Materials Cloud
a platform for open computational science

Presenter: Valeria Granata (THEOS @ EPFL)

MARVEL · MAX DRIVING THE EXASCALE TRANSITION · swissuniversities · FNSNF Swiss National Science Foundation · INTERSECT · MarketPlace · 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

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
is Materials Cloud

HOW
is Materials Cloud
built

WHO
is Materials Cloud
for

Materials Cloud

Students

- Learn with videos and tutorials
- Learn with interactive simulation tools

Experimental scientists

- Run simulations with AiiDAlab
- Browse materials properties

Computational scientists

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

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WHO
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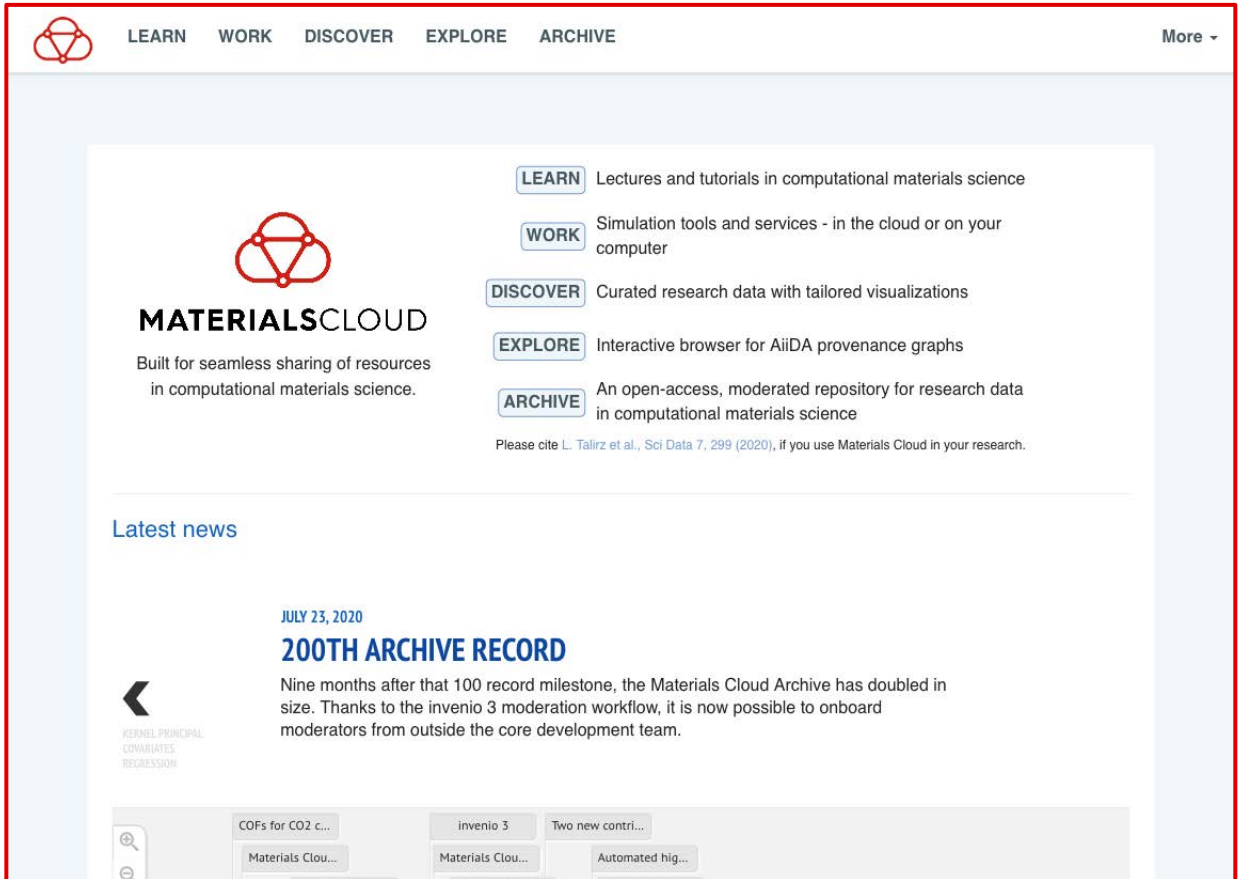
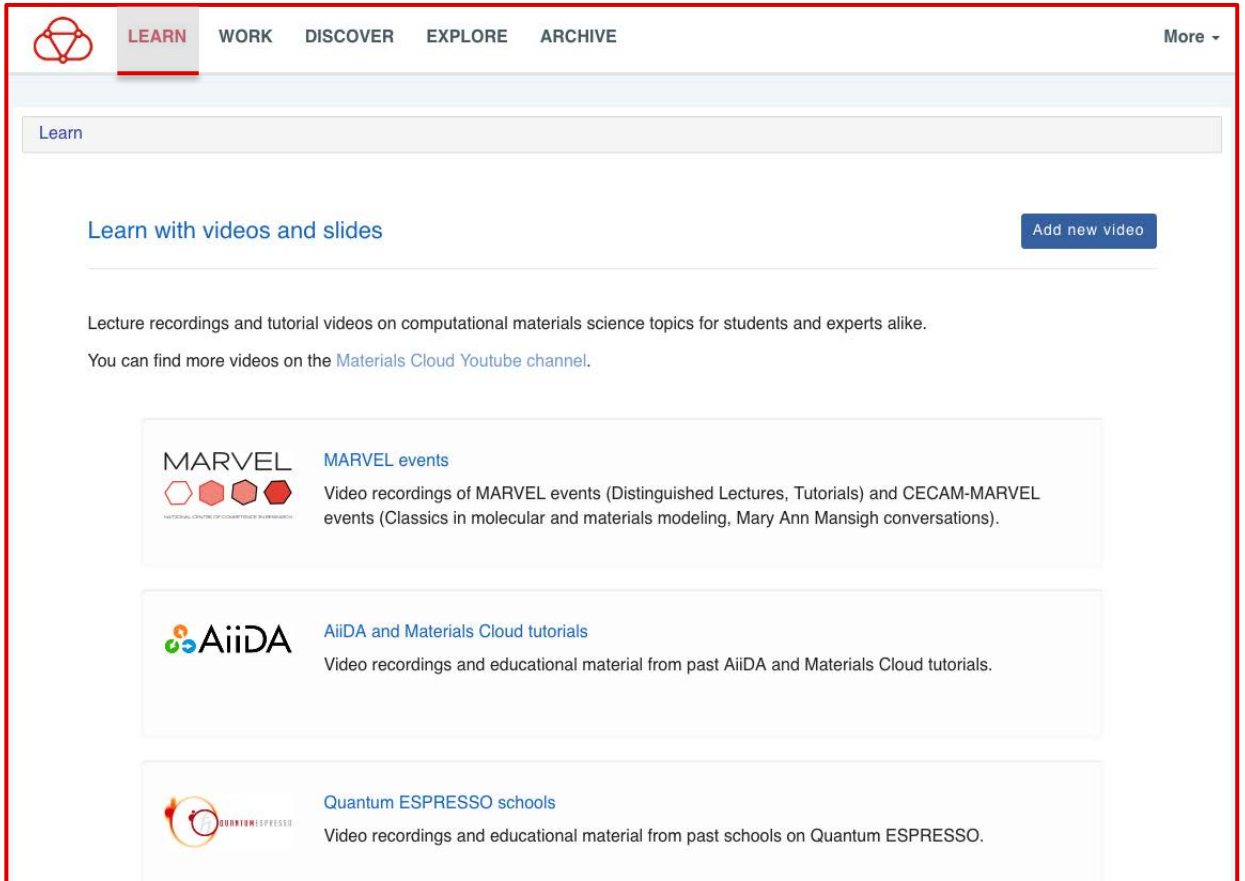
Materials Cloud



