Demo of Materials Cloud and AiiDAlab: integrated platforms for FAIR computational materials science

Giovanni Pizzi (EPFL); Carlo Pignedoli (Empa)

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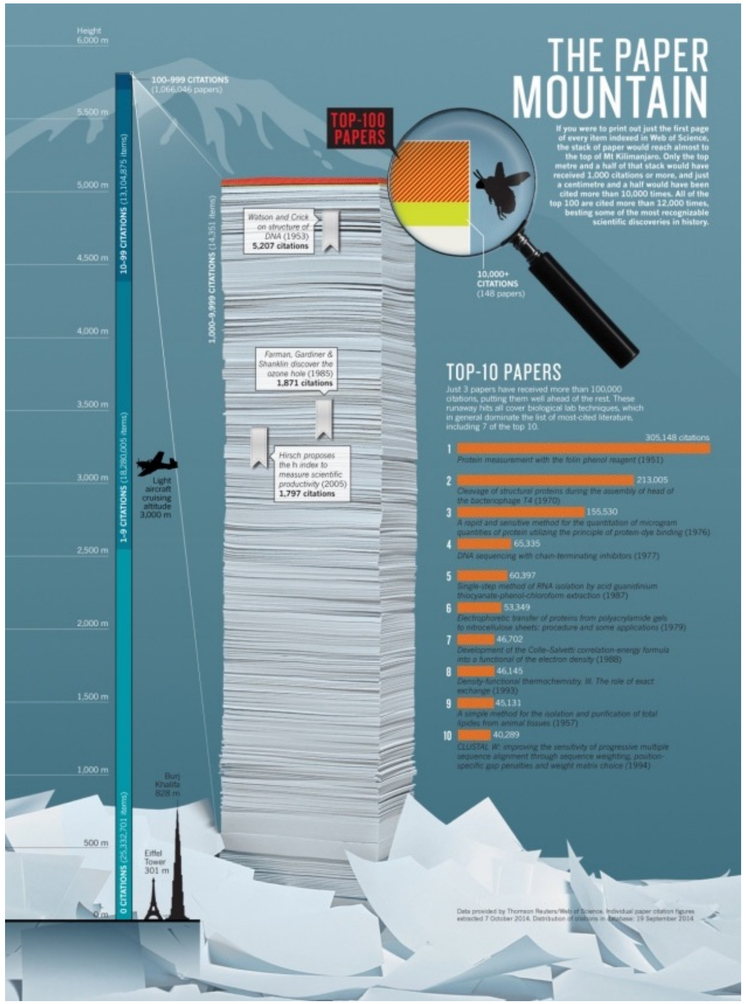
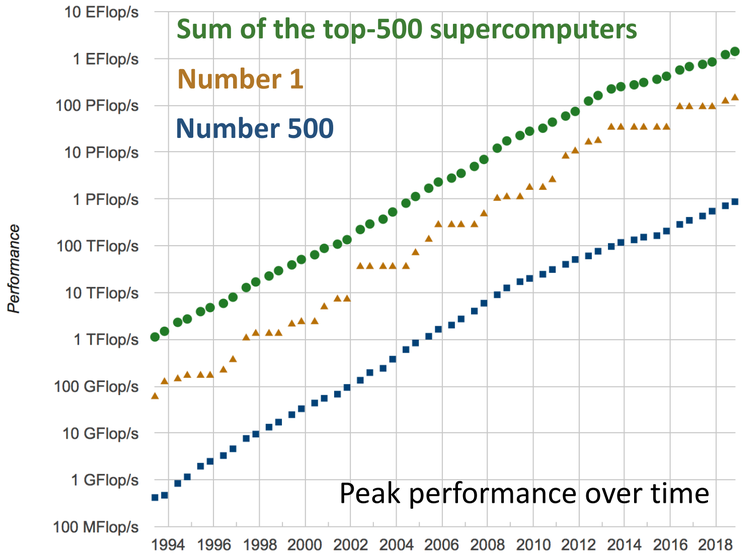
DFT materials simulations



Van Noorden et al., Nature 514, 550 (2014)

Our research: Materials simulations

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



Accuracy and predictive power of quantum engines

150,000x increase in the past 20 years

1 month (2001)

↓

10 seconds (2021)

DFT materials simulations

Van Noorden et al., Nature 514, 550 (2014)

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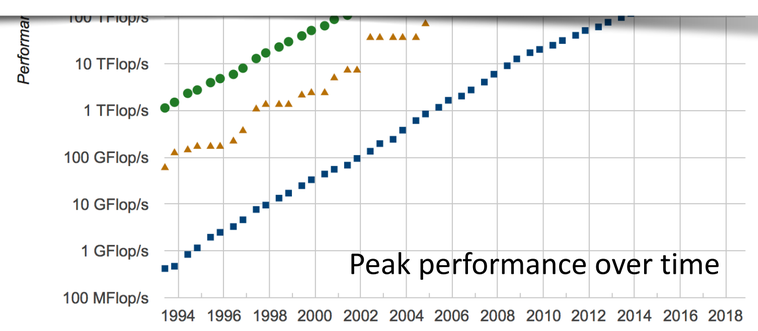
Combined: materials design and discovery via ***high-throughput computations***



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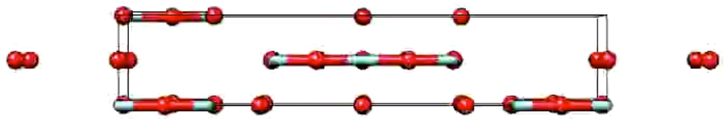
Leverage supercomputers to compute and predict materials properties



Aim: Compute properties for all of them
(and even new, invented ones)
and **discover novel functional materials**

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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

AiiDA

- **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

MIT LICENSED

open source initiative

Scalable workflow engine

Built-in support for HPC

Automated full data provenance

Flexible plugin system

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

S.P. Huber et al., Scientific Data 7, 300 (2020)

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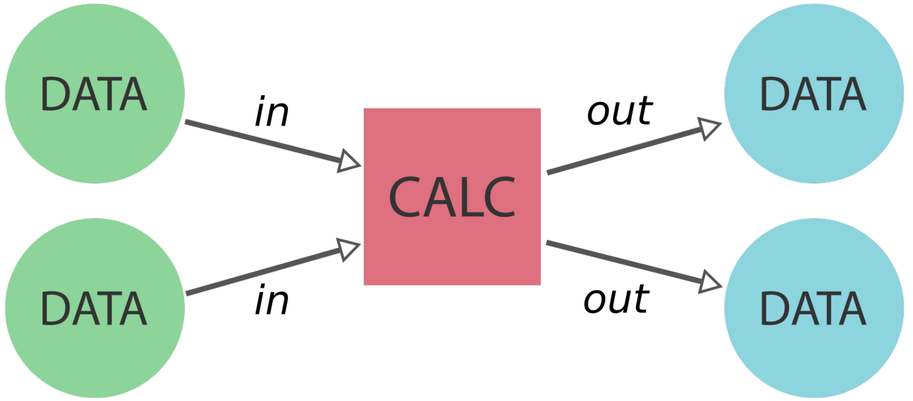
Data provenance

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**



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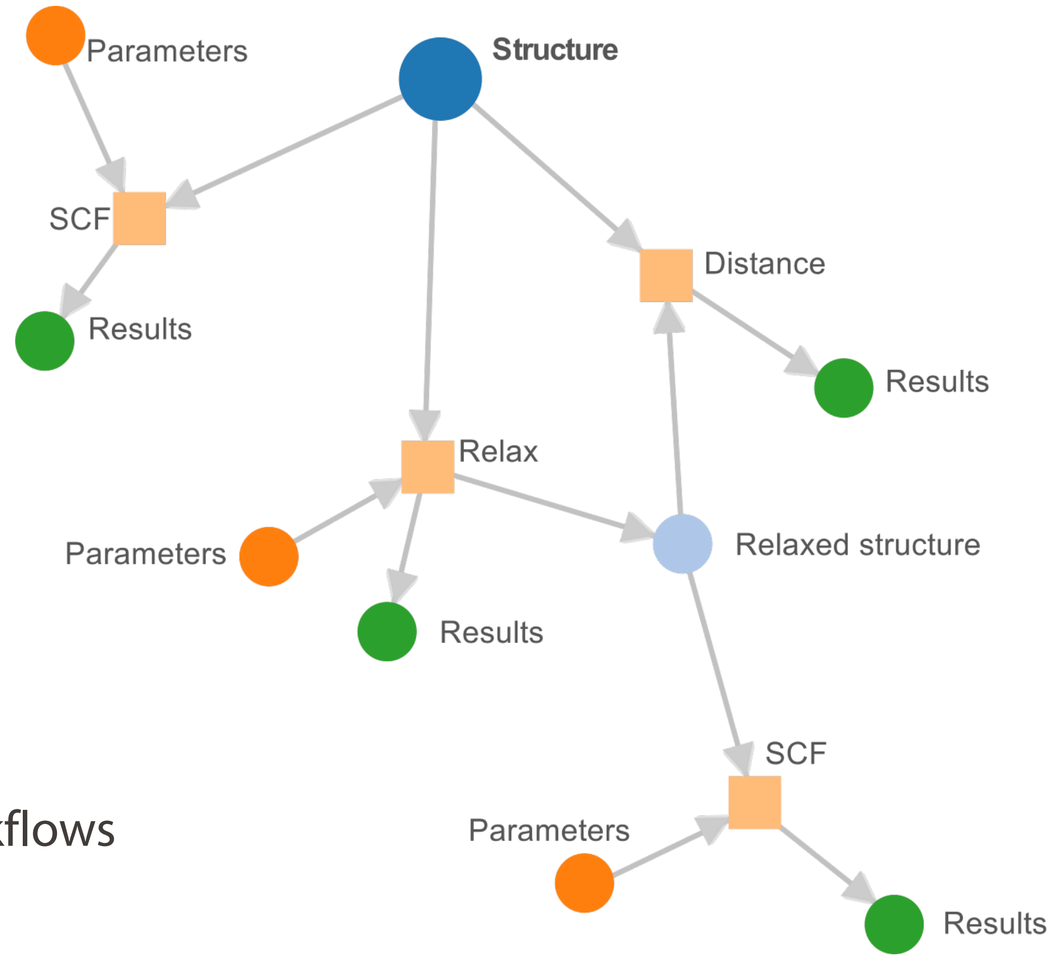

Provenance graphs

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

Data provenance

Simple recipe

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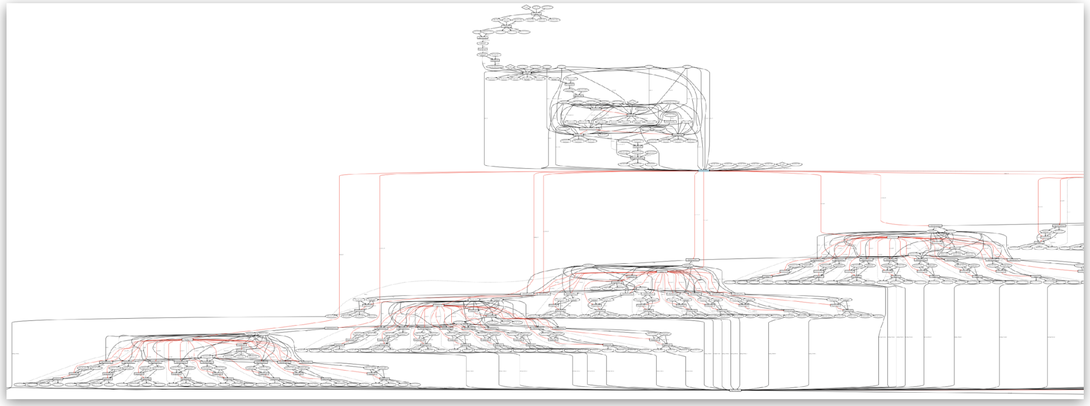
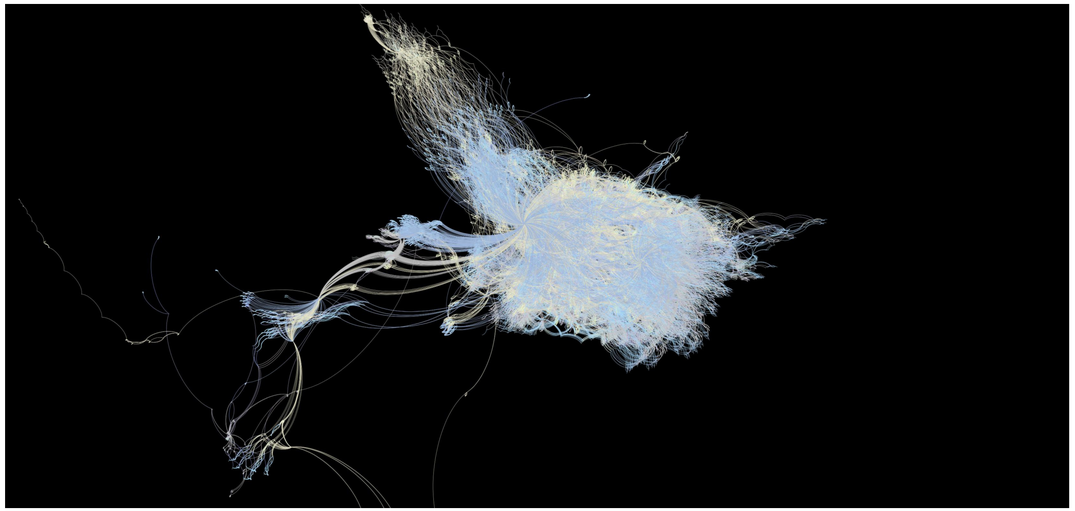


