MATERIALS CLOUD AS AN INCUBATOR FOR FUTURE DIGITAL INFRASTRUCTURES

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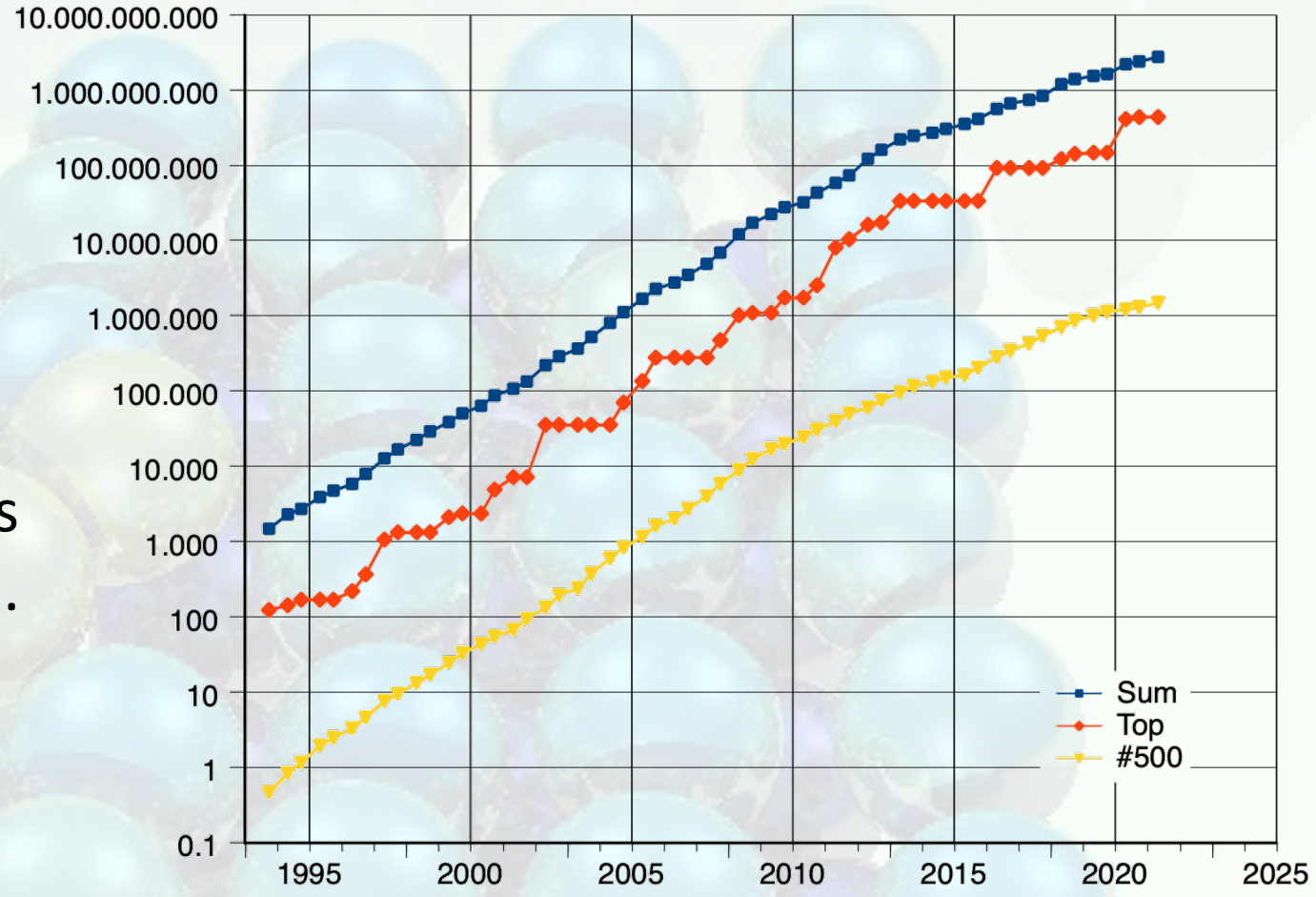
@NASA/JPL

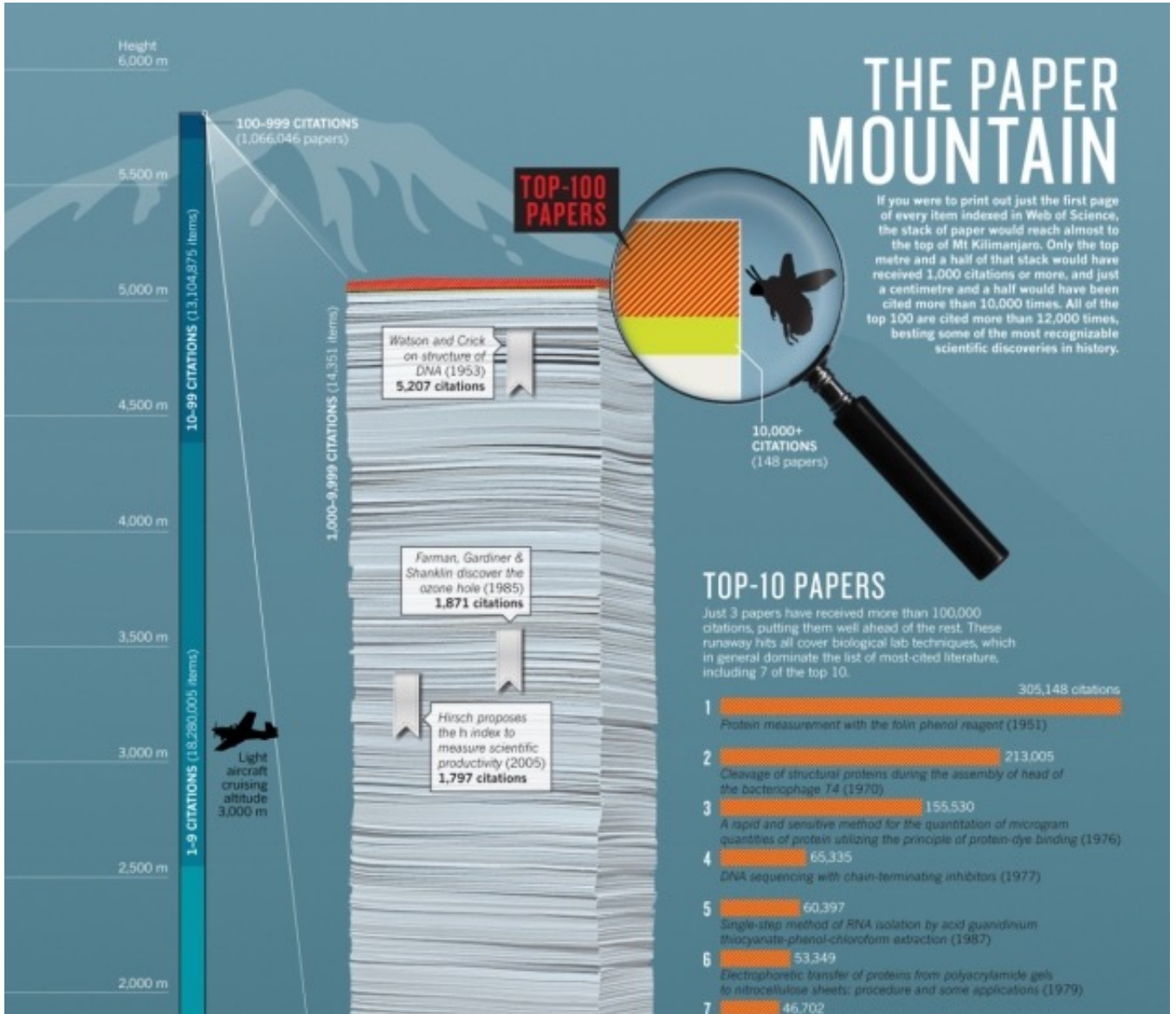
THE RISE OF COMPUTATIONAL SCIENCE

A calculation that took one year in 1994 takes ten seconds in 2023:
3-million-fold increase, or 100% returns every 16 months.

And this is just with bits: neurons are in, and qubits on the horizon.
21st-century science and discovery will greatly benefit from computational science.



THE RISE OF ELECTRONIC-STRUCTURE SIMULATIONS



THE TOP 100 PAPERS:

12 papers on density-functional theory in the top-100 most cited papers in the entire scientific-medical-engineering literature, ever.

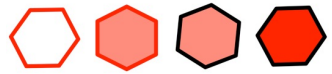
NATURE, OCT 2014

THIS IS BIG SCIENCE… (APS, 2021)

Title	Authors	Journal	# cited
Generalized gradient approximation made simple	Perdew, Burke, Ernzerhof	PRL (1996)	108 099
Development of the Colle-Salvetti correlation-energy formula …	Lee, Yang, Parr	PRB (1988)	77 473
Efficient iterative schemes for ab initio total-energy calculations …	Kresse, Furthmüller	PRB (1996)	58 176
Projector augmented-wave method	Blöchl	PRB (1994)	43 455
Self-consistent equations including exchange and correlation …	Kohn, Sham	PR (1965)	42 795
From ultrasoft pseudopotentials to the projector augmented-wave …	Kresse, Joubert	PRB (1999)	42 485
Special points for Brillouin-zone Integrations	Monkhorst, Pack	PRB (1976)	41 232
Density-functional exchange-energy approximation with correct …	Becke	PRA (1988)	41 142
Inhomogeneous electron gas	Hohenberg, Kohn	PRB (1964)	35 445
Ab initio molecular dynamics for liquid metals	Kresse, Hafner	PRB (1993)	23 192

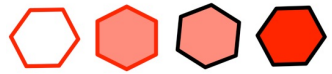
Table 1. Top ten most highly cited articles published by the American Physical Society, all of which deal with density functional theory and its practical application. Data collected from the Web of Science on June 16th, 2021.

https://github.com/ltalirz/livecoms-atomistic-software



…AND THIS IS THE FUNDING FOR BIG SCIENCE

- ESA **7.1 billion €/year** (2023)
- ITER **22 to 65 billion $** (2007-35)
- CERN **1.4 billion CHF/year** (2023)
- Argonne **1.1 billion $/year** (2021)
- James Webb **10 billion $** (2021)