5 Sections
LEARN
WORK
DISCOVER
EXPLORE
ARCHIVE

Materials Cloud - LEARN

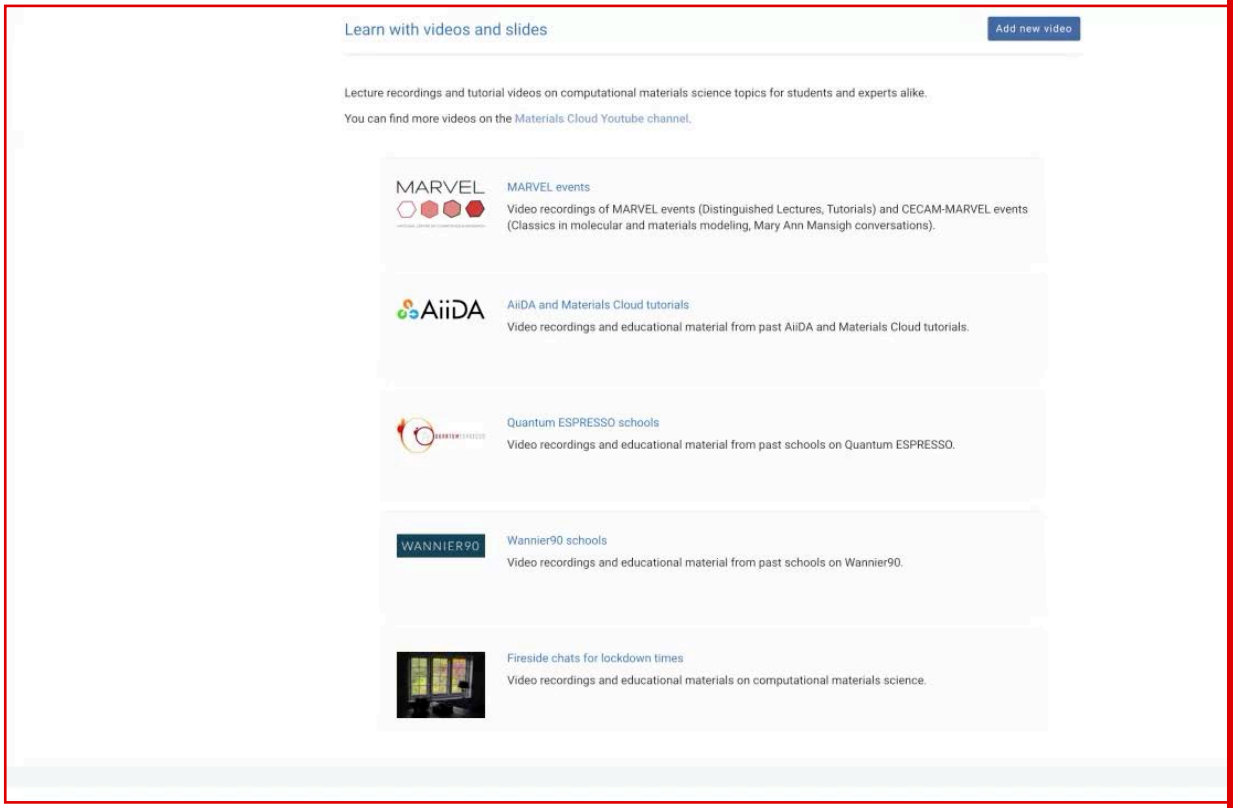


LEARN

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

Learn new theory, methods and codes

Materials Cloud - LEARN



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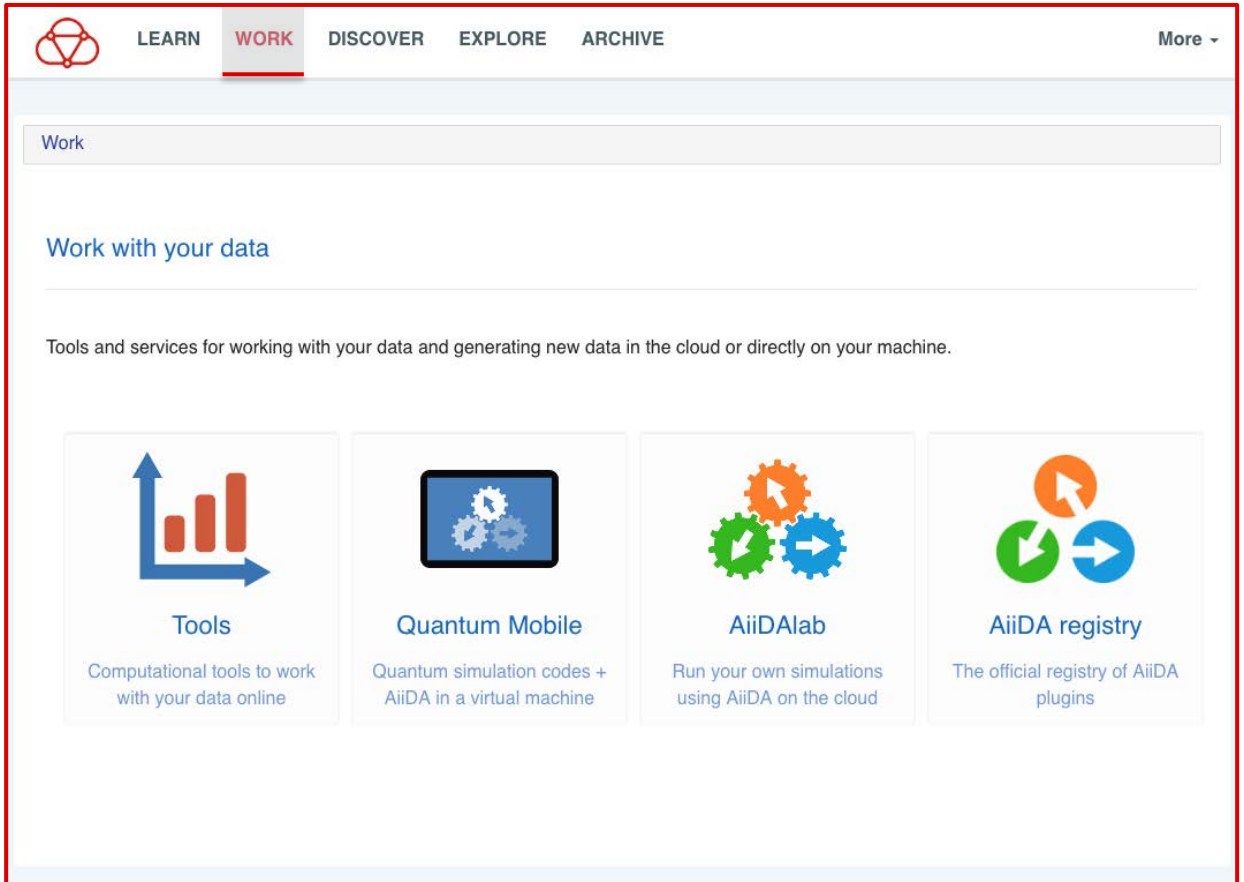


