

# Materials Cloud

a platform for open computational science

Presenter: Valeria Granata (THEOS @ EPFL)



# Materials Cloud

An **Open Science** web portal for sharing resources for computational materials science - online since Dec 2017

Provides simulation codes and analytics tools

Gives access to workflows, processed and curated datasets

Embraces the FAIR principles of sharing of data and workflows, facilitating reproducibility

[www.materialscloud.org](http://www.materialscloud.org)

WHAT  
is Materials  
Cloud

HOW  
is Materials Cloud  
built

WHO  
is Materials Cloud  
for



# Materials Cloud

Built **on the cloud**

- runs on virtual machines in OpenStack
- data is stored in containers of a Swift Object Store (CSCS)

Developed with **open source software**

Leverages **AiiDA**,

a python framework for automated workflows and provenance tracking. AiiDA manages, automates and stores simulations and their results (next talk by Francisco Ramirez)

WHAT  
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for



# Materials Cloud

## Students

- Learn with videos and tutorials

- Learn with interactive simulation tools

## Experimental scientists

- Run simulations with AiiDA Lab

- Browse materials properties

## Computational scientists

- Upload and share their own data, simulation programs and results

WHAT

is Materials Cloud

HOW

is Materials Cloud  
built

WHO

is Materials  
Cloud  
for



# Materials Cloud



LEARN WORK DISCOVER EXPLORE ARCHIVE

More -



## MATERIALSCLOUD

Built for seamless sharing of resources  
in computational materials science.

**LEARN** Lectures and tutorials in computational materials science

**WORK** Simulation tools and services - in the cloud or on your computer

**DISCOVER** Curated research data with tailored visualizations

**EXPLORE** Interactive browser for AiiDA provenance graphs

**ARCHIVE** An open-access, moderated repository for research data in computational materials science

Please cite L. Talirz et al., *Sci Data* 7, 299 (2020), if you use Materials Cloud in your research.

### Latest news

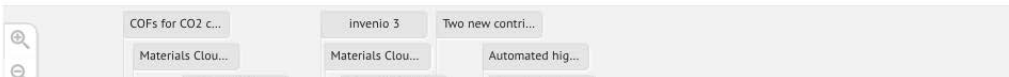
JULY 23, 2020

## 200TH ARCHIVE RECORD

Nine months after that 100 record milestone, the Materials Cloud Archive has doubled in size. Thanks to the invenio 3 moderation workflow, it is now possible to onboard moderators from outside the core development team.



KERNEL PRINCIPAL  
COVARIATES  
REGRESSION



5 Sections  
LEARN  
WORK  
DISCOVER  
EXPLORE  
ARCHIVE



# Materials Cloud - LEARN

LEARN WORK DISCOVER EXPLORE ARCHIVE More ▾

Learn

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** [MARVEL events](#)  
Video recordings of MARVEL events (Distinguished Lectures, Tutorials) and CECAM-MARVEL events (Classics in molecular and materials modeling, Mary Ann Mansigh conversations).

**AiiDA** [AiiDA and Materials Cloud tutorials](#)  
Video recordings and educational material from past AiiDA and Materials Cloud tutorials.

**Quantum ESPRESSO** [Quantum ESPRESSO schools](#)  
Video recordings and educational material from past schools on Quantum ESPRESSO.

## LEARN

Educational materials, video lectures, tutorials, and seminars in computational materials science

Learn new theory, methods and codes



# Materials Cloud - LEARN

Learn with videos and slides

Add new video

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

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MARVEL events

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AiiDA and Materials Cloud tutorials

Video recordings and educational material from past AiiDA and Materials Cloud tutorials.



Quantum ESPRESSO schools

Video recordings and educational material from past schools on Quantum ESPRESSO.



Wannier90 schools

Video recordings and educational material from past schools on Wannier90.



Fireside chats for lockdown times

Video recordings and educational materials on computational materials science.