Molecular dynamics study of Lithium in a solid electrolyte

Graph requirements

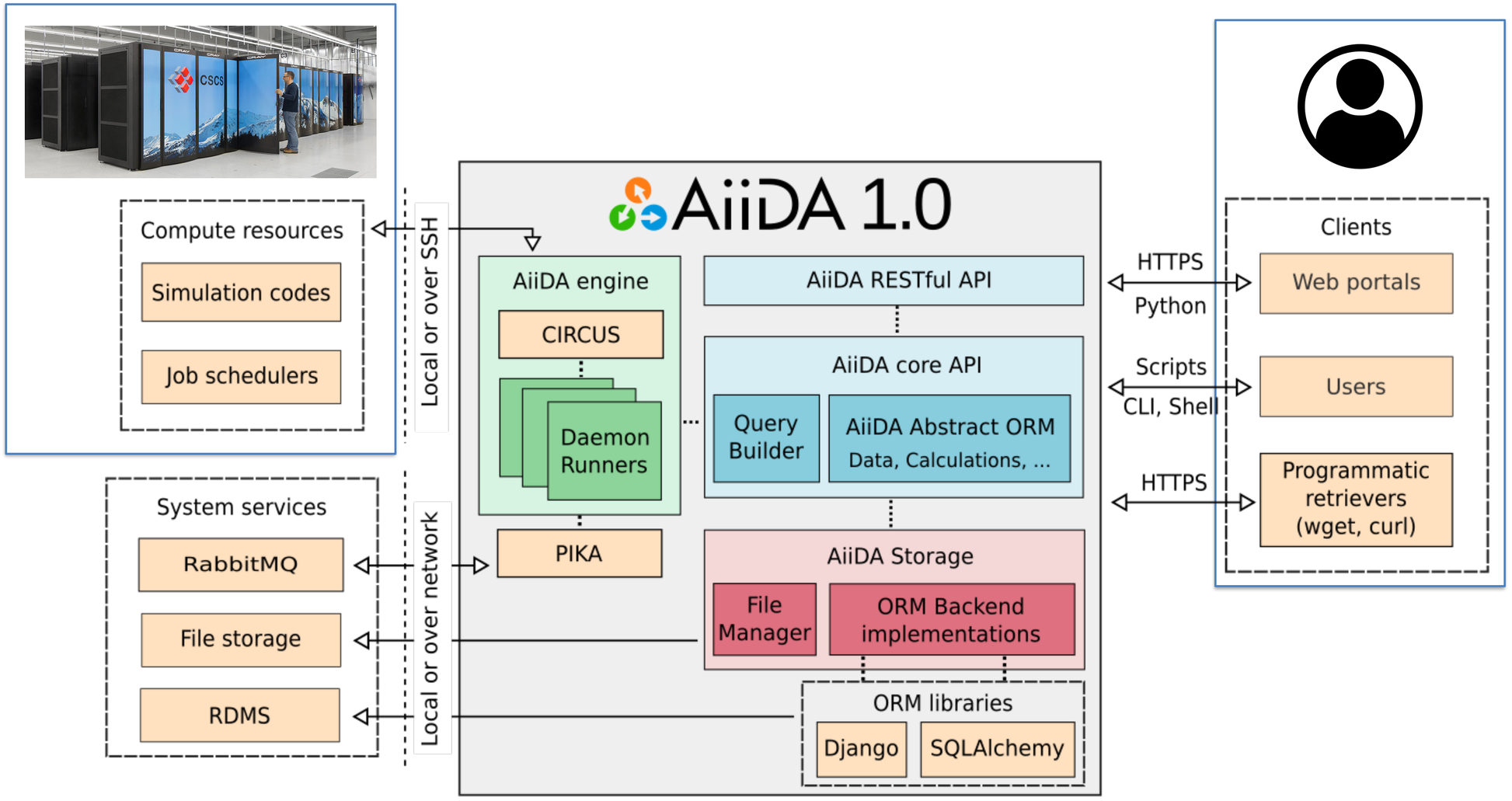
- Needs to be automated
- Needs to be stored *as data is created*

Complexity grows quickly even for simple workflows: impossible to reconstruct *a posteriori*
without a tool like AiiDA

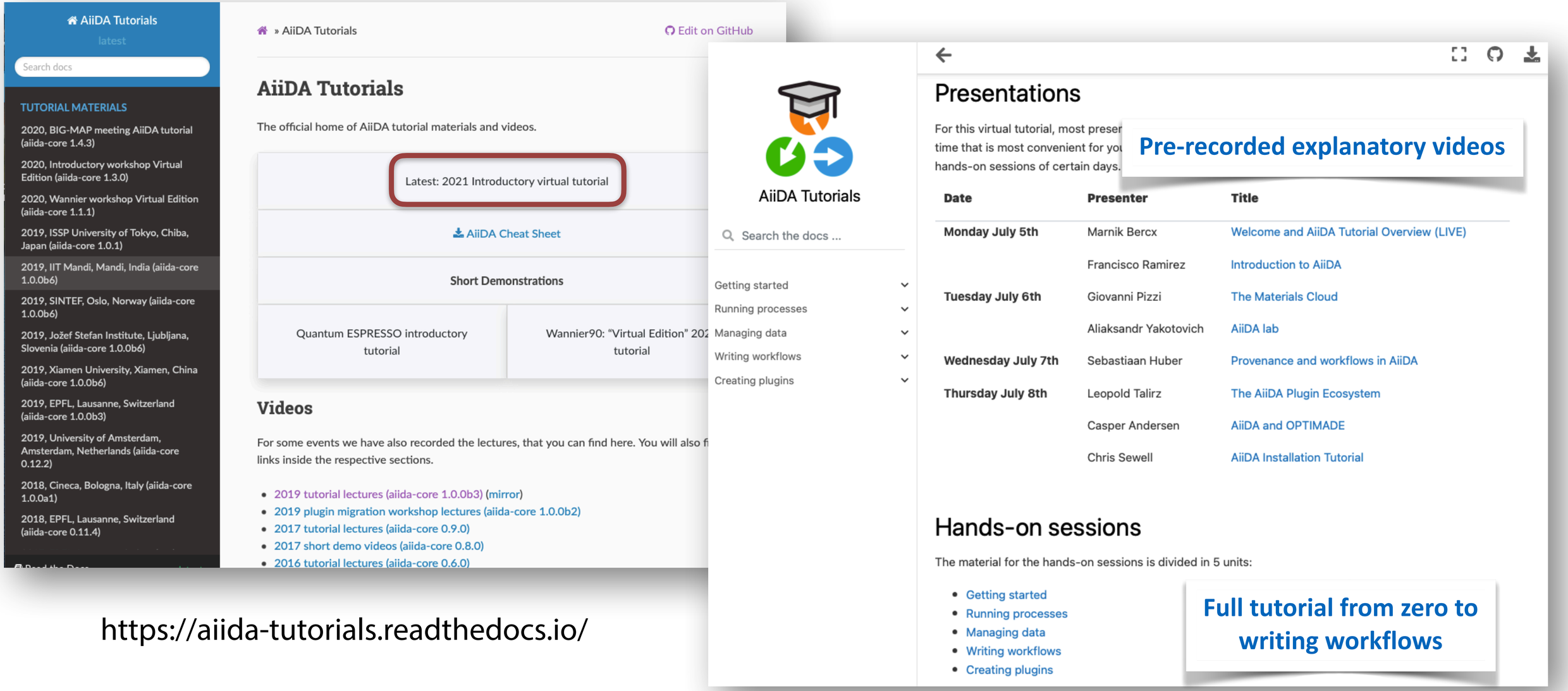


Graphical representation of actual AiiDA database

AiiDA architecture



AiiDA tutorials

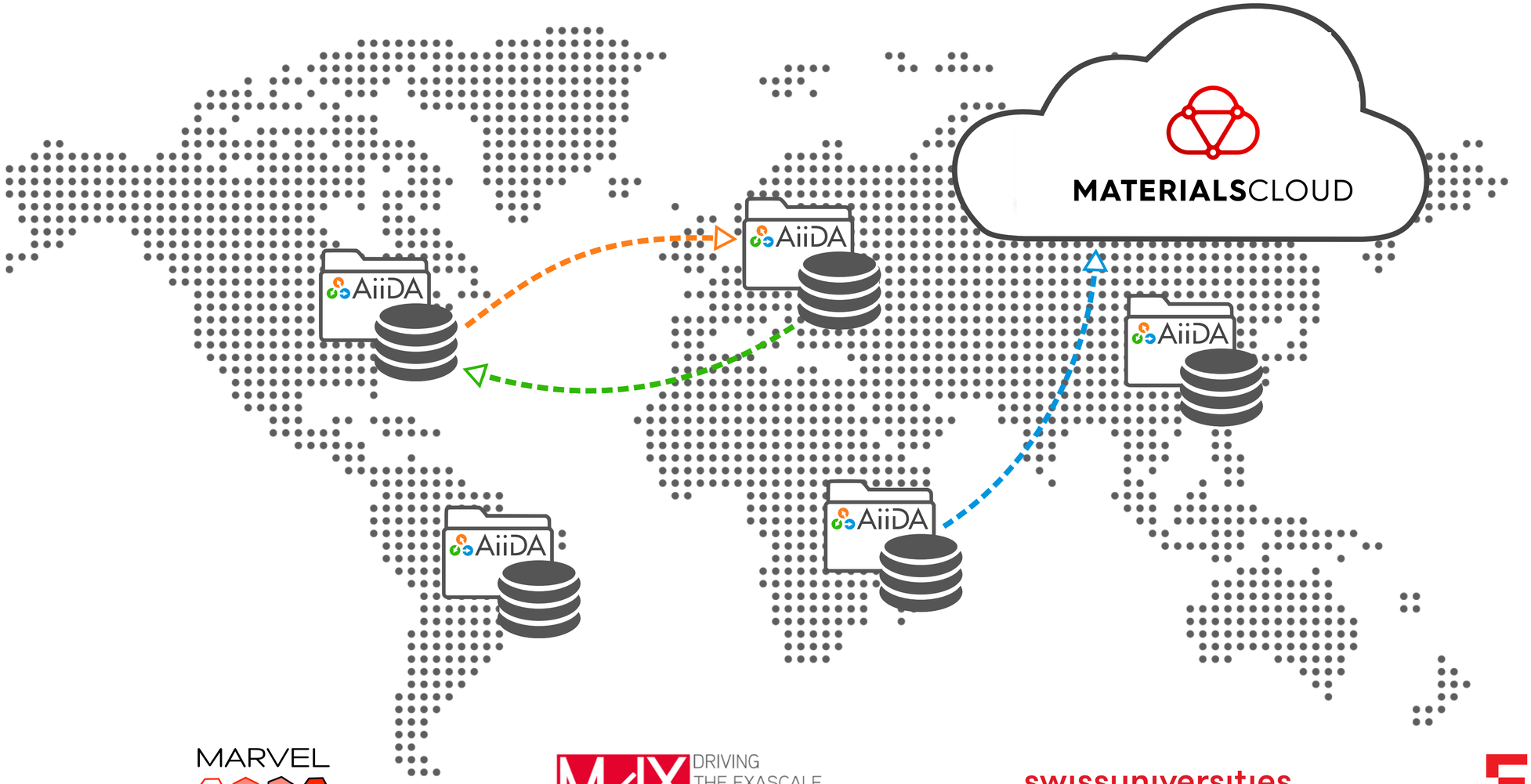


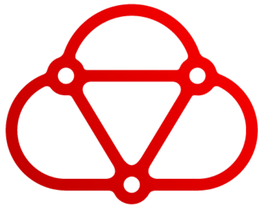
https://aiida-tutorials.readthedocs.io/

FAIR **data** access and sharing

FAIR sharing in AiiDA: data and graphs

- Share directly between private AiiDA instances
- Share on **online repositories**





MATERIALSCLOUD

https://www.materialscloud.org

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

Materials Cloud is also a GO FAIR *implementation network*

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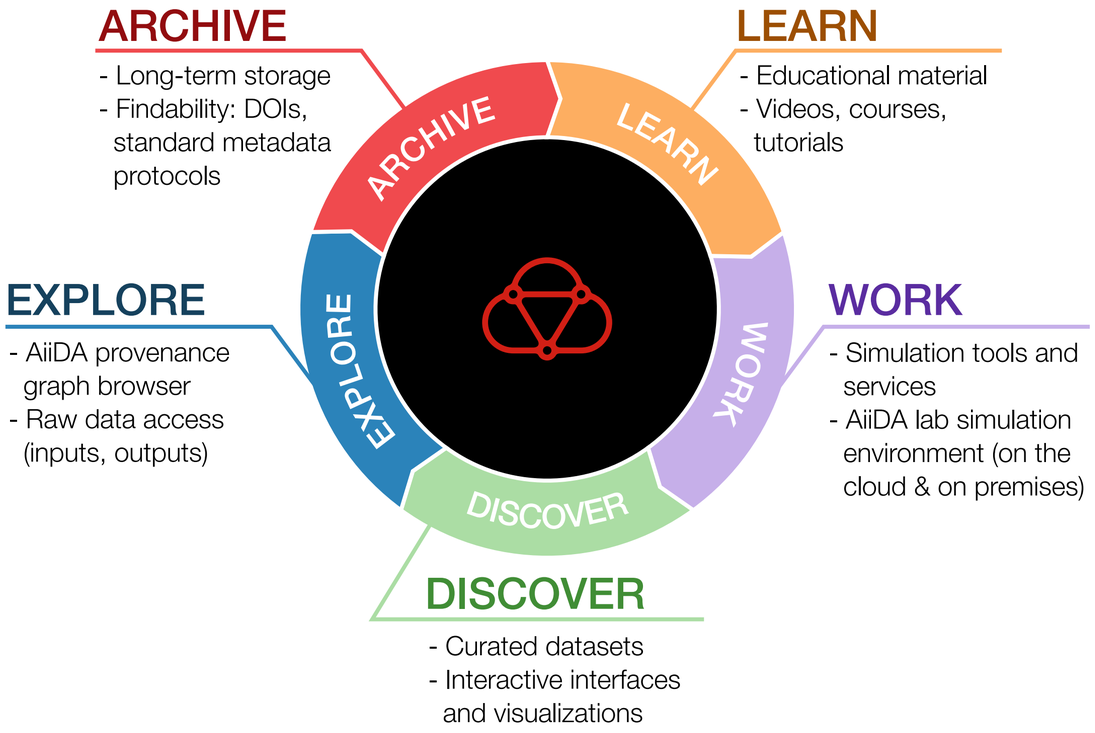
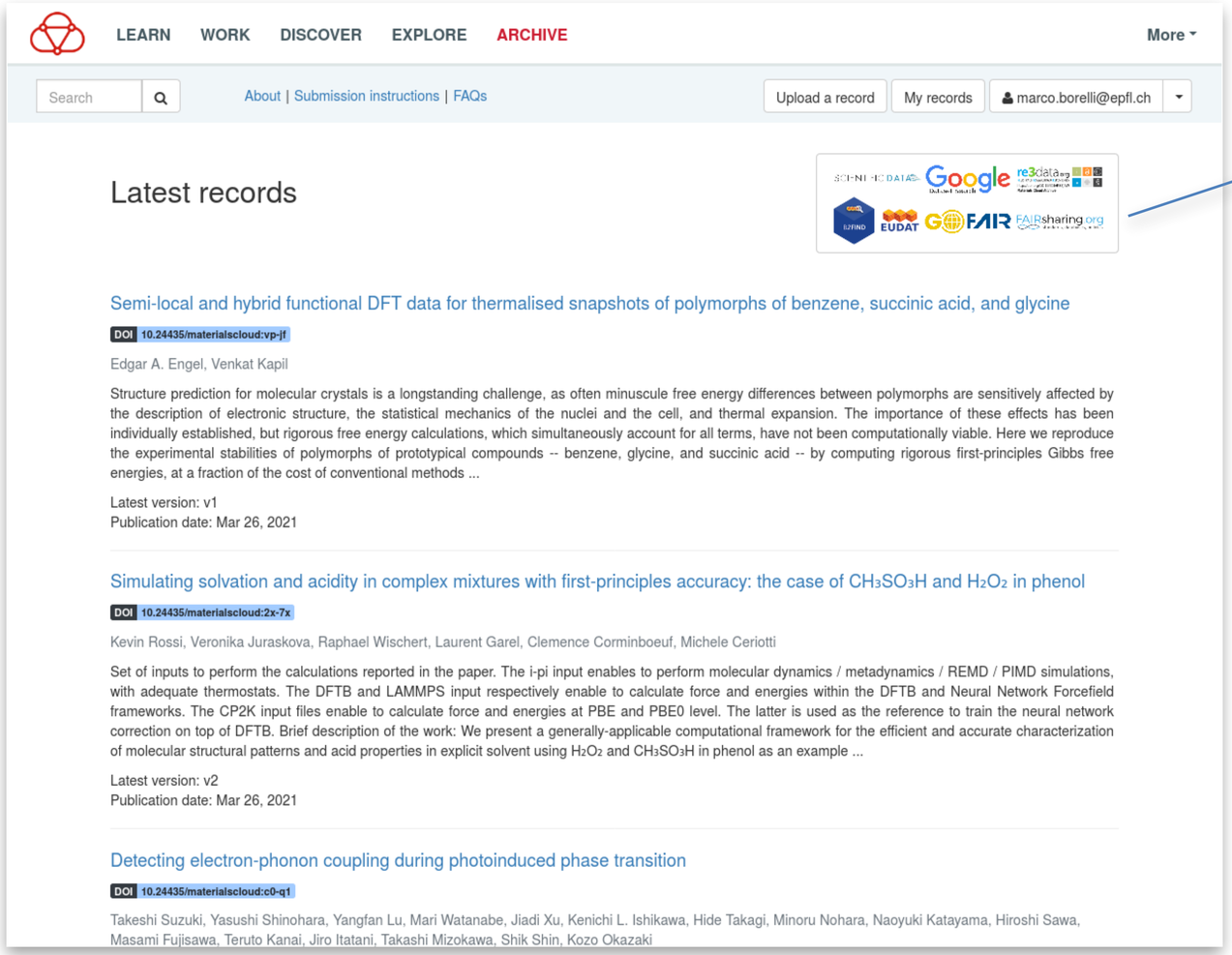
Materials Cloud

