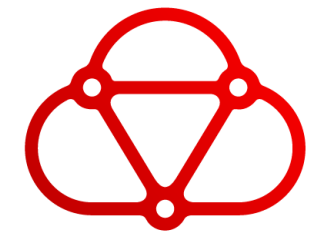




Demo of Materials Cloud and AiiDA Lab: integrated platforms for FAIR computational materials science



MATERIALSCLOUD



Giovanni Pizzi (EPFL); Carlo Pignedoli (Empa)



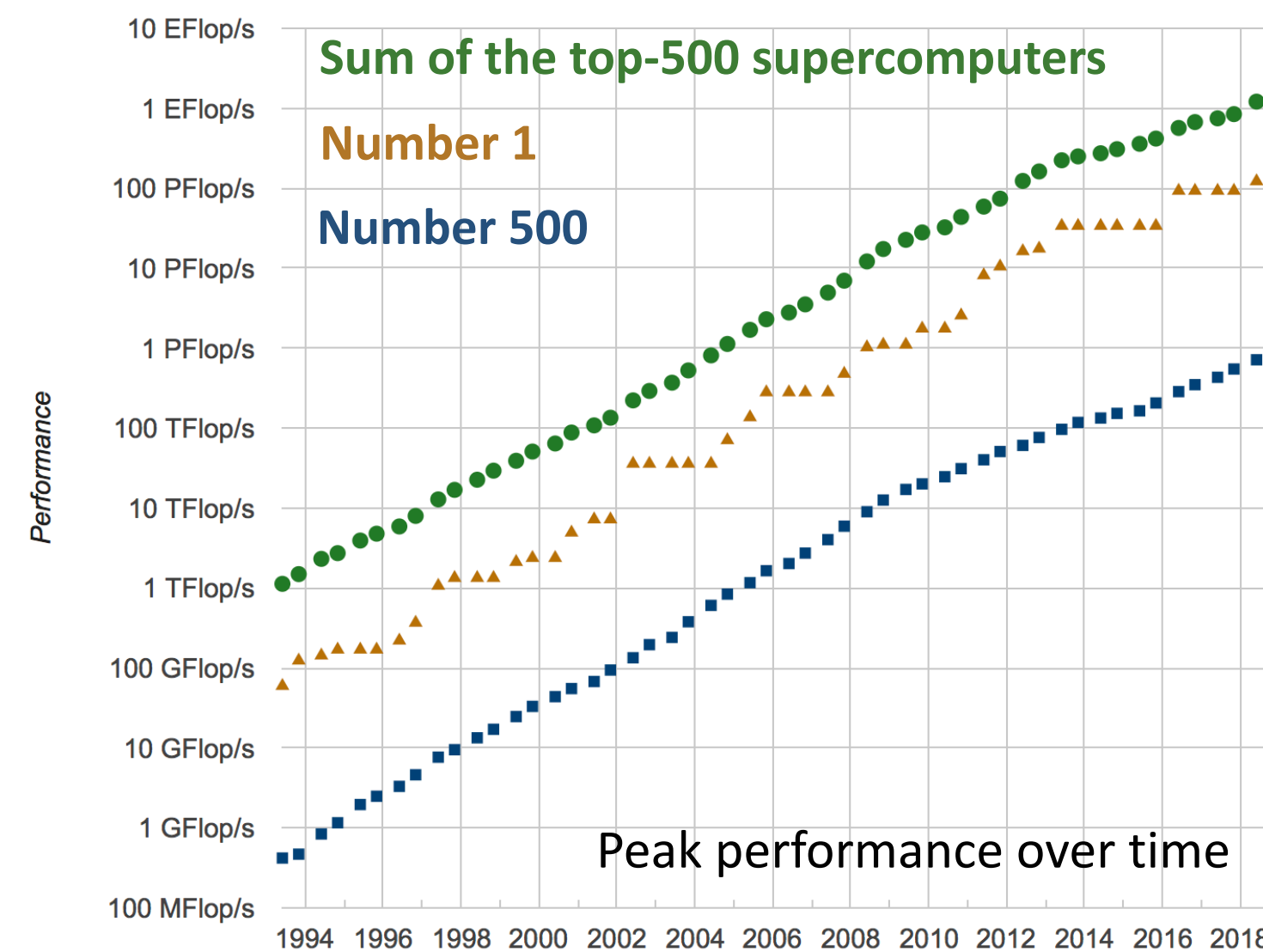
DFT materials simulations

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

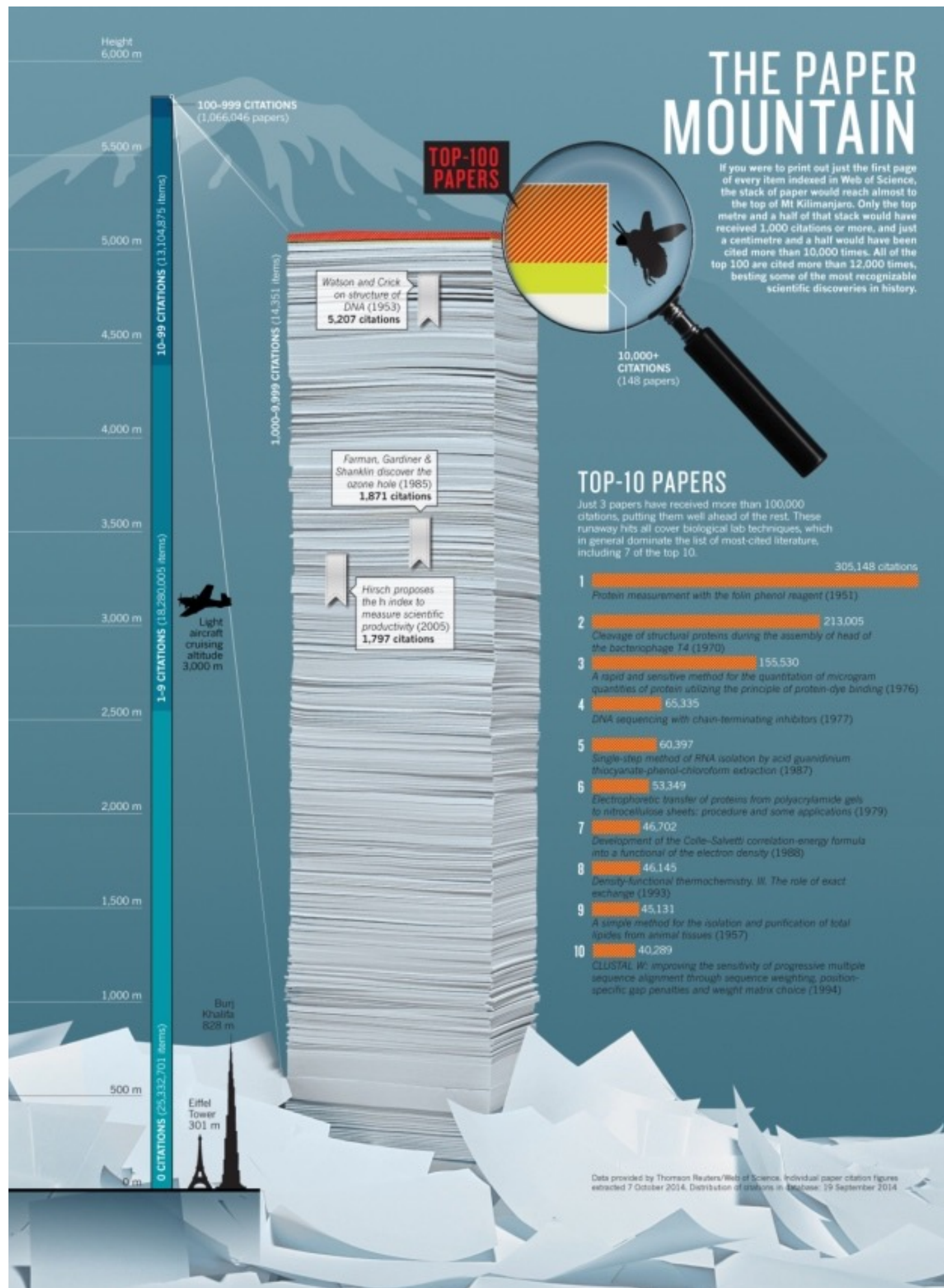


150,000x increase in the past 20 years

1 month (2001)