## LEARN

Educational materials, video lectures, tutorials, and seminars in computational materials science

Learn new theory, methods and codes



# Materials Cloud - WORK

The screenshot shows the Materials Cloud website interface. At the top, there is a navigation bar with the EPFL logo and menu items: LEARN, WORK (highlighted), DISCOVER, EXPLORE, and ARCHIVE. A 'More' dropdown arrow is on the right. Below the navigation bar is a search bar containing the word 'Work'. The main content area is titled 'Work with your data' and includes a subtitle: 'Tools and services for working with your data and generating new data in the cloud or directly on your machine.' Below this are four feature cards:

- Tools**: Computational tools to work with your data online. (Icon: Bar chart)
- Quantum Mobile**: Quantum simulation codes + AiiDA in a virtual machine. (Icon: Laptop with gears)
- AiiDALab**: Run your own simulations using AiiDA on the cloud. (Icon: Three interlocking gears)
- AiiDA registry**: The official registry of AiiDA plugins. (Icon: Three interlocking gears with arrows)

## WORK

Data generation

Tools

Quantum Mobile

AiiDALab

AiiDA registry





# Materials Cloud - WORK

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- Tools**: Computational tools to work with your data online. The icon shows a bar chart with three bars of increasing height and a blue arrow pointing upwards and to the right.
- Quantum Mobile**: Quantum simulation codes + AiiDA in a virtual machine. The icon shows a blue tablet with three white gears on the screen.
- AiiDALab**: Run your own simulations using AiiDA on the cloud. The icon shows three interlocking gears in orange, green, and blue.
- AiiDA registry**: The official registry of AiiDA plugins. The icon shows three interlocking gears in orange, green, and blue, with arrows pointing outwards from each gear.

## Tools

Simple web-based applications that provide interactive visualization and data processing







# Materials Cloud - WORK

LEARN WORK DISCOVER EXPLORE ARCHIVE

Work Tools

Tools [Add new tool](#)

Computational tools offered as a service: no download, no installation, but click-and-run.

-  **Quantum ESPRESSO input generator and structure visualizer**  
**Authors:** Elsa Passaro, Sebastiaan P. Huber, Giovanni Pizzi & Nicola Marzari  
**Description:** A tool to generate the input file of the Quantum ESPRESSO PWscf code and to visualize the corresponding structure.
-  **SeeK-path: the k-path finder and visualizer**  
**Authors:** Yoyo Hinuma, Giovanni Pizzi, Yu Kumagai, Fumiyasu Oba & Isao Tanaka  
**Description:** A k-path finder that provides band paths compatible with space group symmetry, and an interactive 3D visualizer.
-  **ShiftML: chemical shifts in molecular crystals by machine learning**  
**Authors:** Andrea Anelli, Félix Musil, Federico M. Paruzzo, Albert Hofstetter, Sandip De, Edgar Engel, Lyndon Emsley & Michele Ceriotti  
**Description:** A machine learning model to predict the isotropic chemical shielding of molecular crystals containing H, C, N, O and S, including the uncertainty of the prediction, and an interactive 3D visualiser.
-  **AlphaML: machine learning of molecular polarizabilities**  
**Authors:** David M. Wilkins, Andrea Grisafi, Yang Yang, Ka Un Lao, Robert A. DiStasio Jr. & Michele

## Tools

Simple web-based applications that provide interactive visualization and data processing



# Materials Cloud - WORK

The screenshot shows the Materials Cloud website interface. At the top, there is a navigation bar with the EPFL logo on the left and the following menu items: LEARN, WORK (highlighted with a red underline), DISCOVER, EXPLORE, and ARCHIVE. On the far right of the navigation bar is a 'More' dropdown arrow. Below the navigation bar is a search bar containing the text 'Work'. The main content area features a blue link 'Work with your data' followed by a horizontal line. Below this line is a paragraph: 'Tools and services for working with your data and generating new data in the cloud or directly on your machine.' There are four service cards arranged horizontally. The first card is titled 'Tools' and describes 'Computational tools to work with your data online'. The second card, 'Quantum Mobile', is highlighted with a red border and describes 'Quantum simulation codes + AiiDA in a virtual machine'. The third card is titled 'AiiDALab' and describes 'Run your own simulations using AiiDA on the cloud'. The fourth card is titled 'AiiDA registry' and describes 'The official registry of AiiDA plugins'.