FORTUNE COOKIE

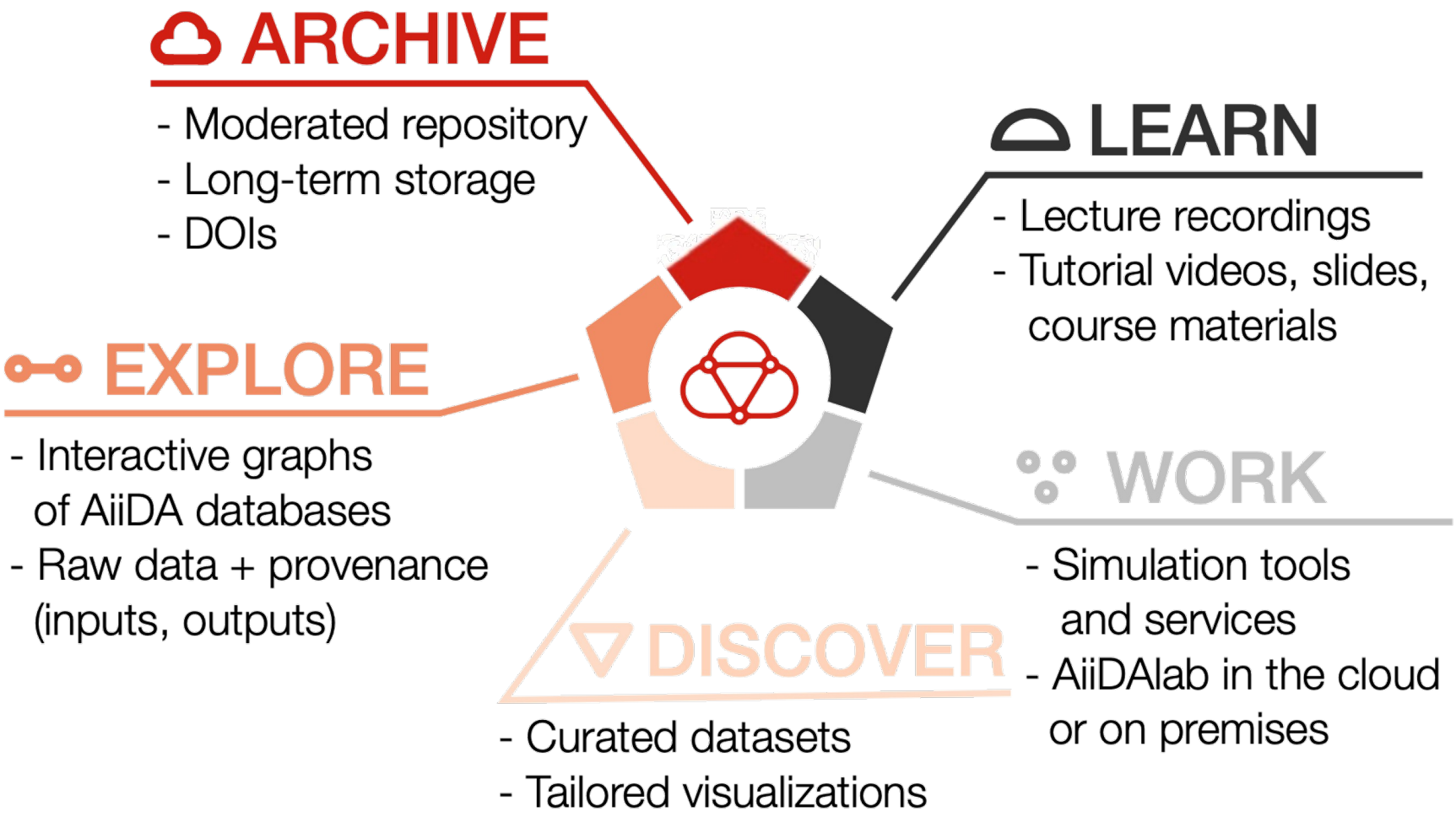
AGAINST SUCH MAJOR IMPACT, THERE IS RATHER MARGINAL FUNDING FOR THE INFRASTRUCTURE, AND NOT MUCH STRATEGY EITHER

2013 VISION

Materials Cloud is built to enable the seamless sharing and dissemination of resources in computational materials science, offering **educational, research, and archiving tools; simulation software and services; and curated and raw data.**

https://www.materialscloud.org

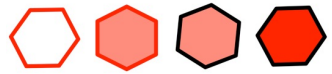
2013 VISION



https://www.materialscloud.org

TARGET AUDIENCES

Section	Content	Target audience	Objective	Access	Submission
LEARN	Video lectures and tutorials	Students and experts in computational materials science	Dissemination of educational and research content	Open, no registration	Partners; other submissions considered
WORK	Online simulations tools and services; redeployable locally	Researchers in computational materials science	Dissemination of open simulation services and tools	Open, with registration for AiiDAlab	Partners; other submissions considered
DISCOVER	Curated datasets of calculated materials properties	Researchers in materials science	Dissemination of calculated materials properties	Open, no registration	Partners; other submissions considered
EXPLORE	AiiDA databases and their graphs	Researchers in computational materials science; data scientists	Exploration and query of the raw data and provenance of AiiDA workflows	Open, no registration	Open, with registration
ARCHIVE	Computational data in any format; experimental data linked to computational data	Researchers in materials science; data scientists	FAIR research data dissemination and storage	Open, no registration	Open, with registration



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 events

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

AiiDA and Materials Cloud tutorials

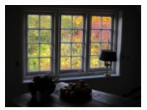
Video recordings and educational material from past AiiDA and Materials Cloud tutorials.

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.

MARVEL Distinguished Lectures

Subsection of: MARVEL events

A series of Distinguished Lectures sponsored by NCCR MARVEL, bringing high-profile researchers in contact with the MARVEL community.

Videos

▶ WATCH

34: Chirality and Topology

Claudia Felser

Date: 2 May 2023

The 34th NCCR MARVEL Distinguished Lecture will be given by Prof. Claudia Felser, Max Planck Institute for Chemical Physics of Solids (Dresden, Germany). She will be presenting a lecture entitled: 'Chirality and Topology'.

Profile link

▶ WATCH

33: Emergent Properties in Flatland: When One Plus One is More than Two

Kristian Sommer Thygesen

Date: 13 December 2022

The 33rd NCCR MARVEL Distinguished Lecture will be given by Prof. Kristian Sommer Thygesen, professor computational atomic-scale materials design at the Technical University of Denmark (DTU). He will be presenting a lecture entitled: 'Emergent Properties in Flatland: When One Plus One is More than Two'

Profile link

▶ WATCH

32: Materials discovery in challenging spaces with machine learning

Heather Kulik

Date: 13 December 2022

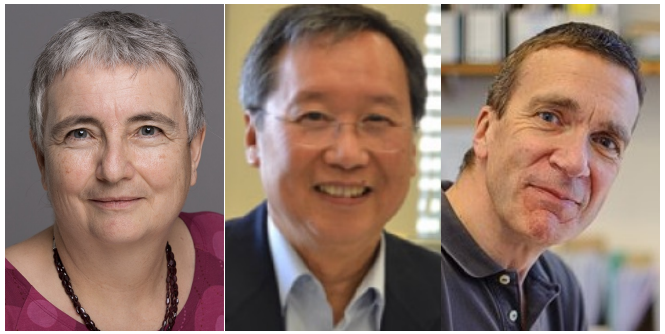
The 32nd NCCR MARVEL Distinguished Lecture will be given by Prof. Heather Kulik, professor of chemical engineering at the MIT. She will be discussing materials discovery in challenging spaces with machine learning, from transition metal complexes to metal-organic frameworks.

Profile link

BROAD ATTENDANCE

MARVEL Distinguished Lectures: Now fully online – great attendance worldwide (Kresse, 670 participants). E.g. 2021-22 Zunger, Perdew, Mertig, Glotzer, Aspuru-Guzik, Chan.

CECAM-MARVEL Classics in Molecular and Materials Modelling: 400-600 participants. For 2021-22:

https://www.materialscloud.org/learn/

MATERIALS CLOUD WORK

Work with your data

Tools and services for working with your data and generating new data in the cloud or directly on your machine.