10 seconds (2021)



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

DFT materials simulations

Our research: Materials simulations

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



Combined: materials design and discovery via high-throughput computations

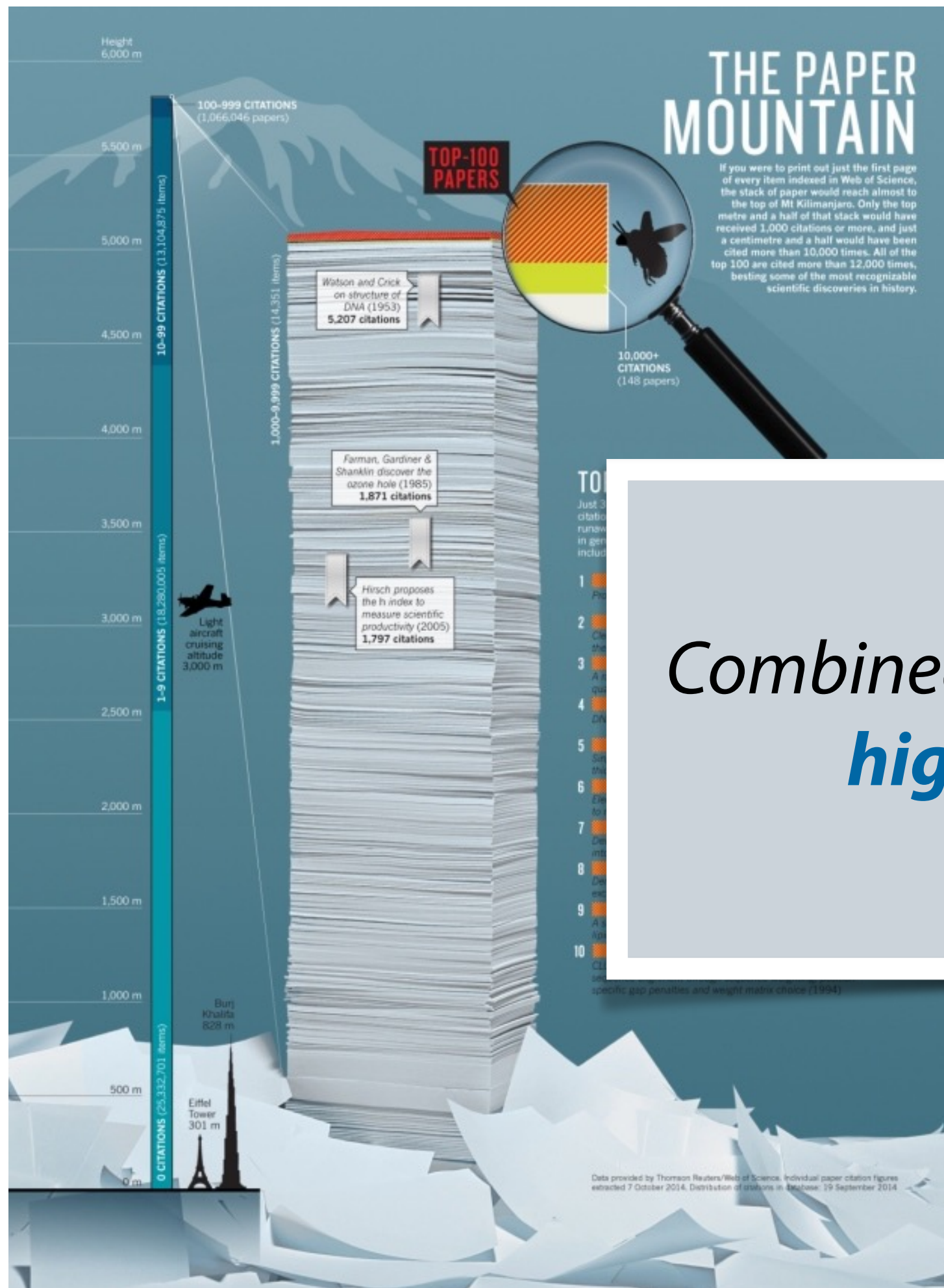
Accuracy and predictive power of quantum engines

150,000x increase in the past 20 years

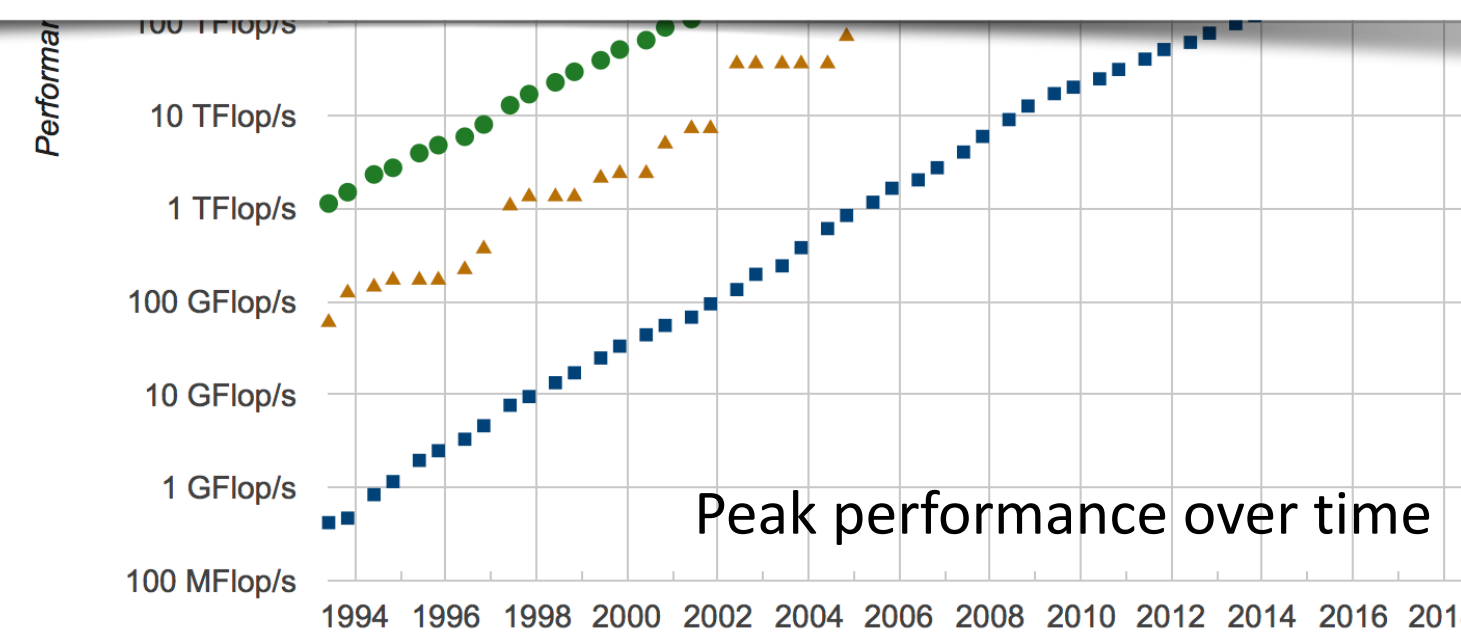
1 month (2001)



