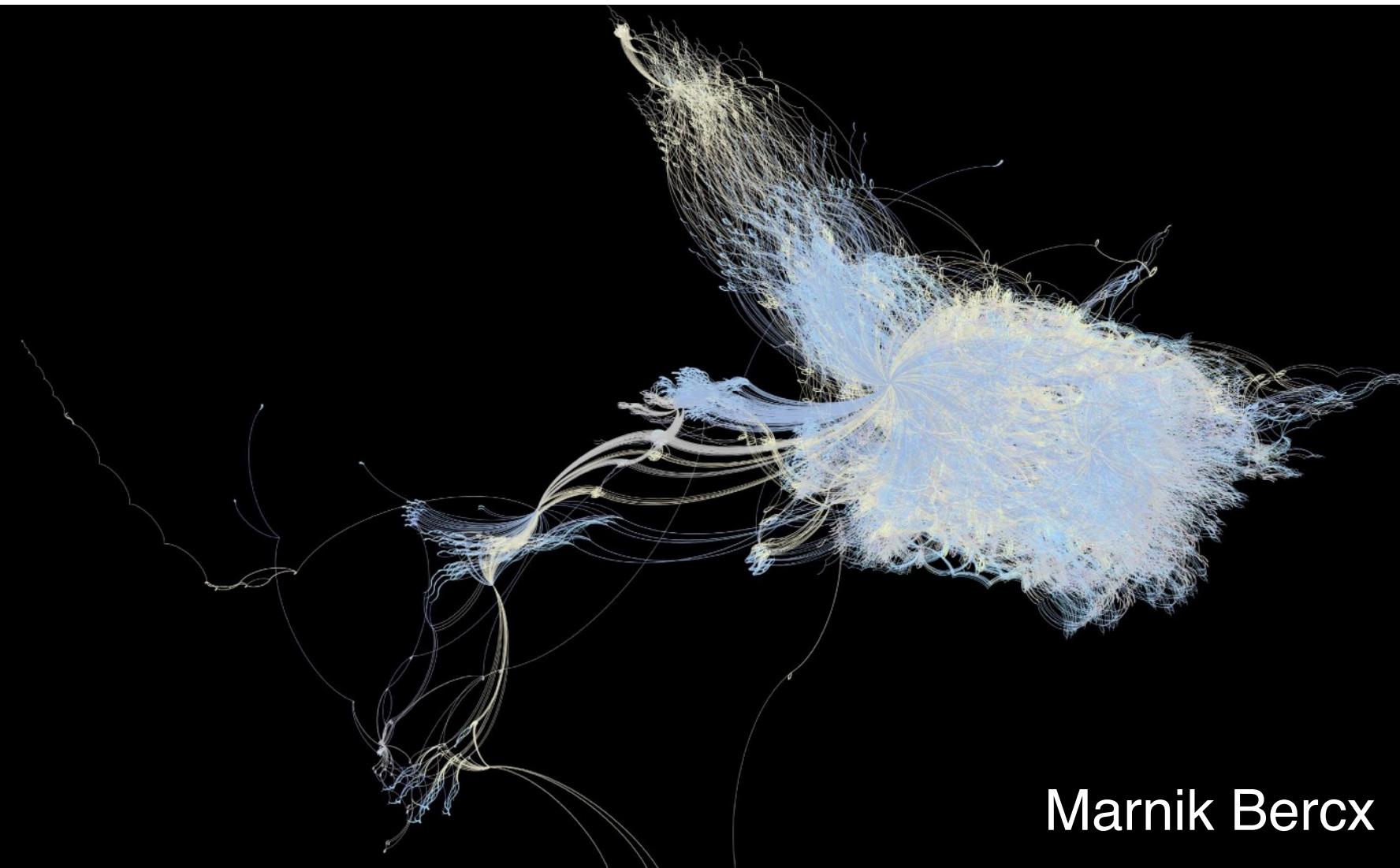


Quantum ESPRESSO School



Marnik Bercx

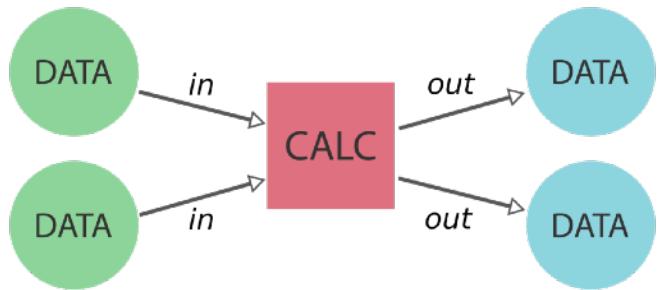
Challenges in high-throughput HPC

- **Workflow automation**
 - Need tools to define complex workflows with advanced error handling
 - An automated, robust and scalable engine to run the workflows
- **Data management**
 - Data should be stored reliably and efficiently
 - Stored data should be interoperable and queryable
- **Reproducibility**
 - All produced data should be reproducible by storing the full provenance

Data provenance

Simple recipe

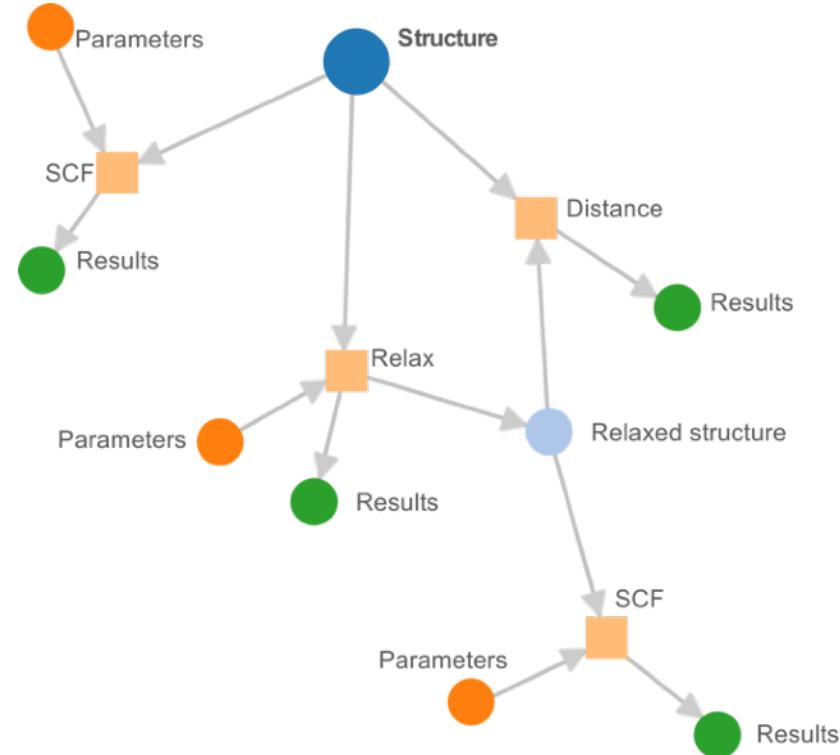
- Store data transformations or '**calculations**'
- Store its **inputs** and their metadata
- Store its **outputs** and their metadata
- Most **crucially** store the **inter-connections**



Data provenance

Simple recipe

- Store data transformations or '**calculations**'
- Store its **inputs** and their metadata
- Store its **outputs** and their metadata
- Most **crucially** store the **inter-connections**



