, policies

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

Authors: Nicolas Mounet^{1*}, Marco Gibertini¹, Philippe Schwaller¹, Davide Campi¹, Andrius Merkys^{1,2}, Antimo Marrazzo¹, Thibault Sohier¹, Ivano E. Castelli¹, Andrea Cepellotti¹, Giovanni Pizzi¹, 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](https://doi.org/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](https://doi.org/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](#)

DOIs assigned

[FAIRsharing.org](https://www.fairsharing.org)
[re3data.org](https://www.re3data.org)

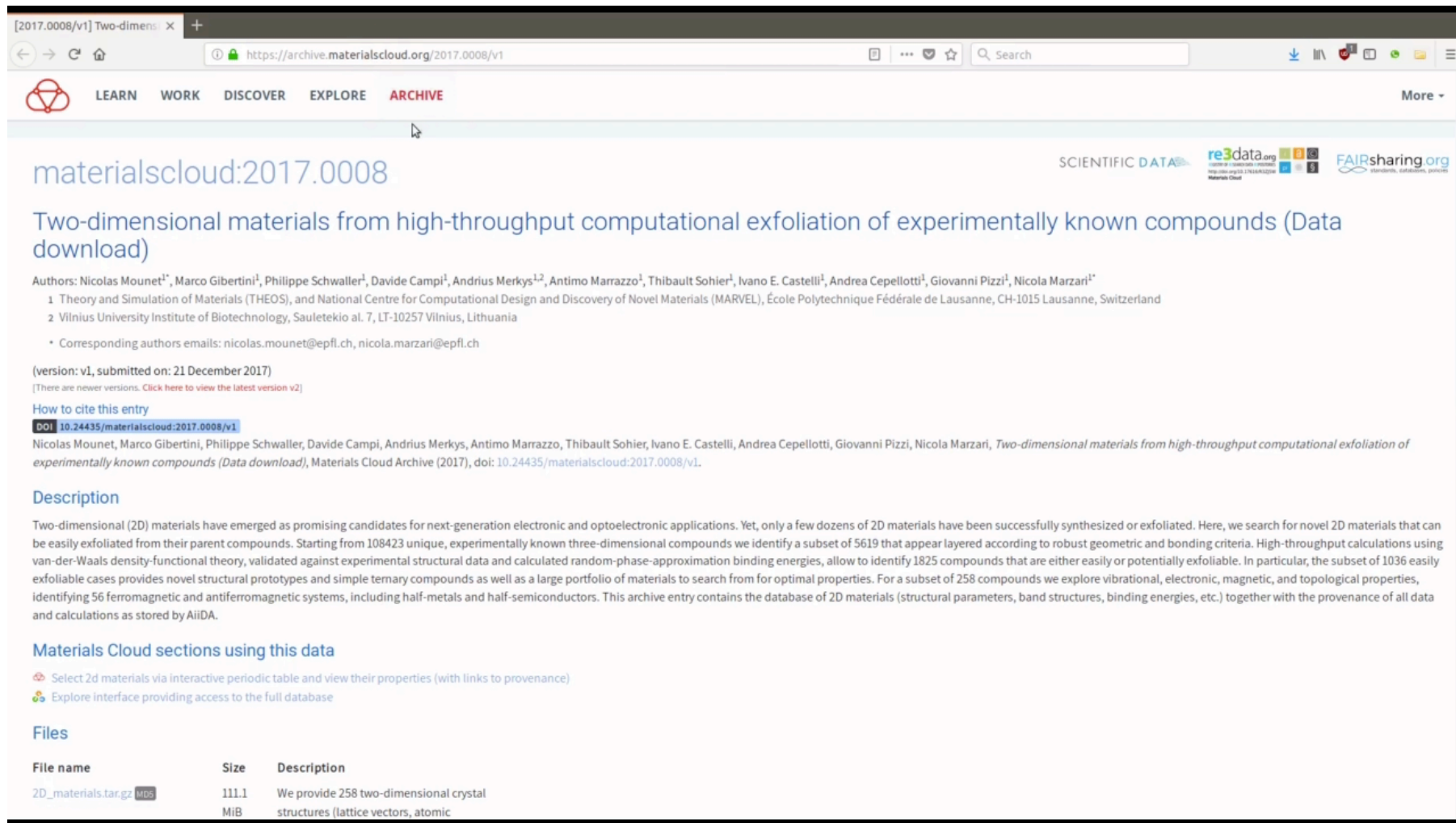
+

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

Direct links to Discover & Explore



Open data sharing: Archive, Discover, Explore



The screenshot shows a web browser window displaying the Materials Cloud Archive page for dataset 'materialscloud:2017.0008'. The page title is 'Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds (Data download)'. The authors listed are Nicolas Mounet^{1*}, Marco Gibertini¹, Philippe Schwaller¹, Davide Campi¹, Andrius Merkys^{1,2}, Antimo Marrazzo¹, Thibault Sohier¹, Ivano E. Castelli¹, Andrea Cepellotti¹, Giovanni Pizzi¹, and Nicola Marzari^{1*}. The page includes a description of the dataset, a 'Description' section, and a 'Files' section with a table of files.