**Quantum Mobile**  
A downloadable virtual machine, pre-installed with AiiDA and codes

Run simulations on the cloud or on your own computer



# Materials Cloud - WORK

The screenshot shows the Materials Cloud website interface. At the top, there is a navigation bar with the EPFL logo and menu items: LEARN, WORK (highlighted), DISCOVER, EXPLORE, and ARCHIVE. A 'More' dropdown is also present. Below the navigation bar, there is a search bar containing the word 'Work'. The main content area is titled 'Work with your data' and includes a subtitle: 'Tools and services for working with your data and generating new data in the cloud or directly on your machine.' There are four cards displayed in a row:

- Tools**: Computational tools to work with your data online. (Icon: Bar chart)
- Quantum Mobile**: Quantum simulation codes + AiiDA in a virtual machine. (Icon: Laptop with gears)
- AiiDALab**: Run your own simulations using AiiDA on the cloud. (Icon: Three interlocking gears with arrows, highlighted with a red border)
- AiiDA registry**: The official registry of AiiDA plugins. (Icon: Three interlocking gears with arrows)

AiiDALab

a pre-configured  
AiiDA setup

Jupyter notebooks  
to look like web  
apps



# Materials Cloud - WORK

calhost:8100/apps/apps/home/start.ipynb

jupyter

Edit App Logout

File Manager Terminal Tasks App Store Help

▼ Quantum ESPRESSO

Latest Version

Quantum ESPRESSO

Manage App URL

▼ AiiDA lab Widgets

Latest Version

**Basic data objects.**

- Dealing with one structure
- AiiDA datatypes viewers

**Codes and computers.**

- Setup computer
- Setup code
- Dealing with codes and computers

**Processes.**

- Process list
- Follow a process

Manage App URL

AiiDA lab

a pre-configured  
AiiDA setup

Jupyter notebooks  
to look like web  
apps



# Materials Cloud - WORK

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AiiDA registry

Access to the  
registered AiiDA  
plugins



# Materials Cloud - ARCHIVE

The screenshot shows the Materials Cloud ARCHIVE website. At the top, there is a navigation bar with the following tabs: LEARN, WORK, DISCOVER, EXPLORE, and ARCHIVE (which is highlighted). To the right of the navigation bar is a 'More' dropdown menu. Below the navigation bar is a search bar with a search icon and a 'Q' button. To the right of the search bar are links for 'FAQ and instructions', 'Upload a record', 'My records', and a user profile for 'valeria.granata@epfl.ch' with a dropdown arrow. The main content area features a 'Latest records' section. The first record is titled 'Unraveling the synergy between metal-organic frameworks and co-catalysts in photocatalytic water splitting'. Below the title is a DOI link: [DOI 10.24435/materialscloud:ge-at](https://doi.org/10.24435/materialscloud:ge-at). The authors listed are Stefano Falletta, Patrick Gono, Zhendong Guo, Stavroula Kampouri, Kyriakos C. Stylianou, and Alfredo Pasquarello. The abstract text describes the investigation of the synergy in photocatalytic water splitting between the metal-organic framework MIL-125-NH2 and two co-catalysts, NiO and Ni2P. The latest version is v1, and the publication date is Oct 14, 2020. A banner for 'SCIENTIFIC DATA' is visible, featuring logos for Google Dataset Search, re3data.org, EUDAT, FAIR, and FAIRsharing.org.