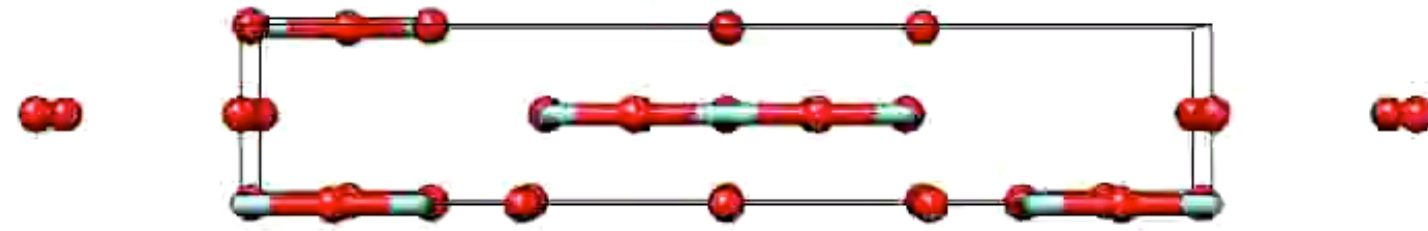
10 seconds (2021)



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



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**



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

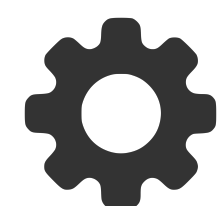
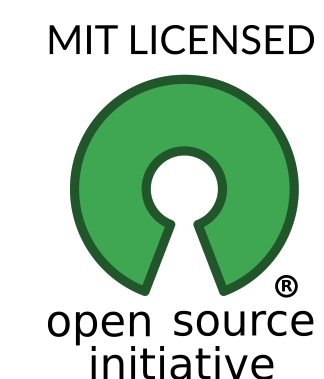
- **COMPUTATIONAL SCIENCE INFRASTRUCTURE**
- **FOR HIGH THROUGHPUT WORKFLOWS**
- **WITH FULL DATA PROVENANCE**



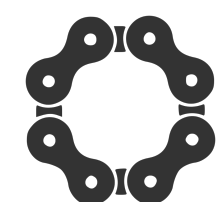
Language: implemented and API in python

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

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



Scalable workflow engine



Built-in support for HPC

Automated full data provenance



Flexible plugin system



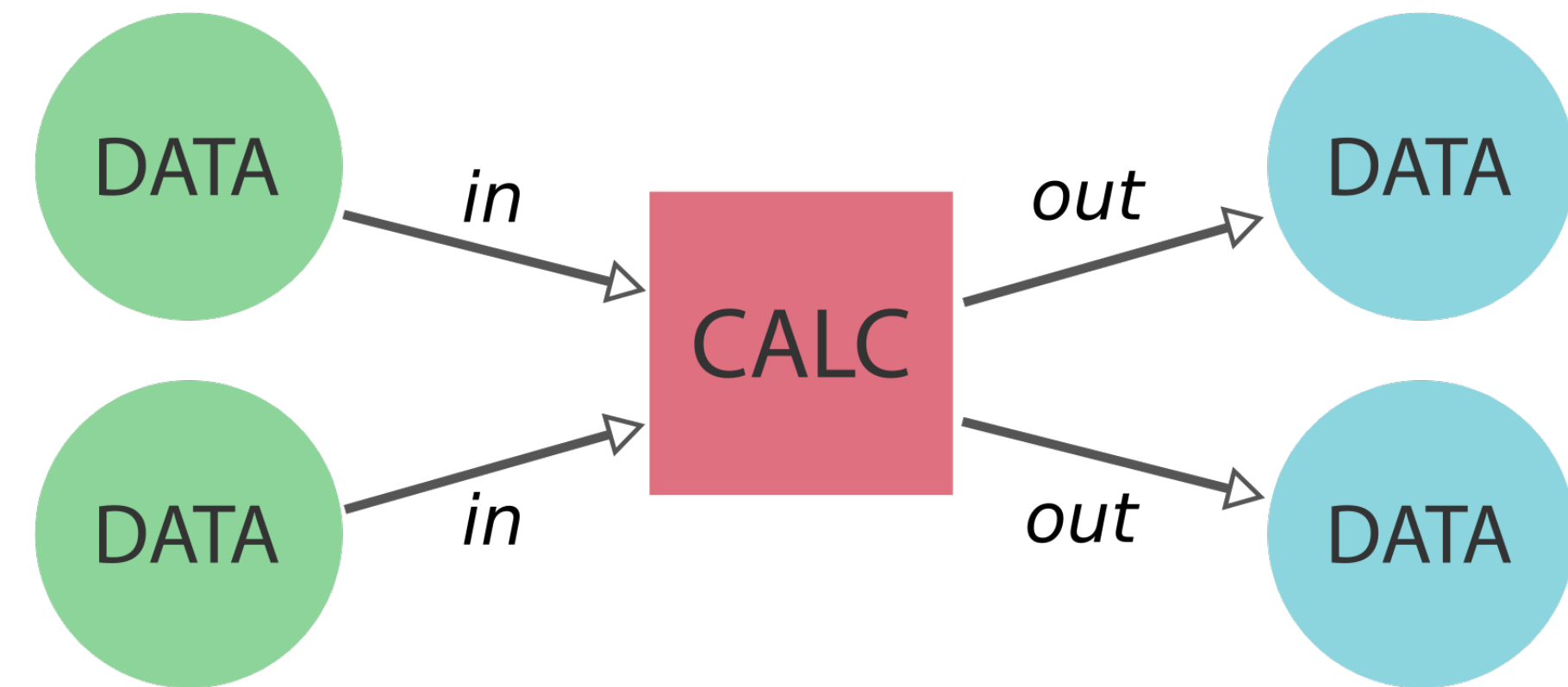
G. Pizzi et al., Comp. Mat. Sci. 111, 218-230 (2016)