Tools

Computational tools to work with your data online

Quantum Mobile

Quantum simulation codes + AiiDA in a virtual machine

AiiDAlab

Run your own simulations using AiiDA on the cloud

AiiDA registry

The official registry of AiiDA plugins

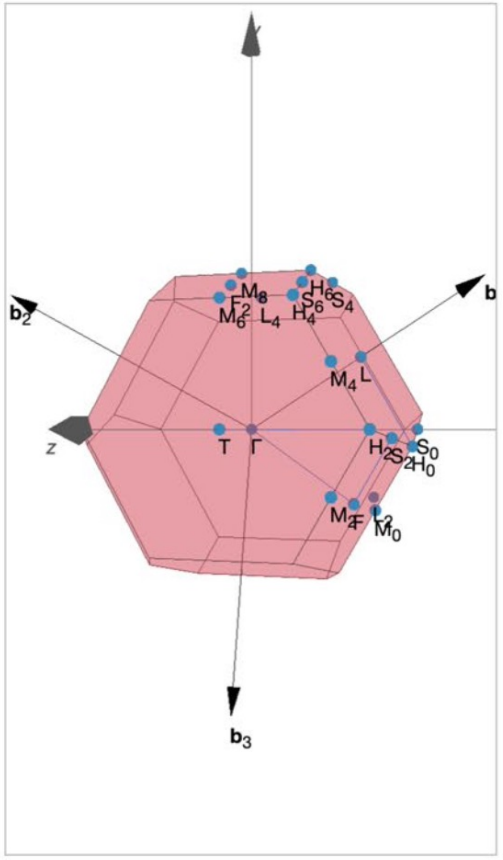
OSSCAR

Open Software Services for Classrooms and Research

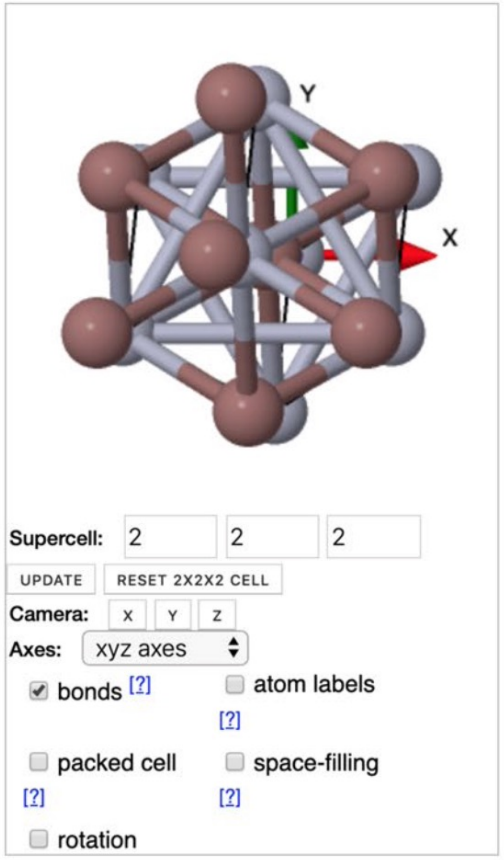
DIRECTLY ACCESSIBLE TOOLS

a

Brillouin Zone

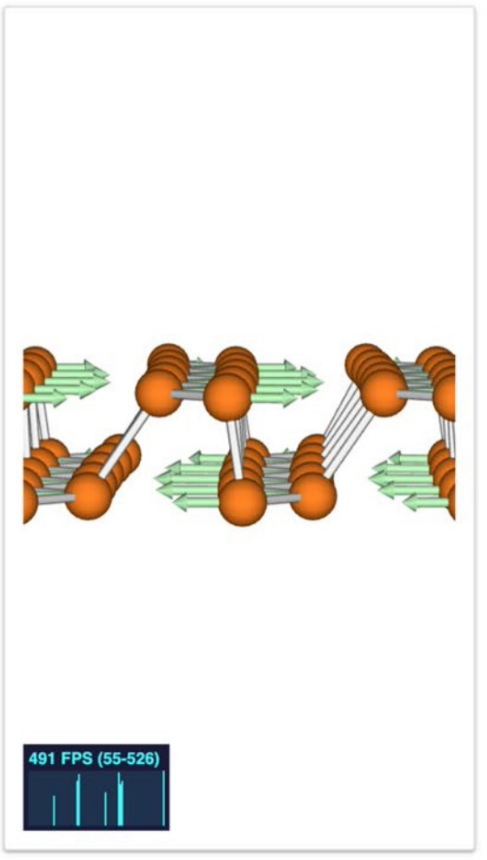


Primitive Cell

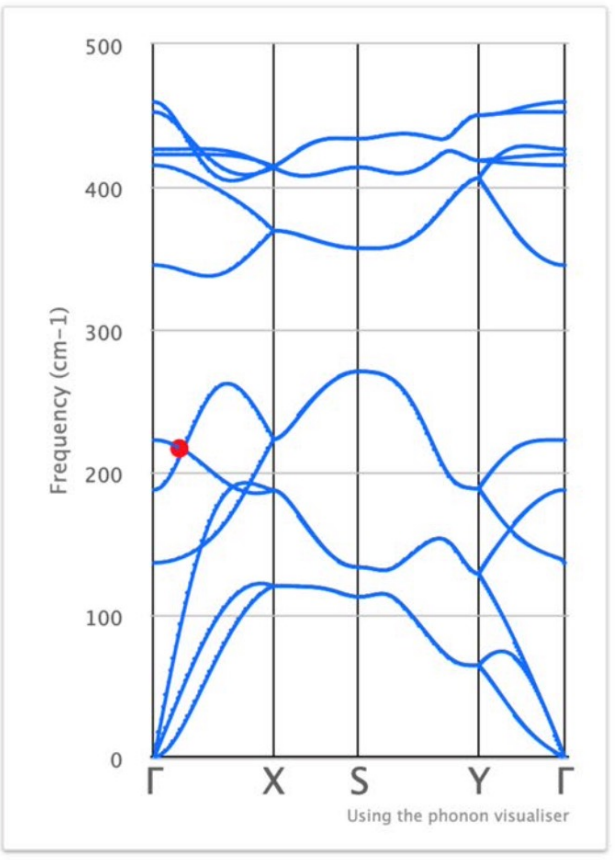


b

Phonon Eigenvectors



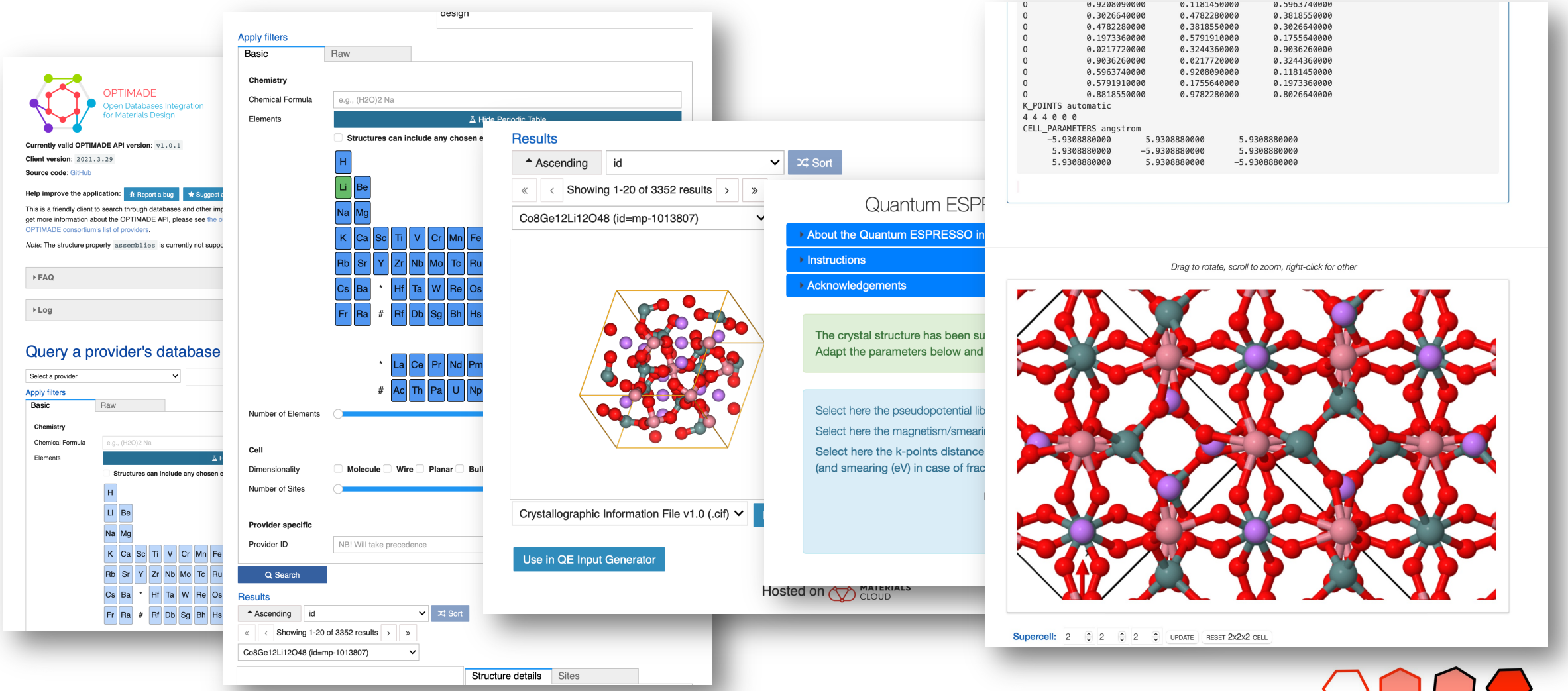
Phonon Band Structure



UNIVERSAL APIs

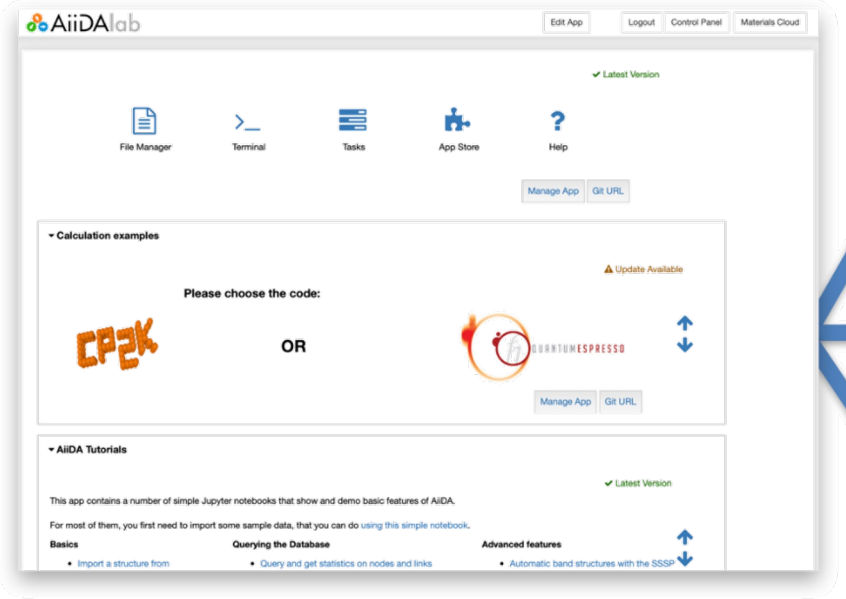
https://optimadeclient.materialscloud.io/

https://www.materialscloud.org/work/tools/qeinputgenerator

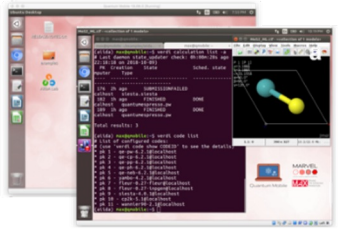


IN THE CLOUD OR ON-PREMISES SIMULATIONS

AiiDAlab



A. V. Yakutovich et al., Comp. Mat. Sci. 188, 110165 (2021)



QUANTUM MOBILE

https://www.materialscloud.org/quantum-mobile

openstack.

https://ailldalab.materialscloud.org/
(@CSCS, also via PRACE-FENIX-ICEI)

kubernetes

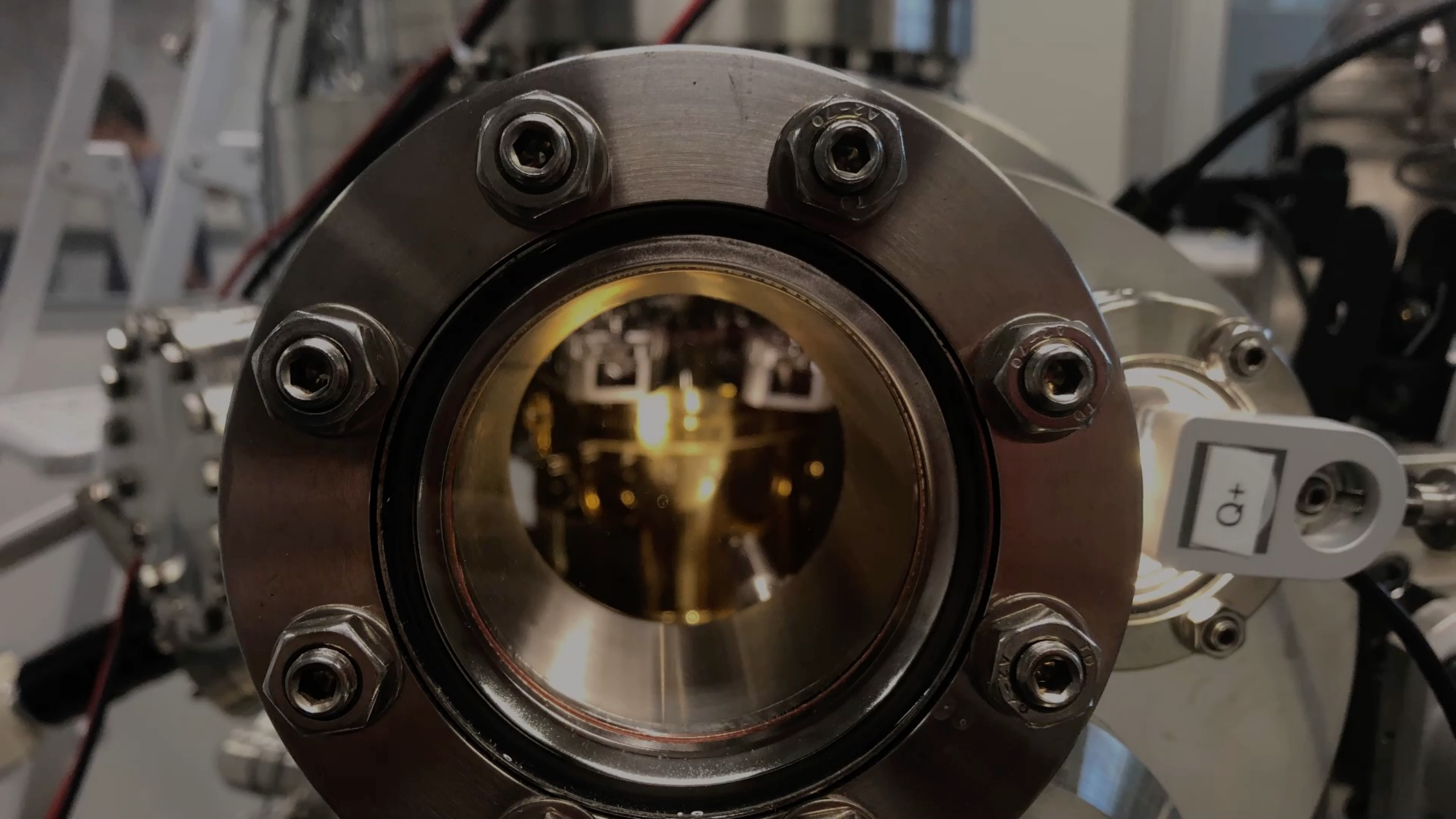
https://ailldalab-demo.materialscloud.org/
(@EOSC/EGI CESNET; plan to move to CSCS)