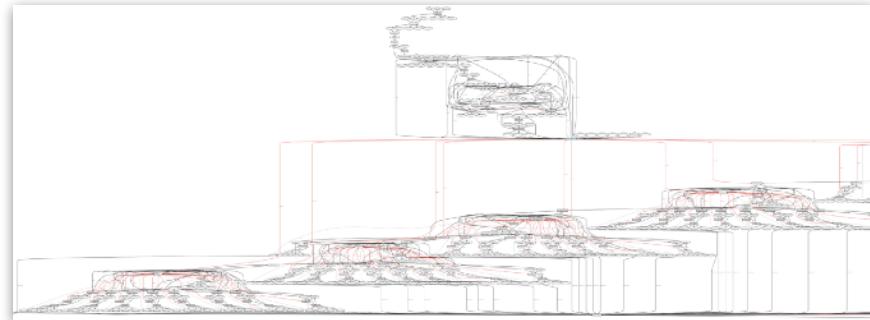
Provenance graphs

- When data gets reused, a directed graph is created
- That quickly grow in complexity even for “simple” workflows

Data provenance

Simple recipe

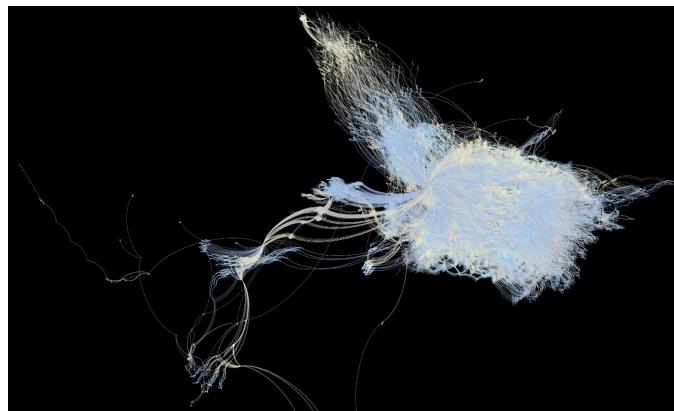
- Store data transformations or '**calculations**'
- Store its **inputs** and their metadata
- Store its **outputs** and their metadata
- Most **crucially** store the **inter-connections**



Molecular dynamics study of Lithium in a solid electrolyte.