WORK

Data generation

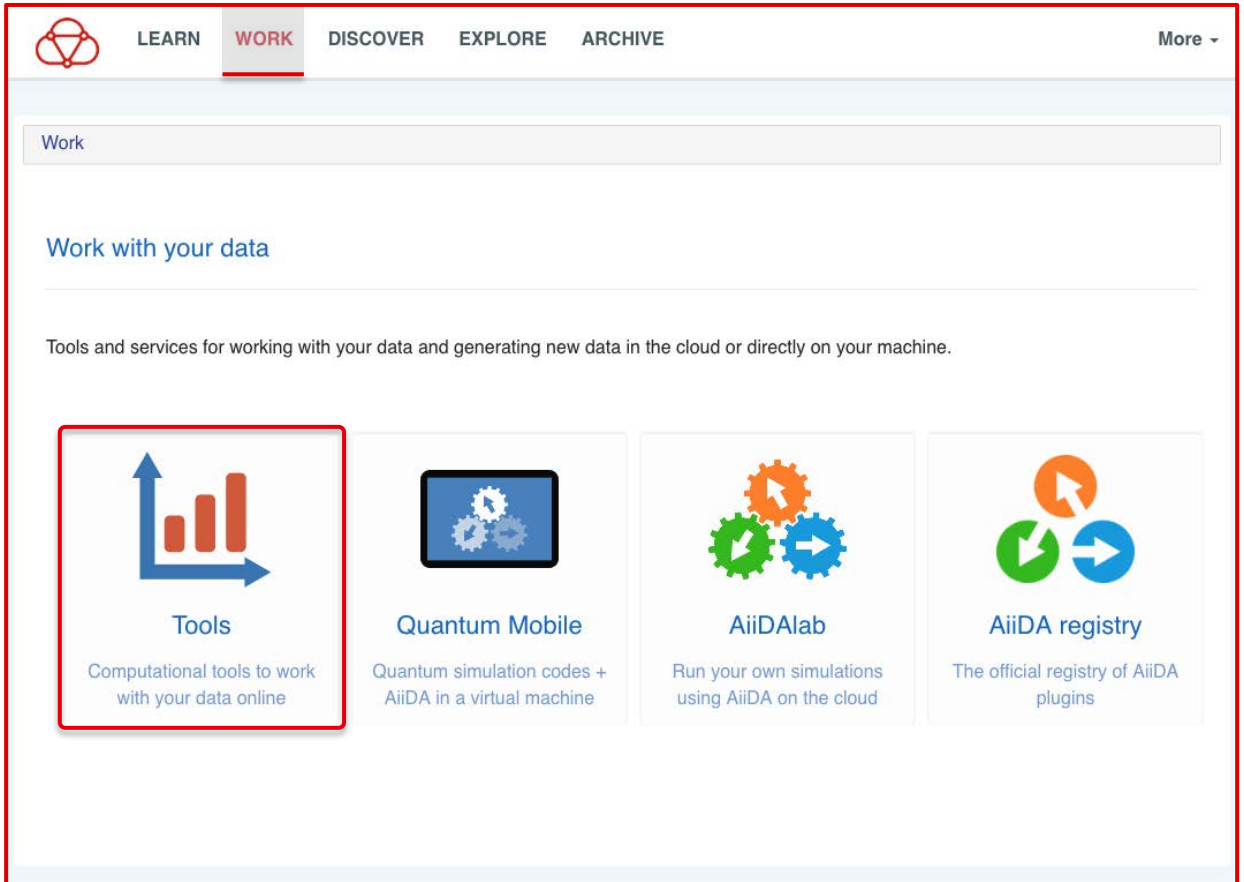
Tools

Quantum Mobile

AiiDAlab

AiiDA registry

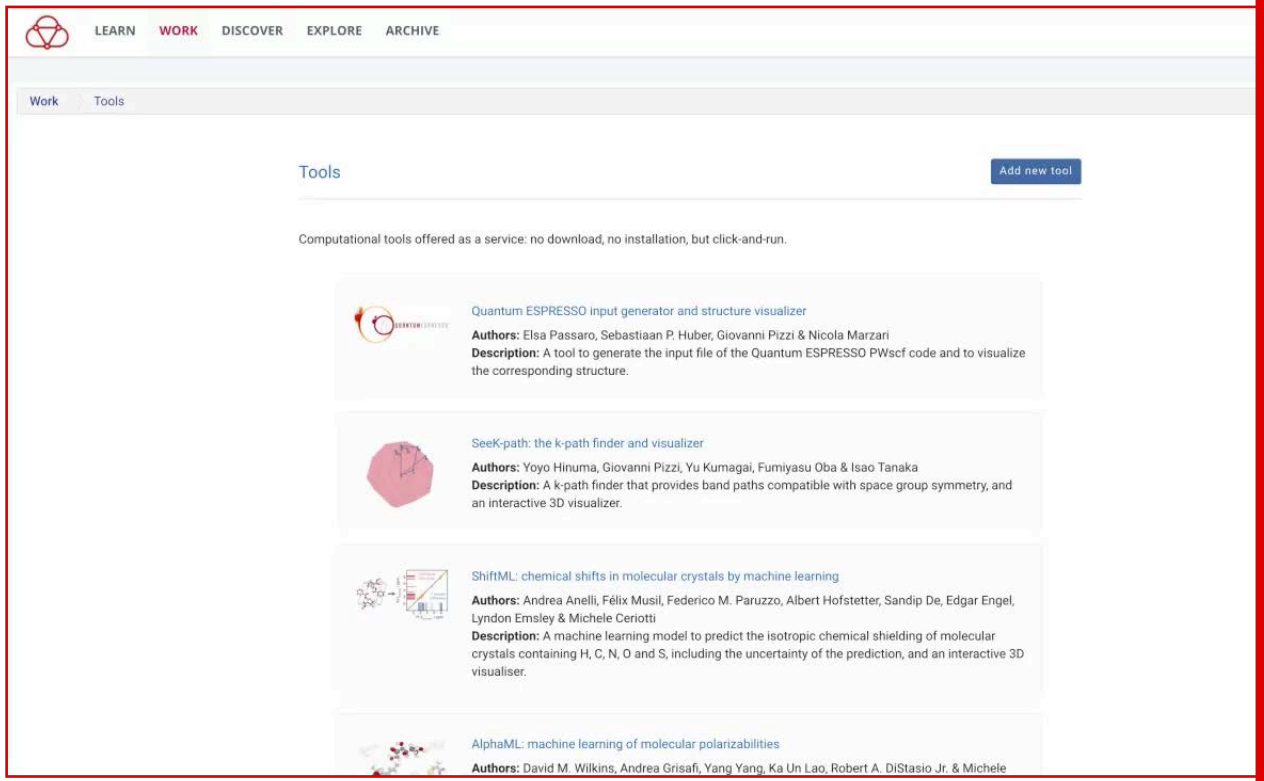
Materials Cloud - WORK



Tools