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



FAIR data sharing: **Archive, Discover, Explore**



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

European Commission

Research and Innovation

Open Research Europe

https://open-research-europe.ec.europa.eu/for-authors/data-guidelines

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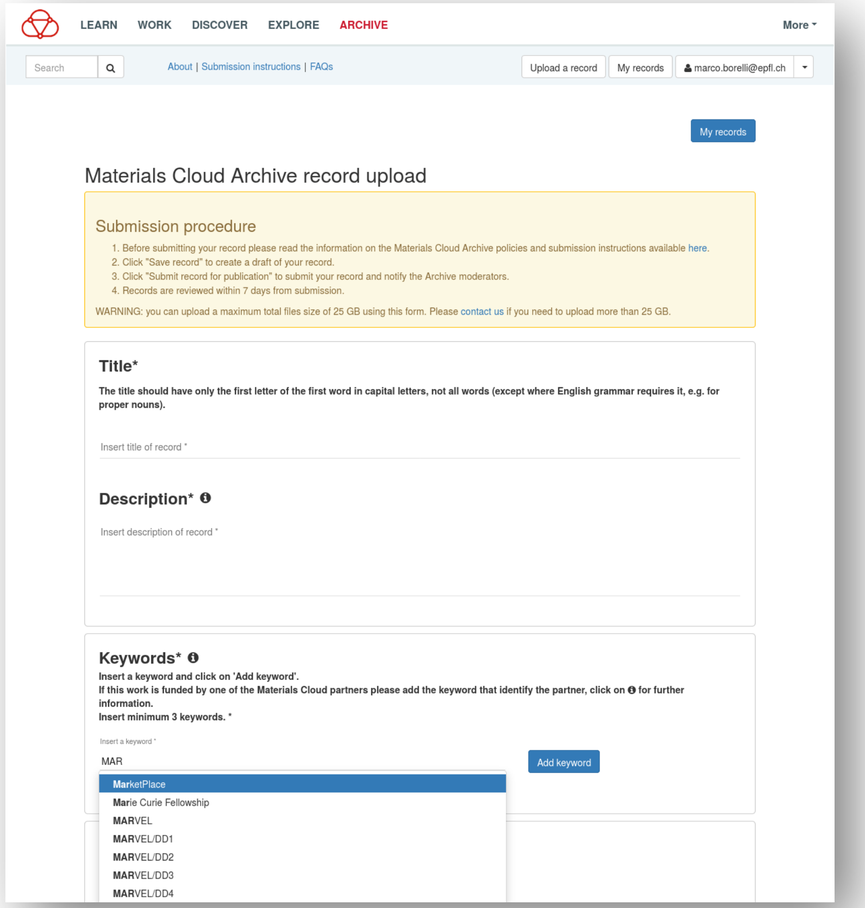
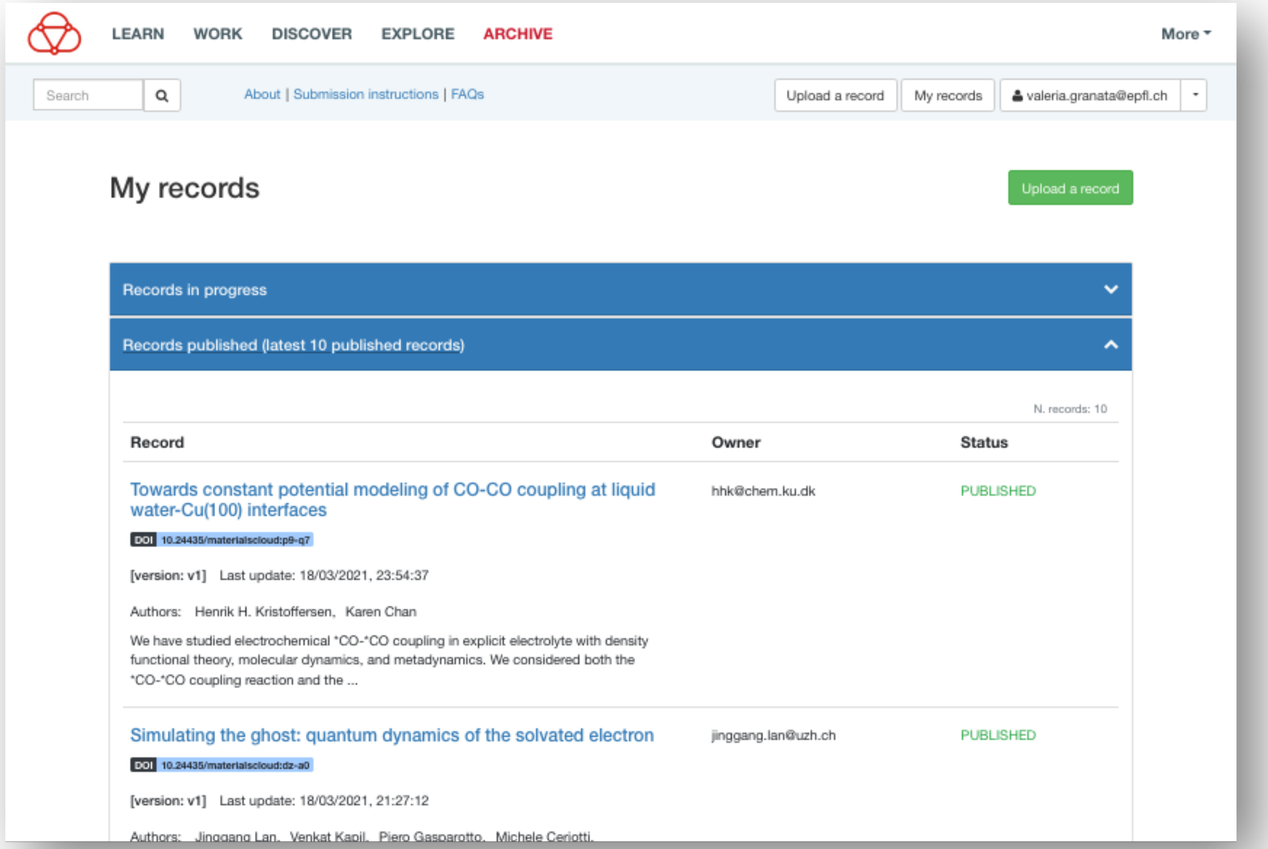
Interface for users submitting data

Submission form



User view (own entries)



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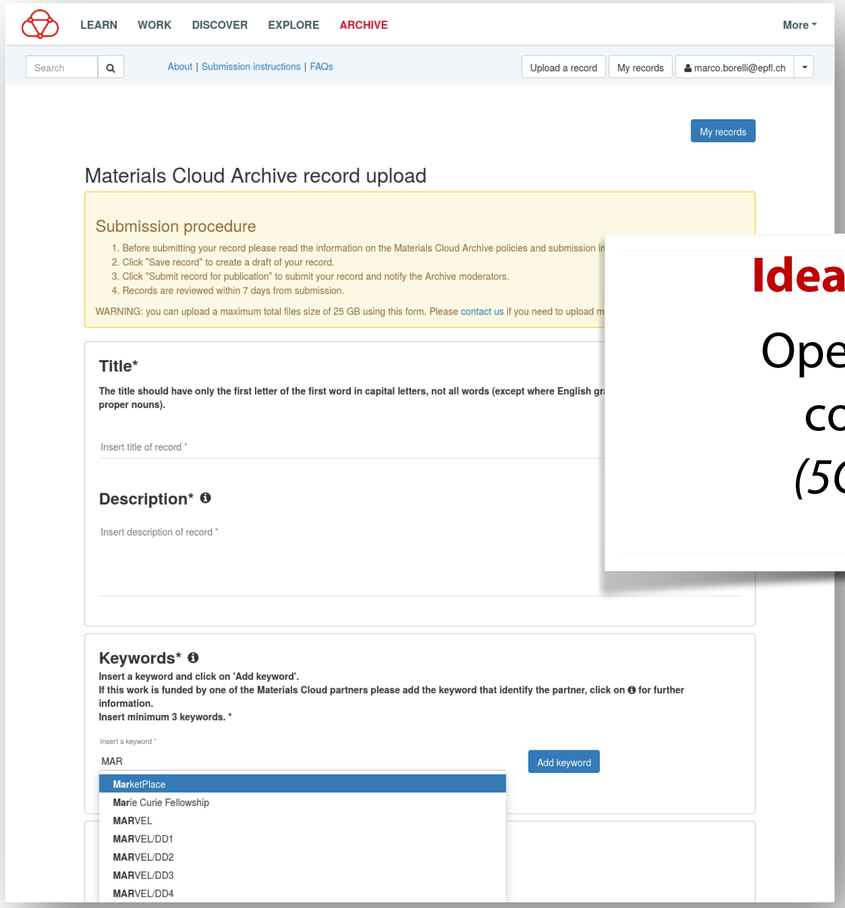

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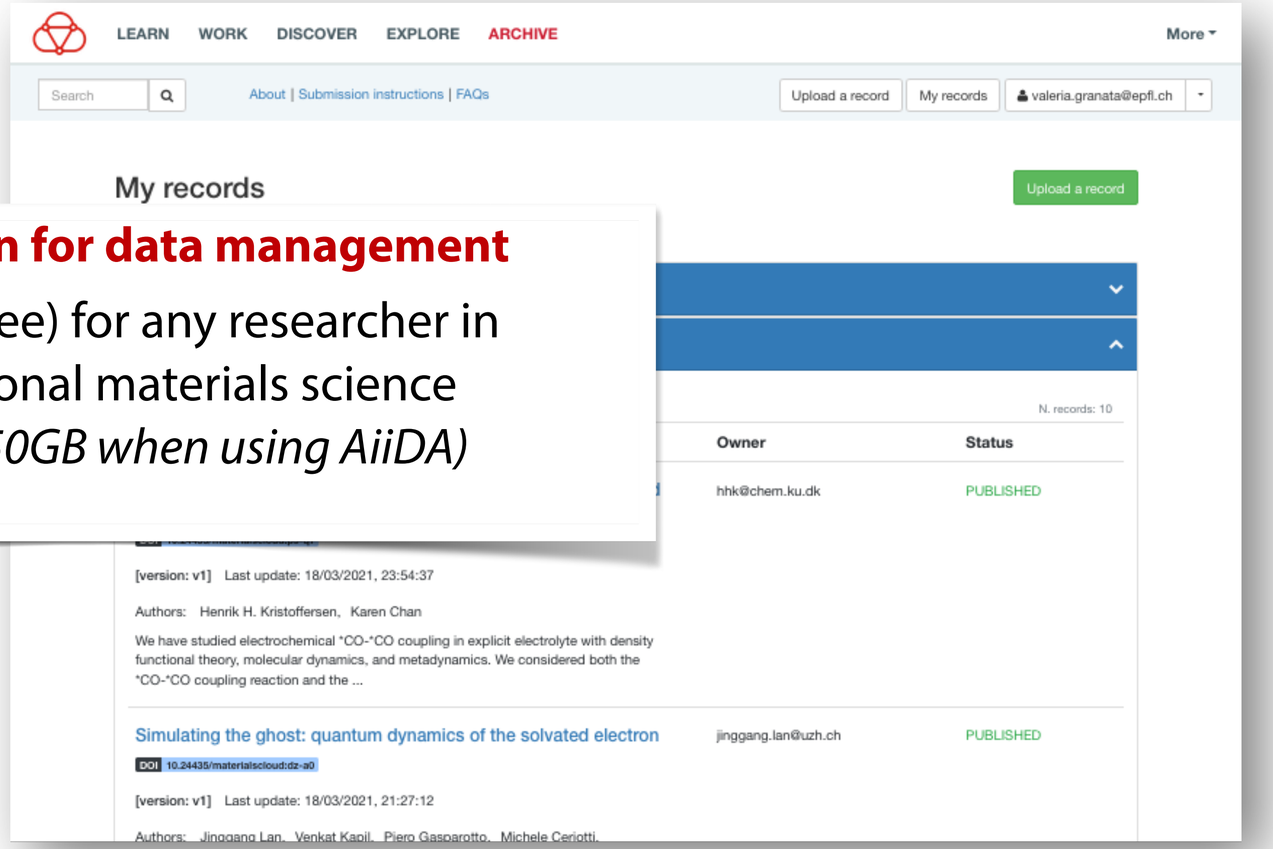