Graph requirements

- Needs to be automated
- Needs to be stored *as data is created*



Graphical representation of actual AiiDA database



- COMPUTATIONAL SCIENCE INFRASTRUCTURE
- FOR HIGH THROUGHPUT WORKFLOWS
- WITH FULL DATA PROVENANCE



Language: implemented and API in python



License: MIT open source <http://www.aiida.net/>

Source: <https://github.com/aiidateam/aiida-core>



Scalable workflow engine

Automated full data provenance



Built-in support for HPC

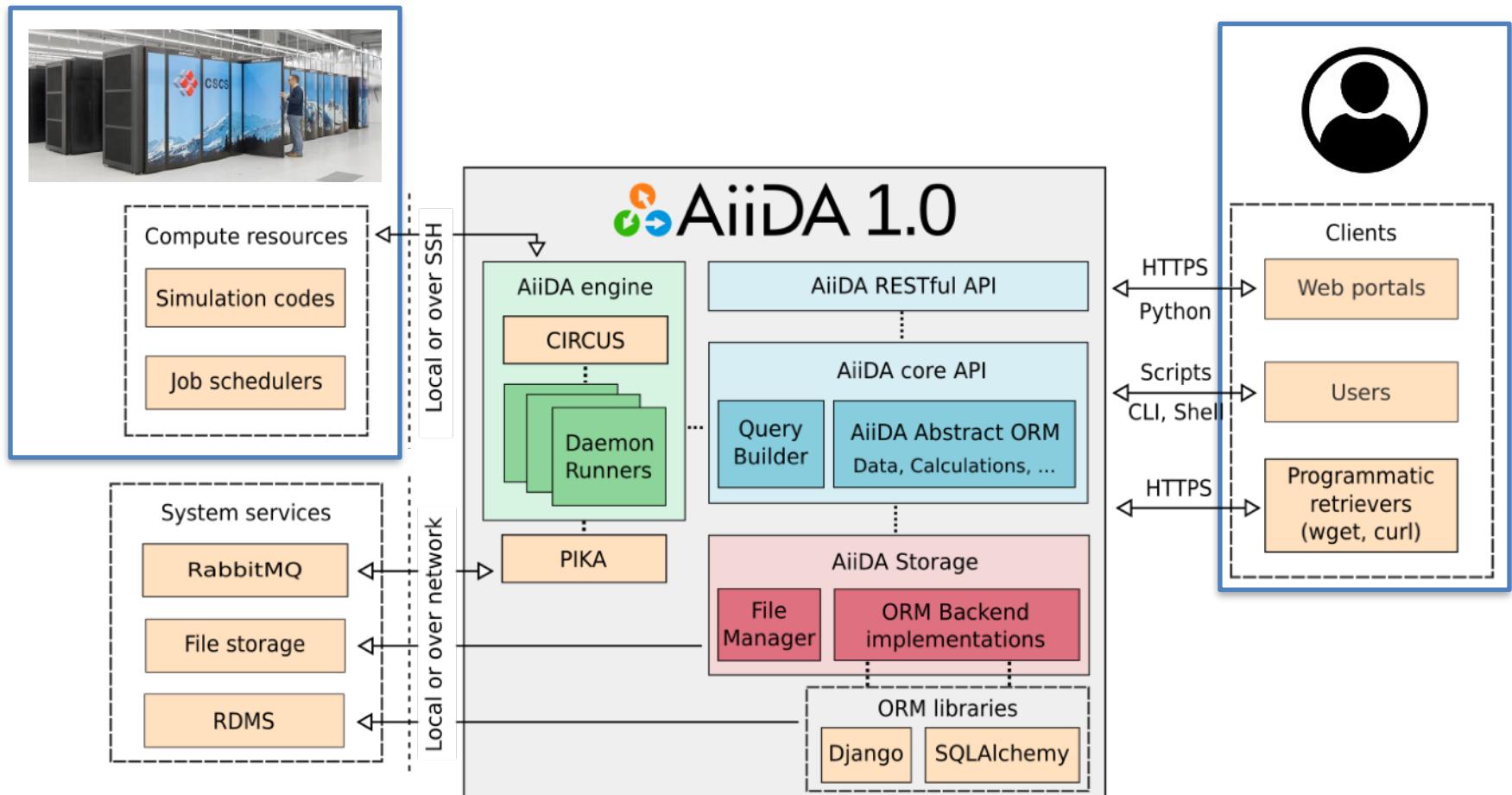


Flexible plugin system



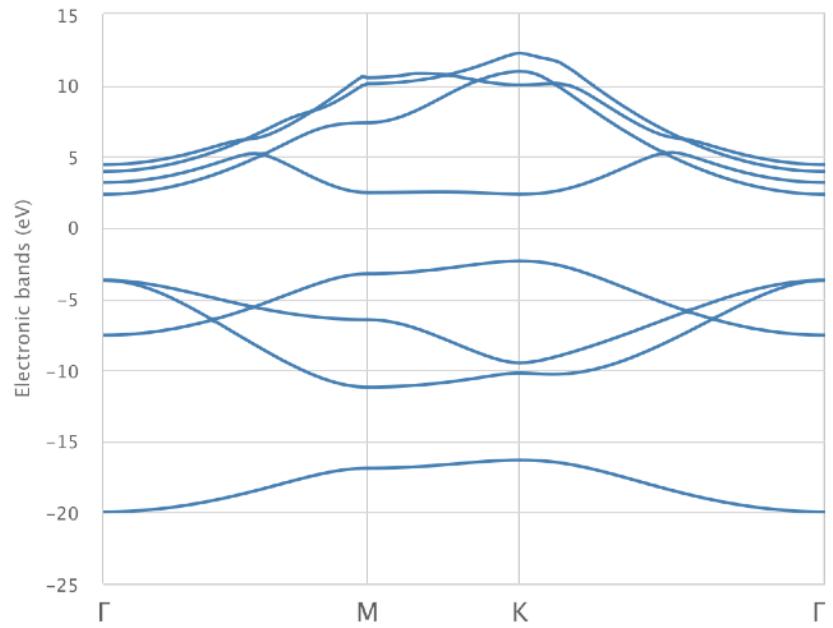
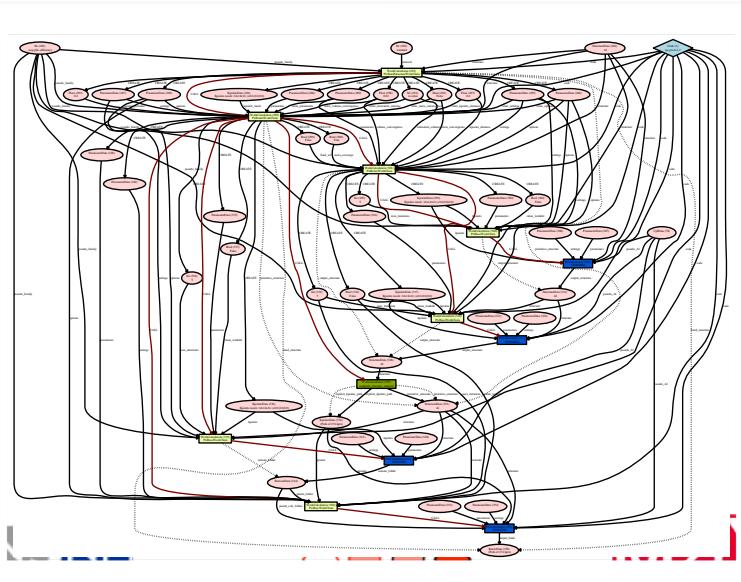
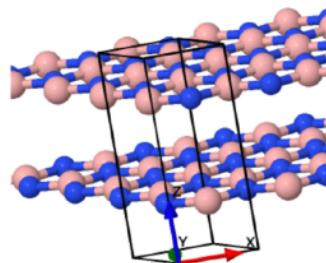
G. Pizzi *et al.*, Comp. Mat. Sci. 111, 218-230 (2016)
S.P. Huber *et al.*, Scientific Data 7, 300 (2020)

AiiDA architecture

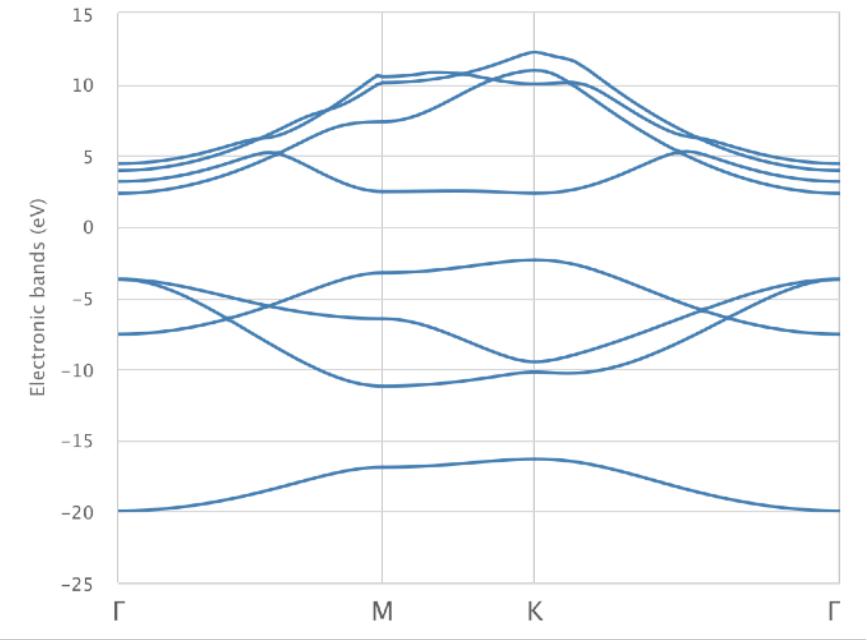
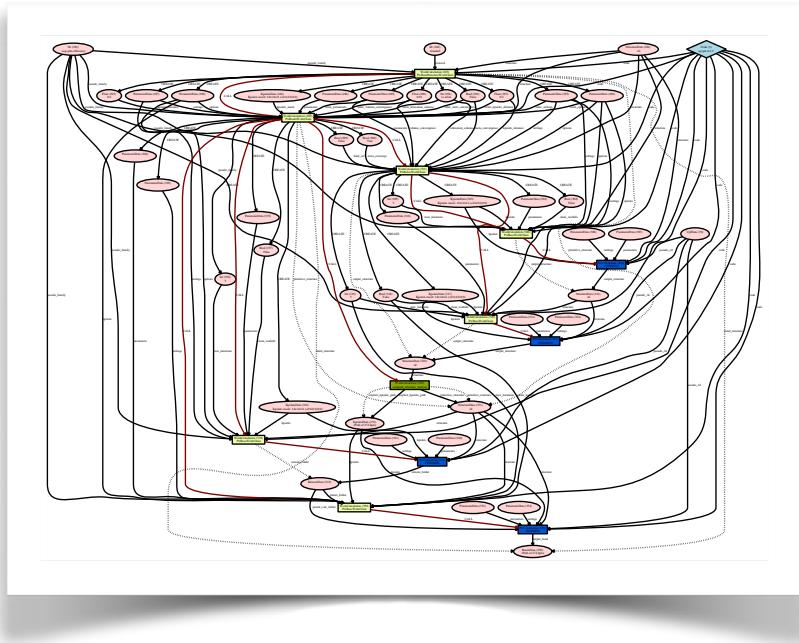