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

Data provenance

Simple recipe

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



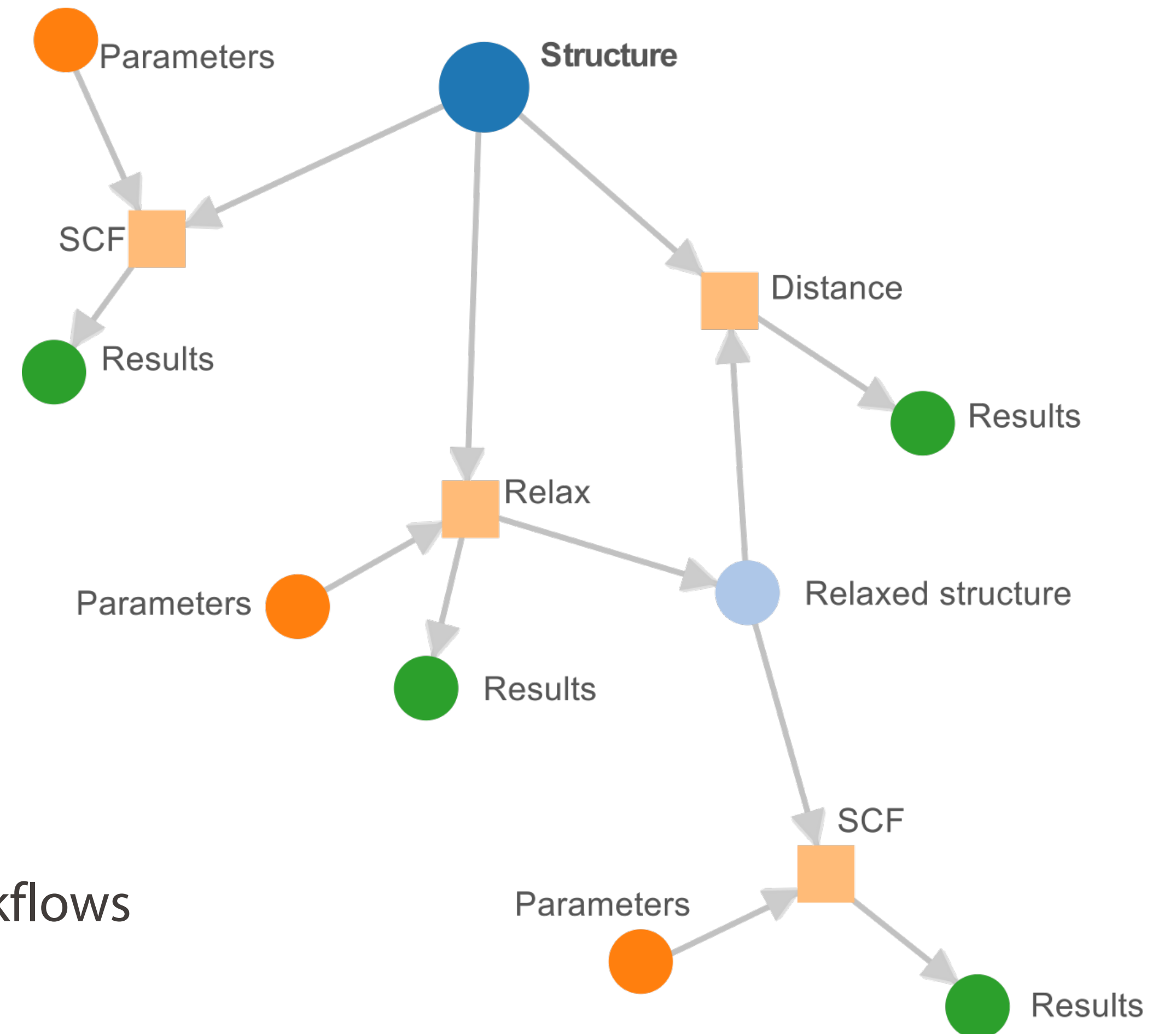
Data provenance

Simple recipe

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

Provenance graphs

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



Data provenance

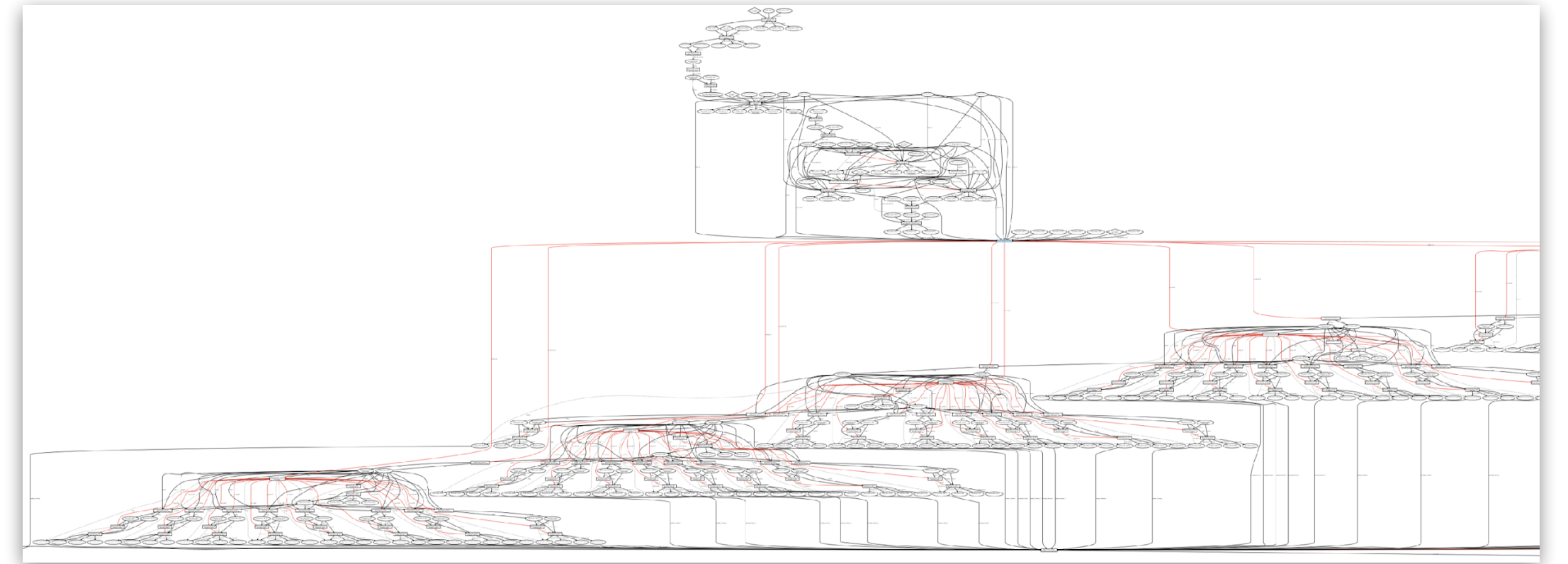
Simple recipe

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

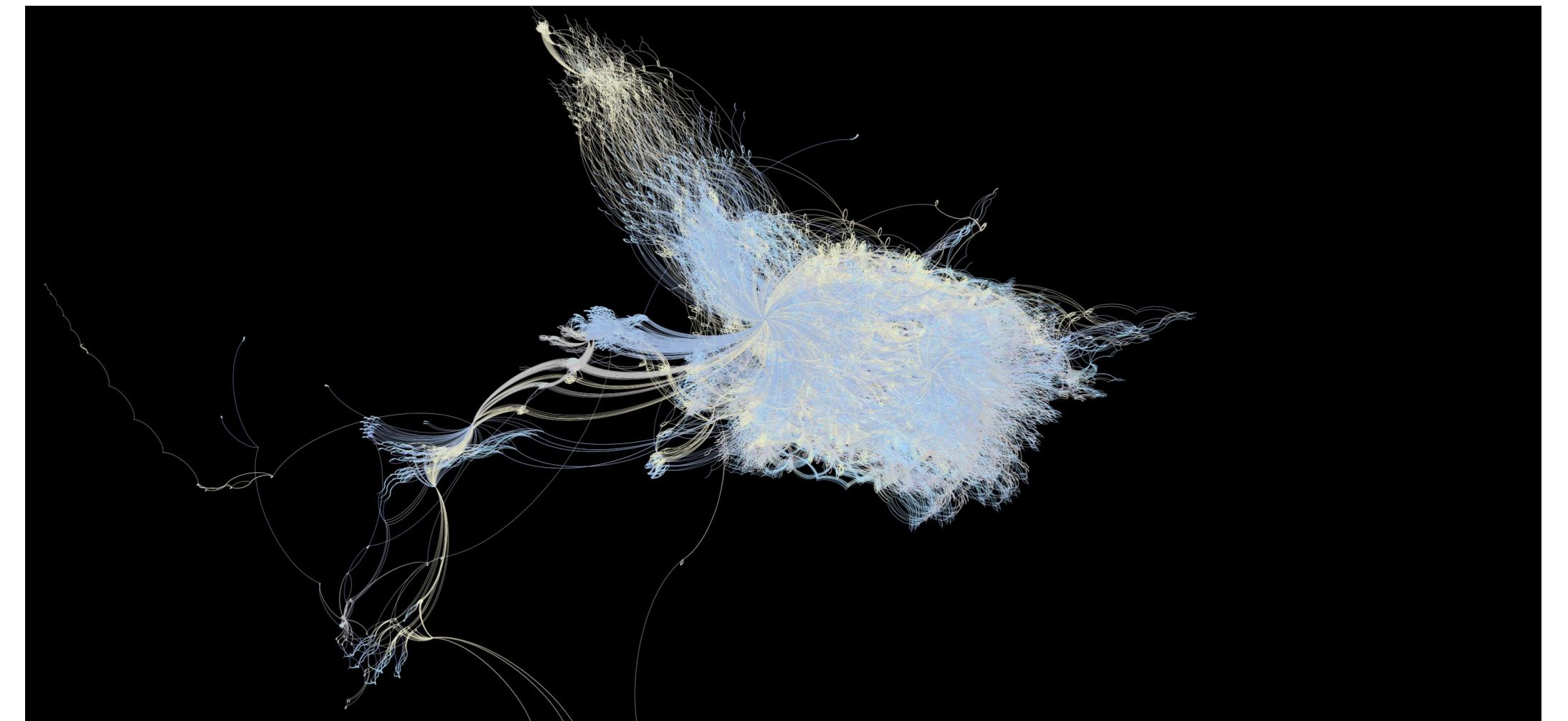
Graph requirements

- 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

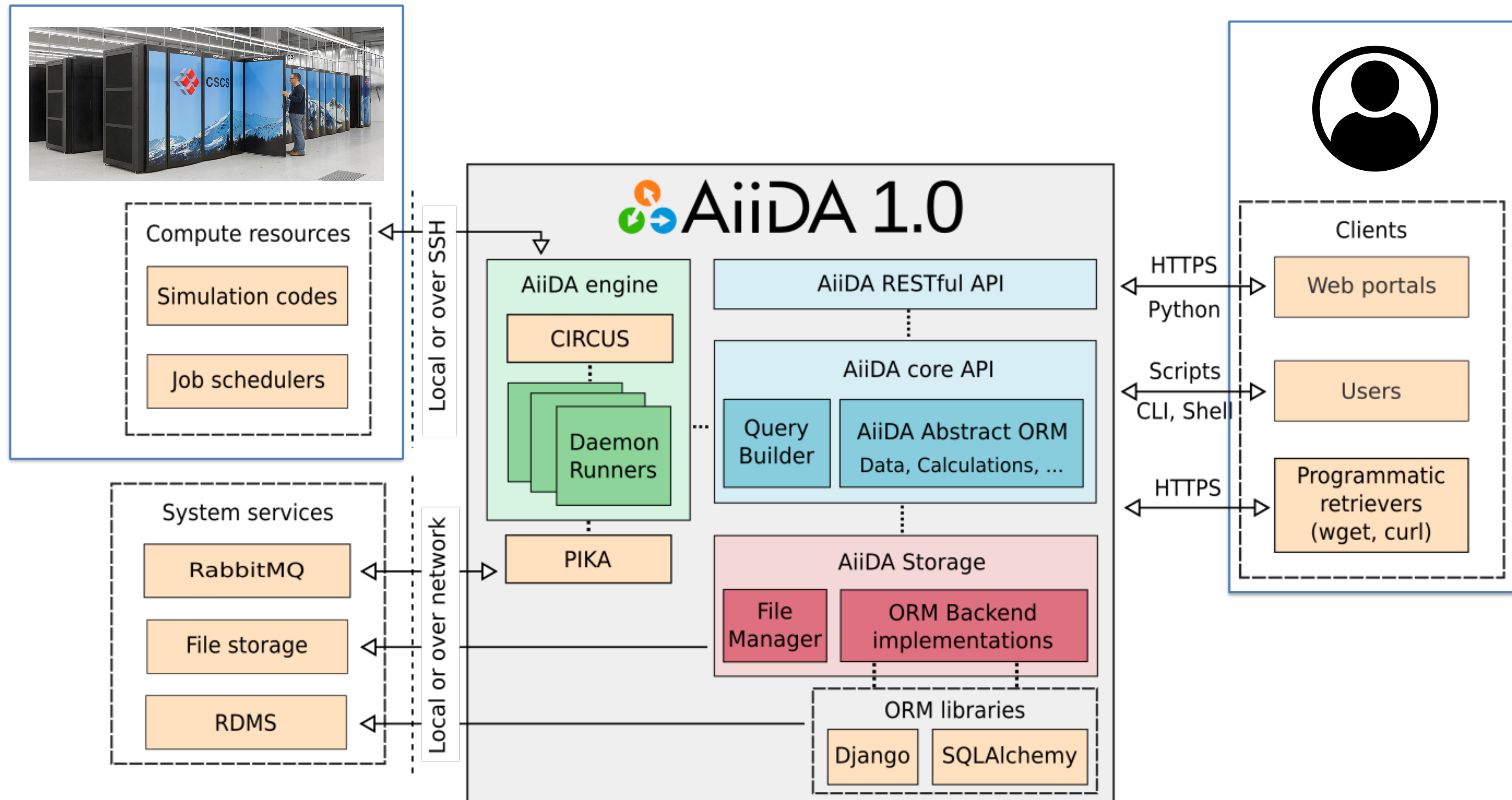


Molecular dynamics study of Lithium in a solid electrolyte



Graphical representation of actual AiiDA database

AiiDA architecture



AiiDA tutorials

The screenshot displays the AiiDA Tutorials website interface. On the left is a sidebar with a search bar and a list of tutorial materials. The main content area features a header with the AiiDA logo and navigation links, followed by a section for 'Latest: 2021 Introductory virtual tutorial' and a 'Short Demonstrations' table. Below this is a 'Videos' section with a list of lecture recordings. On the right, a 'Presentations' table lists dates, presenters, and titles. A 'Hands-on sessions' section lists five units. Three callout boxes highlight key features: 'Pre-recorded explanatory videos', 'Full tutorial from zero to writing workflows', and 'Latest: 2021 Introductory virtual tutorial'.