Custom on-premise deployments

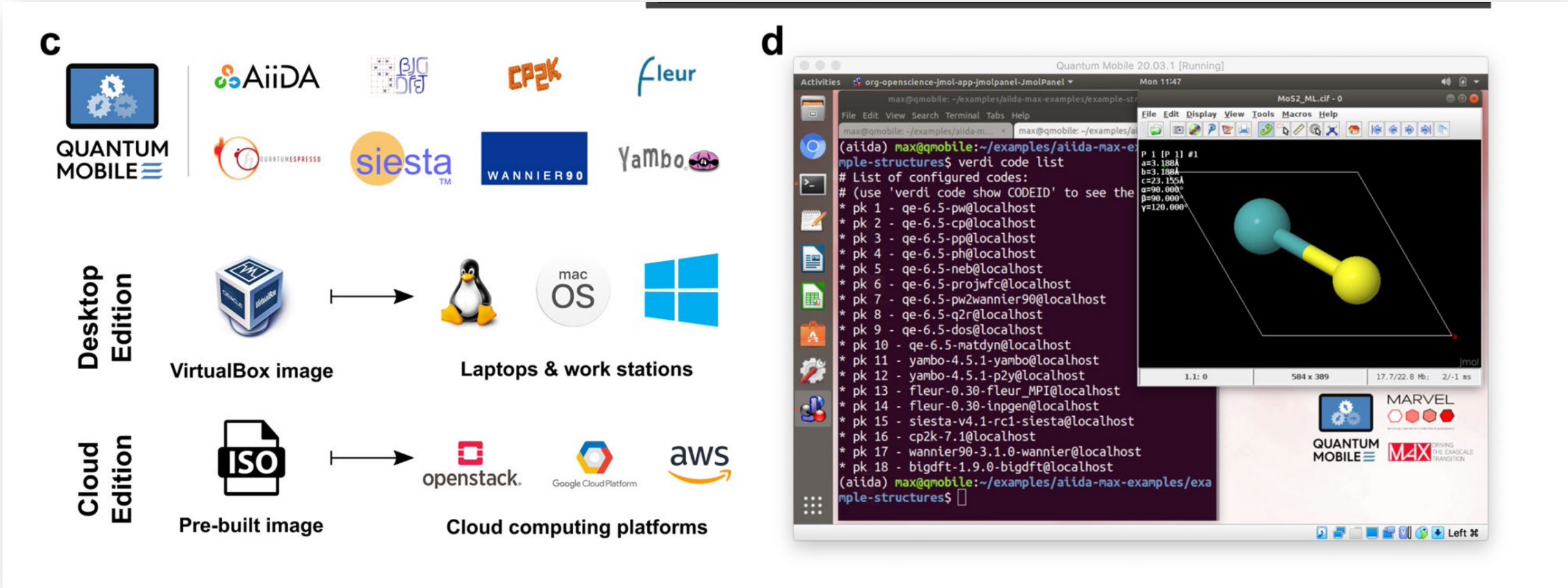
MarketPlace
EU projects

SANDVIK Coromant
Industries (*ongoing*)

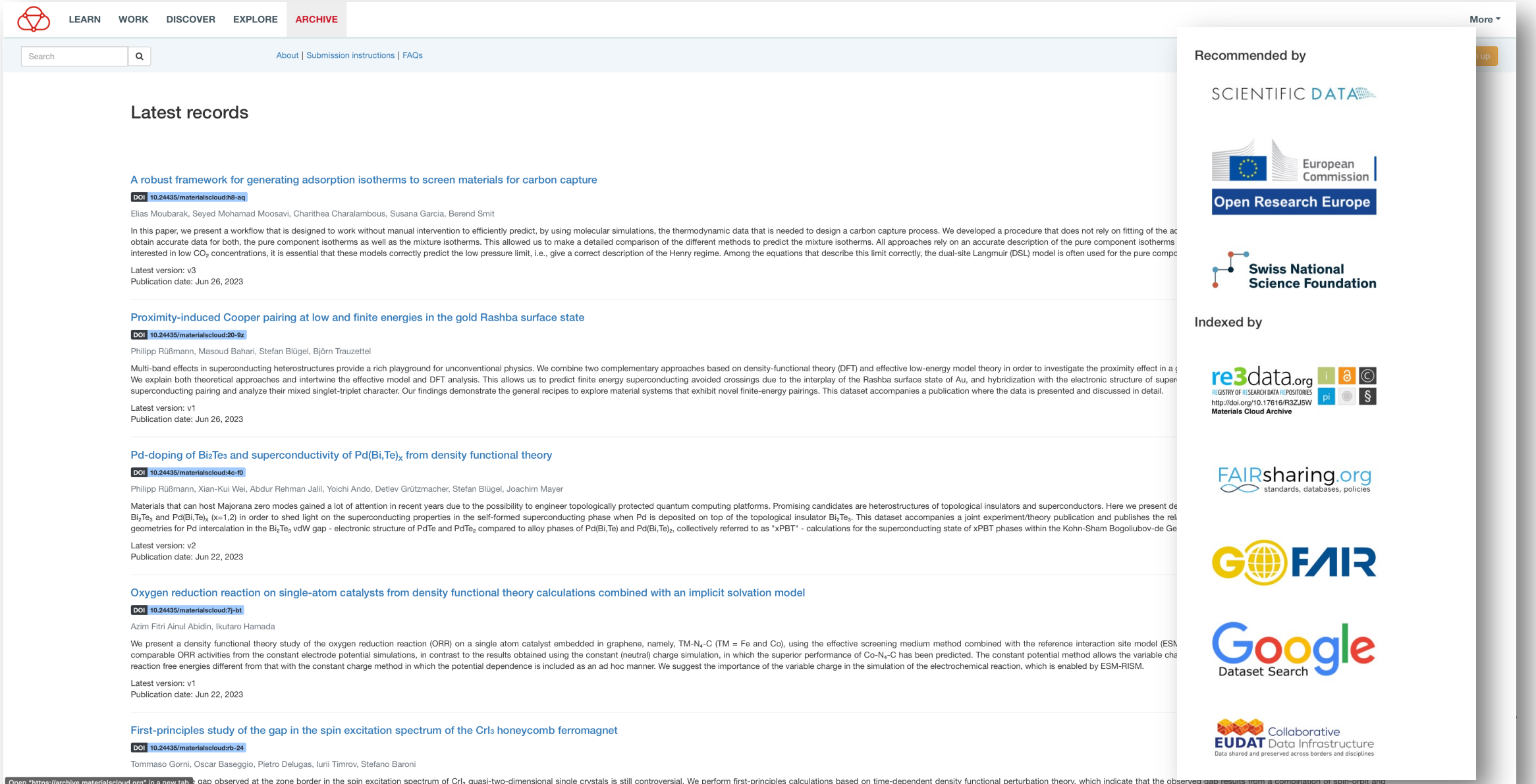
+ documentation and terraform configuration for custom deployment (collaboration with Microsoft)
https://github.com/aiidalab/aiidalab-k8s



AGILE DEPLOYMENT THROUGH THE QUANTUM MOBILE



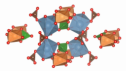
THE DATA STRATEGY: ARCHIVE…



THE DATA STRATEGY: …DISCOVER…

Discover curated data sets

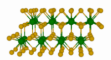
Curated research data sets with tailored visualizations maintained by the Materials Cloud team.



Materials Cloud three-dimensional crystals database (MC3D) DOI 10.24435/materialscloud

Authors: Sebastiaan Huber, Marnik Bercx, Kristjan Eimre, Nicolas Hörmann, Martin U
Marzari, Giovanni Pizzi

Description: Curated set of relaxed three-dimensional crystal structures based on raw
from the experimental databases MPDS, COD, and ICSD.



Materials Cloud two-dimensional crystals database (MC2D) DOI 10.24435/materialscloud:a

DOI 10.24435/materialscloud:36-nd

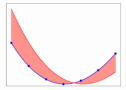
Authors: Davide Campi, Davide Grassano, Nicolas Mounet, Marco Gibertini, Philippe
Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano E. Castelli, Andrea Cepellotti
Kumbhar, Elsa Passaro, Kristjan Eimre, Giovanni Pizzi, Nicola Marzari

Description: Results from screening known 3D crystal structures finding those that ca
computationally exfoliated, producing 2D materials candidates.

Standard solid-state pseudopotentials (SSSP) DOI 10.24435/materialscloud:rz-77

Authors: Gianluca Prandini, Antimo Marrazzo, Ivano E. Castelli, Nicolas Mounet, Snel
Elsa Passaro, Nicola Marzari

Description: A Standard Solid State Pseudopotentials (SSSP) library optimized for pr
efficiency.



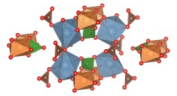
Verification of the precision of DFT implementations via AiiDA common workflows

DOI 10.24435/materialscloud:s4-3h

Authors: E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Bröder, M. Callsen, S. C
Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, M. Fornari, A. Garcia, L. Genovese, M
Giantomassi, S. P. Huber, H. Janssen, G. Kastlunger, M. Krack, G. Kresse, T. D. Kühn
Lejaeghere, G. K. H. Madsen, M. Marsman, N. Marzari, G. Michalicek, H. Mirhosseini,
Müller, G. Petretto, C. J. Pickard, S. Poncé, G. Rignanese, O. Rubel, T. Ruh, M. Sluydt
Vanpoucke, S. Vijay, M. Wolloch, D. Wortmann, A. V. Yakutovich, J. Yu, A. Zadoks, B.

Description: Reference and verification datasets of equations of state calculated with
density-functional-theory (DFT) codes and computational approaches, using the AiiDA common
workflows (ACWF) infrastructure.

Materials Cloud three-dimensional crystals database (MC3D)



DOI 10.24435/materialscloud:rw-t0

Curated set of relaxed three-dimensional crystal structures based on raw CIF data from the experimental databases MPDS, COD, and ICSD.