Turn-key workflows in AiiDA

- 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**

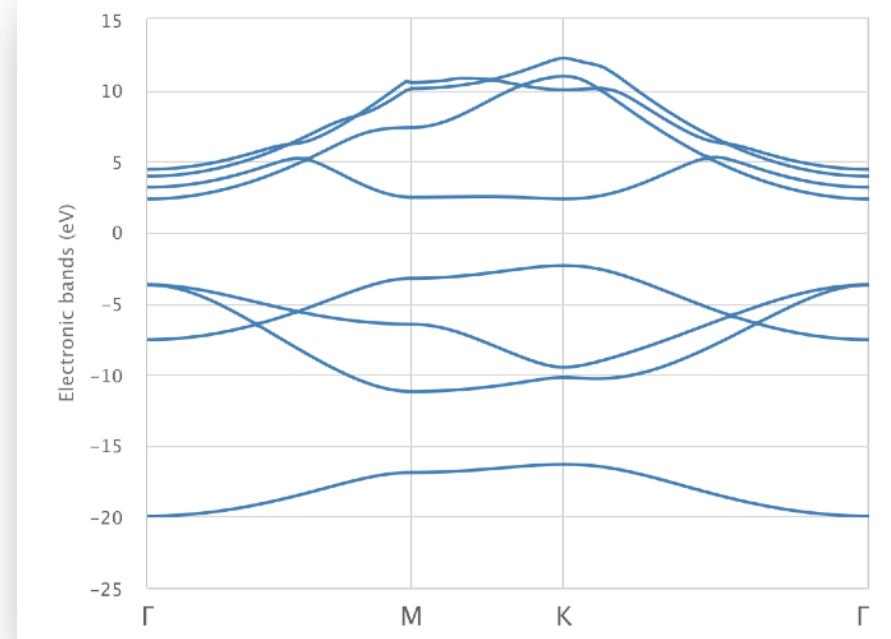
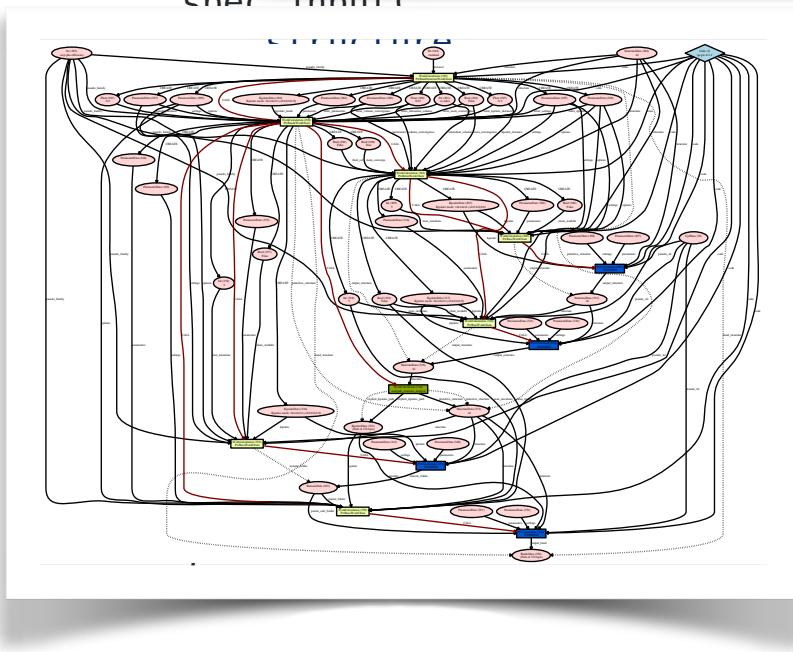
Turn-key workflows in AiiDA

- Turn-key solution:

```
class BandStructureWorkChain(AiiDAWorkChain):
    @classdef
    def __init__(self, spec):
        super().__init__(spec=spec)

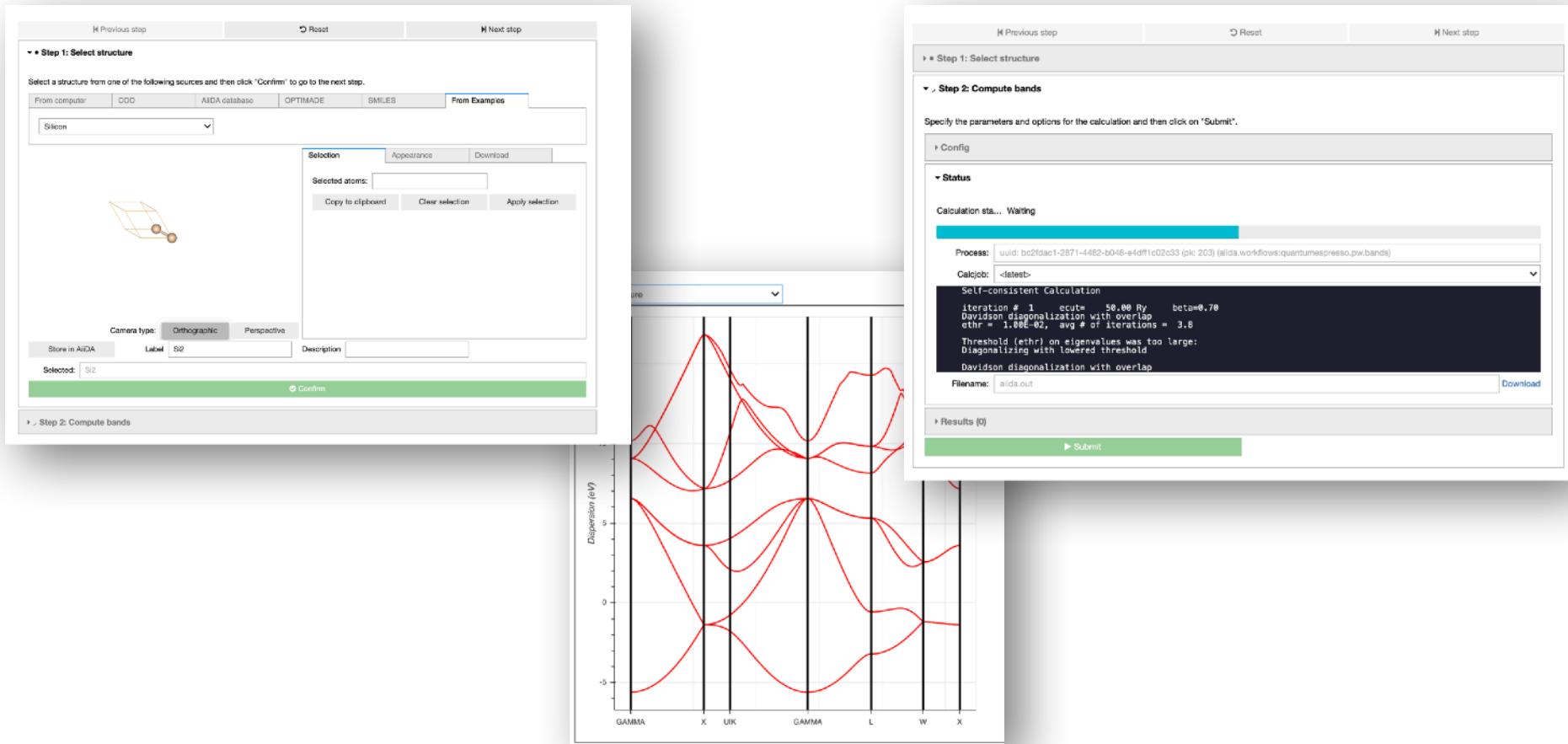
    def run(self):
        code = self.inputs.code
        structure = self.inputs.structure
        # ...
```

ledge on
fixing, ...



Easy access to these simulations on the cloud

- Easy access to these advanced HPC capabilities to everybody: AiiDA lab



Sharing in AiiDA: codes, plugins and workflows



Calculation

Data

Parsers

Transport
and
scheduler

Workflows

Importers &
exporters

The screenshot shows the AiiDA Plugin Registry homepage. It features the AiiDA logo and the text "PLUGIN REGISTRY". Below this, there is a button "[View on GitHub/register your package]".