Search docs

TUTORIAL MATERIALS

- 2020, BIG-MAP meeting AiiDA tutorial (aiida-core 1.4.3)
- 2020, Introductory workshop Virtual Edition (aiida-core 1.3.0)
- 2020, Wannier workshop Virtual Edition (aiida-core 1.1.1)
- 2019, ISSP University of Tokyo, Chiba, Japan (aiida-core 1.0.1)
- 2019, IIT Mandi, Mandi, India (aiida-core 1.0.0b6)
- 2019, SINTEF, Oslo, Norway (aiida-core 1.0.0b6)
- 2019, Jožef Stefan Institute, Ljubljana, Slovenia (aiida-core 1.0.0b6)
- 2019, Xiamen University, Xiamen, China (aiida-core 1.0.0b6)
- 2019, EPFL, Lausanne, Switzerland (aiida-core 1.0.0b3)
- 2019, University of Amsterdam, Amsterdam, Netherlands (aiida-core 0.12.2)
- 2018, Cineca, Bologna, Italy (aiida-core 1.0.0a1)
- 2018, EPFL, Lausanne, Switzerland (aiida-core 0.11.4)

AiiDA Tutorials

The official home of AiiDA tutorial materials and videos.

Latest: 2021 Introductory virtual tutorial

[AiiDA Cheat Sheet](#)

Short Demonstrations

Quantum ESPRESSO introductory tutorial	Wannier90: "Virtual Edition" 2021 tutorial
--	--

Videos

For some events we have also recorded the lectures, that you can find here. You will also find links inside the respective sections.

- 2019 tutorial lectures (aiida-core 1.0.0b3) (mirror)
- 2019 plugin migration workshop lectures (aiida-core 1.0.0b2)
- 2017 tutorial lectures (aiida-core 0.9.0)
- 2017 short demo videos (aiida-core 0.8.0)
- 2016 tutorial lectures (aiida-core 0.6.0)

Presentations

For this virtual tutorial, most presentations are pre-recorded explanatory videos that you can watch at any time that is most convenient for you. There will also be some hands-on sessions of certain days.

Date	Presenter	Title
Monday July 5th	Marnik Bercx	Welcome and AiiDA Tutorial Overview (LIVE)
	Francisco Ramirez	Introduction to AiiDA
Tuesday July 6th	Giovanni Pizzi	The Materials Cloud
	Aliaksandr Yakotovich	AiiDA lab
Wednesday July 7th	Sebastian Huber	Provenance and workflows in AiiDA
Thursday July 8th	Leopold Talirz	The AiiDA Plugin Ecosystem
	Casper Andersen	AiiDA and OPTIMADE
	Chris Sewell	AiiDA Installation Tutorial

Hands-on sessions

The material for the hands-on sessions is divided in 5 units:

- Getting started
- Running processes
- Managing data
- Writing workflows
- Creating plugins

Pre-recorded explanatory videos

Full tutorial from zero to writing workflows

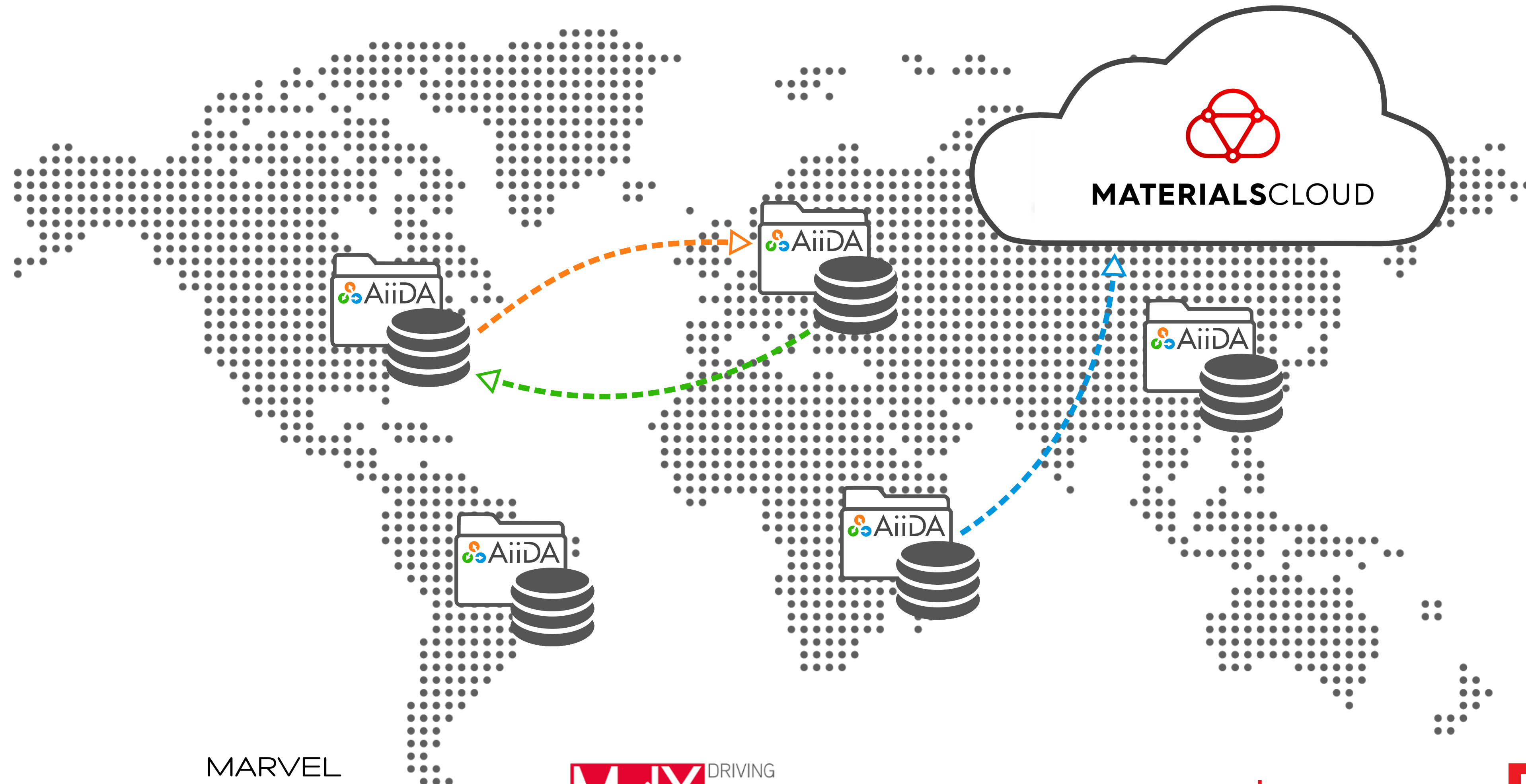
<https://aiida-tutorials.readthedocs.io/>