## ARCHIVE

A moderated repository for research data from computational materials science

Built within the CERN Invenio framework (v3)



# Materials Cloud - ARCHIVE

materialscloud:2020.86

## Relative abundance of Z2 topological order in exfoliable two-dimensional insulators

Artimo Manzato<sup>1,2</sup>, Marco Gibertini<sup>1,2</sup>, Davide Campi<sup>1</sup>, Nicolas Mounet<sup>1</sup>, Nicola Marzari<sup>1</sup>  
<sup>1</sup> Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Optimization in Materials (MARVEL), Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland  
<sup>2</sup> Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest Ansermet, CH-1205 Geneva, Switzerland  
 Corresponding authors emails: artimo.manzato@epfl.ch

DOI: 10.24435/materialscloud:cm-7p [version v2]  
 Publication date: Jul 31, 2020

### How to cite this record

Artimo Manzato, Marco Gibertini, Davide Campi, Nicolas Mounet, Nicola Marzari, Relative abundance of Z2 topological order in exfoliable two-dimensional insulators, Materials Cloud Archive 2020.86 (2020), doi: 10.24435/materialscloud:cm-7p.

### Description

Quantum spin Hall insulators (QSIs) make up a class of two-dimensional materials with a finite electronic band gap in the bulk and gapless helical edge states. Some of the phenomena that can be hosted in these materials, from one-dimensional low-dissipation electronic transport to spin filtering, could be promising for many technological applications in the fields of electronics, spintronics, and topological quantum computing. Nevertheless, the rarity of two-dimensional materials that can exhibit nontrivial topological order at room temperature hinders development. In this publication, we report on our screening of a comprehensive database we recently identified of 1825 monolayers that can be exfoliated from experimentally known compounds to search for novel quantum spin Hall insulators. In this entry we provide the AiiDA database with the calculations of the DFT band structures (both with and without spin-orbit coupling) and the DFPT phonon dispersions for the QSH candidates that we identify. All the data are also displayed in the dedicated DISCOVER section "2D topological insulators": <https://www.materialscloud.org/discover/2dtopo/discover/tables>.

### Materials Cloud sections using this data

- Discover interface providing interactive scatter plots
- Explore interface providing access to the full database

### Files

File name	Size	Description
README.txt	875 Bytes	README where the content of the AiiDA export files is explained in more detail, including the group names.
band_structures_QSH_withoutSOC_MCarchive.aiiida	38.1 MIB	The AiiDA export file containing the DFT band structures without spin-orbit coupling
band_structures_QSH_withSOC_MCarchive.aiiida	41.2 MIB	The AiiDA export file containing the DFT band structures with spin-orbit coupling
phonons_QSH_MCarchive.aiiida	52.6 MIB	The AiiDA export file containing the DFPT phonon dispersions for the QSH candidates (except jacutingaite)
Phonons_QSH_phonons.dat	48.2 KIB	The file containing the DFPT phonon dispersions for jacutingaite

### License

Files and data are licensed under the terms of the following license: [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/).

### External references

#### Journal reference

A. Manzato, M. Gibertini, D. Campi, N. Mounet, N. Marzari, Relative Abundance of Z2 Topological Order in Exfoliable Two-Dimensional Insulators, Nano Lett. 2019, 19, 12, 8421-8440 doi:10.1021/acs.nanolett.9b02999

### Keywords

[DFT](#) [DFPT](#) [top materials](#) [quantum spin Hall](#) [topological insulator](#) [spin-orbit](#) [MARVEL003](#) [PIMAC](#) [SHP](#)

### Version history:

2020.86 [version v2] [This version] Jul 31, 2020 DOI: 10.24435/materialscloud:cm-7p  
 2019.0081.v1 [version v1] Nov 20, 2019 DOI: 10.24435/materialscloud:2019.0081.v1

DOI: 10.24435/materialscloud:cm-7p [version v2]

Publication date: Jul 31, 2020

## Materials Cloud sections using this data

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File name	Size	Description
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band_structures_QSH_withoutSOC_MCarchive.aiiida <a href="#">MDS</a>	38.1 MIB	The AiiDA export file containing the DFT band structures without spin-orbit coupling
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phonons_QSH_MCarchive.aiiida <a href="#">MDS</a>	52.6 MIB	The AiiDA export file containing the DFPT phonon dispersions for the QSH candidates (except jacutingaite)
Pt4Hg2Se6_phonons.dat <a href="#">MDS</a>	48.2 KIB	The file containing the DFPT phonon dispersions for jacutingaite

ARCHIVE





# Materials Cloud - DISCOVER



LEARN
WORK
DISCOVER
EXPLORE
ARCHIVE

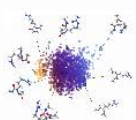
More ▾

Discover

Discover curated data sets

Add DISCOVER section

Curated research data sets with tailored visualizations contributed by authors affiliated with the [Materials Cloud partners](#).