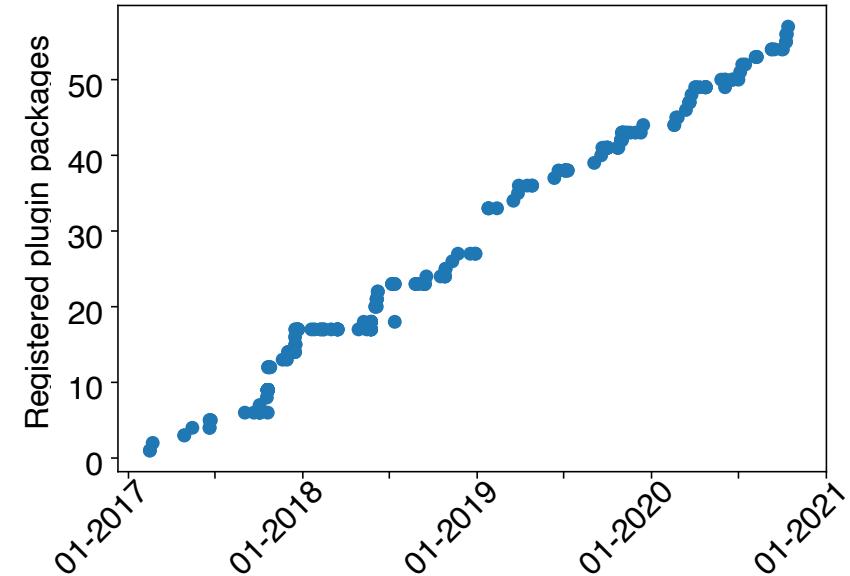
Registered plugin packages: 58

Calculations	98 plugins in 39 packages
Parsers	84 plugins in 40 packages
Data	79 plugins in 24 packages
Workflows	95 plugins in 27 packages
Console scripts	19 plugins in 14 packages
Other	95 plugins in 26 packages

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



swissuniversities



Code interoperability: common workflow interfaces

- **Ultimate goal:** robust, cross-validated and accessible

Simulations with unified interfaces

Common workflows for computing materials properties using different quantum engines

Sebastiaan P. Huber,^{1,*} Emanuele Bosoni,² Marnik Bercx,¹ Jens Bröder,^{3,4} Augustin Degomme,⁵ Vladimir Dikan,² Kristjan Eimre,⁶ Espen Flage-Larsen,⁷ Alberto Garcia,² Luigi Genovese,⁵ Dominik Gresch,⁸ Conrad Johnston,⁹ Guido Petretto,¹⁰ Samuel Poncé,¹ Gian-Marco Rignanese,¹⁰ Christopher J. Sewell,¹ Vasily Tseplyaev,^{3,4} Martin Uhrin,¹ Aliaksandr V. Yakutovich,^{11,1} Austin Zadoks,¹ Pezhman Zarabadi-Poor,^{12,13} Bonan Zhu,^{14,13} Nicola Marzari,¹ and Giovanni Pizzi^{1,†}

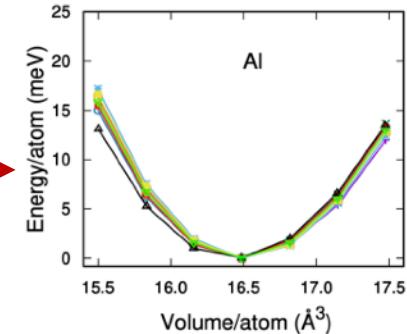
Ready to be submitted

<https://github.com/aiidateam/aiida-common-workflows/>

\$ aiida-common-workflows launch eos **siesta** --structure=Al --protocol=precise

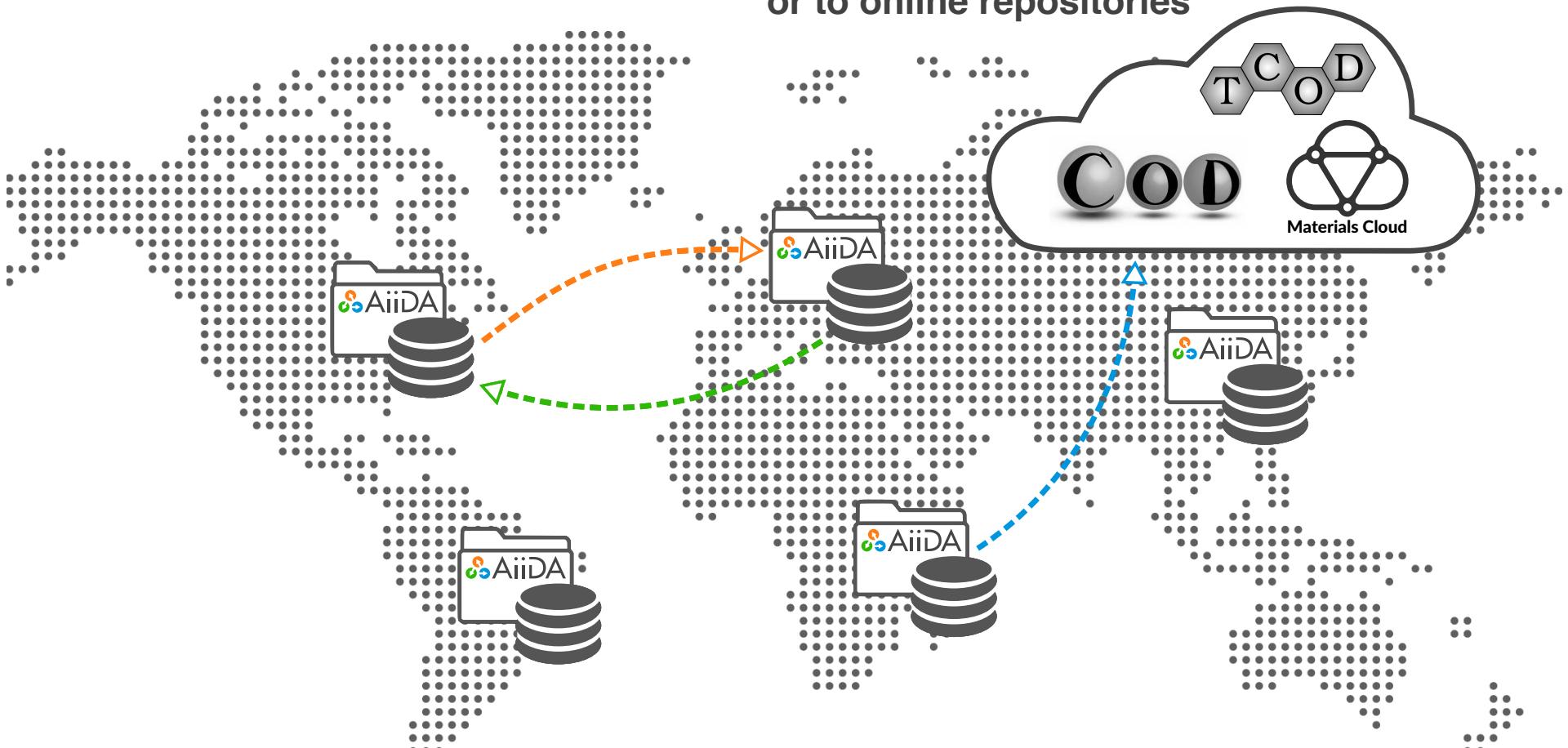
Implementations
for 11 quantum
codes

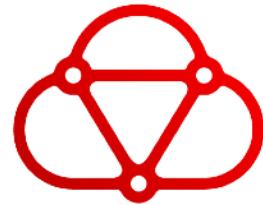
EOS only for the
9 with PBC;
relax and
dissociation
for all 11