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

Materials Cloud - WORK



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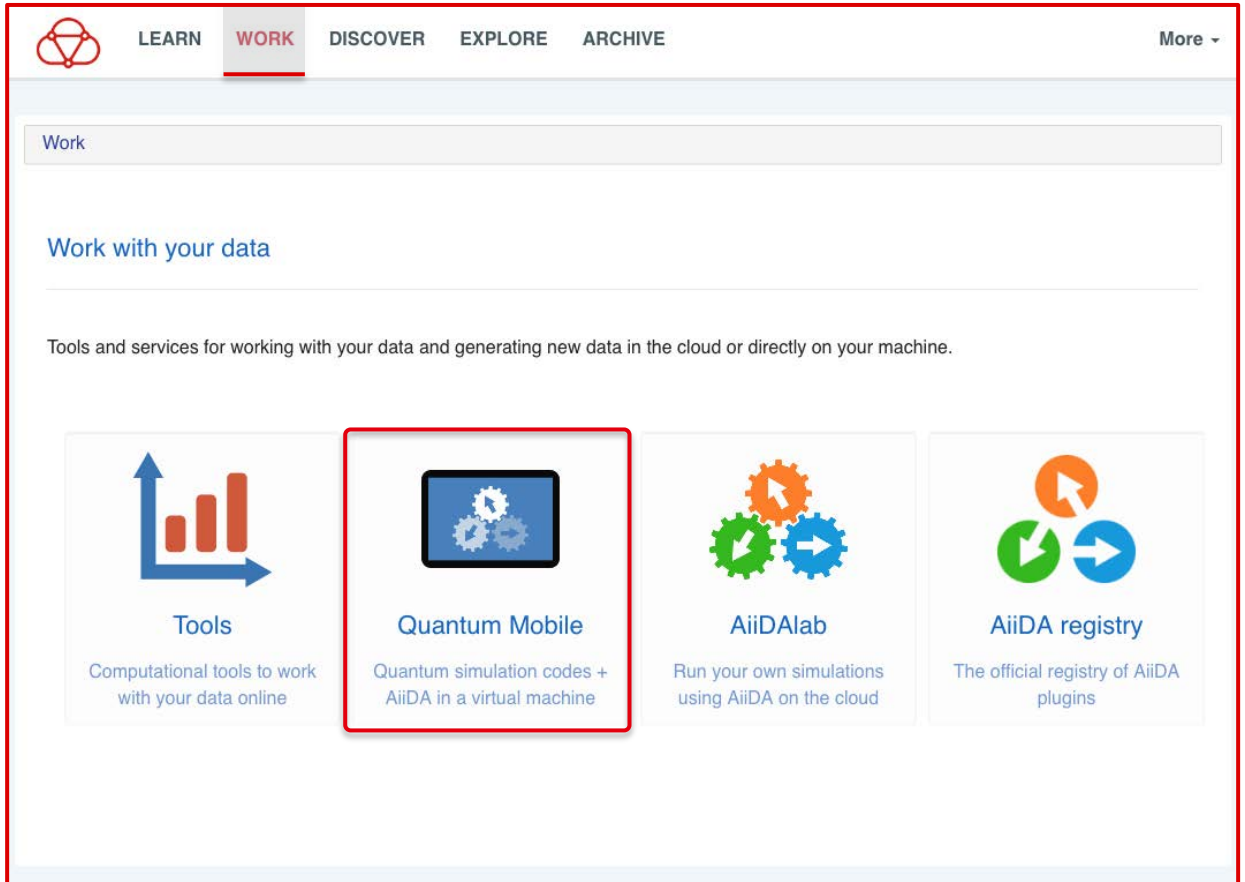
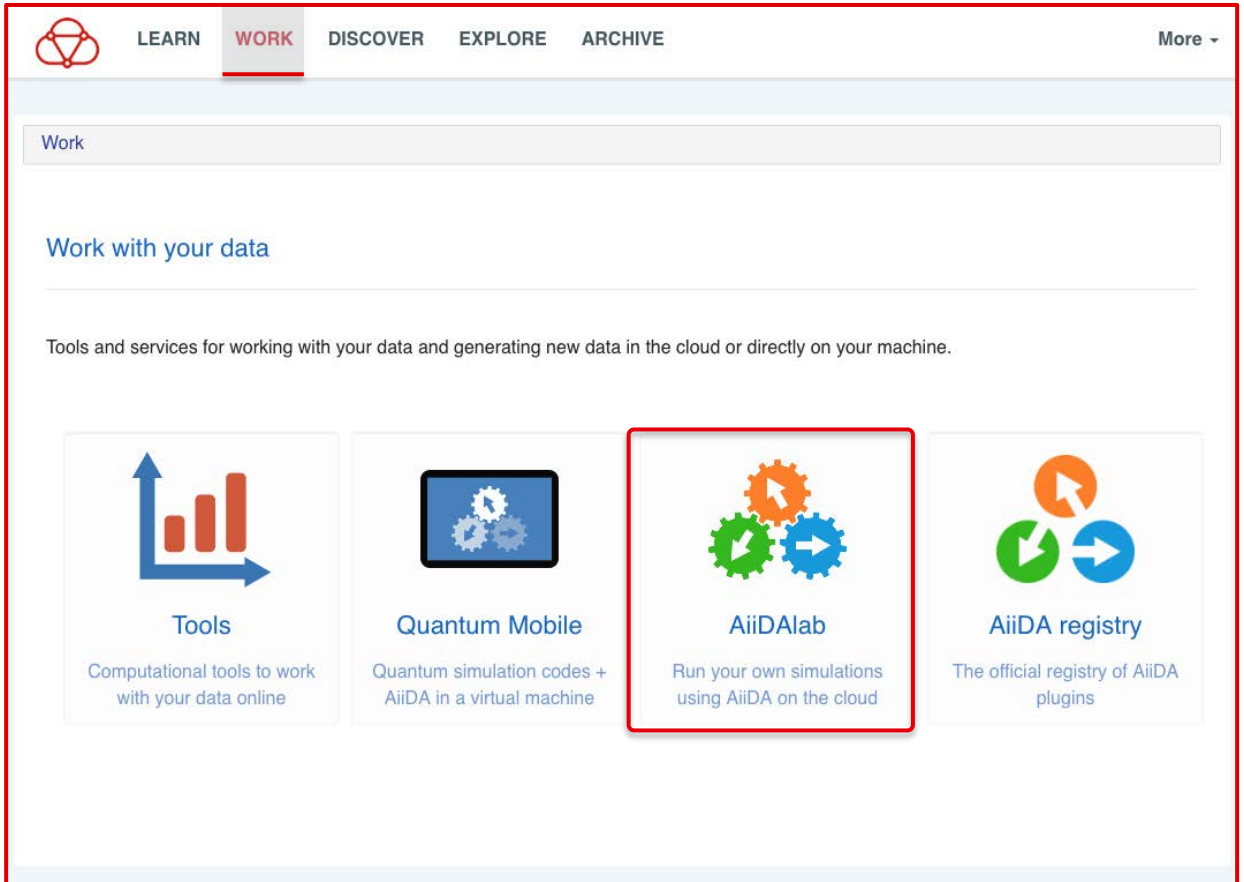