Ideal solution for data management

Open (and free) for any researcher in computational materials science

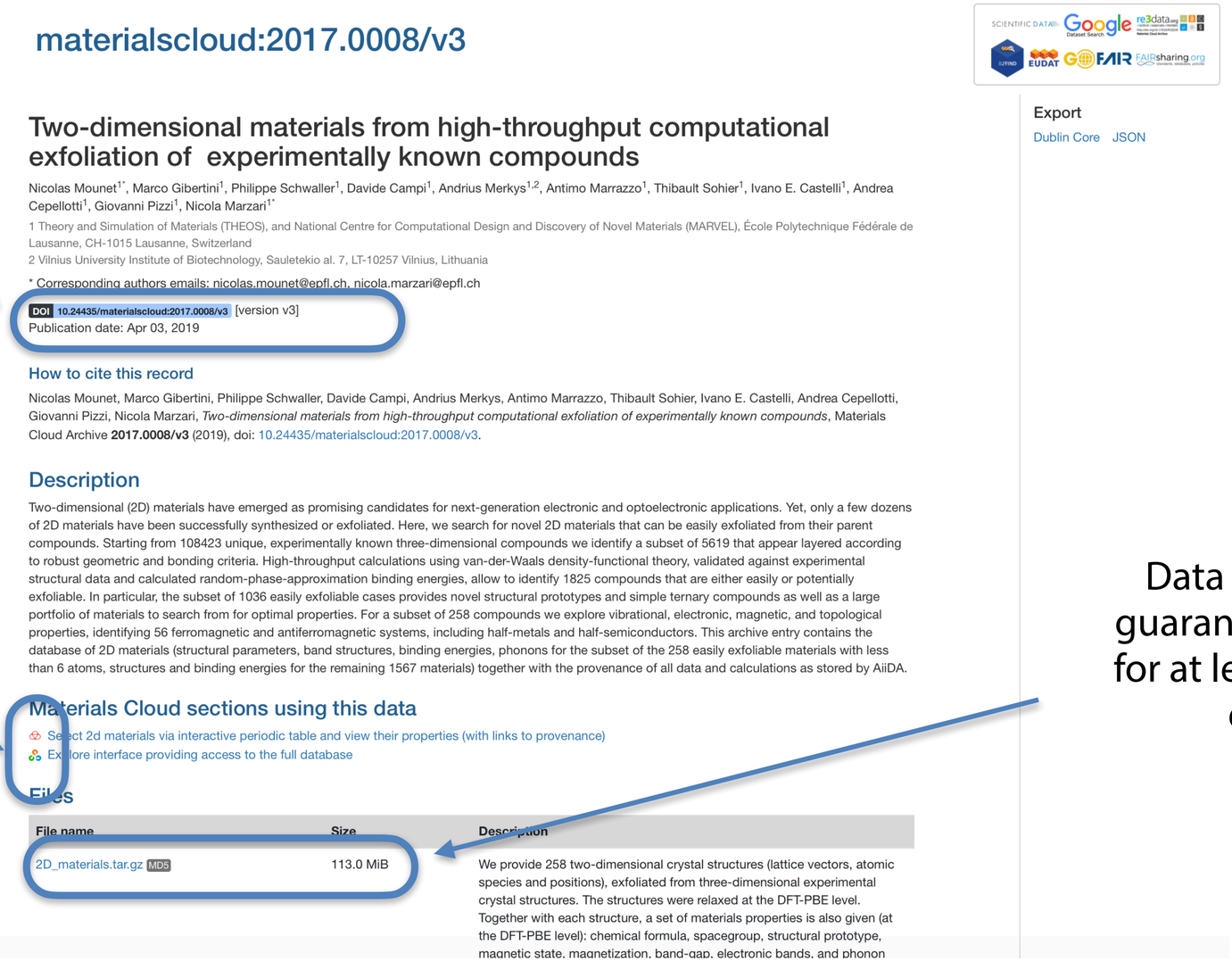
(5GB limit, 50GB when using AiiDA)

Open data sharing: **Archive, Discover, Explore**

DOIs assigned

Direct links to Discover & Explore

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



materialscloud:2017.0008/v3

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

Nicolas Mounet[1*], Marco Gibertini[1], Philippe Schwaller[1], Davide Campi[1], Andrius Merkys[1,2], Antimo Marrazzo[1], Thibault Sohier[1], Ivano E. Castelli[1], Andrea Cepellotti[1], Giovanni Pizzi[1], Nicola Marzari[1*]

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DOI 10.24435/materialscloud:2017.0008/v3 [version v3]
Publication date: Apr 03, 2019

Export
Dublin Core JSON

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.

Description

Two-dimensional (2D) materials have emerged as promising candidates for next-generation electronic and optoelectronic applications. Yet, only a few dozens of 2D materials have been successfully synthesized or exfoliated. Here, we search for novel 2D materials that can be easily exfoliated from their parent compounds. Starting from 108423 unique, experimentally known three-dimensional compounds we identify a subset of 5619 that appear layered according to robust geometric and bonding criteria. High-throughput calculations using van-der-Waals density-functional theory, validated against experimental structural data and calculated random-phase-approximation binding energies, allow to identify 1825 compounds that are either easily or potentially exfoliable. In particular, the subset of 1036 easily exfoliable cases provides novel structural prototypes and simple ternary compounds as well as a large portfolio of materials to search from for optimal properties. For a subset of 258 compounds we explore vibrational, electronic, magnetic, and topological properties, identifying 56 ferromagnetic and antiferromagnetic systems, including half-metals and half-semiconductors. This archive entry contains the database of 2D materials (structural parameters, band structures, binding energies, 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.

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

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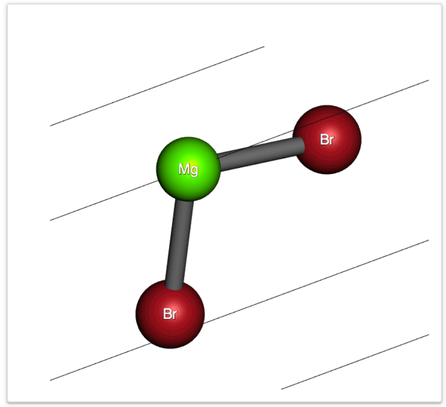
Open data sharing: **Archive, Discover, Explore**

DISCOVER

Compound: $MgBr_2$



Info and properties

See definitions...

Formula: $MgBr_2$
Spacegroup: P-3m1
Pointgroup: -3m
Prototype: CdI2
Band gap [eV]: 4.8

Magnetic properties:
- Magnetic State: non-magnetic
- Tot. Magnetization [μB/cell]: -
- Abs. Magnetization [μB/cell]: -

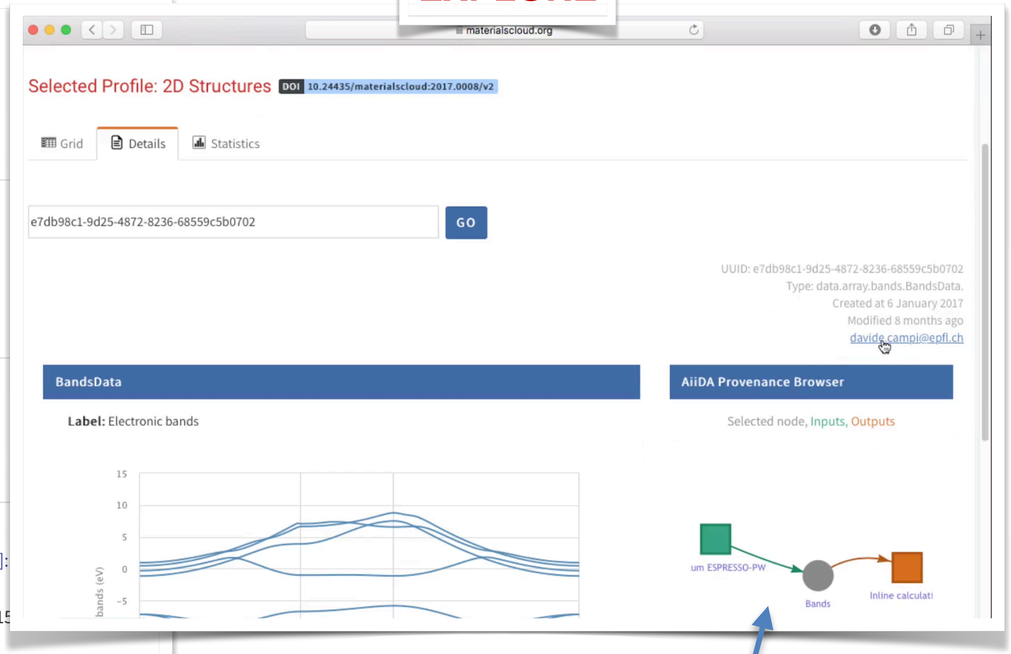
Binding Energies:
- DF2-C09 Binding energy [meV/Å^2]: (From parent COD 9009107)
- rVV10 Binding energy [meV/Å^2]: 15 (From parent COD 9009107)

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

EXPLORE



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

Data management plans (DMP) 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

- **+ reproducible** thanks to *full provenance*

- We provide DMP templates for researchers using Materials Cloud

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

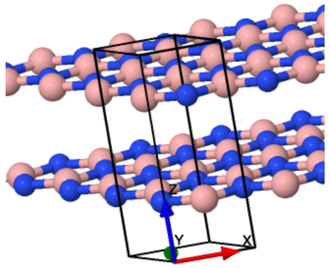
Feel free to contact us with any questions regarding the use of the Materials Cloud Archive as part of your data management plan.

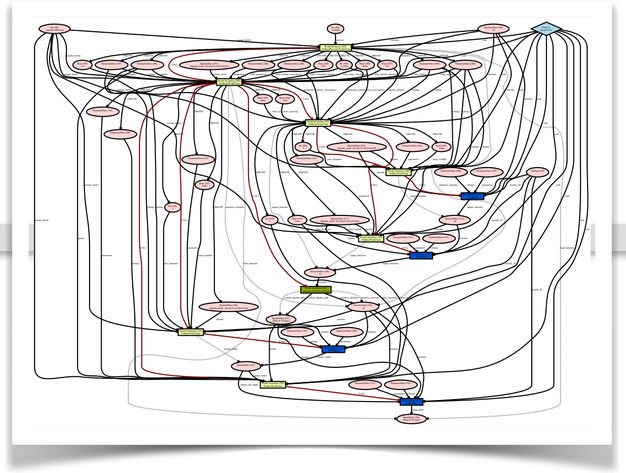
Funding Body	DMP template (using AiiDA)	DMP template (no AiiDA)
SNF	.docx .odt .pdf	.docx .odt .pdf
H2020	.docx .odt .pdf	.docx .odt .pdf

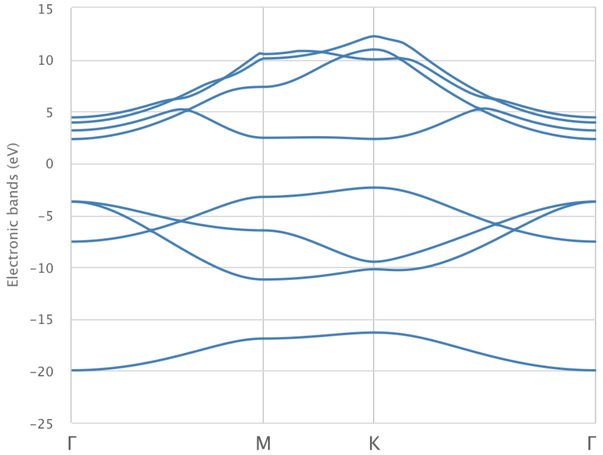
Beyond FAIR *data* sharing: FAIR **simulation** access

Workflows to generate data

- Given a material, we compute advanced quantities: often non-trivial, result of a complex workflow

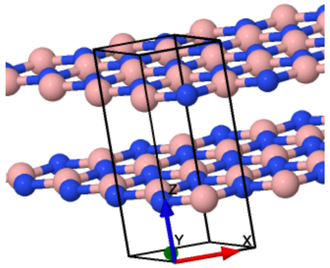


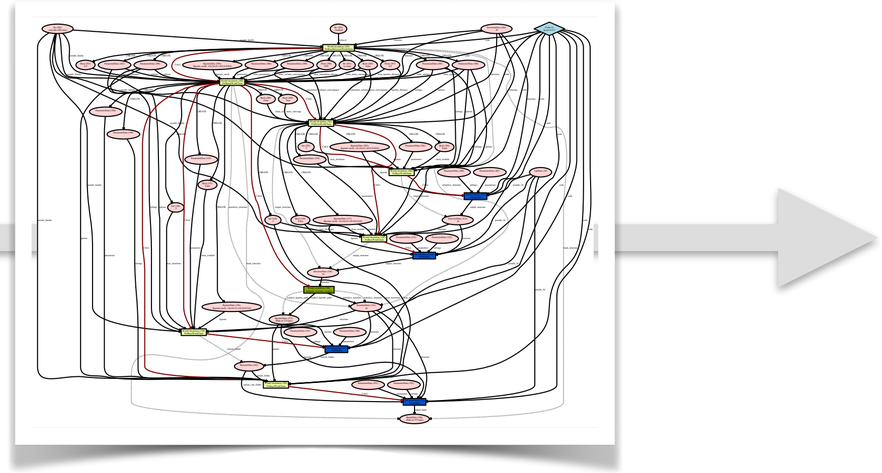


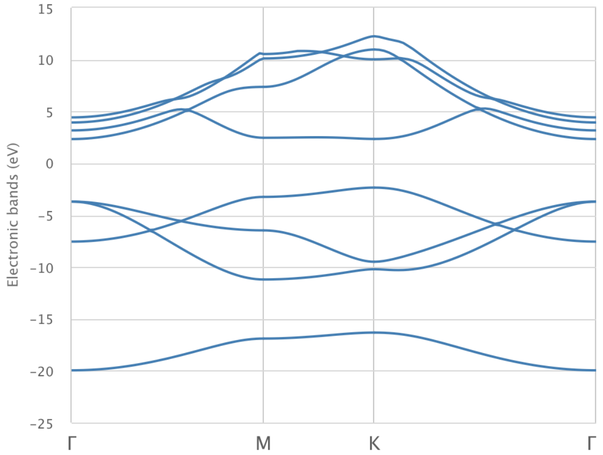


- AiiDA provenance graph: explain know how the structure was computed and to **reproduce that single specific calculation:** *log of "what happened in the past"*
- **AiiDA workflow engine**: Flexible python interface to encode complex scientific steps
  - Provides robustness (connection drops, ...) and allows to easily implement "error handlers" for common code-specific errors (crashes, non-convergence, end-of-walltime, ...)
  - Added bonus: automated provenance tracking and reproducibility

Mini-example of simple calculation submission








```
PwBandsWorkChain = WorkflowFactory('quantumespresso.pw.bands')
code = load_code('pw.x@daint')
structure = StructureData(ase=ase.io.read('BN.xsf'))
builder = PwBandsWorkChain.get_builder_from_protocol(code=code, structure=structure)
... # Possible overrides
workchain_node = submit(builder)
```

FAIR sharing in AiiDA beyond data: codes, plugins and workflows

Calculation | **Data** | **Parsers** | **Transport and scheduler** | **Workflows** | **Importers & exporters**

AiiDA PLUGIN REGISTRY

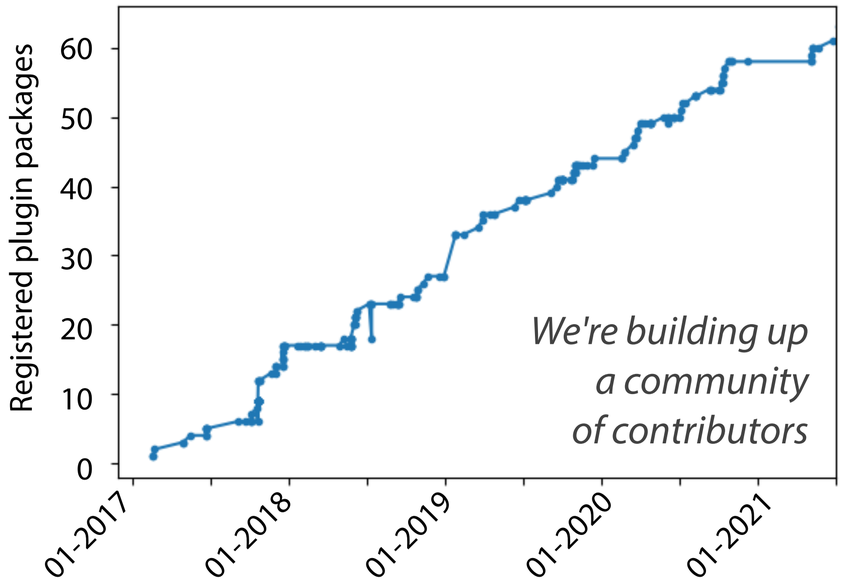
[View on GitHub/register your package]