Use | About | REST API

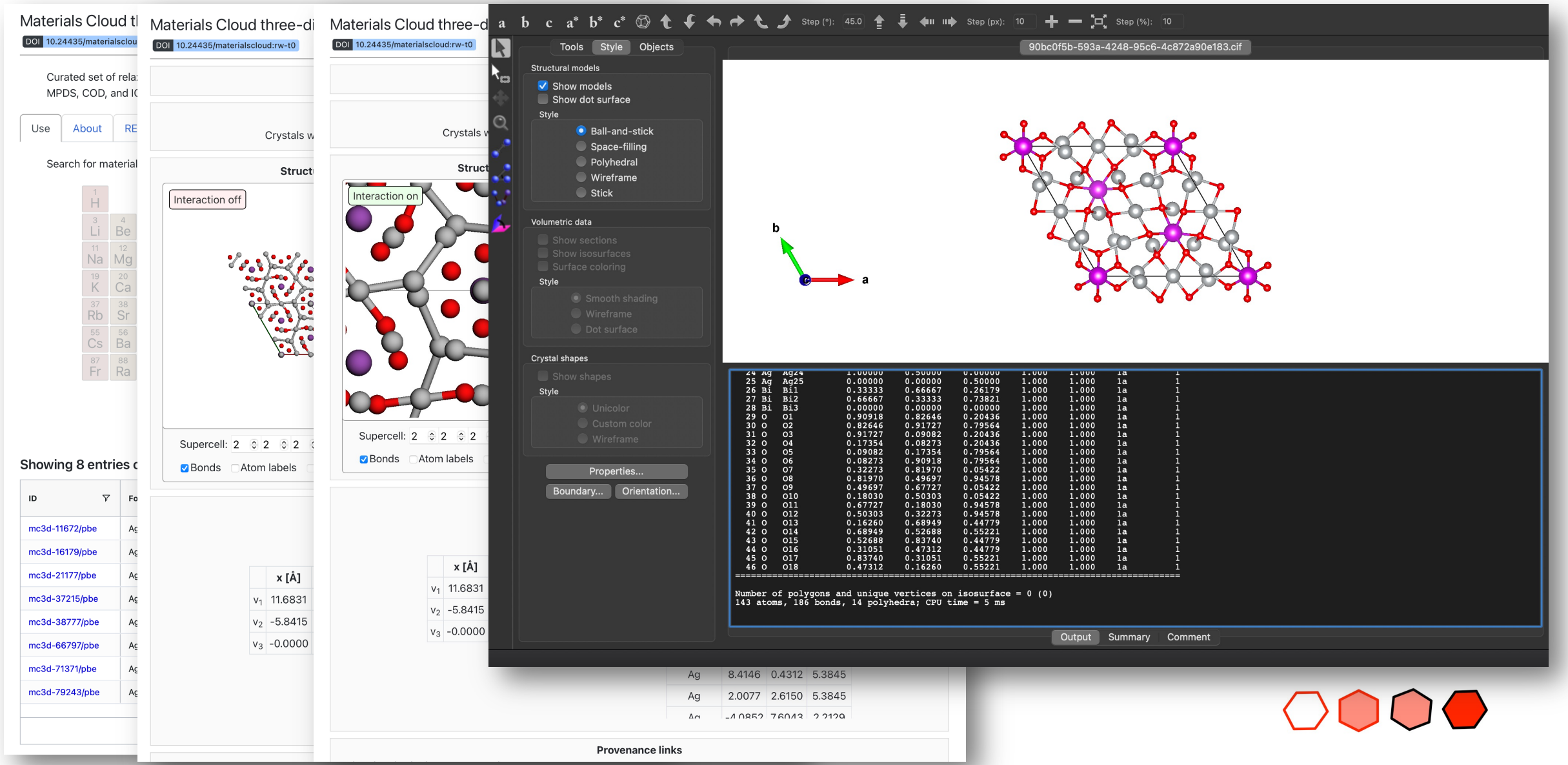
Search for materials:

Elements filtering mode:
- (•) Include/exclude
- ( ) Only selected

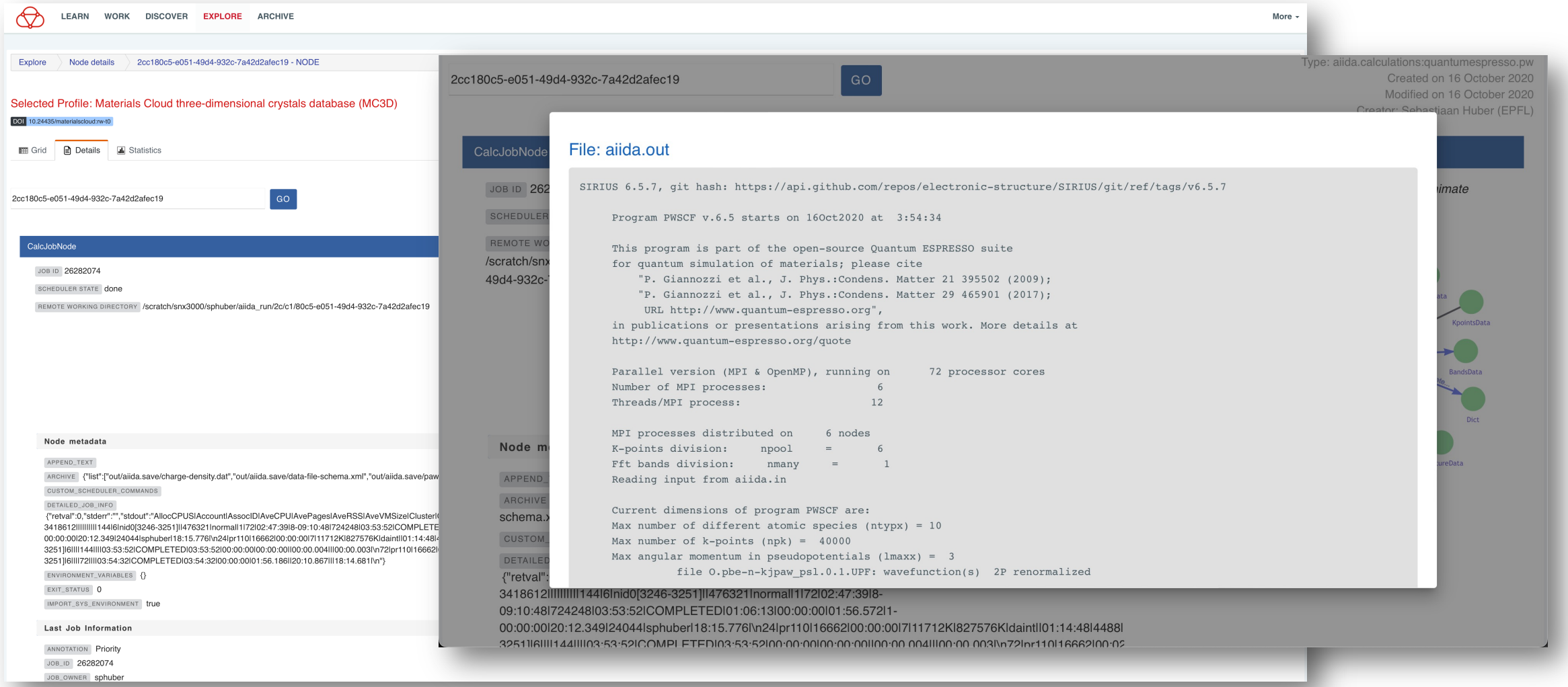
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