Quantum Mobile

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

Run simulations on the cloud or on your own computer

Materials Cloud - WORK

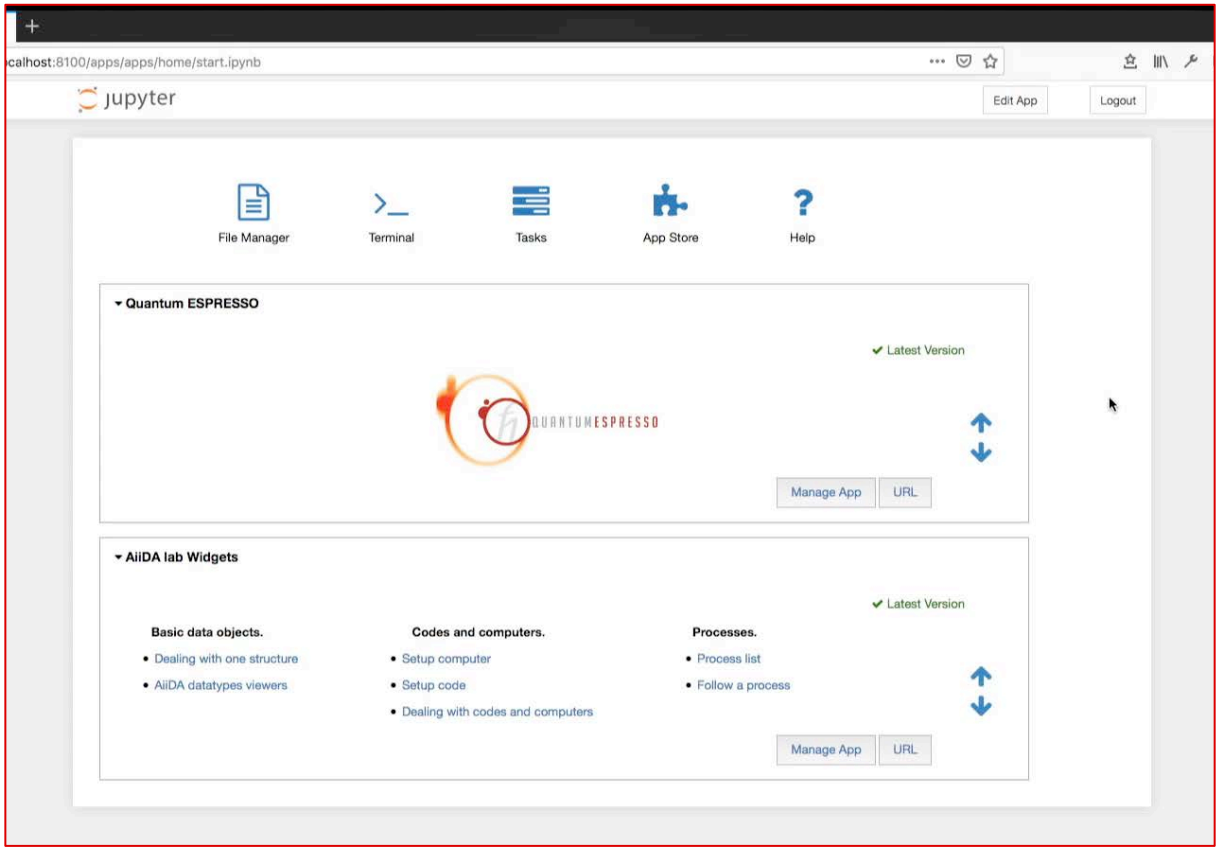


AiiDAlab

a pre-configured AiiDA setup

Jupyter notebooks to look like web apps

Materials Cloud - WORK



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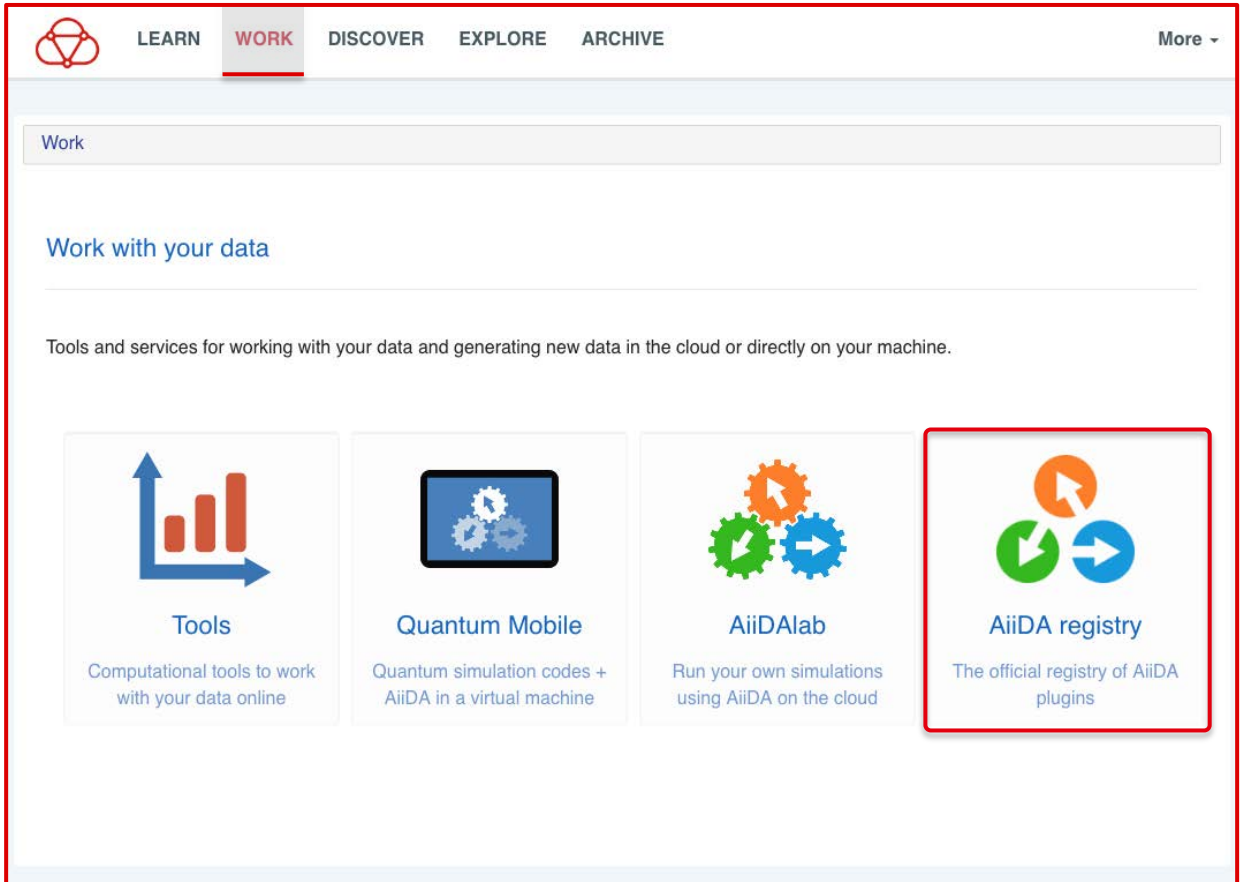
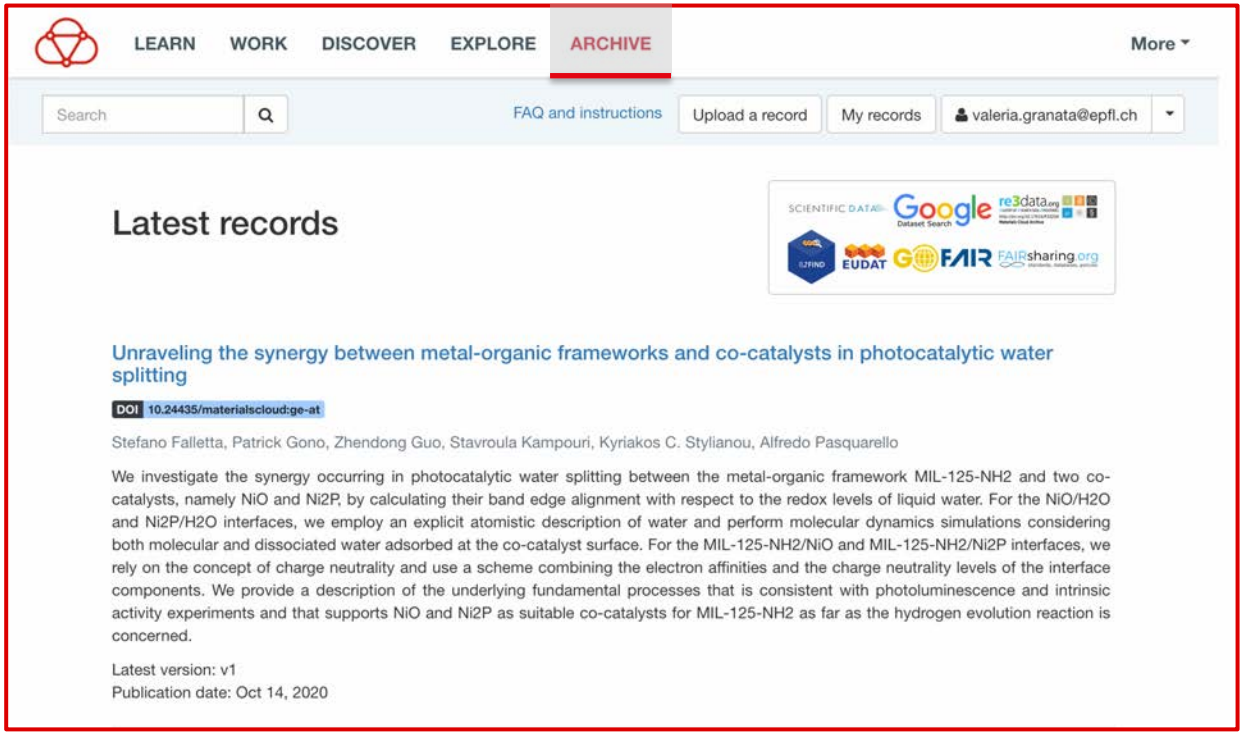