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





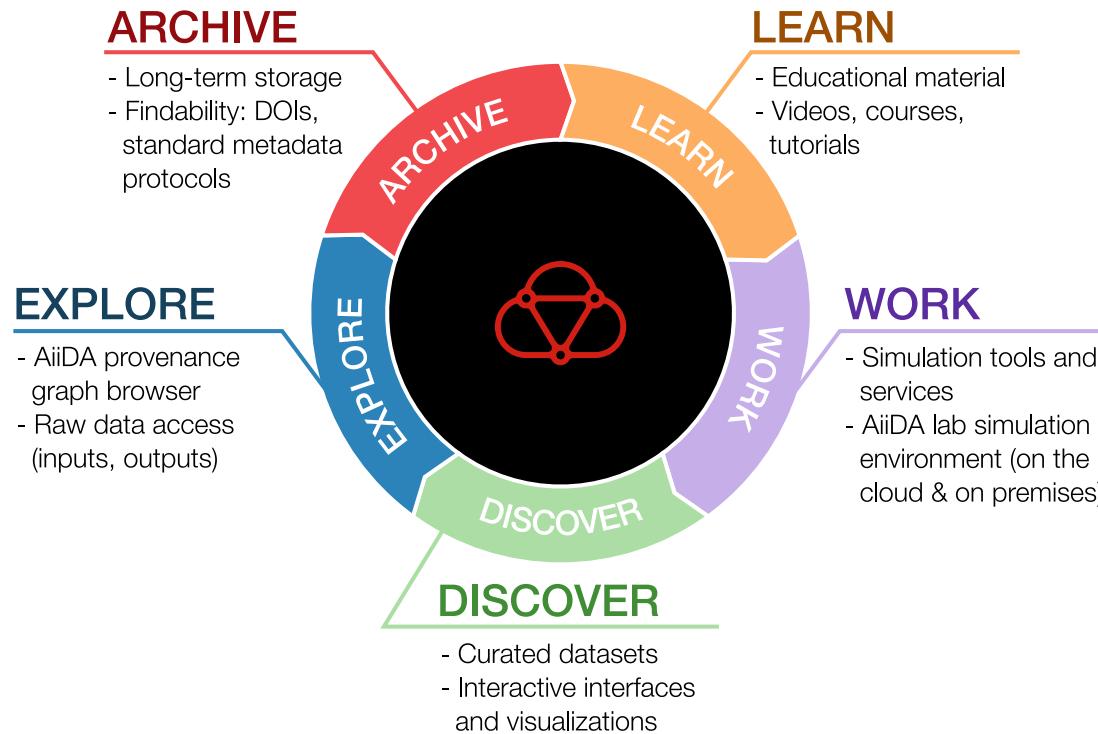
MATERIALS CLOUD

<https://www.materialscloud.org>

L. Talirz et al., Scientific Data 7, 299 (2020)

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*



Materials Cloud Learn: Educational platform

Learn with videos and slides

Add new video

Lecture recordings and tutorial videos on computational materials science topics for students and experts alike.

You can find more videos on the [Materials Cloud Youtube channel](#).

MARVEL
NATIONAL CENTRE OF COOPERATION IN RESEARCH

MARVEL events
Video recordings of MARVEL events (Classics in molecular simulation)

AiiDA
AiiDA and Materials Cloud tutorials
Video recordings and educational material

Quantum ESPRESSO school
Video recordings and educational material

WANNIER90
Wannier90 schools
Video recordings and educational material

Quantum Simulations of Sustainable Energy Materials
Prof. Emily Carter

Prof. Emily A. Carter
Quantum Simulations of Sustainable Energy Materials
MARVEL NCCR

00:20:38 01:04:02

Viscosity and Surface Tension of Liquid Li

Viscosity (mPa) vs Temperature (K)

Surface tension (mN/m)	453 K (melting point)	470 K	520 K	570 K
OFDFT-MD	364	345	339	
Experiment	398 [1]	trend: decreasing		

[1] Phys. Rev. **128**, 6 (1962)

Mohan Chen, Joseph R. Vella, Frank H. Stillinger, Emily A. Carter, Athanassios Z. Panagiotopoulos, Pablo G. Debenedetti, AIChE Journal, **6**, 2841 (2015).

Viscosity and Surface tension of Liquid Li

Liquid Li Theory versus Experiment

Liquid Li with OFDFTMD

Liquid Li with OFDFTMD

Liquid Li with OFDFTMD

Liquid Li with OFDFTMD

Data generation: Materials Cloud Work

The screenshot shows the Materials Cloud interface with a red header bar containing 'LEARN', 'WORK' (highlighted in red), 'DISCOVER', 'EXPLORE', and 'ARCHIVE'. Below the header are four service cards:

- Tools**: Computational tools to work with your data online. It features a bar chart icon.
- Quantum Mobile**: Quantum simulation codes + AiiDA in a virtual machine. It features a blue square icon with three gears.
- AiiDA lab**: Run your own simulations using AiiDA on the cloud. It features a green, orange, and blue gear icon.
- AiiDA registry**: The official registry of AiiDA plugins. It features a green, orange, and blue circular arrow icon.

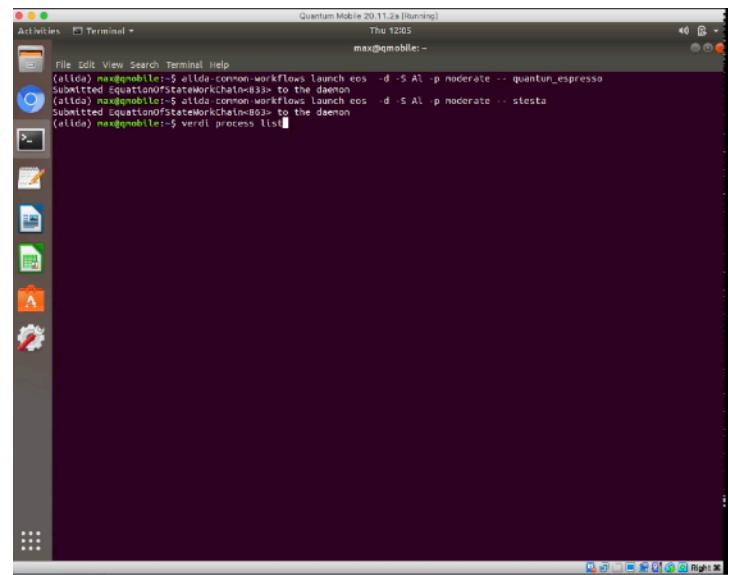
Quantum Mobile

- **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** (courses, tutorials, ...)

"Quantum Mobile" virtual machine (VM)



Testimonials



Compared to [courses of] previous years, the overhead due to technical problems and misunderstandings has been greatly reduced. Quantum Mobile is **absolutely the right tool to have**.

Stefaan Cottenier, compmatphys.org

Quantum Mobile is really a fantastic tool! I do think that it really gives a **gigantic help for the organisation of Schools** focusing on simulation codes.