Kernel principal covariates regression

DOI [10.24435/materialscloud:ay-eq](https://doi.org/10.24435/materialscloud:ay-eq)

**Authors:** Benjamin A. Helfrecht, Rose K. Cersonsky, Guillaume Fraux & Michele Ceriotti

**Description:** Illustration of the Kernel Principal Covariates Regression method on various datasets.




Automated high-throughput wannierisation

DOI [10.24435/materialscloud:dd-nz](https://doi.org/10.24435/materialscloud:dd-nz)

**Authors:** Valerio Vitale, Giovanni Pizzi, Antimo Marrazzo, Snehal Kumbhar, Elsa Passaro, Jonathan R. Yates, Nicola Marzari & Arash A. Mostofi

**Description:** Validation results of an automated protocol for generating maximally-localized Wannier functions in a high-throughput framework.



Covalent organic frameworks for carbon capture

DOI [10.24435/materialscloud:2020.0029/v1](https://doi.org/10.24435/materialscloud:2020.0029/v1)

**Authors:** Kathryn S. Deeg, Daiane Damasceno Borges, Daniele Ongari, Nakul Rampal, Leopold

DISCOVER

Curated data

3D visualization of structures

Structure properties, band structure

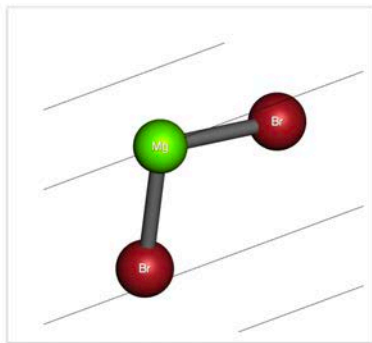
Link to Explore section

■ Swiss Research Data Day 2020 - October 2020



# Materials Cloud - DISCOVER

## Compound: MgBr<sub>2</sub>



### Info and properties

See definitions...

Formula: MgBr<sub>2</sub>  
 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<sup>2</sup>]: 10.2  
 (From parent COD 9009107)  
 rV10 Binding energy [meV/Å<sup>2</sup>]: 15.3  
 (From parent COD 9009107)

### Delta in interlayer distance (vdW vs revPBE):

$\Delta_{DF2}$  [%]: 17.1  
 (From parent COD 9009107)  
 $\Delta_{rV10}$  [%]: 18.3  
 (From parent COD 9009107)

### Band structure



Link to EXPLORE  
Section

UUID of provenance  
graph

DISCOVER

Curated data

3D visualization of  
structures

Structure properties,  
band structure

Link to Explore  
section



# Materials Cloud - EXPLORE

The screenshot shows the Materials Cloud website's 'EXPLORE' section. At the top, there is a navigation bar with 'LEARN', 'WORK', 'DISCOVER', 'EXPLORE' (highlighted), and 'ARCHIVE'. A 'More' dropdown menu is visible on the right. Below the navigation bar, there is a search bar containing the word 'Explore'. The main content area features a blue button labeled 'Add EXPLORE section' and a heading 'Explore the full provenance'. A descriptive paragraph states: 'An interactive browser for exploring AiiDA provenance graphs uploaded to the Materials Cloud Archive.' Below this, there are three featured items:

- Browse your own AiiDA database**: Includes an icon of three arrows forming a circle. **Description:** Use the REST API built into AiiDA to connect to your own AiiDA database. Your data stays inside your browser and is not transmitted to Materials Cloud.
- Automated high-throughput wannierisation**: Includes an icon of a globe with arrows. **DOI:** 10.24435/materialscloud:dd-nz. **Authors:** Valerio Vitale, Giovanni Pizzi, Antimo Marrazzo, Jonathan R. Yates, Nicola Marzari & Arash A. Mostofi. **Description:** Validation results of an automated protocol for generating maximally-localized Wannier functions in a high-throughput framework.
- Covalent organic frameworks for carbon capture**: Includes an icon of a molecular structure. **DOI:** 10.24435/materialscloud:2020.0029/M1