AiiDA registry

Access to the registred AiiDA plugins

Materials Cloud - ARCHIVE

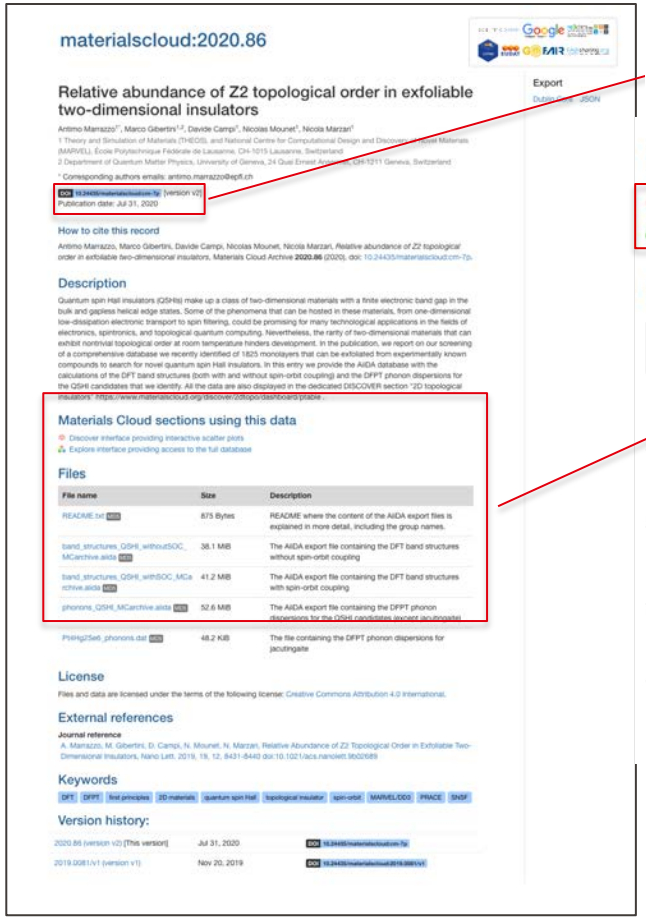


ARCHIVE

A moderated repository for research data from computational materials science

Built within the CERN Invenio framework (v3)

Materials Cloud - ARCHIVE



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

ARCHIVE

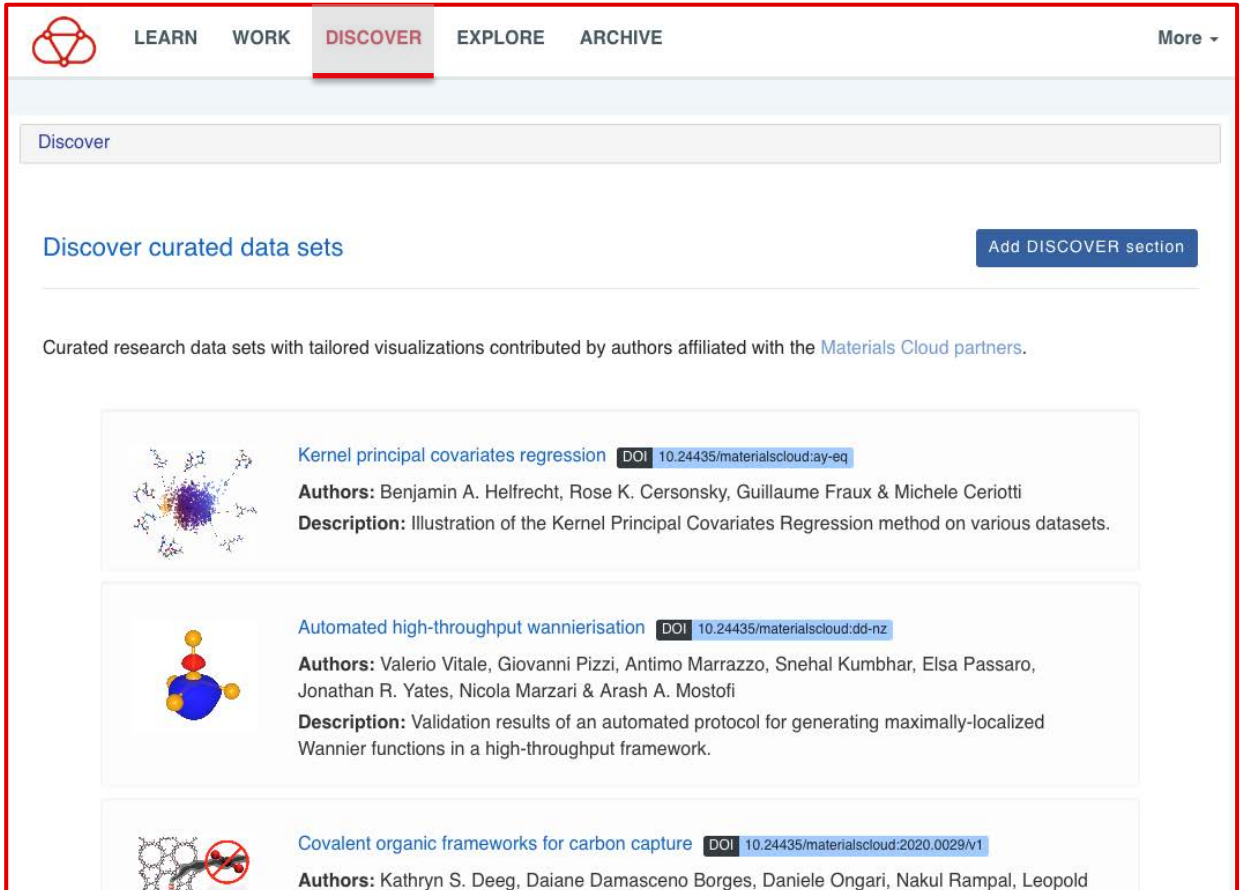
Materials Cloud sections using this data

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

Files

File name	Size	Description
README.txt MD5	875 Bytes	README where the content of the AiiDA export files is explained in more detail, including the group names.
band_structures_QSHI_withoutSOC_MCarchive.aiida MD5	38.1 MiB	The AiiDA export file containing the DFT band structures without spin-orbit coupling
band_structures_QSHI_withSOC_MCarchive.aiida MD5	41.2 MiB	The AiiDA export file containing the DFT band structures with spin-orbit coupling
phonons_QSHI_MCarchive.aiida MD5	52.6 MiB	The AiiDA export file containing the DFPT phonon dispersions for the QSHI candidates (except jacutingaite)
Pt4Hg2Se6_phonons.dat MD5	48.2 KiB	The file containing the DFPT phonon dispersions for jacutingaite