materialscloud:2017.0008

Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds (Data download)

Authors: Nicolas Mounet^{1*}, Marco Gibertini¹, Philippe Schwaller¹, Davide Campi¹, Andrius Merkys^{1,2}, Antimo Marrazzo¹, Thibault Sohier¹, Ivano E. Castelli¹, Andrea Cepellotti¹, Giovanni Pizzi¹, 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

(version: v1, submitted on: 21 December 2017)
[There are newer versions. [Click here to view the latest version v2](#)]

How to cite this entry
DOI: [10.24435/materialscloud:2017.0008/v1](https://doi.org/10.24435/materialscloud:2017.0008/v1)

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 (Data download)*, Materials Cloud Archive (2017), doi: [10.24435/materialscloud:2017.0008/v1](https://doi.org/10.24435/materialscloud:2017.0008/v1).


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 for 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

Files

File name	Size	Description
2D_materials.tar.gz 	111.1 MIB	We provide 258 two-dimensional crystal structures (lattice vectors, atomic



DATA MANAGEMENT PLANS AND FAIR PRINCIPLES

- Combination of **AiiDA + Materials Cloud** (Discover, Explore, Archive): **FAIR-compliant sharing**
- **Findable**: DOIs with standardized metadata
- **Accessible**: web interface to browse data, calculations and provenance, curated data in Discover section
- **Interoperable**: data linked via the AiiDA directed graph; data structures reusable between different codes
- **Reusable**: downloadable data, encourage open (CC) licences, reproduce in the AiiDA Lab thanks to *full provenance*
- We provide **DMP templates** for researchers using Materials Cloud (Swiss SNSF, EU H2020, and more in the future)

Below, we provide templates for data management plans using the Materials Cloud Archive (with and without AiiDA).

Funding Body	DMP template (using  AiiDA)	DMP template (no AiiDA)
SNSF	.docx .odt .pdf	.docx .odt .pdf



Acknowledgements and funding



SNSF NCCR “MARVEL”

Discovery of new materials via simulations and dissemination of curated data



H2020 Centre of Excellence “MaX”

Scaling towards exascale machines and high-throughput efficiency

swissuniversities

Swissuniversities P-5 “Materials Cloud”

Scaling the web platform, extending to more disciplines



EPFL Open Science Fund “OSSCAR”

Creating a hub of computational resources geared also towards education and teaching

Moreover: *H2020 Marketplace* (providing data and simulation services in a EU Marketplace platform also for industry); *H2020 Intersect* (develop AiiDA workflows to compute transport properties of materials)



AiiDA and the Materials Cloud



Acknowledgements

The Materials Cloud And AiiDA teams



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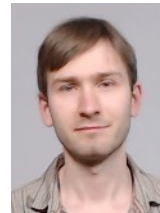
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The CSCS support teams

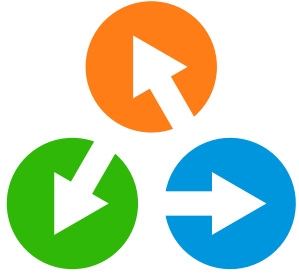
Summary

- **AiiDA**: the reproducibility and automation engine
 - Define turn-key workflows, automate them on supercomputers
 - Keep track of the **provenance** in the form of a graph
 - Share data, plugins and workflows
- **Materials Cloud**: the dissemination portal
 - **AiiDA Lab**: data generation platform, both on the cloud or locally (Quantum Mobile VM)
 - **Archive**: Findable long-term storage + **Discover** (curated data) + **Explore** (raw AiiDA data): **FAIR sharing**
 - Supports researchers in data management and DMPs

Open Science: not only *open data, codes and workflows*,
but also ***straightforward access to them***



Contacts



Website: <http://www.aiida.net>

Docs: <http://aiida-core.readthedocs.io>

Git repo: https://github.com/aiidateam/aiida_core/

Plugin registry: <http://aiidateam.github.io/aiida-registry>



<https://www.facebook.com/aiidateam>



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Materials Cloud: <http://www.materialscloud.org>

- **AiiDA Lab:** <http://aiidalab.materialscloud.org>

- **Archive:** <http://archive.materialscloud.org>

Quantum Mobile: <http://www.materialscloud.org/work/quantum-mobile>