Andrea Marini, founder of the Yambo code

Data generation: Materials Cloud Work

The screenshot shows a navigation bar with links: LEARN, WORK (highlighted in red), DISCOVER, EXPLORE, ARCHIVE, and More. Below the navigation bar are four service cards:

- Tools**: Computational tools to work with your data online.
- Quantum Mobile**: Quantum simulation codes + AiiDA in a virtual machine.
- AiiDA lab**: Run your own simulations using AiiDA on the cloud. This card is highlighted with a red border.
- 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 ESPRESSO app: making simulations accessible

The screenshot shows a Jupyter Notebook interface running on a web browser. The title bar indicates it's a Jupyter Notebook at ab63397873ac.eu.ngrok.io/apps/apps/home/start.ipynb. The main content area displays the AiiDA lab interface with several sections:

- File Manager**: Shows a file icon.
- Terminal**: Shows a terminal icon.
- Tasks**: Shows a tasks icon.
- App Store**: Shows an app store icon.
- Help**: Shows a help icon.

(title) metadata.json file is not present: This section contains the Quantum ESPRESSO logo and a message indicating no metadata file is present. It includes a "Manage App" button and a "Modified" status indicator with up and down arrows.

OPTIMADE Client: This section contains the OPTIMADE logo and text describing it as "Open Databases Integration for Materials Design". It includes a "Manage App" button, a "URL" button, and an "Update available" status indicator with up and down arrows.

AiiDAlab Base Widgets: This section is currently empty.

Open data sharing: Archive, Discover, Explore

The screenshot shows the MaterialsCloud website interface. At the top, there are navigation links: LEARN, WORK, DISCOVER, EXPLORE, and ARCHIVE. Below this is a search bar and a user profile dropdown for marco.borelli@epfl.ch. A blue arrow points from the text "Recommended data repository by Nature's journal Scientific Data" to the FAIRsharing.org logo in the header. The main content area displays three research records:

- Semi-local and hybrid functional DFT data for thermalised snapshots of polymorphs of benzene, succinic acid, and glycine**
DOI: 10.24435/materialscloud.v2-x-7x
Edgar A. Engel, Venkat Kapil
Structure prediction for molecular crystals is a longstanding challenge, as often minuscule free energy differences between polymorphs are sensitively affected by the description of electronic structure, the statistical mechanics of the nuclei and the cell, and thermal expansion. The importance of these effects has been individually established, but rigorous free energy calculations, which simultaneously account for all terms, have not been computationally viable. Here we reproduce the experimental stabilities of polymorphs of prototypical compounds – benzene, glycine, and succinic acid – by computing rigorous first-principles Gibbs free energies, at a fraction of the cost of conventional methods ...
Latest version: v1
Publication date: Mar 26, 2021
- Simulating solvation and acidity in complex mixtures with first-principles accuracy: the case of CH₃SO₃H and H₂O₂ in phenol**
DOI: 10.24435/materialscloud.v2-x-7x
Kevin Rossi, Veronika Juraskova, Raphael Wissert, Laurent Garot, Clemence Cominbeauf, Michele Coriolet
Set of inputs to perform the calculations reported in the paper. The -pi input enables to perform molecular dynamics / metadynamics / REMD / PIMD simulations, with adequate thermostats. The DFTB and LAMMPS input respectively enable to calculate force and energies within the DFTB and Neural Network Forcefield frameworks. The CP2K input files enable to calculate force and energies at PBE and PBEC level. The latter is used as the reference to train the neural network correction on top of DFTB. Brief description of the work: We present a generally-applicable computational framework for the efficient and accurate characterization of molecular structural patterns and acid properties in explicit solvent using H₂O₂ and CH₃SO₃H in phenol as an example ...
Latest version: v2
Publication date: Mar 26, 2021
- Detecting electron-phonon coupling during photoinduced phase transition**
DOI: 10.24435/materialscloud.v2-1
Takeshi Suzuki, Yasushi Shirohara, Yangfan Lu, Mari Watanabe, Jiali Xu, Kenichi L. Ishikawa, Hidetaka Takegi, Minoru Nohara, Naoyuki Katsuyama, Hiroshi Sawa, Masami Fujisawa, Teruo Kanai, Jiro Itaya, Takashi Mizokawa, Shik Shin, Kozo Okazaki

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

Indexed by **Google Dataset Search**
and by EUDAT/EOSC's **B2FIND**

Registered on **[FAIRsharing.org](#)**
and **[re3data.org](#)**

New! Recommended by the new
"Open Research Europe" journal



Research and Innovation

Open Research Europe

[https://open-research-europe.ec.europa.eu/
for-authors/data-guidelines](https://open-research-europe.ec.europa.eu/for-authors/data-guidelines)

Open data sharing: Archive, Discover, Explore

Submission form

The screenshot shows the 'Materials Cloud Archive record upload' section of the submission form. It includes fields for 'Title*', 'Description*', 'Keywords*', 'References*', and 'Affiliation'. A sidebar lists MARVEL partners: MaxPlanc, Marie Curie Fellowships, MARVEL, MARVEL001, MARVEL002, MARVEL003, MARVEL004, MARVEL005, MARVEL006, MARVEL Inst, MARVEL007, MARVEL008, MARVEL009, and MARVEL-NPC. At the bottom, there's a note about EPFL's affiliation.

User view (own entries)

The screenshot shows the 'My records' page with sections for 'Records in progress' and 'Records published (latest 10 published records)'. It displays two entries:

Record	Owner	Status
Towards constant potential modeling of CO-CO coupling at liquid water-Cu(100) interfaces DOI: 10.24435/materialscloud:99-07 [version: v1] Last update: 18/03/2021, 23:54:37 Authors: Henrik H. Kristoffersen, Karen Chan We have studied electrochemical "CO-CO coupling in explicit electrolyte with density functional theory, molecular dynamics, and metadynamics. We considered both the "CO-CO coupling reaction and the ...	hhk@chem.ku.dk	PUBLISHED
Simulating the ghost: quantum dynamics of the solvated electron DOI: 10.24435/materialscloud:99-08 jinggang.lan@uzh.ch	jinggang.lan@uzh.ch	PUBLISHED

Ideal solution for data management

Open (and free) for any researcher in computational materials science
(*5GB limit, 50GB when using AiiDA*)

Open data sharing: Archive, Discover, Explore

DOIs assigned

materialscloud:2017.0008/v3

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

Nicolas Mounet¹, Marco Gibertini¹, Philippe Schwaller¹, Davide Campi¹, Andrius Merkys^{1,2}, Antimo Marrazzo¹, Thibault Sohier¹, Ivano E. Castelli¹, Andrea Cepellotti¹, Giovanni Pizzi¹, Nicola Marzari¹

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, Saulėtekio a. 7, LT-10257 Vilnius, Lithuania

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

DOI: [10.24435/materialscloud:2017.0008/v3](https://doi.org/10.24435/materialscloud:2017.0008/v3) [version v3]

Publication date: Apr 03, 2019

How to cite this record

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 **2017.0008/v3** (2019), doi: [10.24435/materialscloud:2017.0008/v3](https://doi.org/10.24435/materialscloud:2017.0008/v3).

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 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, phonons for the subset of the 258 easily exfoliable materials with less than 6 atoms, structures and binding energies for the remaining 1567 materials) together with the provenance of all data and calculations as stored by AiIDA.