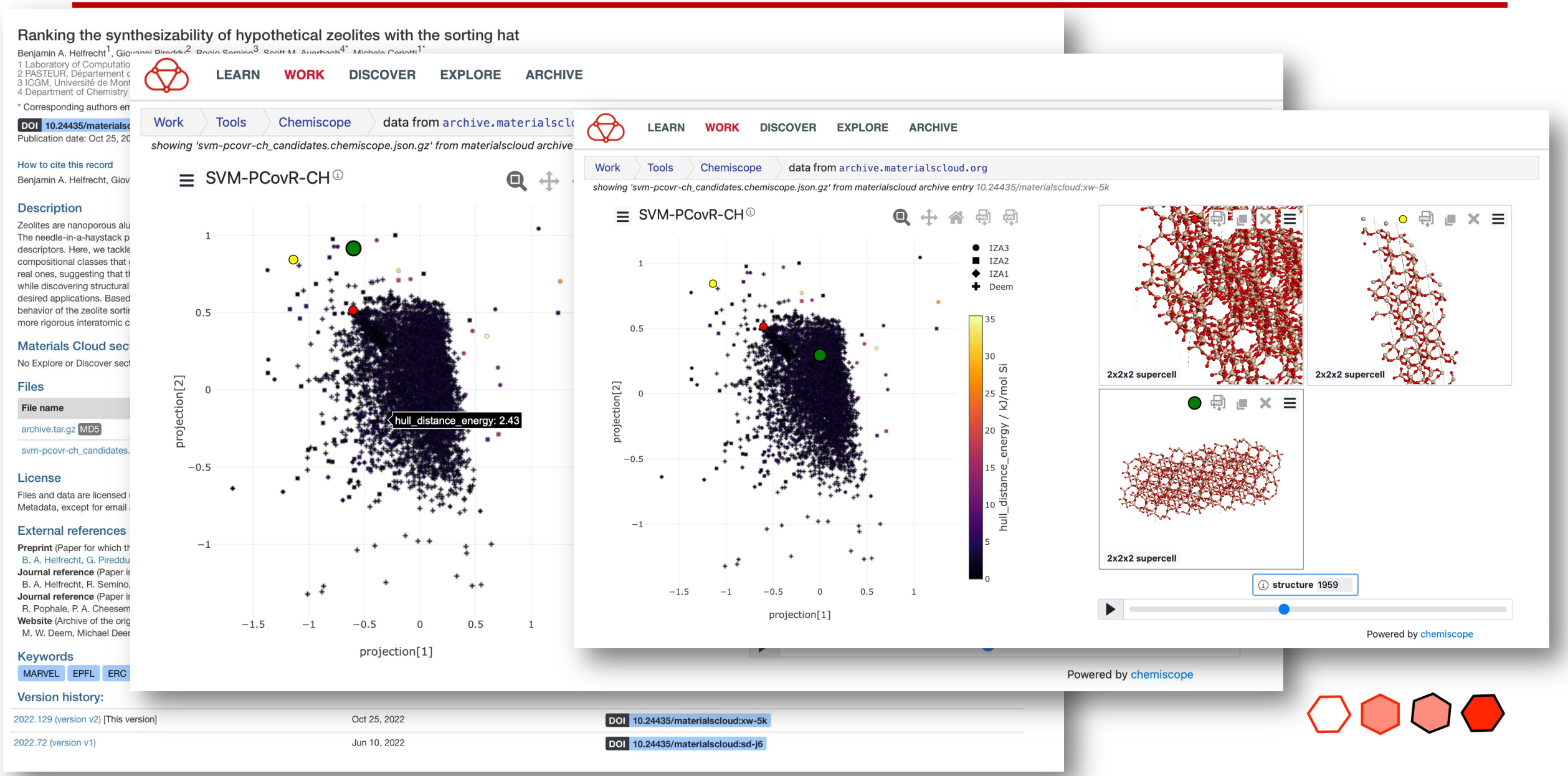
THE DATA STRATEGY: …DISCOVER…



THE DATA STRATEGY: …EXPLORE

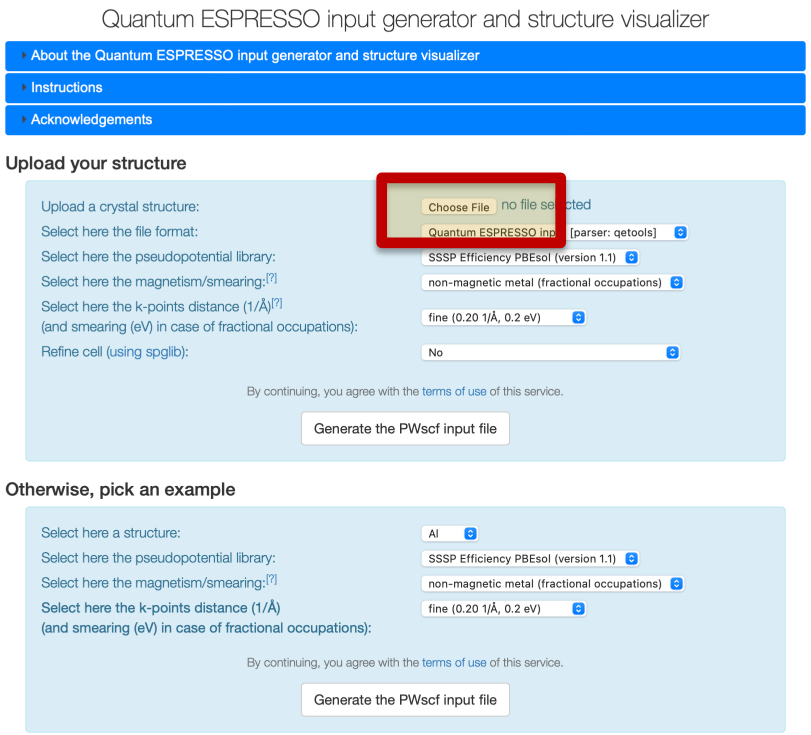


INTEROPERABILITY: FROM ARCHIVE TO IN-CLOUD ANALYSIS



INTEROPERABILITY: ON-PREMISES SIMULATIONS

Quantum ESPRESSO input generator, or full simulations services in AiiDAlab



INTEROPERABILITY: INTEGRATION WITH MATERIALS CLOUD TOOLS

Summary of the input parameters

Pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Smearing/magnetism: non-magnetic metal (fractional occupations)

K-points distance: 0.2 $Å^{-1}$

The input parameters provided by this tool are accurate safe choices. Optimized choices that allow for faster runs with comparable accuracy can be achieved by expert users.

Additionally, the input file provided here does not guarantee that the Quantum ESPRESSO calculation will always converge successfully. Indeed, this is just the first step of the automated workflows released within the aiida-quantumespresso package. These implement advanced strategies to reduce the failure rate of the code by changing the input parameters to achieve convergence.

If you don't have AiiDA installed, you can anyway try out the workflows inside the Quantum Mobile virtual machine, by using the "Quantum ESPRESSO" app inside the AiiDAlab interface.

If you use the results of this tool in a publication, please cite the following works:

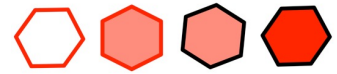
- SSSP (for the pseudopotential library)
  G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, npj Computational Materials **4**, 72 (2018).
  WEB: http://materialscloud.org/sssp.
- Pseudopotentials:
  - bi_pbesol_v1.uspp.F.UPF,
  - cl_pbesol_v1.4.uspp.F.UPF,
  - s_pbesol_v1.4.uspp.F.UPF,
    from GBRV: K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, *Comput. Mater. Sci.* **81**, 446 (2014).
    DOI: 10.1016/j.commatsci.2013.08.053, WEB: http://www.physics.rutgers.edu/gbrv, LICENSE: GNU General Public License (version 3).
  - Ag_ONCV_PBEsol-1.0.upf,
    from SG15: M. Schlipf and F. Gygi, *Comp. Phys. Comm.* **196**, 36 (2015).
    DOI: 10.1016/j.cpc.2015.05.011, WEB: http://www.quantum-simulation.org/potentials/sg15_oncv, LICENSE: Creative Commons Attribution-ShareAlike 4.0 International License (CC BY-SA 4.0).
  - Al.pbesol-n-kjpaw_psl.1.0.0.UPF,
    from Pslibrary 1.0.0: A. Dal Corso, *Comput. Mater. Sci.* **95**, 337 (2014).
    DOI: 10.1016/j.commatsci.2014.07.043, WEB: http://www.quantum-espresso.org/pseudopotentials, LICENSE: GNU General Public License (version 2 or later).

Download zip of input file and pseudopotentials | **Change parameters** | **Choose a different structure**

Quantum ESPRESSO PWscf input

Copy to clipboard

```
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   3.4000000000d-04
  forc_conv_thr =   1.0000000000d-04
  outdir = './out/'
  prefix = 'aiida'
  pseudo_dir = './pseudo/'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =   1.4699723600d-02
  ecutrho =   3.6000000000d+02
  ecutwfc =   5.0000000000d+01
```



INTEROPERABILITY: INTEGRATION WITH MATERIALS CLOUD TOOLS

Summary of the input parameters

Pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Smearing/magnetism: non-magnetic metal (fractional occupations)

K-points distance: 0.2 $Å^{-1}$

The input parameters provided by this tool are accurate safe choices. Optimized choices that allow for faster runs with comparable accuracy can be achieved by expert users.

Additionally, the input file provided here does not guarantee that the Quantum ESPRESSO calculation will always converge successfully. Indeed, this is just the first step of the automated workflows released within the aiida-quantumespresso package. These implement advanced strategies to reduce the failure rate of the code by changing the input parameters to achieve convergence.

If you don't have AiiDA installed, you can anyway try out the workflows inside the Quantum Mobile virtual machine, by using the "Quantum ESPRESSO" app inside the AiiDAlab interface.

If you use the results of this tool in a publication, please cite the following works:

- SSSP (for the pseudopotential library)
  G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, npj Computational Materials **4**, 72 (2018).
  WEB: http://materialscloud.org/sssp.
- Pseudopotentials:
  - bi_pbesol_v1.uspp.F.UPF,
  - cl_pbesol_v1.4.uspp.F.UPF,
  - s_pbesol_v1.4.uspp.F.UPF,
    from GBRV: K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, *Comput. Mater. Sci.* **81**, 446 (2014).
    DOI: 10.1016/j.commatsci.2013.08.053, WEB: http://www.physics.rutgers.edu/gbrv, LICENSE: GNU General Public License (version 3).
  - Ag_ONCV_PBEsol-1.0.upf,
    from SG15: M. Schlipf and F. Gygi, *Comp. Phys. Comm.* **196**, 36 (2015).
    DOI: 10.1016/j.cpc.2015.05.011, WEB: http://www.quantum-simulation.org/potentials/sg15_oncv, LICENSE: Creative Commons Attribution-ShareAlike 4.0 International License (CC BY-SA 4.0).
  - Al.pbesol-n-kjpaw_psl.1.0.0.UPF,
    from Pslibrary 1.0.0: A. Dal Corso, *Comput. Mater. Sci.* **95**, 337 (2014).
    DOI: 10.1016/j.commatsci.2014.07.043, WEB: http://www.quantum-espresso.org/pseudopotentials, LICENSE: GNU General Public License (version 2 or later).

Download zip of input file and pseudopotentials | **Change parameters** | **Choose a different structure**

Quantum ESPRESSO PWscf input

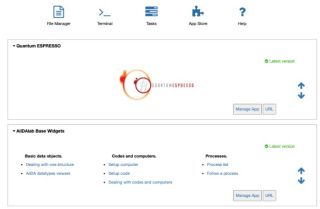
Copy to clipboard

```
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   3.4000000000d-04
  forc_conv_thr =   1.0000000000d-04
  outdir = './out/'
  prefix = 'aiida'
  pseudo_dir = './pseudo/'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =   1.4699723600d-02
  ecutrho =   3.6000000000d+02
  ecutwfc =   5.0000000000d+01
```

AiiDAlab

AiiDAlab

AiiDAlab provides you with a dedicated and intuitive simulation environment directly in the cloud or on remote or local resources.
With AiiDAlab you can run and manage complex, robust, and reliable workflows with tailored lightweight web applications, all from your browser. In addition, you can easily create your own applications, all running on top of AiiDA workflows.



Features

1. A cloud platform where you launch and monitor AiiDA workflows, and analyze the results.
2. Dedicated applications with intuitive graphical user interfaces.
3. Sharing of apps and workflows via the AiiDAlab App Store.
4. Fast development of new apps as Jupyter notebooks.
5. Open technologies throughout - host your own AiiDAlab!

Publication

We kindly ask you to cite the following publication if you use AiiDAlab

A. V. Yakutovich et al., Comp. Mat. Sci. 188, 110165 (2021).
DOI:10.1016/j.commatsci.2020.110165

Documentation

AiiDAlab documentation can be found on the following web page.

Apps

The list of available apps can be found at the AiiDAlab App Store.

Open Source

AiiDAlab is open source. We invite you to explore the repositories in our GitHub organization.

Official deployments

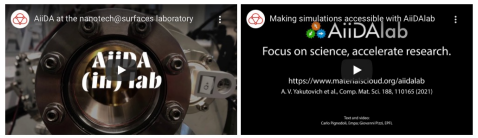
Status	Login	Description & Access policies
UP	Login	**Open** AiiDAlab demonstrator running on the kubernetes cluster hosted at CESNET (under a EOSC-hub Early Adopter Programme grant)
UP	Login	MARVEL/MaX AiiDAlab for researchers affiliated with Materials Cloud partners, running on the OpenStack cluster hosted at the Swiss National Supercomputing Centre (CSCS) under a PRACE-FENIX grant (production instance)

We acknowledge support from PRACE, FENIX and EOSC for the deployment of AiiDAlab.

Additionally, you can host AiiDAlab yourself on-premises or in the cloud (see the documentation).

Testimonials

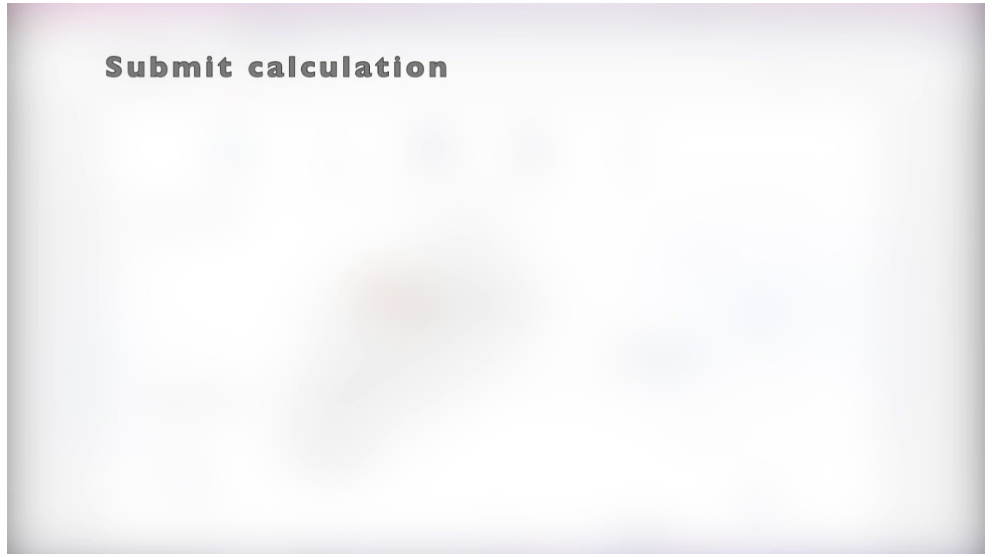
Read the interview with Dr. Carlo A. Pignedoli from Empa, describing how AiiDAlab is used in a mixed theoretical/experimental research group.