Registered plugin packages: 66

Calculations	109 plugins in 46 packages
Parsers	94 plugins in 47 packages
Data	82 plugins in 23 packages
Workflows	129 plugins in 31 packages
Console scripts	19 plugins in 14 packages
Other	94 plugins in 24 packages

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

- Plugins collected in the AiiDA plugin registry
- **100+ codes currently supported,** 120+ workflows
- Many are **community-contributed**



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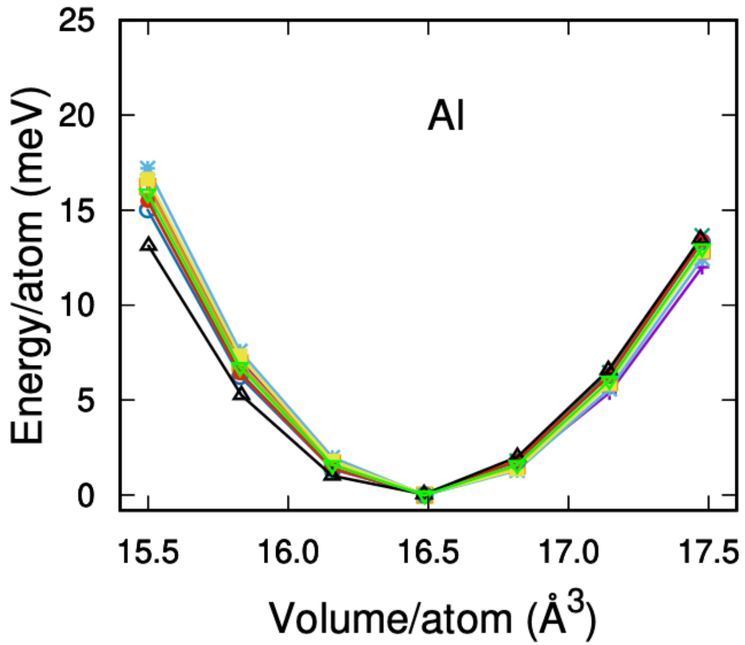
The need for turn-key solutions

- Like in a car: many end-users, drive without need to know how the engine works
  - Engines are "robust"
  - Just turn the key and drive
- I still need a driving license, but:
  - many needs addressed by driving my own car
  - no need to learn again to drive if I change car brand

A first goal

- As a non-expert, be able to ask

"Please run an **equation of state** with code
[Quantum ESPRESSO|SIESTA|FLEUR|VASP|CASTEP|...]
on the XXX supercomputer, using YY nodes,
and **automatically choose numerical parameters**
(basis set size/cutoff, k-points, ...) to get converged results."



- As an expert:
  - check the automatic parameters
  - adapt them if needed
  - check details of already-run simulations (by someone else): via provenance tracking

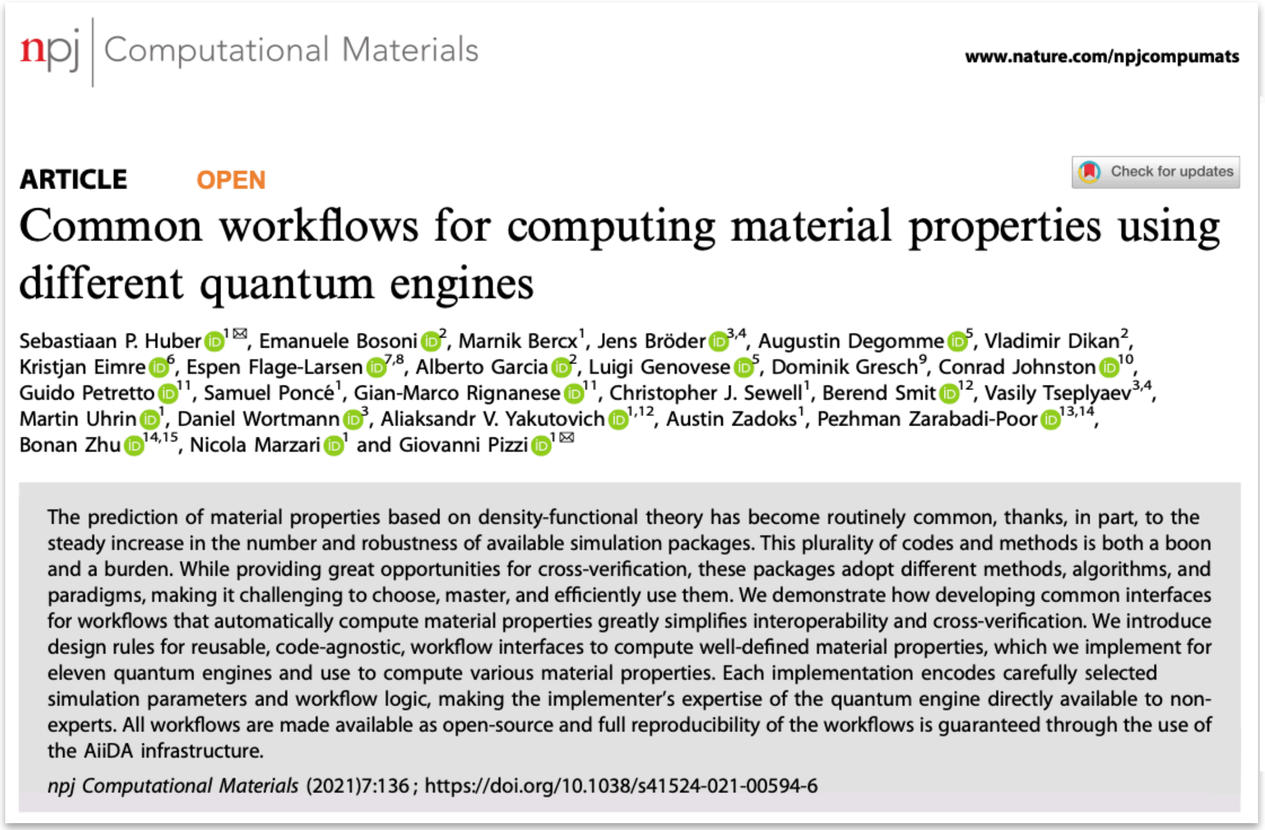
What are the challenges?

- Have turn-key solutions to calculate common materials properties
  Robust, with automatic error recovery, and automatic parameter choice
- Accessible to non-experts, without losing control for experts
  Automatic choice of numerical parameters
- Interoperability among several quantum engines
  Same input and output formats, and data types

Biggest challenge: all of the above at the same time

Code interoperability: common workflow interfaces

- Robust, cross-verified and accessible simulations with unified interface
- Effort started in the MaX CoE, but open to many more contributions



npj | Computational Materials

www.nature.com/npjcompumats

ARTICLE OPEN

Check for updates

Common workflows for computing material 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[7,8], Alberto Garcia[2], Luigi Genovese[5], Dominik Gresch[9], Conrad Johnston[10], Guido Petretto[11], Samuel Poncé[1], Gian-Marco Rignanese[11], Christopher J. Sewell[1], Berend Smit[12], Vasily Tseplyaev[3,4], Martin Uhrin[1], Daniel Wortmann[3], Aliaksandr V. Yakutovich[1,12], Austin Zadoks[1], Pezhman Zarabadi-Poor[13,14], Bonan Zhu[14,15], Nicola Marzari[1] and Giovanni Pizzi[1✉]

The prediction of material properties based on density-functional theory has become routinely common, thanks, in part, to the steady increase in the number and robustness of available simulation packages. This plurality of codes and methods is both a boon and a burden. While providing great opportunities for cross-verification, these packages adopt different methods, algorithms, and paradigms, making it challenging to choose, master, and efficiently use them. We demonstrate how developing common interfaces for workflows that automatically compute material properties greatly simplifies interoperability and cross-verification. We introduce design rules for reusable, code-agnostic, workflow interfaces to compute well-defined material properties, which we implement for eleven quantum engines and use to compute various material properties. Each implementation encodes carefully selected simulation parameters and workflow logic, making the implementer's expertise of the quantum engine directly available to non-experts. All workflows are made available as open-source and full reproducibility of the workflows is guaranteed through the use of the AiiDA infrastructure.

npj Computational Materials (2021)7:136 ; https://doi.org/10.1038/s41524-021-00594-6

abinit — Guido Petretto, Samuel Poncé, Austin Zadoks, Gian-Marco Rignanese

BigDFT — Augustin Degomme, Luigi Genovese

CASTEP — Bonan Zhu

CP2K — Aliaksandr V. Yakutovich, Berend Smit

VASP — Espen Flage-Larsen

AiiDA — Sebastiaan P. Huber, Emanuele Bosoni, Giovanni Pizzi, Nicola Marzari, Dominik Gresch, Christopher J. Sewell, Martin Uhrin

Jens Bröder

www.flapw.de

fleur — Vasily Tseplyaev, Daniel Wortmann

QUANTUM ESPRESSO — Marnik Bercx

siesta — Vladimir Dikan, Alberto Garcia

ORCA — Pezhman Zarabadi-Poor

NWCHEM — HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE — Conrad Johnston

Kristjan Eimre

S. P. Huber et al., npj Comput. Mater. 7, 136 (2021)

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

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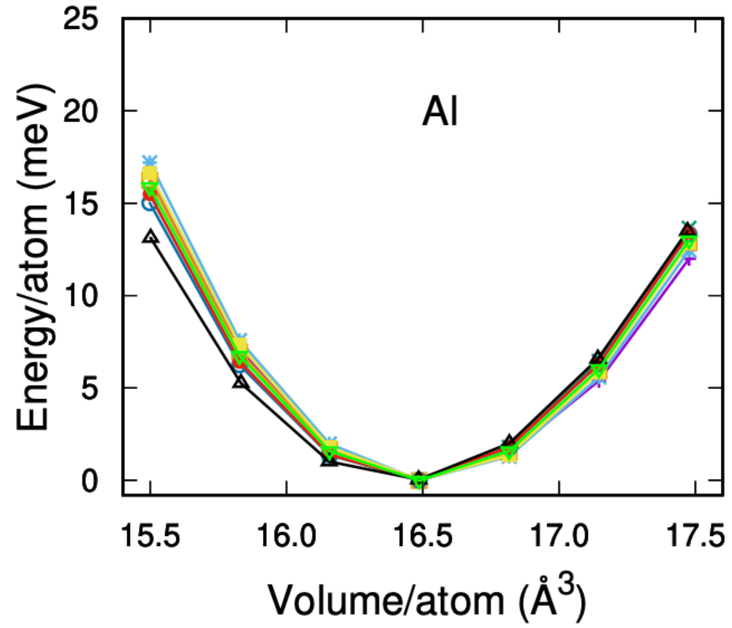
Code interoperability: common workflow interfaces

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



From common workflow interfaces to common workflows

- We now have code-specific common workflow interfaces (e.g. for relaxation) with common interface
- We can now **implement (only once!) common workflows** using the workflows with common interfaces:
  - Dissociation curves
  - Equation of states (EOS)
  - Phonons
  - ...

Equation of states: results

- Tested (simple cases) for:
  - insulators
  - metals
  - magnetic systems
    - ferromagnetic
    - antiferromagnetic

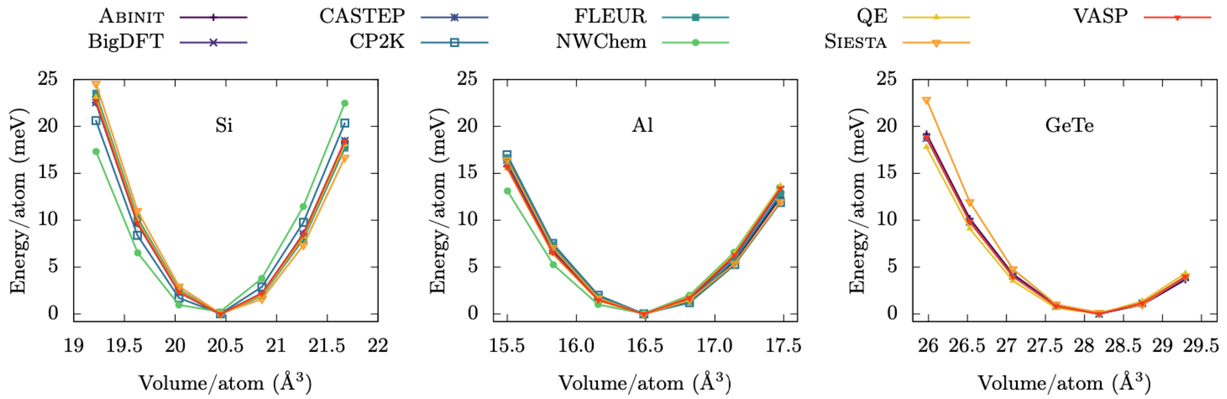
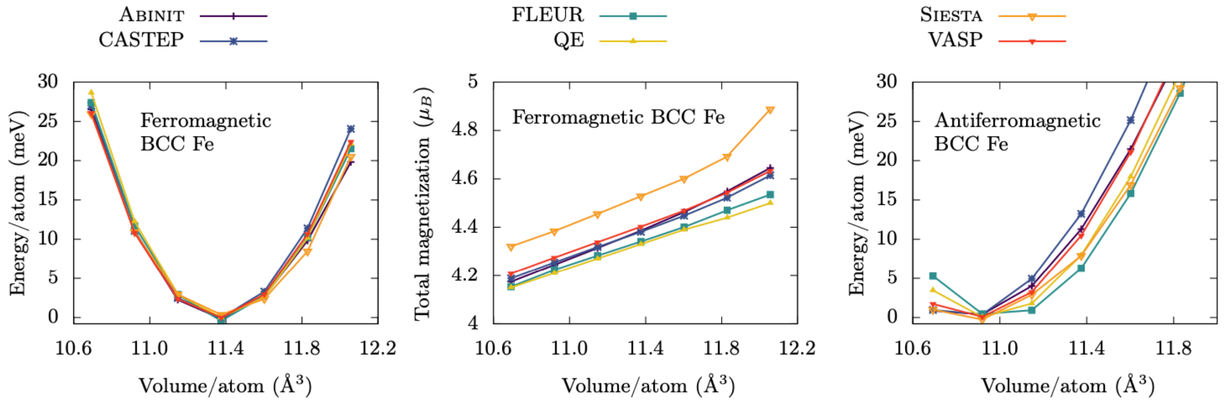
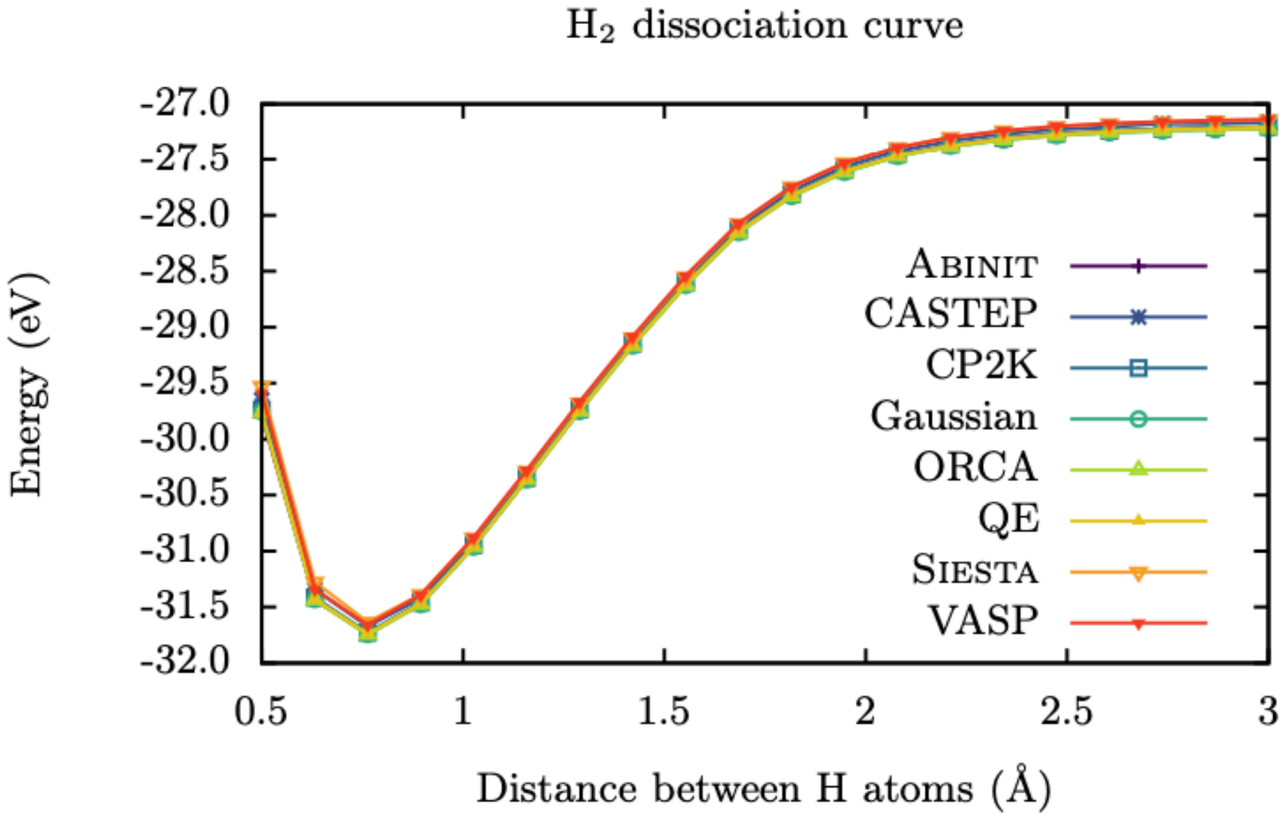