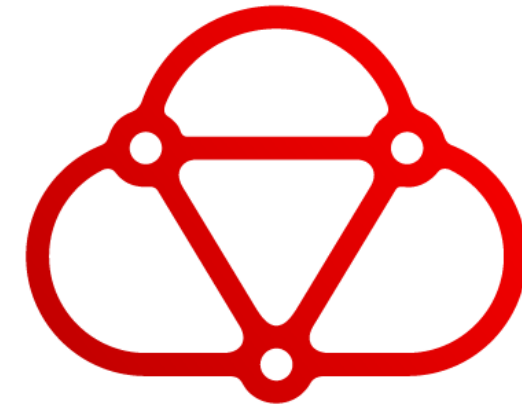
FAIR data access and sharing



FAIR sharing in AiiDA: data and graphs

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





MATERIALSCLOUD

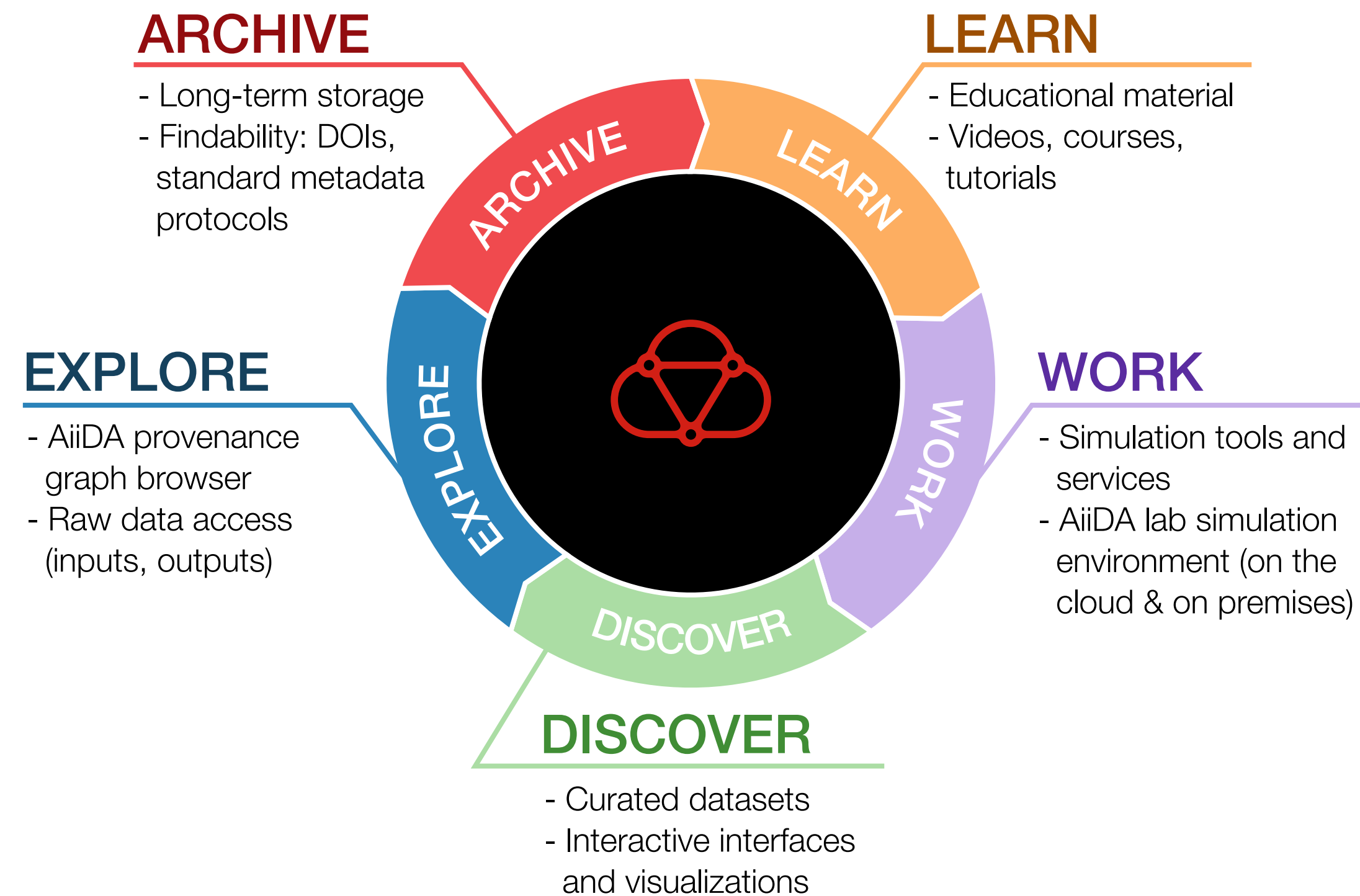
<https://www.materialscloud.org>

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

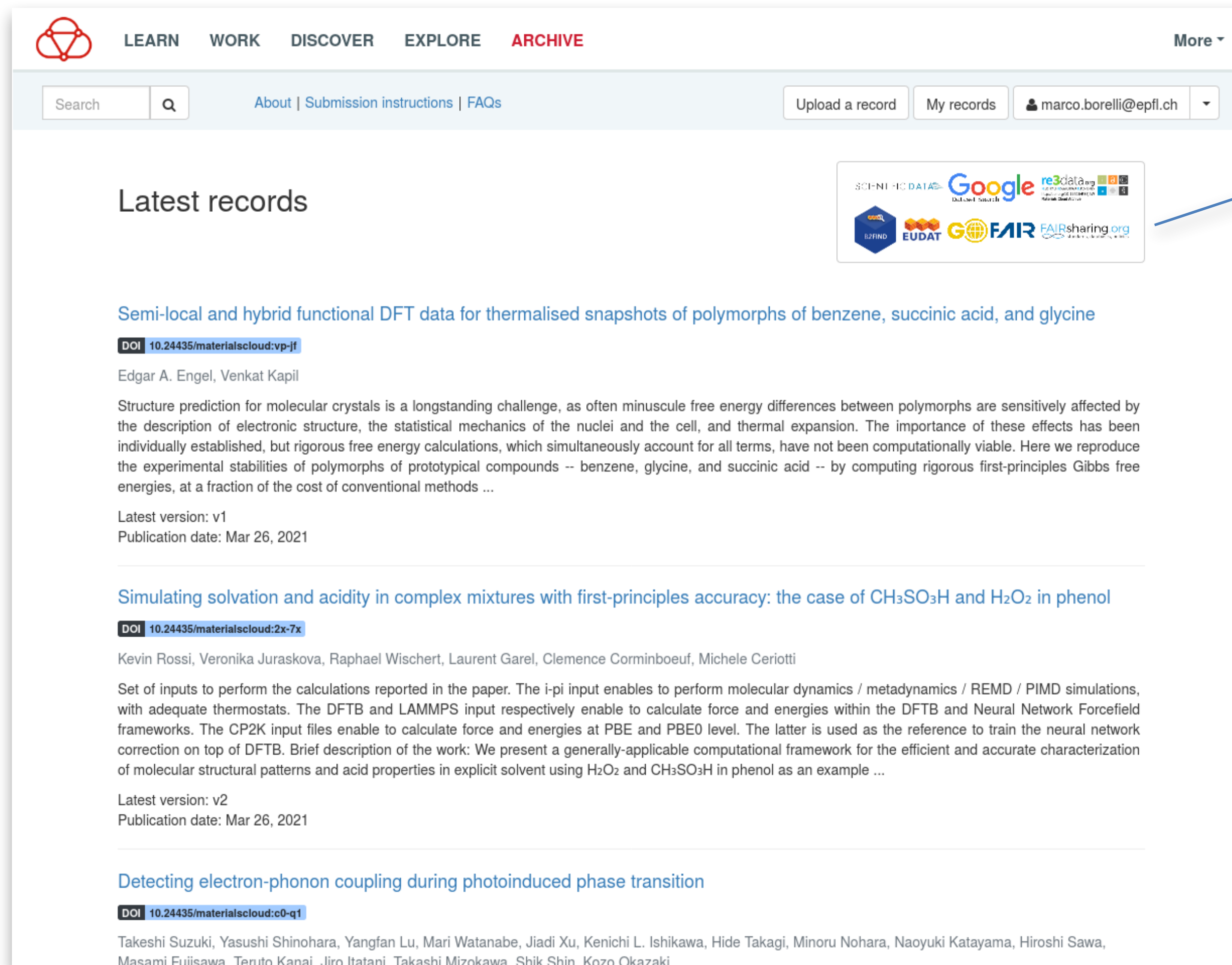
Materials Cloud is also a  implementation network