Direct links
to Discover &
Explore

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 MD5	113.0 MiB	We provide 258 two-dimensional crystal structures (lattice vectors, atomic species and positions), exfoliated from three-dimensional experimental crystal structures. The structures were relaxed at the DFT-PBE level. Together with each structure, a set of materials properties is also given (at the DFT-PBE level): chemical formula, spacegroup, structural prototype, magnetic state, magnetization, band-gap, electronic bands, and phonon



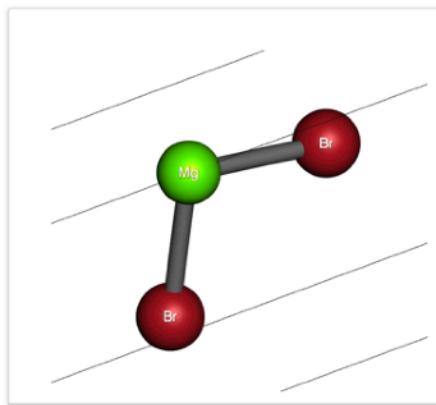
Export
Dublin Core JSON

Data (and metadata)
guaranteed to be
online for at least
10 years after
deposition

Open data sharing: Archive, Discover, Explore

DISCOVER

Compound: MgBr₂



Info and properties

[See definitions...](#)

Formula: MgBr₂

Spacegroup: P-3m1

Pointgroup: -3m

Prototype: CdI2

Band gap [eV]: 4.8 

Magnetic properties:

Magnetic State: non-magnetic

Tot. Magnetization [μ B/cell]: -

Abs. Magnetization [μ B/cell]: -

Binding Energies:

DF2-C09 Binding energy [meV/ \AA^2]: 10.2 

(From parent COD 9009107)

rVV10 Binding energy [meV/ \AA^2]: 15.3 

(From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):

Δ_{DF2} [%]: 17.1 

(From parent COD 9009107)

Δ_{rVV10} [%]: 18.3 

(From parent COD 9009107)

Band structure

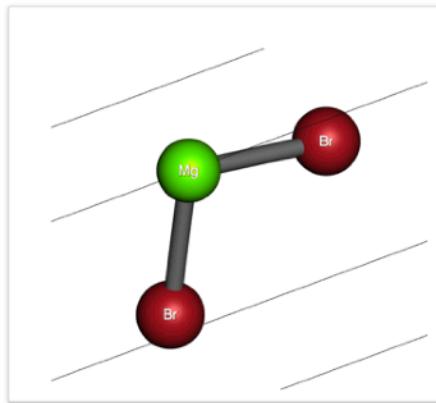
UUID links to jump to the
provenance graph in the
EXPLORE section



Open data sharing: Archive, Discover, Explore

DISCOVER

Compound: MgBr₂



Info and properties

[See definitions...](#)

Formula: MgBr₂

Spacegroup: P-3m1

Pointgroup: -3m

Prototype: CdI2

Band gap [eV]: 4.8 

Magnetic properties:

Magnetic State: non-magnetic

Tot. Magnetization [$\mu\text{B}/\text{cell}$]: -

Abs. Magnetization [$\mu\text{B}/\text{cell}$]: -

Binding Energies:

DF2-C09 Binding energy [meV/ \AA^2]:

(From parent COD 9009107)

rVV10 Binding energy [meV/ \AA^2]: 15

(From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):

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

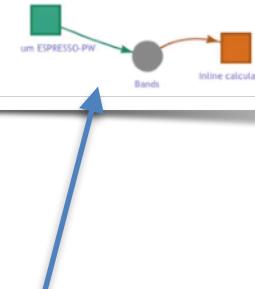
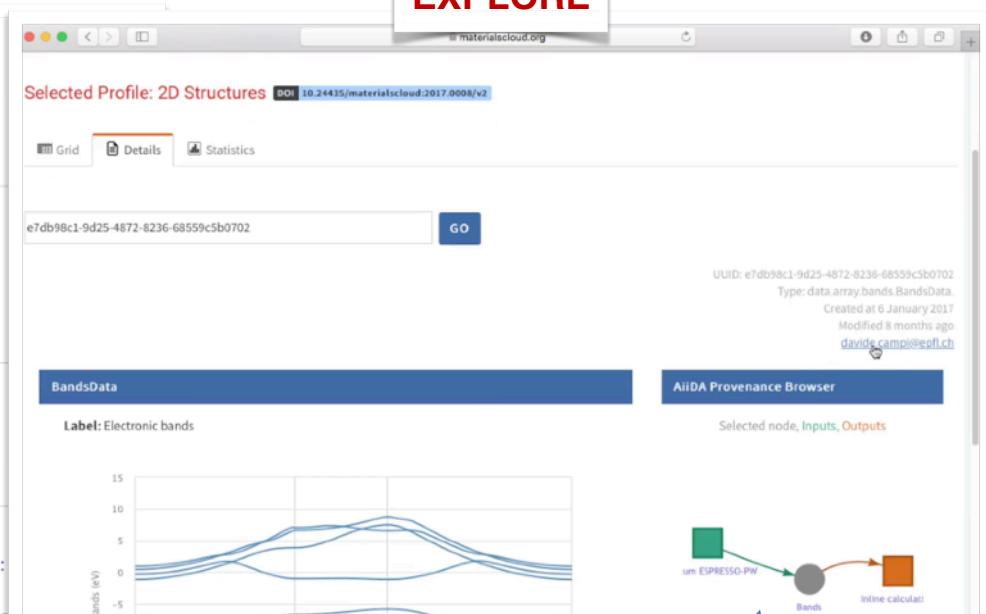
$\Delta_{\text{rVV10}} [\%]$: 18.3  (From parent COD 9009107)

Band structure



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

EXPLORE



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

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
- We provide DMP templates for researchers using Materials Cloud

- Interoperable:** data linked via the AiiDA directed graph; data structures reusable between different codes
- Reusable:** downloadable data, encourage open (CC) licences, reproduce in the AiiDAlab thanks to *full provenance*

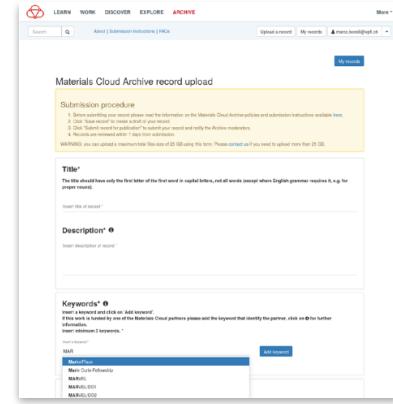
Below, we provide templates for data management plans using the Materials Cloud Archive (with and without AiiDA).

Feel free to contact us with any questions regarding the use of the Materials Cloud Archive as part of your data management plan.

Funding Body	DMP template (using  AiiDA)	DMP template (no AiiDA)
SNF	.docx .odt .pdf	.docx .odt .pdf
H2020	.docx .odt .pdf	.docx .odt .pdf

Conclusion and final take-home messages

- There is a **very simple data management strategy** for data associated with your papers via the **Materials Cloud Archive** (even if you don't use AiiDA) - this is **really easy**
- For AiiDA-driven efforts, workflows for **QE (or NWchem/Gaussian/ ORCA)** are the **next entry with low barriers** (via common workflows)



AiiDA and Materials Cloud teams

The Materials Cloud And AiiDA teams



Carl Simon
Adorf
(EPFL)



Casper W.
Andersen
(EPFL)



Marco
Borelli
(EPFL)



Valeria
Granata
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