EXPLORE  
Raw data

Access to AiiDA  
databases

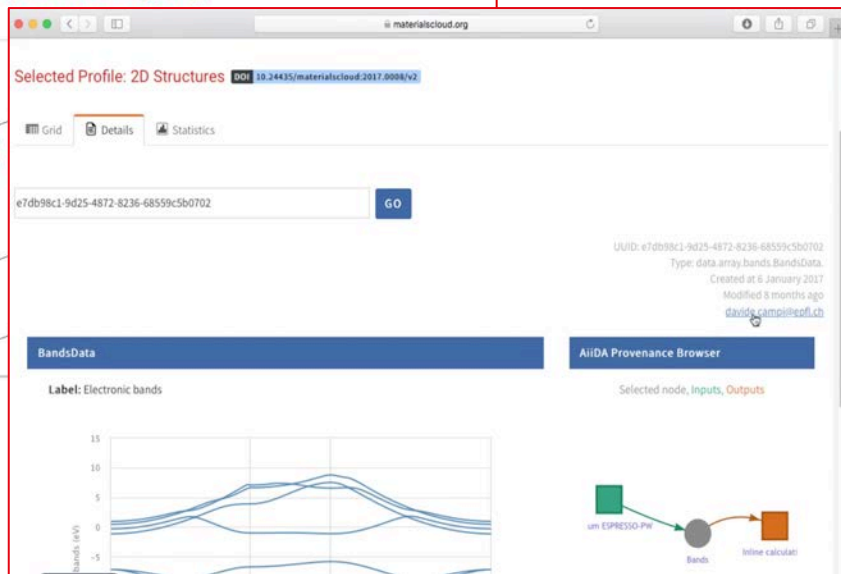
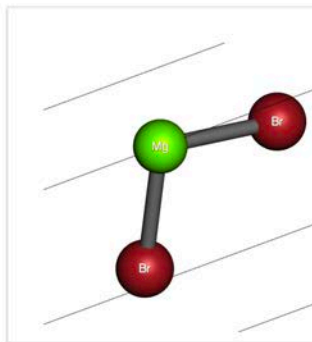
Browse the AiiDA  
provenance graphs