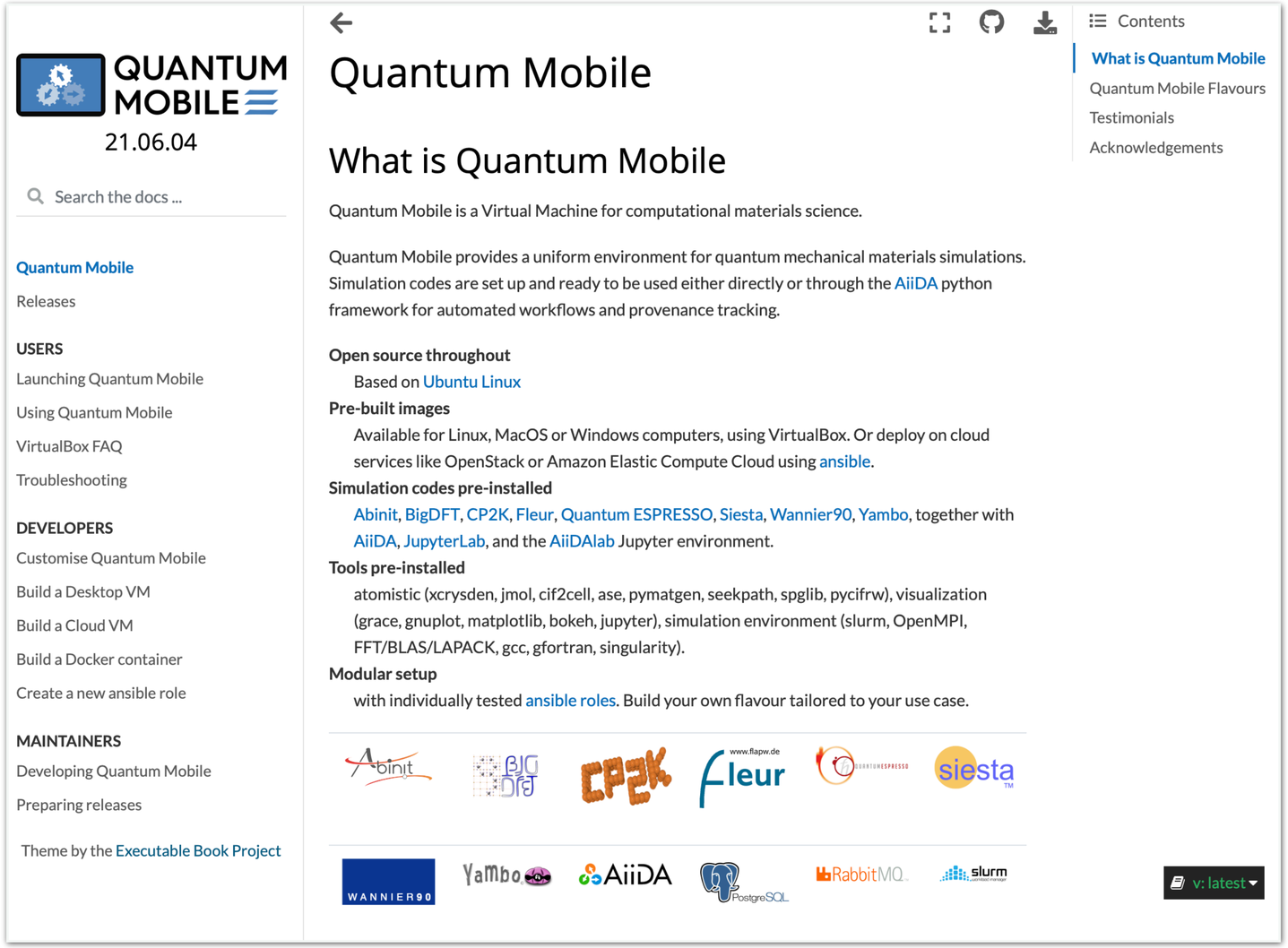
Figure 7. **EOS for Si, Al and GeTe.** Results obtained with the code-agnostic `EquationOfStateWorkflow`. For each code, the energy is shifted to set the minimum energy to zero. The EOS has been computed with all codes discussed in this work, except ORCA and Gaussian, which are mainly specialized for non-periodic systems. In addition, for GeTe, results are missing for BigDFT, CP2K, FLEUR and NWChem (see Table II in the Supplementary Information for more details). The label QE stands for QUANTUM ESPRESSO.



Dissociation curve: results

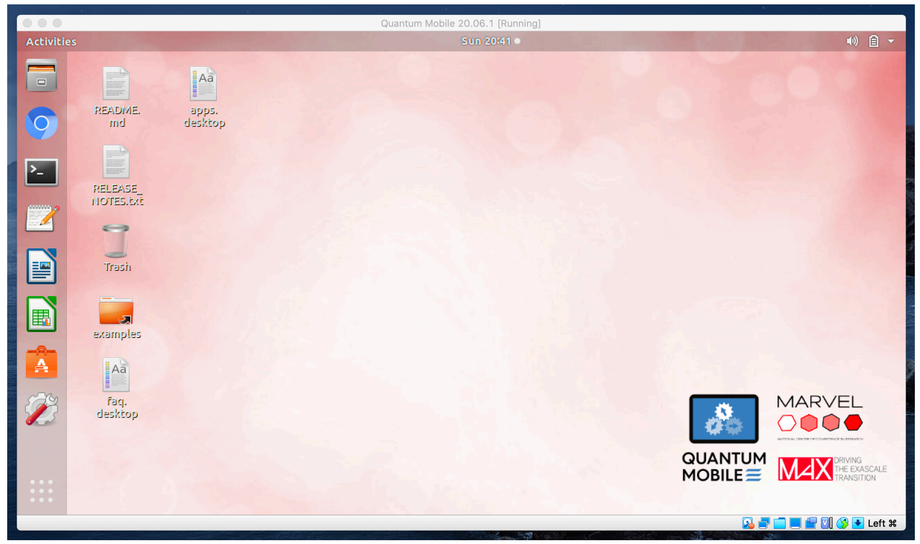


Making it easy to use: Quantum Mobile



- It contains:
  - AiiDA
  - Quantum codes (all those that are free - some only work in serial for now)
  - AiiDA plugins and workflows (all, open-sources)
  - AiiDA common workflows code (since v21.05.1)
  - ...and much more

"Quantum Mobile" virtual machine (VM)



QUANTUM MOBILE

Testimonials

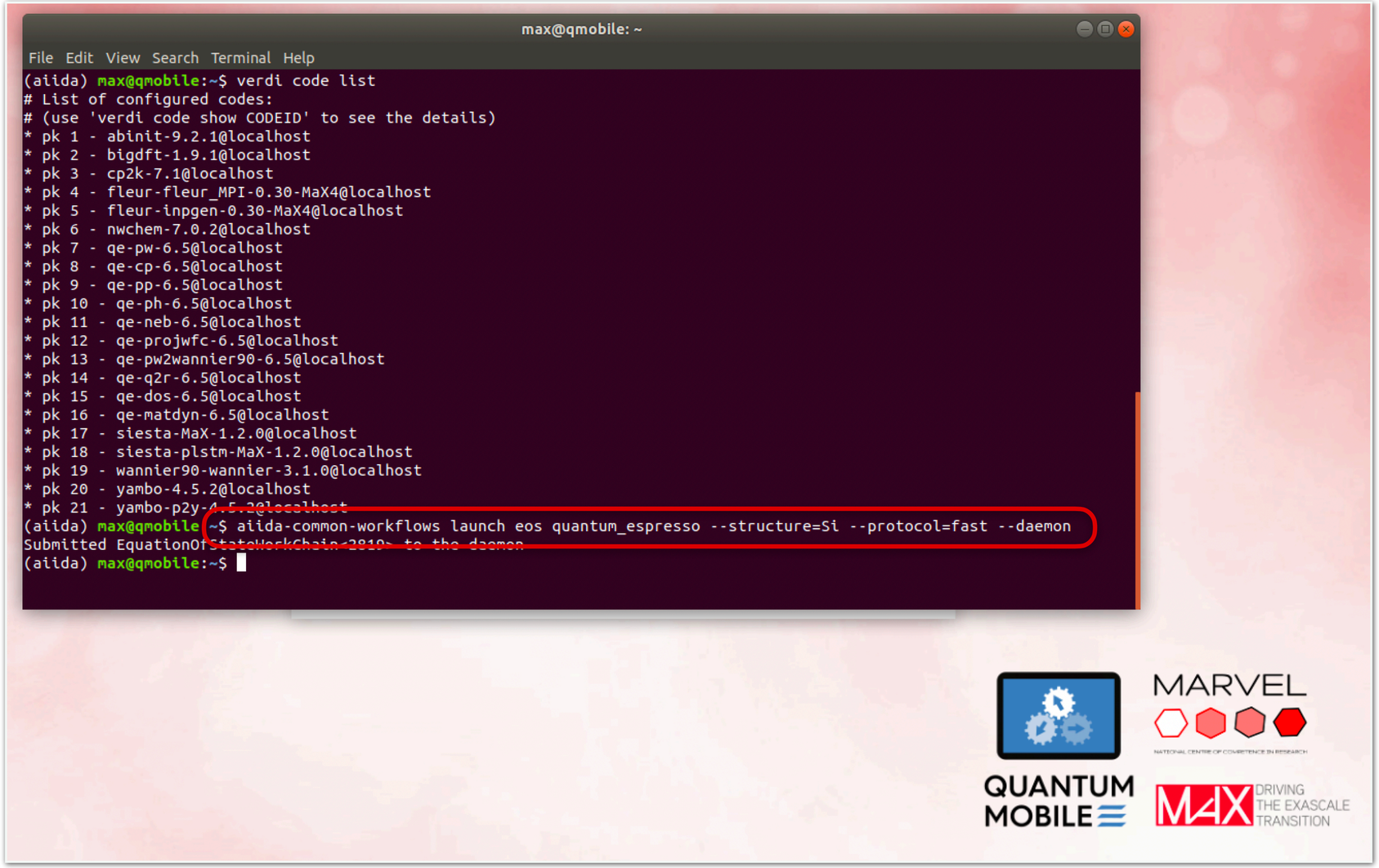
Compared to [courses of] previous years, the overhead due to technical problems and misunderstandings has been greatly reduced. Quantum Mobile is **absolutely the right tool to have.**