Materials Cloud - DISCOVER



DISCOVER

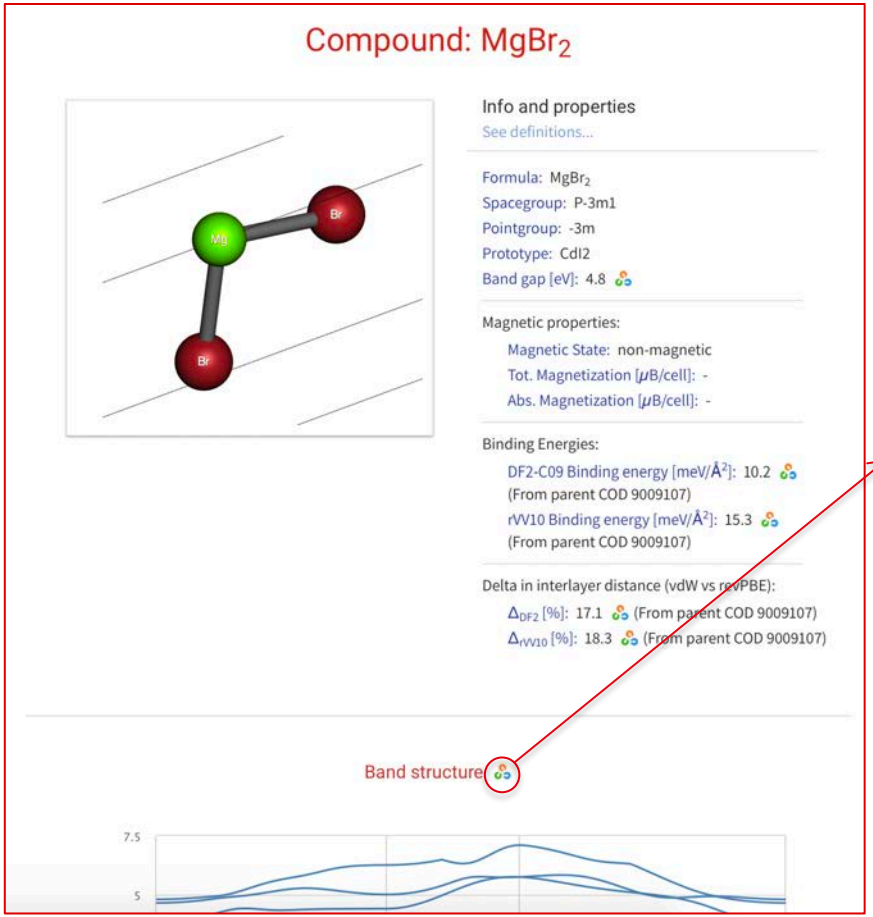
Curated data

3D visualization of structures

Structure properties, band structure

Link to Explore section

Materials Cloud - DISCOVER



Link to EXPLORE Section

UUID of provenance graph

DISCOVER

Curated data

3D visualization of structures

Structure properties, band structure

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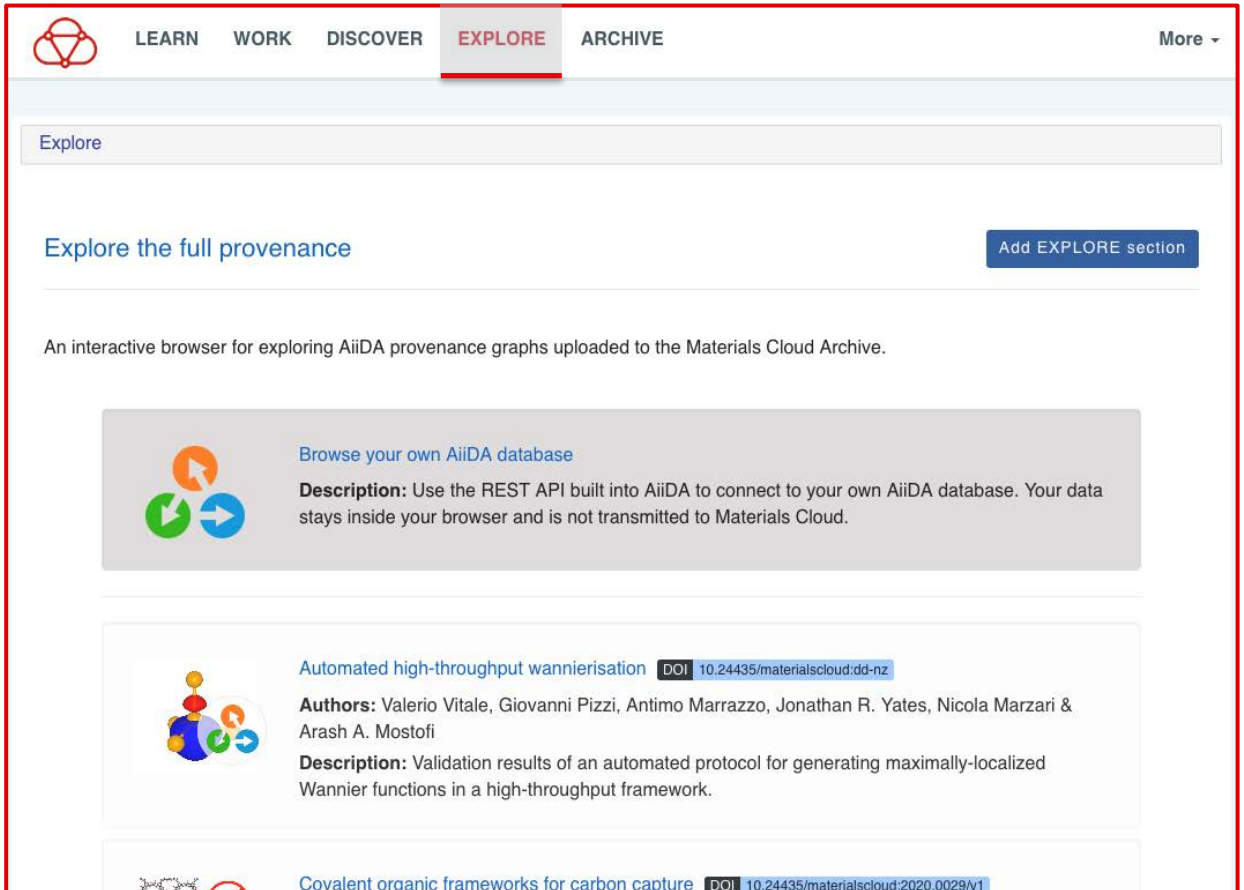