Find input, output  
data and  
calculations to  
generate results

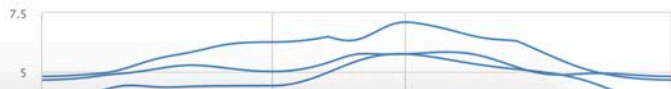


# Materials Cloud - EXPLORE

Compound:  $\text{MgBr}_2$



Band structure



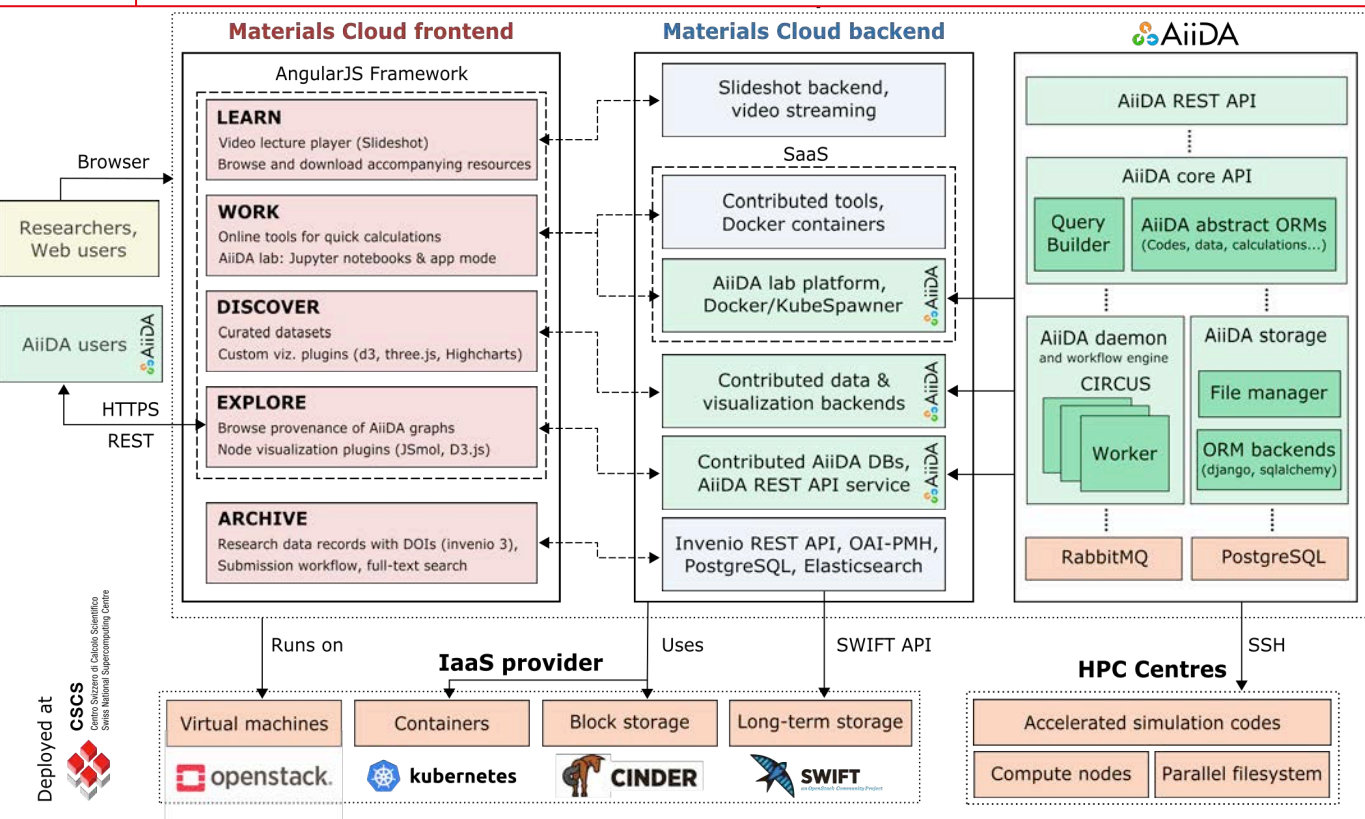
EXPLORE  
Raw data

Access to AiiDA  
databases

Browse the AiiDA  
provenance graphs

Find input, output  
data and  
calculations to  
generate results

# Architecture and technologies



Frontend

Backend

AiiDA

Infrastructure



# Data Management Plans (DMPs) and FAIR principles

Combination of AiiDA + Materials Cloud (Discover, Explore, Archive):  
FAIR-compliant sharing