For more information and feedback on AiiDAlab, please contact aiidalab@materialscloud.org.

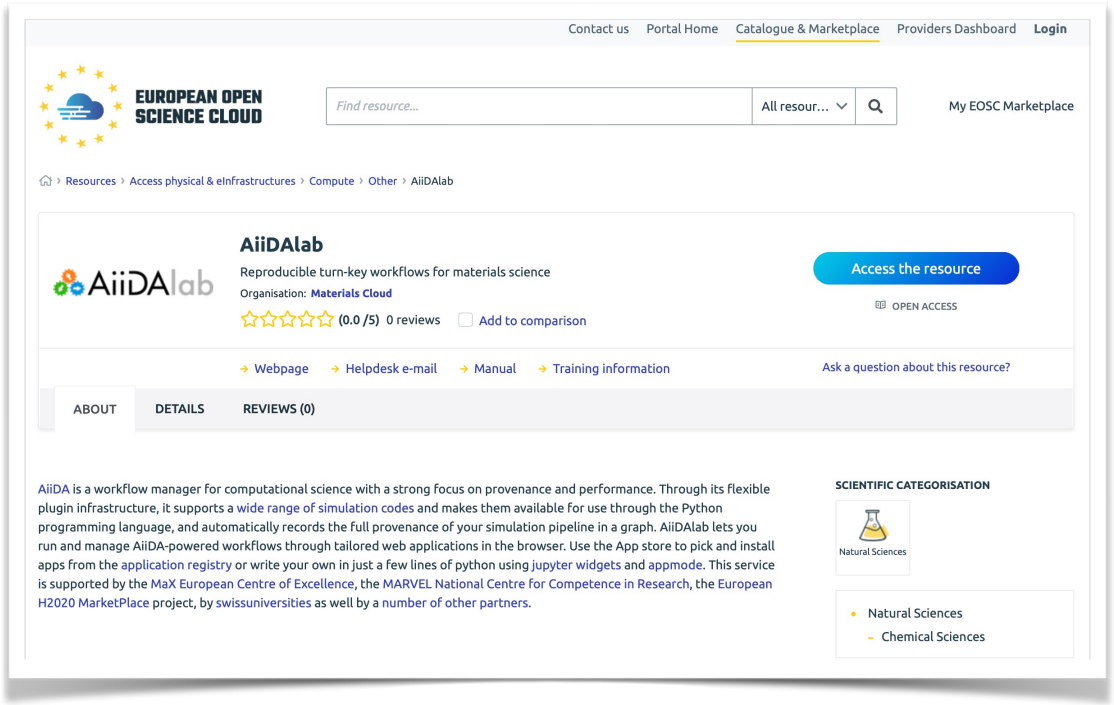
Acknowledgements

The AiiDAlab is supported by the Materials Cloud partners.



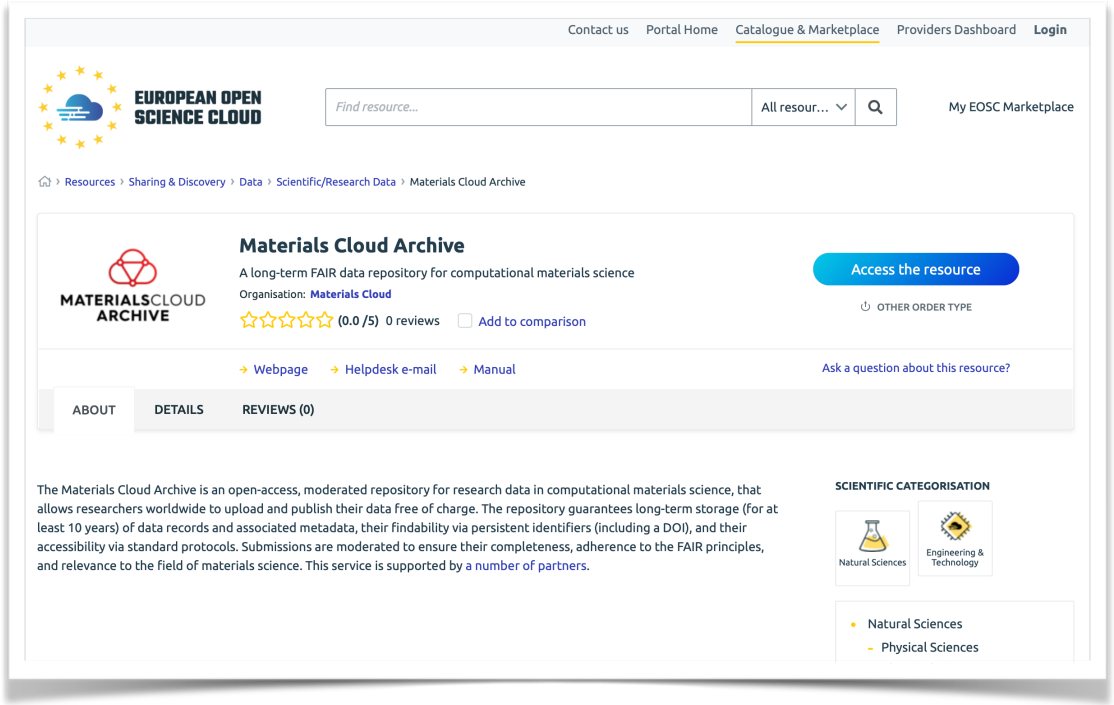
INTEGRATION WITH THE EUROPEAN COMMISSION

Cloud simulations

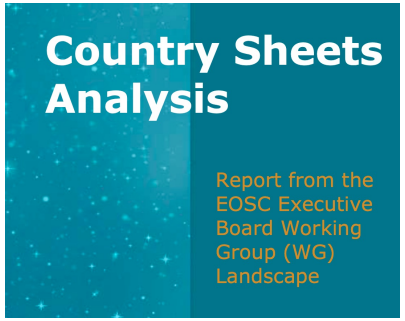


https://marketplace.eosc-portal.eu/services/aiida-lab

Repository and long-term storage



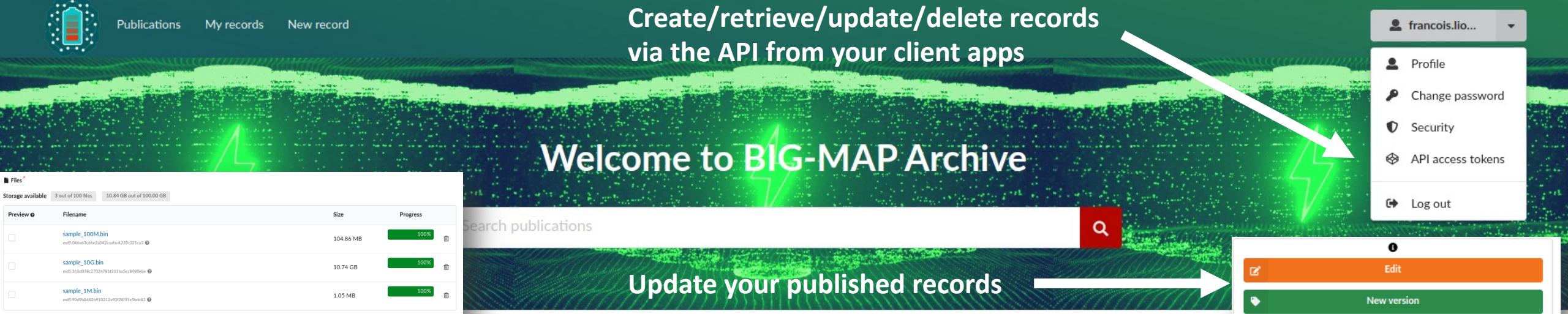
https://marketplace.eosc-portal.eu/services/materials-cloud-archive



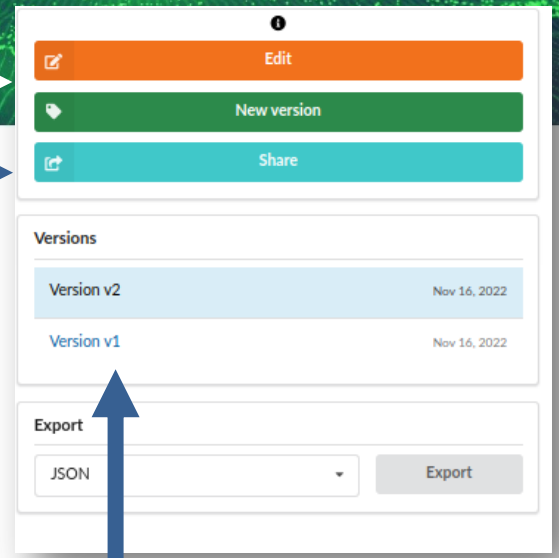
Example of good practice

HPC and EOSC collaboration and training

Materials design at eXascale (MAX) is currently collaborating with EOSC and has already participated in key events throughout 2019, including the EOSC-hub Week. Such tools as AiiDA and Materials Cloud Archive are paving the way for new computational materials science and for granting streamlined access to HPC. MAX also performs tutorials using Virtual Machines, in particular the Quantum Mobile.



Update your published records



Collaborate with others

A Repository for Sharing Files within the BIG-MAP Community

Easily upload files (up to 100 GB per record)

Open for BIG-MAP participants from Dec 1 2022.

InvenioRDM v9 Community feature, from early 2023, will allow a second private tier for Battery 2030+ participants

Later, push button to publish on Materials Cloud Archive

Upload
Upload files up to 100 GB in size & of any format.

Publish
Make your files available to other BIG-MAP members.

Search
Search for records with ease.

Download
Download files of published records.

Leverage API
Exchange files with the archive from your own client applications.

Update
Create new versions of your published records.