Stefaan Cottenier, compmatphys.org

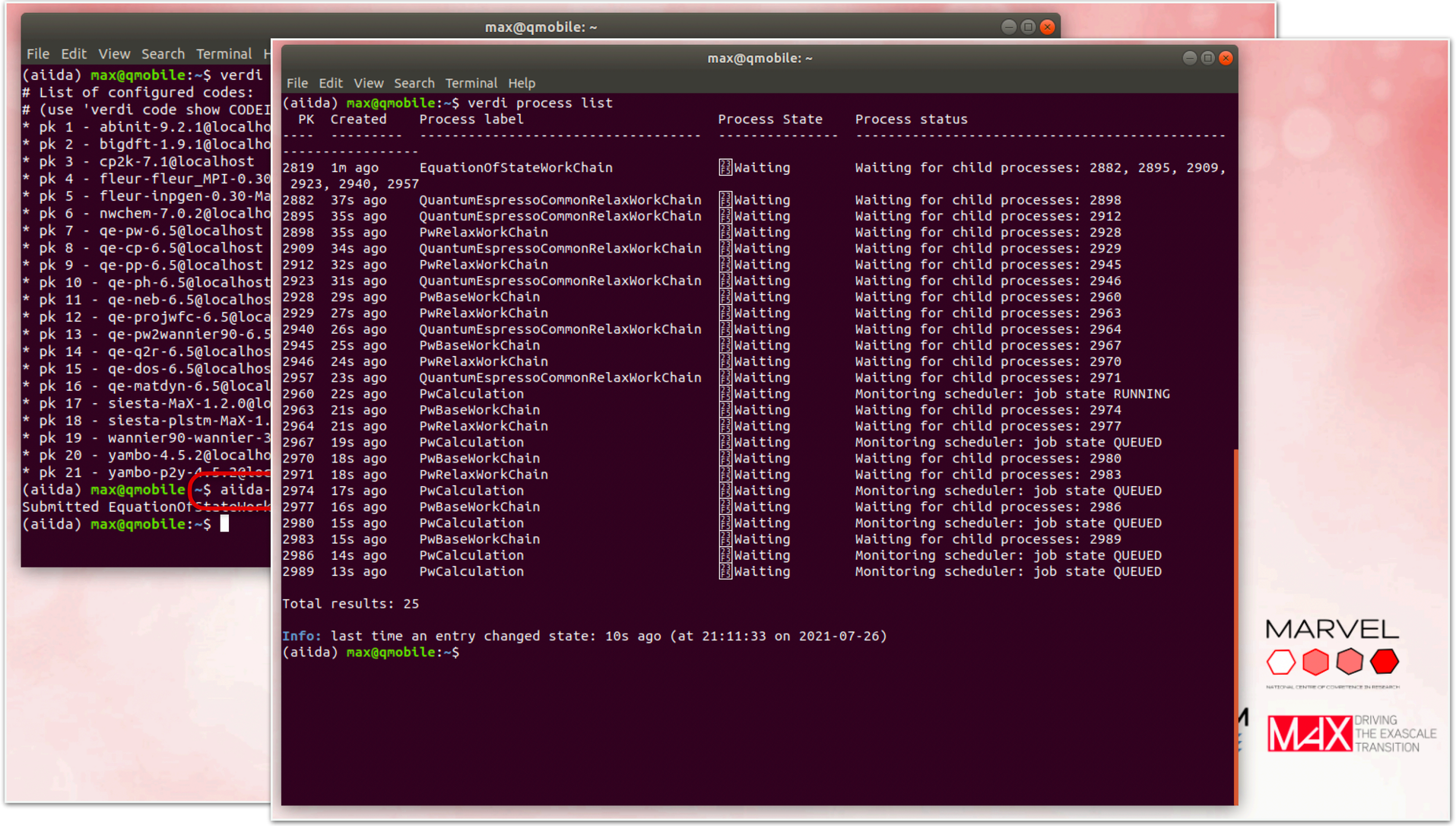
Quantum Mobile is really a fantastic tool! I do think that it really gives a **gigantic help for the organisation of Schools** focusing on simulation codes.

Andrea Marini, founder of the Yambo code

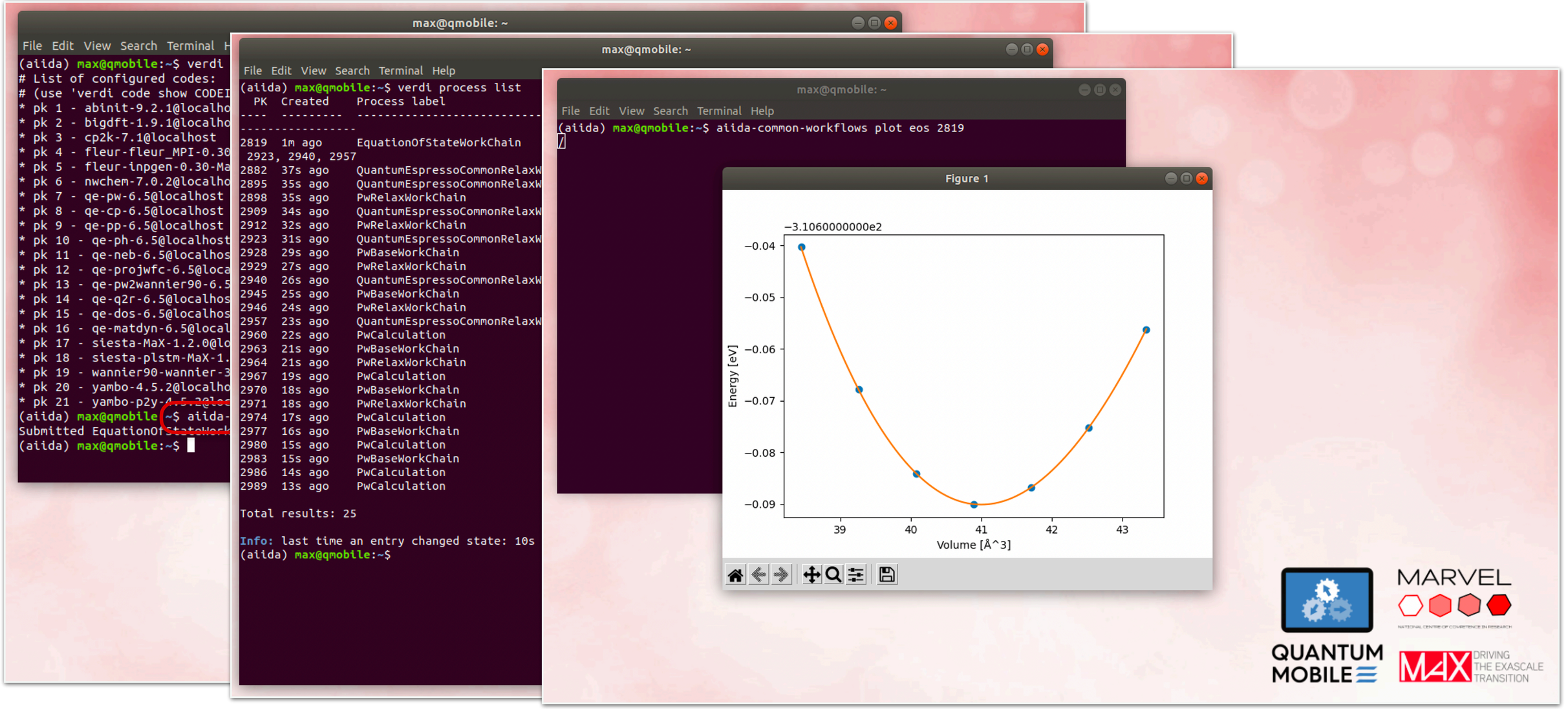
Running in Quantum Mobile



Running in Quantum Mobile



Running in Quantum Mobile



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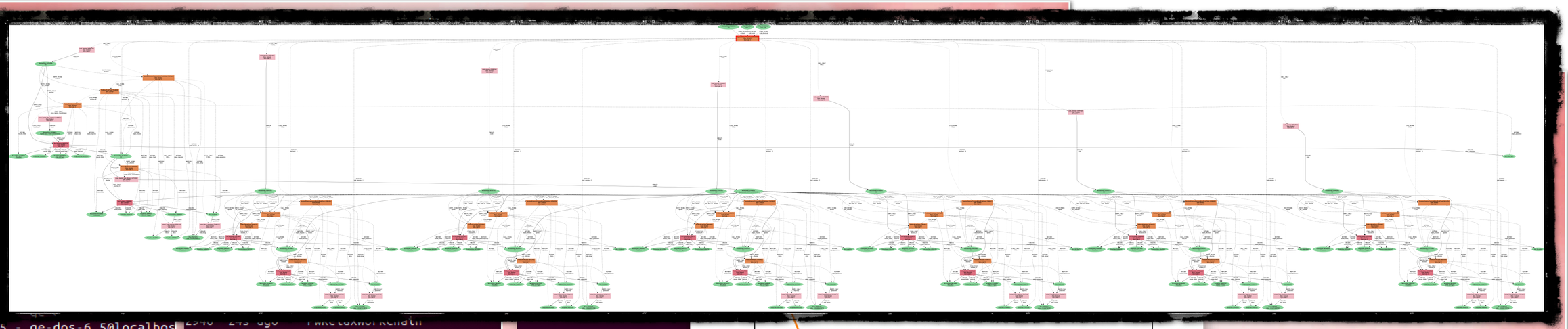
Running in Quantum Mobile

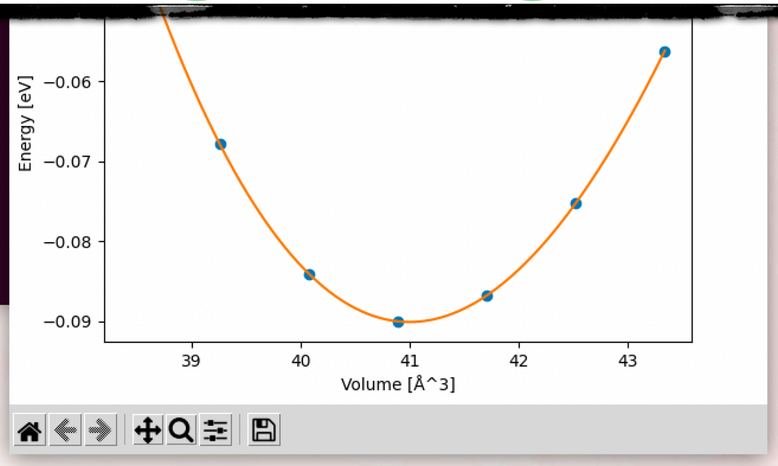


```
(aiida
# List
# (use
* pk 1
* pk 2
* pk 3
* pk 4
* pk 5
* pk 6
* pk 7
* pk 8
* pk 9
* pk 1
* pk 1
* pk 1
* pk 1
* pk 1
* pk 15 - qe-dos-6.5@localhos
* pk 16 - qe-matdyn-6.5@local
* pk 17 - siesta-MaX-1.2.0@lo
* pk 18 - siesta-plstm-MaX-1.
* pk 19 - wannier90-wannier-3
* pk 20 - yambo-4.5.2@localho
* pk 21 - yambo-p2y-4.5.2@loc
(aiida) max@qmobile:~$ aiida-
Submitted EquationOfStateWork
(aiida) max@qmobile:~$
```

```
2957  23s ago    QuantumEspressoCommonRelaxW
2960  22s ago    PwCalculation
2963  21s ago    PwBaseWorkChain
2964  21s ago    PwRelaxWorkChain
2967  19s ago    PwCalculation
2970  18s ago    PwBaseWorkChain
2971  18s ago    PwRelaxWorkChain
2974  17s ago    PwCalculation
2977  16s ago    PwBaseWorkChain
2980  15s ago    PwCalculation
2983  15s ago    PwBaseWorkChain
2986  14s ago    PwCalculation
2989  13s ago    PwCalculation

Total results: 25

Info: last time an entry changed state: 10s
(aiida) max@qmobile:~$
```



QUANTUM MOBILE

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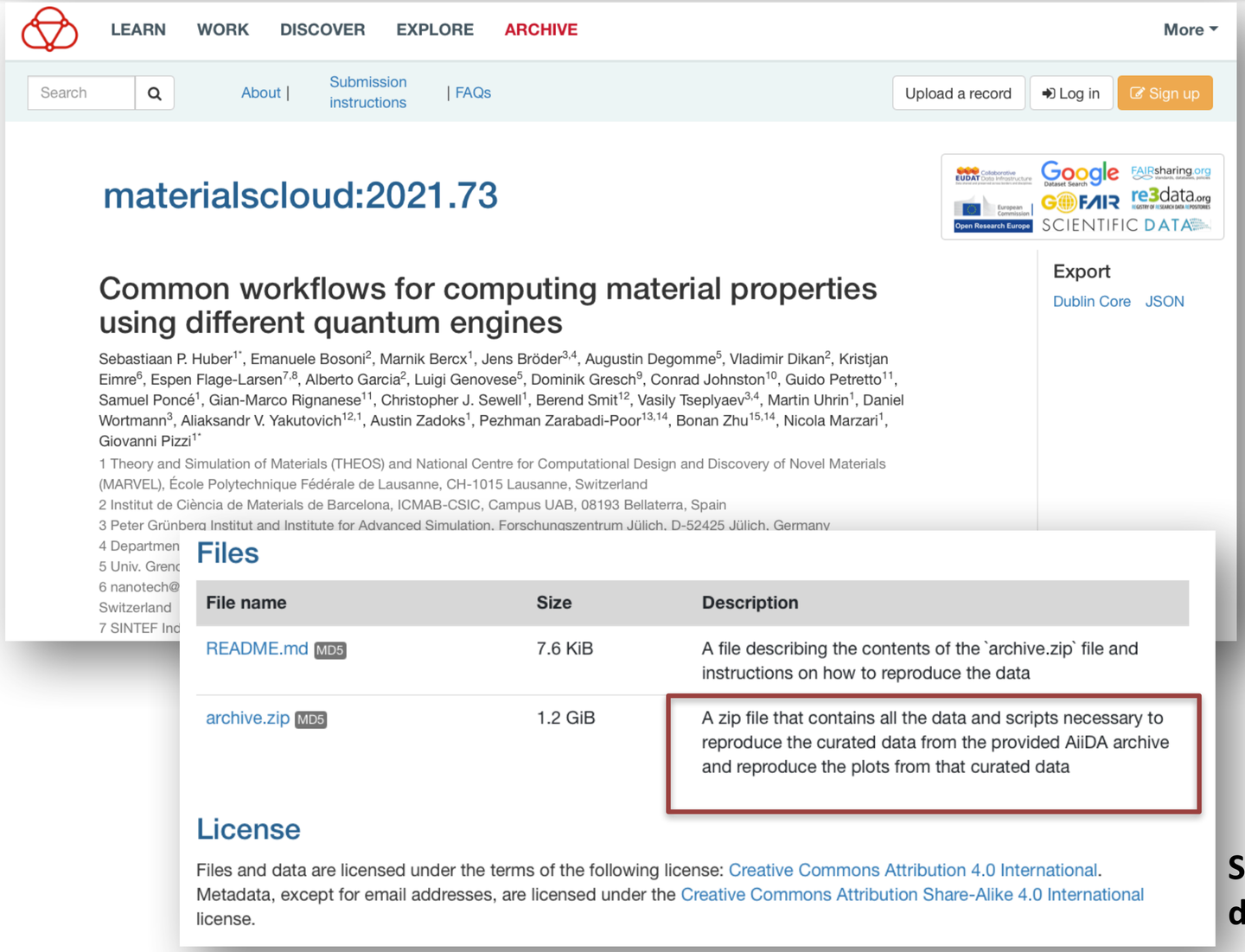
All data is available and reproducible!



S. P. Huber et al., Materials Cloud Archive 2021.73 (2021), doi: 10.24435/materialscloud:nz-01.

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All data is available and reproducible!