**Findable:** DOIs with standardized metadata

**Interoperable:** data linked via the AiiDA directed graph; data structures reusable between different codes

**Accessible:** web interface to browse data, calculations and provenance, curated data in Discover section

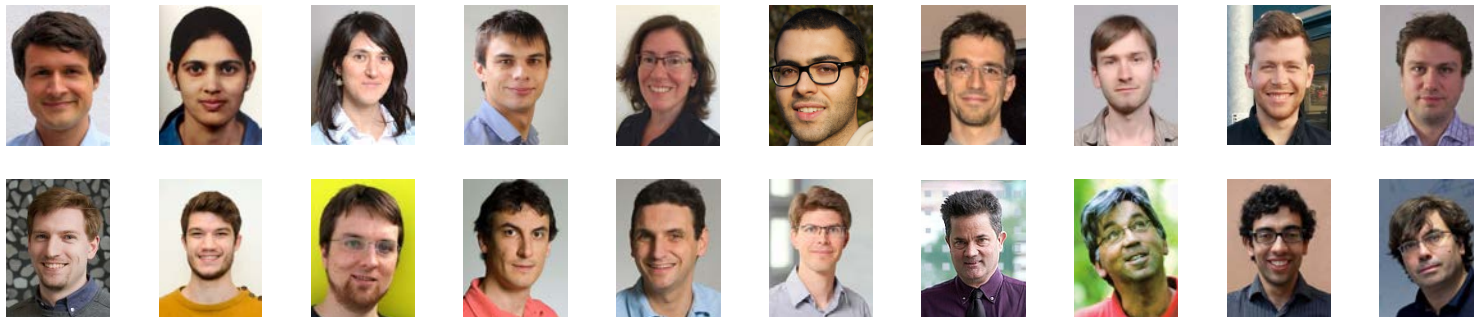
**Reusable:** downloadable data, encourage open (CC) licences, reproduce in the AiiDA Lab thanks to full provenance

We provide **DMP templates** for researchers using Materials Cloud

Funding Body	DMP template (using  AiiDA)	DMP template (no AiiDA)
SNF	<a href="#">.docx</a> <a href="#">.odt</a> <a href="#">.pdf</a>	<a href="#">.docx</a> <a href="#">.odt</a> <a href="#">.pdf</a>
H2020	<a href="#">.docx</a> <a href="#">.odt</a> <a href="#">.pdf</a>	<a href="#">.docx</a> <a href="#">.odt</a> <a href="#">.pdf</a>



# Materials Cloud team and contributors



## Materials Cloud, a platform for open computational science

Leopold Talirz, Snehal Kumbhar, Elsa Passaro, Aliksandr V. Yakutovich, Valeria Granata, Fernando Gargiulo, Marco Borelli, Martin Uhrin, Sebastiaan P. Huber, Spyros Zoupanos, Carl S. Adorf, Casper W. Andersen, Ole Schütt, Carlo A. Pignedoli, Daniele Passerone, Joost VandeVondele, Thomas C. Schulthess, Berend Smit, Giovanni Pizzi, Nicola Marzari

Materials Cloud is a platform designed to enable open and seamless sharing of resources for computational science, driven by applications in materials modelling. It hosts 1) archival and dissemination services for raw and curated data, together with their provenance graph, 2) modelling services and virtual machines, 3) tools for data analytics, and pre-/post-processing, and 4) educational materials. Data is citable and archived persistently, providing a comprehensive embodiment of the FAIR principles that extends to computational workflows. Materials Cloud leverages the AiiDA framework to record the provenance of entire simulation pipelines (calculations performed, codes used, data generated) in the form of graphs that allow to retrace and reproduce any computed result. When an AiiDA database is shared on Materials Cloud, peers can browse the interconnected record of simulations, download individual files or the full database, and start their research from the results of the original authors. The infrastructure is agnostic to the specific simulation codes used and can support diverse applications in computational science that transcend its initial materials domain.

Talirz, L., Kumbhar, S., Passaro, E. *et al.* Materials Cloud, a platform for open computational science. *Sci Data* 7, 299 (2020)

DOI: 10.1038/s41597-020-00637-5

# Acknowledgments



SNSF MARVEL NCCR (I: 2014-18, II: 2018-22, EPFL Lead house) for the Open Science Platform

H2020 MaX Centre of Excellence (I: 2015-18, II: 2018-21) for convergence of HPC, HTC and HPDA via AiiDA

H2020 MarketPlace (2018-22, EPFL co-PI) for providing materials simulation services and data

H2020 Intersect (2019-21, EU; CNR lead PI, EPFL and ICN2 co-PI) for automated modelling of complex devices via AiiDA

Private collaboration with a **major European company** (2019-2020) for AiiDA-powered materials discovery for Li-ion batteries

Swissuniversities P-5 Materials Cloud (2019-20) for transitioning Materials Cloud to self-sustaining service

EPFL Open Science Fund "OSSCAR" (2019-21) for creating an educational hub for research and teaching





# Thank you

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valeria.granata@epfl.ch

[www.materialscloud.org](http://www.materialscloud.org)