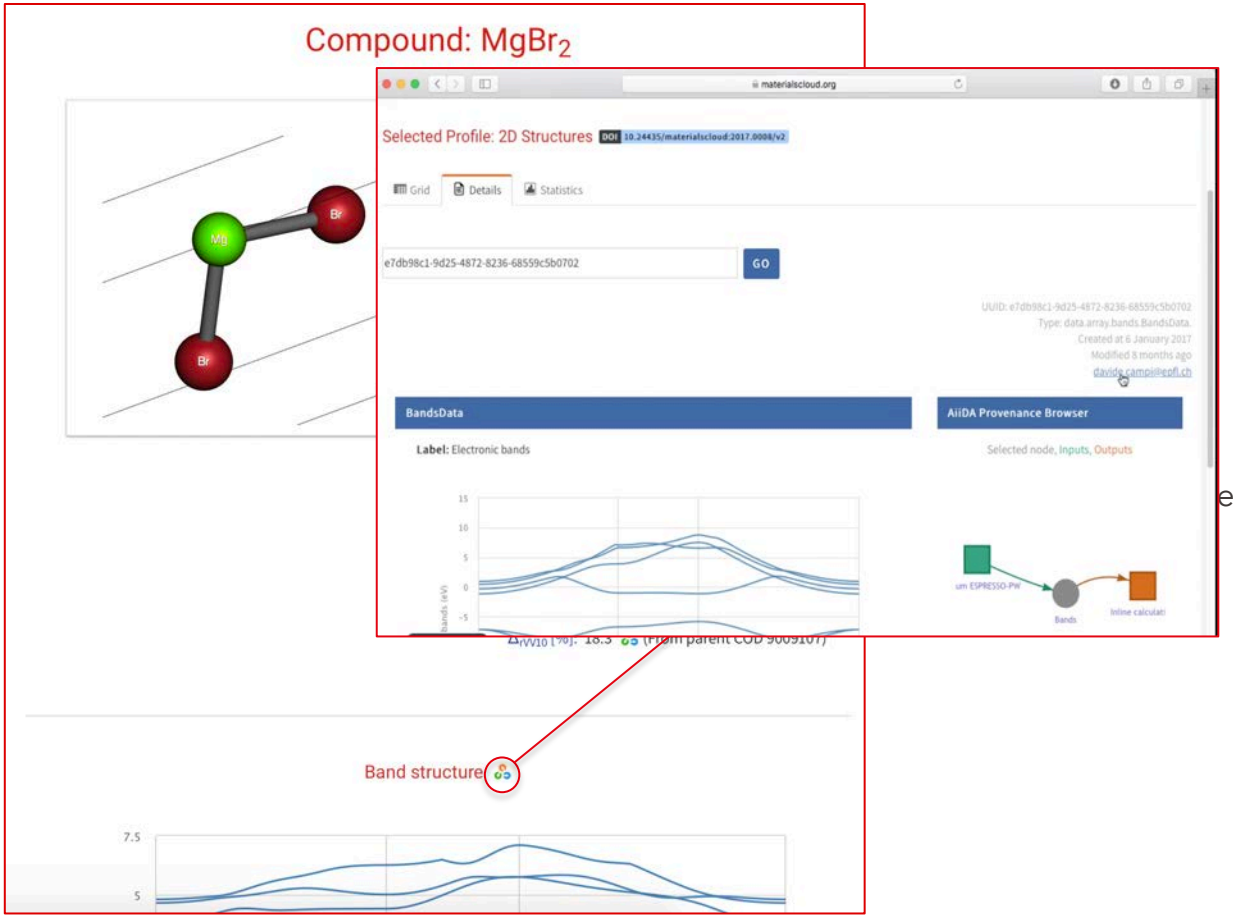
EXPLORE
Raw data

Access to AiiDA databases

Browse the AiiDA provenance graphs

Find input, output data and calculations to generate results

Materials Cloud - EXPLORE



EXPLORE
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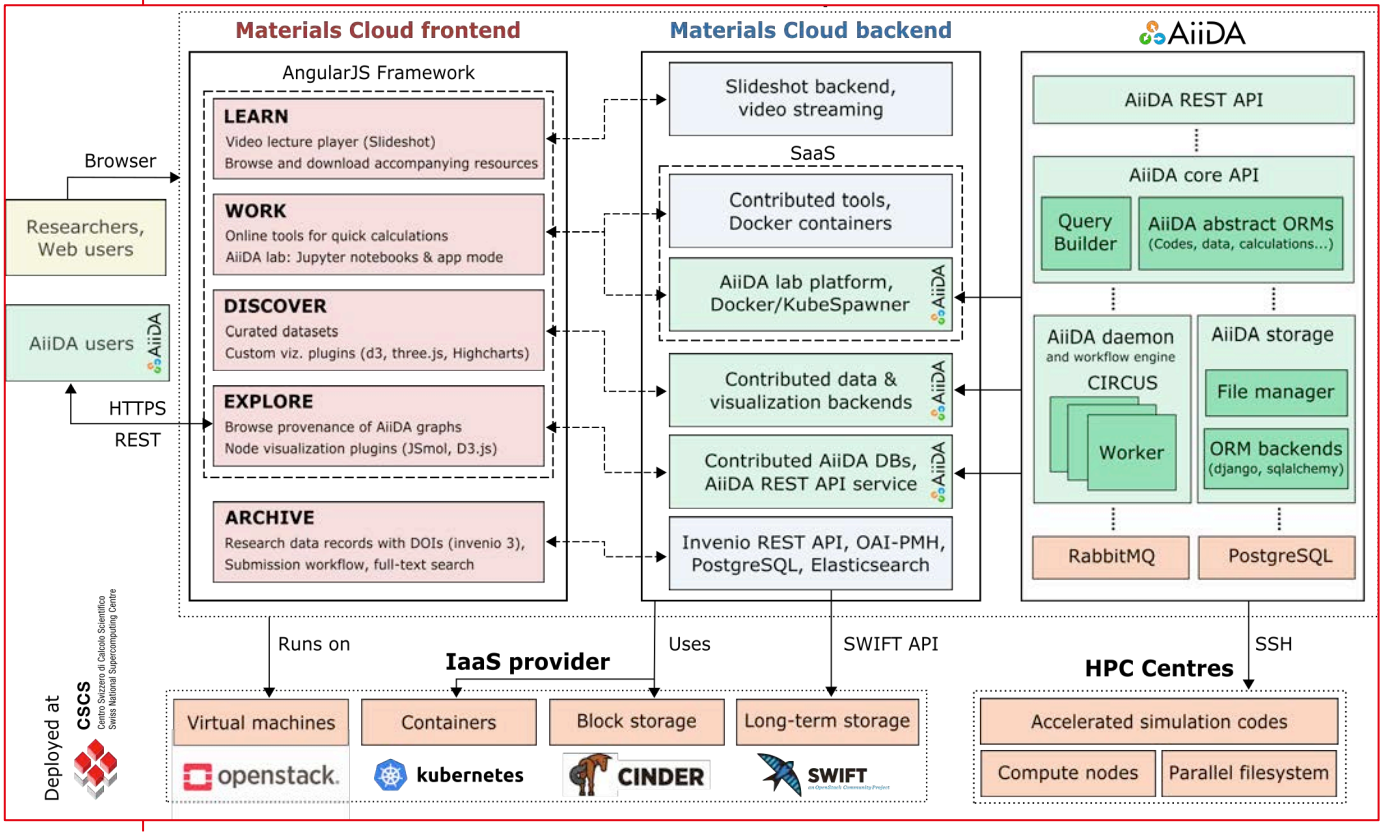
Architecture and technologies



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

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

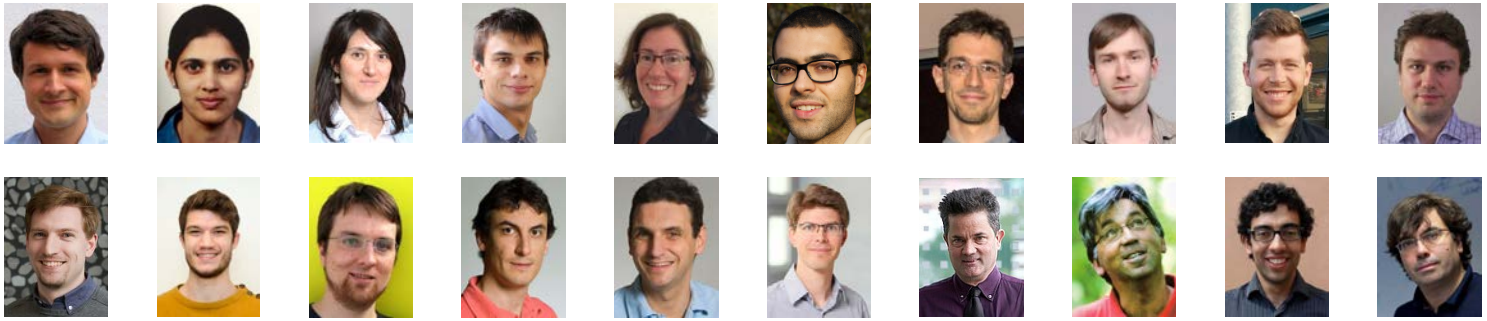
Interoperable: data linked via the AiiDA directed graph; data structures reusable between different codes

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

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

Materials Cloud team and contributors



Materials Cloud, a platform for open computational science

Leopold Talirz, Snehal Kumbhar, Elsa Passaro, Aliaksandr 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)

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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

info@materialscloud.org
valeria.granata@epfl.ch

www.materialscloud.org