You can import the data in the Quantum Mobile, and visualise it e.g. within Materials Cloud

CASTEP

```
#
# type: uuid: 2fe6c185-bc8d-435d-b081-5b6caacf819b (pk: 198)
# pk: 198
# linkname: pseudo__Ge
# uuid: 2fe6c185-bc8d-435d-b081-5b6caacf819b
# label: C19
# description:
#
#
# type: uuid: 2fe6c185-bc8d-435d-b081-5b6caacf819b (pk: 19
# pk: 198
# linkname: pseudo__Te
# uuid: 2fe6c185-bc8d-435d-b081-5b6caacf819b
# label: C19
# description:
#
# END OF HEADER
%BLOCK LATTICE_CART
      4.3248011860       0.0000000000       0.0000000000
      2.2580861359       3.6884891624       0.0000000000
      2.2580861359       1.2652390711       3.4646965804
%ENDBLOCK LATTICE_CART
%BLOCK POSITIONS_ABS
Ge                       6.7381887318       3.7755068400
Te                       2.1027847261       1.1782213934
%ENDBLOCK POSITIONS_ABS
kpoints_mp_grid     : 19 19 19
fix_vol             : True
snap_to_symmetry    : True
symmetry_generate   : True
%BLOCK SPECIES_POT
Ge    C19
Te    C19
%ENDBLOCK SPECIES_POT
```

SIESTA

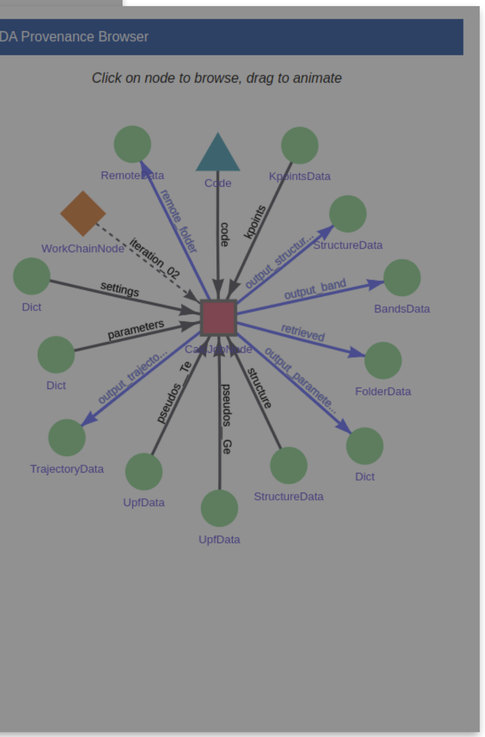
File: aiida.fdf

```
atomiccoordinatesformat Ang
electronictemperature 25 meV
geometrymustconverge T
latticeconstant 1.0 Ang
maxscfiterations 100
maxwalltime 36000
mdconstantvolume True
mdmaxforcetol 0.005 eV/Ang
mdmaxstresstol 0.7 GPa
mdnumcgsteps 100
mdtypeofrun cg
mdvariablecell True
meshsizes [48 48 48]
numberofatoms 2
numberofspecies 2
scfdmtolerance 1e-05
scfmixerhistory 5
scfmixerweight 0.1
solutionmethod diagon
systemlabel aiida
systemname aiida
usetreetimer T
writeforces True
xcauthors PBE
xcfunctional GGA
xmlwrite T
#
# -- Basis Set Info follows
#
pao-basis-size DZP
%block pao-basis
Ge 3
  n=4  0  2
 5.323265        0.0
```

Quantum ESPRESSO

File: aiida.in

```
&CONTROL
  calculation = 'vc-relax'
  etot_conv_thr =   1.0000000000d-05
  forc_conv_thr =   5.0000000000d-05
  max_seconds =   4.1040000000d+04
  outdir = './out/'
  prefix = 'aiida'
  pseudo_dir = './pseudo/'
  restart_mode = 'from_scratch'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =   1.0000000000d-02
  ecutrho =   3.6000000000d+02
  ecutwfc =   4.5000000000d+01
  ibrav = 0
  nat = 2
  nosym = .false.
  ntyp = 2
  occupations = 'smearing'
  smearing = 'cold'
/
&ELECTRONS
  conv_thr =   2.0000000000d-10
  electron_maxstep = 80
  mixing_beta =   4.0000000000d-01
/
&IONS
/
&CELL
  cell_dofree = 'shape'
  press_conv_thr =   5.0000000000d-01
```



...

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S. P. Huber et al., Materials Cloud Archive 2021.73 (2021), doi: 10.24435/materialscloud:nz-01.

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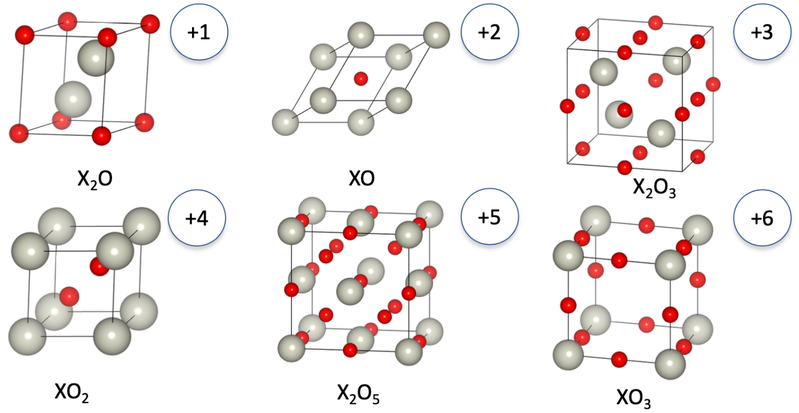
Current plans: second phase of collaboration

Project now continuing with an even larger group of collaborators

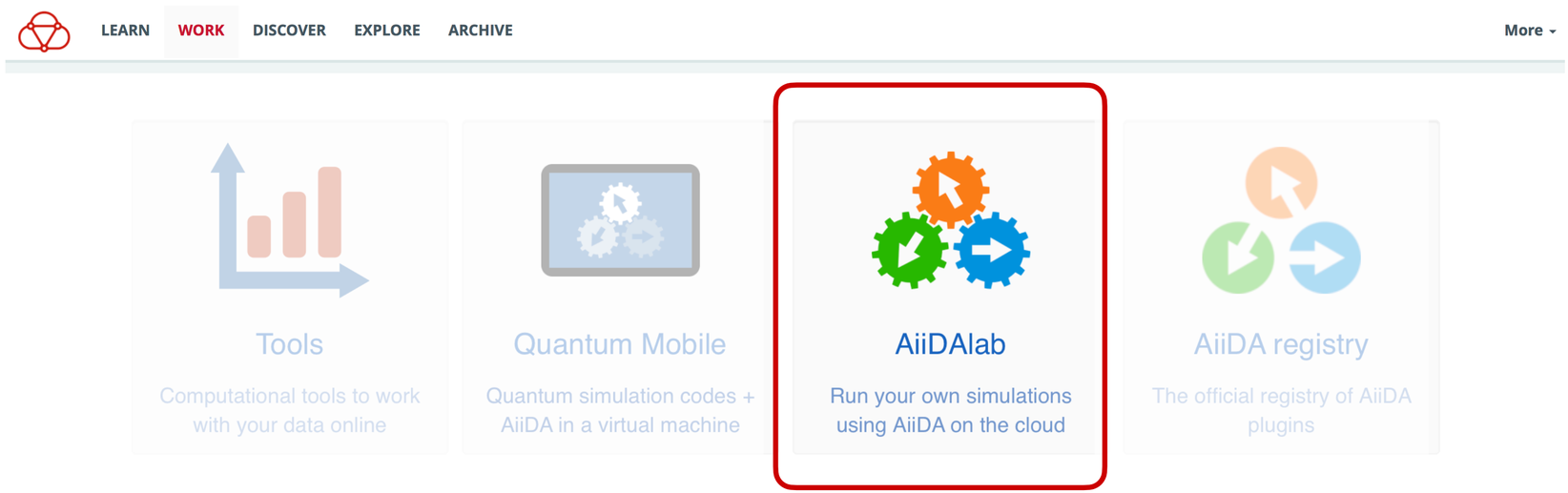
- New codes (JuKKR, GPAW, Wien2K)
- Common workflow interfaces for band-structure and (P)DOS
- Common workflow interfaces for Born-effective charges and dielectric constant
- Common phonon workflow based on phonopy
- Cross-validation on 500+ oxides
- AiiDAlab GUI
- …



Follow-up of the work of S. Cottenier (see talk of yesterday), comparing of various oxide configurations across all codes involved

Not only testing accuracy, but also releasing automated recipes to run with that accuracy!

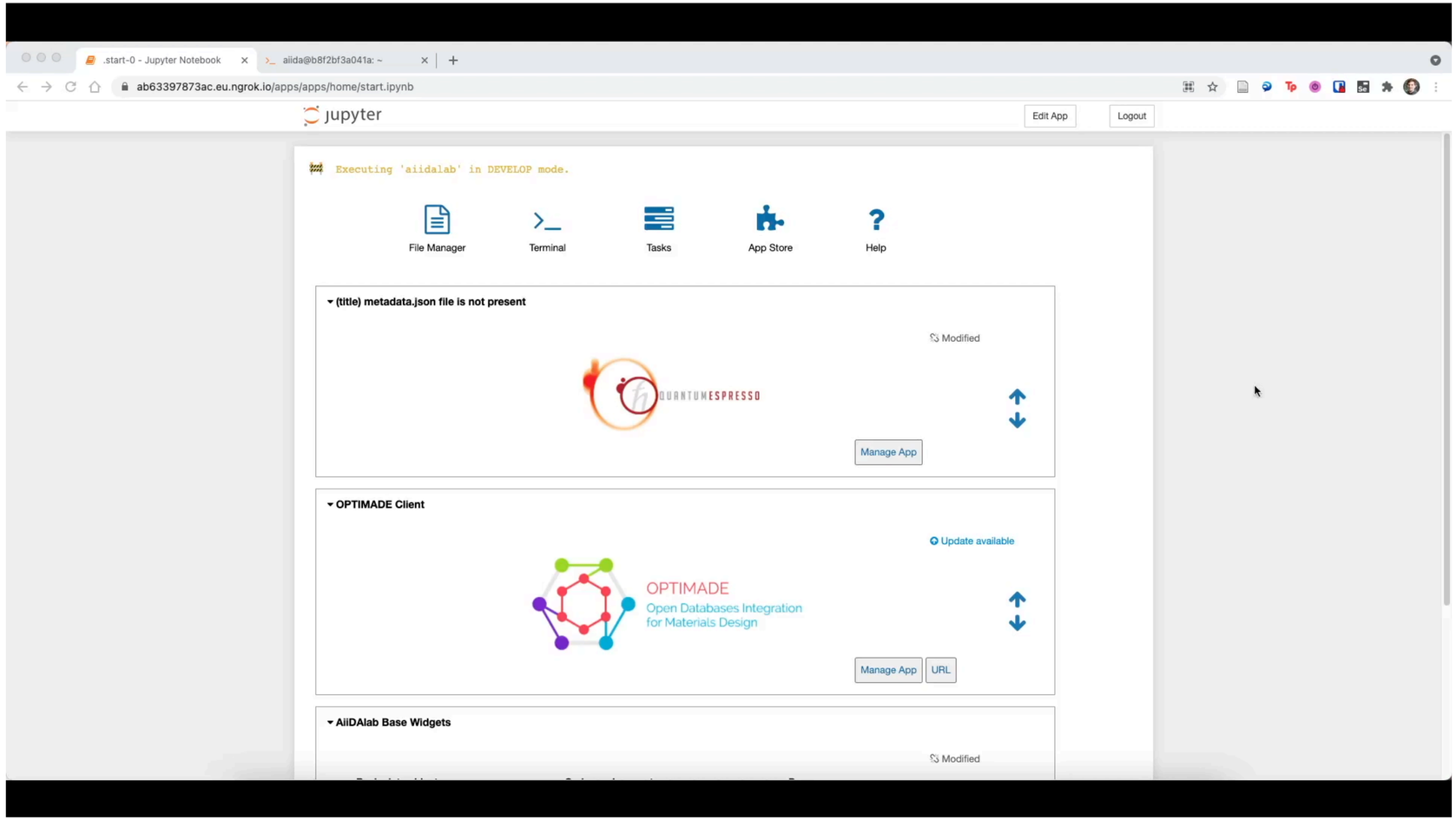
Data generation: Materials Cloud **Work**



AiiDAlab

- Comes with a preconfigured AiiDA setup, **ideal interface for turn-key workflows** to run directly in the browser
- Custom **AppMode** extension to make notebooks look&feel like real web apps: only python for development, no coding skills to use
- Easy to redeploy: JupyterHub + DockerSpawner on bare metal or VMs, but also kubernetes for scalability

Easy access to these advanced HPC capabilities to everybody



https://www.materialscloud.org/work/aiidalab

Making simulations accessible:
AiiDAlab experience at EMPA (CH)

https://www.youtube.com/watch?v=x4mWFjSoAO4

https://www.materialscloud.org/work/aiidalab

AiiDA and Materials Cloud teams

The Materials Cloud
And AiiDA teams


Carl Simon Adorf (EPFL)


Casper W. Andersen (EPFL)


Marnik Bercx (EPFL)


Marco Borelli (EPFL)


Valeria Granata (EPFL)


Sebastiaan P. Huber (EPFL)


Leonid Kahle (EPFL)


Martin Uhrin (EPFL)


Elsa Passaro (EPFL)


Flaviano Dos Santos (EPFL)


Francisco F. Ramirez (EPFL)


Leopold Talirz (EPFL)


Aliaksandr Yakutovich (EPFL)


Chris Sewell (EPFL)


Louis Ponet (EPFL)


Giovanni Pizzi (EPFL)


Berend Smit (EPFL)


Joost VandeVondele (ETHZ,CSCS)


Thomas Schulthess (ETHZ,CSCS)


Nicola Marzari (EPFL)

Contributors for the 40+ plugins: Quantum ESPRESSO, Wannier90, CP2K, FLEUR, YAMBO, SIESTA, VASP, CASTEP, CRYSTAL, …

Contributors to aiida-core and former AiiDA team members —
Oscar Arbelaez, Michael Atambo, Valentin Bersier, Marco Borelli, Jocelyn Boullier, Jens Bröder, Ivano E. Castelli, Andrea Cepellotti, Keija Cui, Vladimir Dikan, Marco Dorigo, Y.-W. Fang, Fernando Gargiulo, Marco Gibertini, Davide Grassano, Dominik Gresch, Conrad Johnston, Rico Häuselmann, Daniel Hollas, Eric Hontz, Jianxing Huang, Christoph Koch, Espen Flage-Larsen, Ian Lee, Daniel Marchand, Antimo Marrazzo, Andrius Merkys, Simon Pintarelli, Nicolas Mounet, Tiziano Müller, Gianluca Prandini, Philip Rüßmann, Riccardo Sabatini, Ole Schütt, Phillippe Schwaller, Andreas Stamminger, Atsushi Togo, Daniele Tomerini, Nicola Varini, Martin Uhrin, Jason Yu, Austin Zadoks, Bonan Zhu, Mario Zic, Spyros Zoupanos

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Common workflows for computing material properties using different quantum engines

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+all new collaborators for the follow-up (currently running) project!

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Acknowledgements and funding

SNSF NCCR "MARVEL"

Discovery of new materials via simulations and dissemination of curated data

H2020 Centre of Excellence "MaX"

Scaling towards exascale machines and high-throughput efficiency

Swissuniversities P-5 "Materials Cloud"

Scaling the web platform, extending to more disciplines

Moreover:

H2020 NEP (starting 2021)

H2020 OpenModel (starting 2021)

Summary

- AiiDA+Materials Cloud: FAIR access to simulation data
- In addition: AiiDA+common workflows: FAIR simulations
  - Open-source, robust turn-key workflows for materials properties
  - Common interface among 11 quantum engines (more coming)
  - Easy to use, but flexible for experts, designed to be interfaced to GUIs
  - Basis of verification studies (oxides set), and starting point for more common workflows