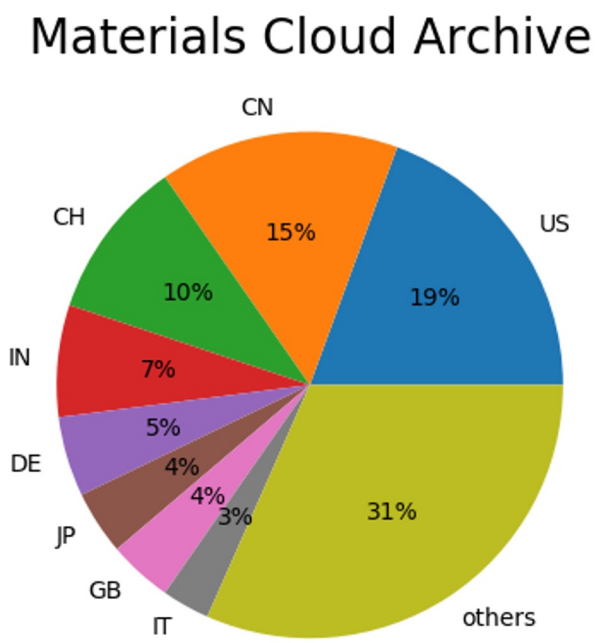
Easily navigate between different versions of your published records

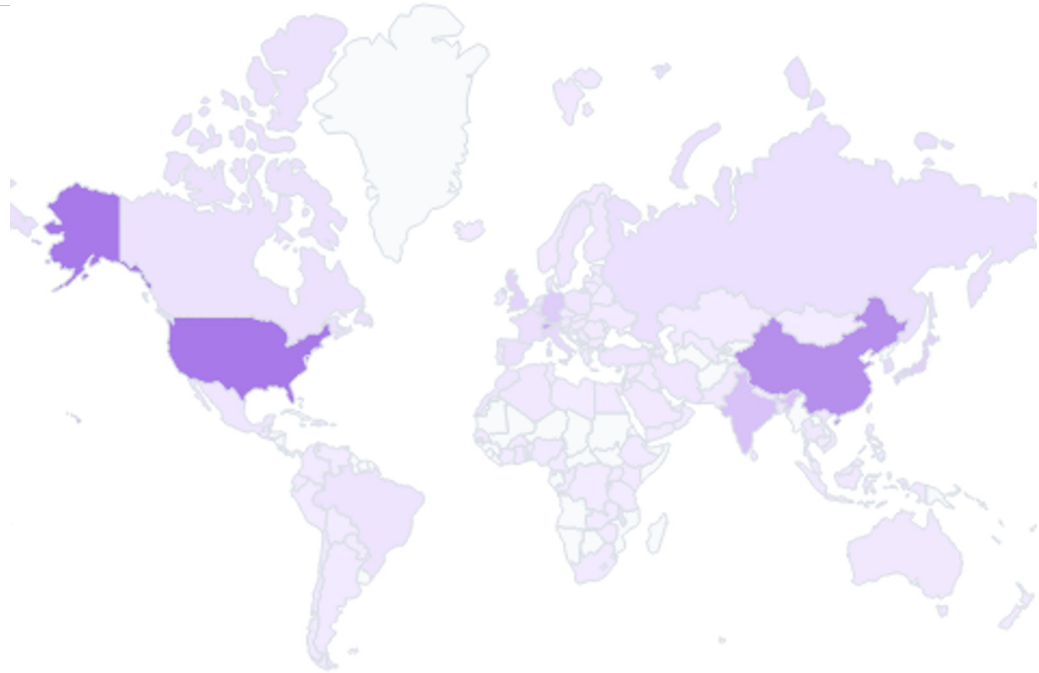
Available at https://archive.big-map.eu/

BATTERY 2030+

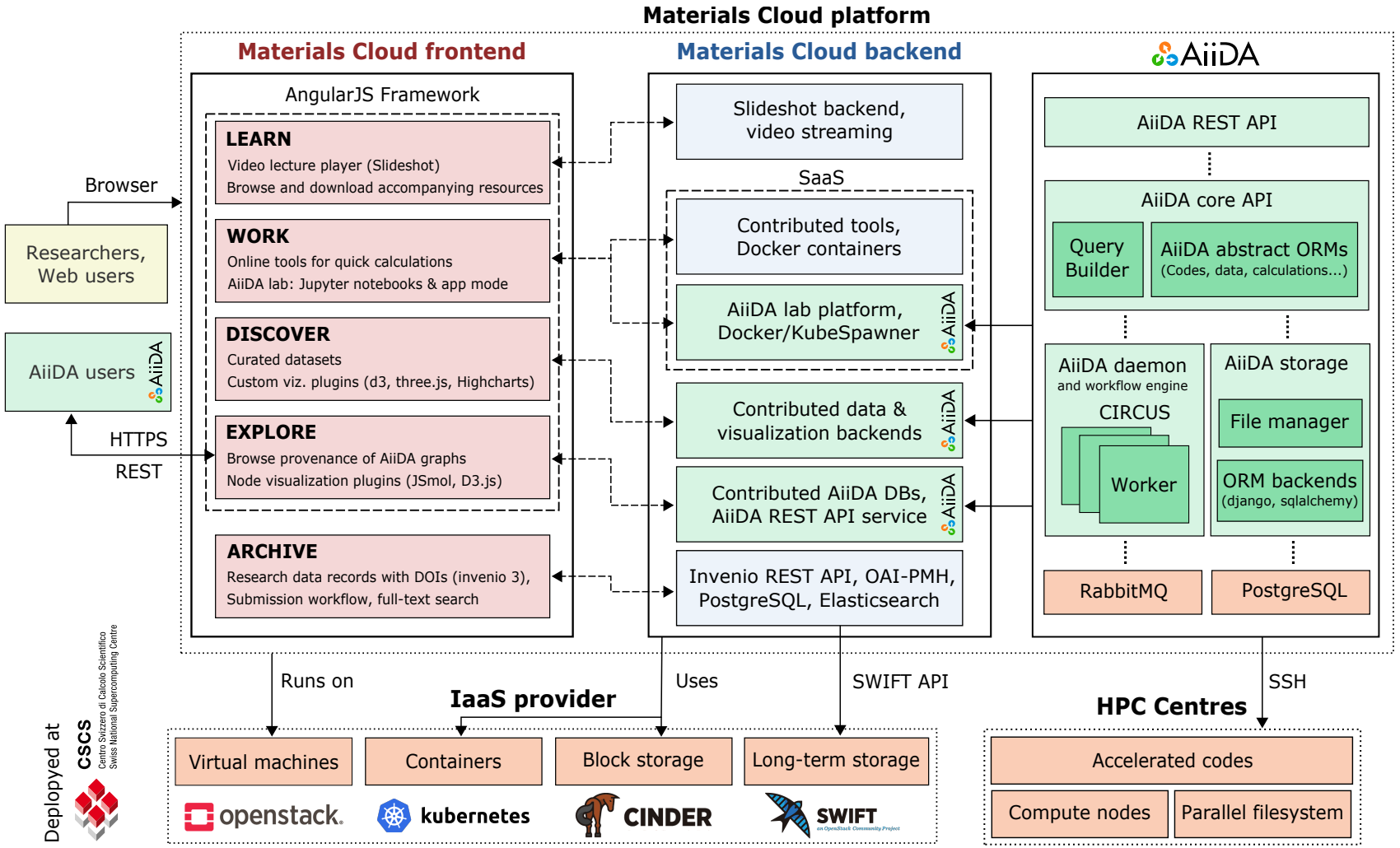
ACCESS AND STATISTICS

- 16,000 unique visitors monthly; 2,500 to the Archive
- No cookies, all open access





MATERIALS CLOUD DEPLOYMENT



Recommended by

SCIENTIFIC DATA

European Commission
Open Research Europe

Swiss National Science Foundation

Indexed by

re3data.org
REGISTRY OF RESEARCH DATA REPOSITORIES
http://doi.org/10.17616/R3ZJ5W
Materials Cloud Archive

FAIRsharing.org
standards, databases, policies

GO FAIR

Google Dataset Search

EUDAT Collaborative Data Infrastructure
Data shared and preserved across borders and disciplines

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

CONCLUSIONS – THE NEED FOR DIGITAL INFRASTRUCTURES

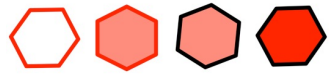
- Computational science is central to the entire scientific and technological effort in the 21st century – no other enabler can compete in terms of speed and acceleration

- Not many policymakers, or even the scientific community at large, have understood its structural needs, and long-term opportunity

- As a side note, it is a powerfully democratic force, that can be shared worldwide at the flick of a switch.

BROADER FINAL THOUGHTS

- Switzerland could do a fantastic job in leveraging competencies and resources if we **move from Institution-wide efforts to domain-wide efforts** - i.e., not having an EPFL, an ETHZ, a PSI, etc... repository, but flagship efforts on domains (synchrotron, XPS, catalysis, planets, computational, etc...). This is what the community needs - **having data on the same topic fragmented across institutions makes them rarely useful or usable.**
- **Data can be shown to be valuable when others feel the need to use those** - curation and accessibility are key. Raw experimental and computational data without extensive curation are useless. Key is:
  - **to develop "universal" domain-specific APIs that can be used to interrogate repositories across institutions/centres/etc...** - these are agreed upon by experts in a domain, and ideally engaging international groups like the research data alliance (RDA) or at least key european players.
  - **to insist on curation of data**, where these are accompanied by extensive material that makes it usable, if in a niche domain, or using standard protocols if in a flagship domain
  - people will happily contribute to a domain-wide repository, but **if it's institution-wide it will remain a niche effort**. I would strongly suggest to pool resources across institutions, and consider opening our repositories to the wider community. In many endeavours the cost is the personnel, not the data storage (in other, linked to major facilities, is the opposite)



ACKNOWLEDGEMENTS

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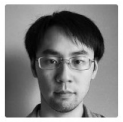

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Executive Committee

The Executive Committee of Materials Cloud is currently formed by:

- Kristjan Eimre (EPFL, Switzerland) [2022-] (representative of the Materials Cloud developers)
- Sara Bonella (EPFL and CECAM, Switzerland) [2020-]
- Carlo Pignedoli (Empa, Switzerland) [2020-]
- Nicola Marzari (EPFL, Switzerland) [2018-]
- Elisa Molinari (Unimore and CNR Nano, Italy) [2018-]
- Giovanni Pizzi (PSI, Switzerland) [2018-]
- Berend Smit (EPFL, Switzerland) [2018-]
- Joost VandeVondele (ETHZ and CSCS, Switzerland) [2018-]
- Tejs Vegge (DTU, Denmark) [2020-]

Materials Cloud@HPC Board

The Materials Cloud@HPC Board, created in late 2020, is currently formed by:

- Fabio Affinito (CINECA, Italy)
- Pekka Manninen (CSC, Finland)
- Giovanni Pizzi (PSI, Switzerland) (Materials Cloud representative)
- Dirk Pleiter (JSC, Germany)
- Joost VandeVondele (CSCS, Switzerland)

FUNDING

http://theossrv1.epfl.ch
Theory and Simulation of Materials (2011 onwards)

http://nccr-marvel.ch
Swiss National Centre for Computational Design and Discovery of Novel Materials (2014-26)

http://max-centre.eu
H2020 Centre of Excellence MaX: Materials Design at the Exascale (2015-26)

https://www.psi.ch/en/lms
Laboratory for Materials Simulations (2021 onwards)

https://www.big-map.eu
H2020 Battery Interface Genome – Materials Acceleration Platform (Battery 2030+, 2020-23, …)

https://www.uni-bremen.de/mapex
U Bremen Excellence Chair (2018-25)

H2020 Nanoscience Foundries and Fine Analysis
H2020 European Materials Modelling Council
H2020 Marketplace
H2020 Intersect
H2020 DOME 4.0
H2020 OpenModel
H2020 NEP
H2020 EPFL Fellows
H2020 EPFL Innovators
H2020 Marie Curie
EPFL Open Science
NCCR Catalysis
PASC
PRACE
Constellium
IBM
Innosuisse
Robert Bosch StiftungSolvay
Samsung
Richemont Varinor