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



The screenshot shows the Materials Cloud website with a navigation bar (LEARN, WORK, DISCOVER, EXPLORE, ARCHIVE) and a search bar. The 'Latest records' section features three entries:

- Semi-local and hybrid functional DFT data for thermalised snapshots of polymorphs of benzene, succinic acid, and glycine**
DOI: 10.24435/materialscloud:vp-jf
Edgar A. Engel, Venkat Kapil
Structure prediction for molecular crystals is a longstanding challenge, as often minuscule free energy differences between polymorphs are sensitively affected by the description of electronic structure, the statistical mechanics of the nuclei and the cell, and thermal expansion. The importance of these effects has been individually established, but rigorous free energy calculations, which simultaneously account for all terms, have not been computationally viable. Here we reproduce the experimental stabilities of polymorphs of prototypical compounds -- benzene, glycine, and succinic acid -- by computing rigorous first-principles Gibbs free energies, at a fraction of the cost of conventional methods ...
Latest version: v1
Publication date: Mar 26, 2021
- Simulating solvation and acidity in complex mixtures with first-principles accuracy: the case of CH₃SO₃H and H₂O₂ in phenol**
DOI: 10.24435/materialscloud:2x-7x
Kevin Rossi, Veronika Juraskova, Raphael Wischert, Laurent Garel, Clemence Corminboeuf, Michele Ceriotti
Set of inputs to perform the calculations reported in the paper. The i-pi input enables to perform molecular dynamics / metadynamics / REMD / PIMD simulations, with adequate thermostats. The DFTB and LAMMPS input respectively enable to calculate force and energies within the DFTB and Neural Network Forcefield frameworks. The CP2K input files enable to calculate force and energies at PBE and PBE0 level. The latter is used as the reference to train the neural network correction on top of DFTB. Brief description of the work: We present a generally-applicable computational framework for the efficient and accurate characterization of molecular structural patterns and acid properties in explicit solvent using H₂O₂ and CH₃SO₃H in phenol as an example ...
Latest version: v2
Publication date: Mar 26, 2021
- Detecting electron-phonon coupling during photoinduced phase transition**
DOI: 10.24435/materialscloud:c0-q1
Takeshi Suzuki, Yasushi Shinohara, Yangfan Lu, Mari Watanabe, Jiadi Xu, Kenichi L. Ishikawa, Hide Takagi, Minoru Nohara, Naoyuki Katayama, Hiroshi Sawa, Masami Fujisawa, Teruto Kanai, Jiro Itatani, Takashi Mizokawa, Shik Shin, Koza Okazaki

Recommended data repository
by Nature's journal [Scientific Data](#)

Indexed by [Google Dataset Search](#)
and by EUDAT/EOSC's [B2FIND](#)

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

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



Research and Innovation

Open Research Europe

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

Interface for users submitting data

Submission form

The screenshot shows the 'Materials Cloud Archive record upload' form. At the top, there is a navigation bar with 'LEARN', 'WORK', 'DISCOVER', 'EXPLORE', and 'ARCHIVE' (highlighted in red). A search bar and user profile 'marco.borelli@epfl.ch' are also visible. The main content area is titled 'Materials Cloud Archive record upload' and includes a 'Submission procedure' section with four numbered steps. Below this are three main input fields: 'Title*' with a note about capitalization, 'Description*' with a help icon, and 'Keywords*' with a note to add at least three keywords. A dropdown menu for keywords is open, showing options like 'MarketPlace', 'Marie Curie Fellowship', 'MARVEL', and 'MARVEL/DD1' through 'MARVEL/DD4'. An 'Add keyword' button is located to the right of the dropdown.

User view (own entries)

The screenshot shows the 'My records' page. It features a navigation bar similar to the submission form, but with the user profile 'valeria.granata@epfl.ch'. The main heading is 'My records' with an 'Upload a record' button. Below the heading, there are two expandable sections: 'Records in progress' and 'Records published (latest 10 published records)'. The 'Records published' section shows a table with 10 records. The first two records are visible:

Record	Owner	Status
Towards constant potential modeling of CO-CO coupling at liquid water-Cu(100) interfaces DOI: 10.24435/materialscloud:p9-q7 [version: v1] Last update: 18/03/2021, 23:54:37 Authors: Henrik H. Kristoffersen, Karen Chan We have studied electrochemical *CO-*CO coupling in explicit electrolyte with density functional theory, molecular dynamics, and metadynamics. We considered both the *CO-*CO coupling reaction and the ...	hhk@chem.ku.dk	PUBLISHED
Simulating the ghost: quantum dynamics of the solvated electron DOI: 10.24435/materialscloud:dz-a0 [version: v1] Last update: 18/03/2021, 21:27:12 Authors: Jinqiang Lan, Venkat Kapil, Piero Gasparotto, Michele Ceriotti	jingqiang.lan@uzh.ch	PUBLISHED

Interface for users submitting data

Submission form

The screenshot shows the 'Materials Cloud Archive record upload' form. It includes a navigation bar with 'LEARN', 'WORK', 'DISCOVER', 'EXPLORE', and 'ARCHIVE'. A search bar and navigation links are present. The form contains a 'Submission procedure' section with four steps, a 'Title*' field with instructions, a 'Description*' field, and a 'Keywords*' section with a dropdown menu showing options like 'MarketPlace', 'Marie Curie Fellowship', 'MARVEL', and 'MARVEL/DD1' through 'MARVEL/DD4'. An 'Add keyword' button is also visible.

User view (own entries)

The screenshot shows the 'My records' user view. It features a navigation bar and a search bar. A table lists records with columns for 'Owner' and 'Status'. A detailed view of a record is shown below the table, including version information, authors, and abstract text.

Owner	Status
hhk@chem.ku.dk	PUBLISHED
jinggang.lan@uzh.ch	PUBLISHED

Record Details:
[version: v1] Last update: 18/03/2021, 23:54:37
Authors: Henrik H. Kristoffersen, Karen Chan
We have studied electrochemical *CO-*CO coupling in explicit electrolyte with density functional theory, molecular dynamics, and metadynamics. We considered both the *CO-*CO coupling reaction and the ...
DOI: 10.24435/materialscloud:dz-a0
[version: v1] Last update: 18/03/2021, 21:27:12
Authors: Jinggang Lan, Venkat Kapil, Piero Gasparotto, Michele Ceriotti

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

materialscloud:2017.0008/v3

DOIs assigned

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

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

¹ Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

² Vilnius University Institute of Biotechnology, Sauletekio al. 7, LT-10257 Vilnius, Lithuania

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

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

How to cite this record

Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Davide Campi, Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano E. Castelli, Andrea Cepellotti, Giovanni Pizzi, Nicola Marzari, *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, Materials Cloud Archive **2017.0008/v3** (2019), doi: 10.24435/materialscloud:2017.0008/v3.

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



Export

Dublin Core JSON

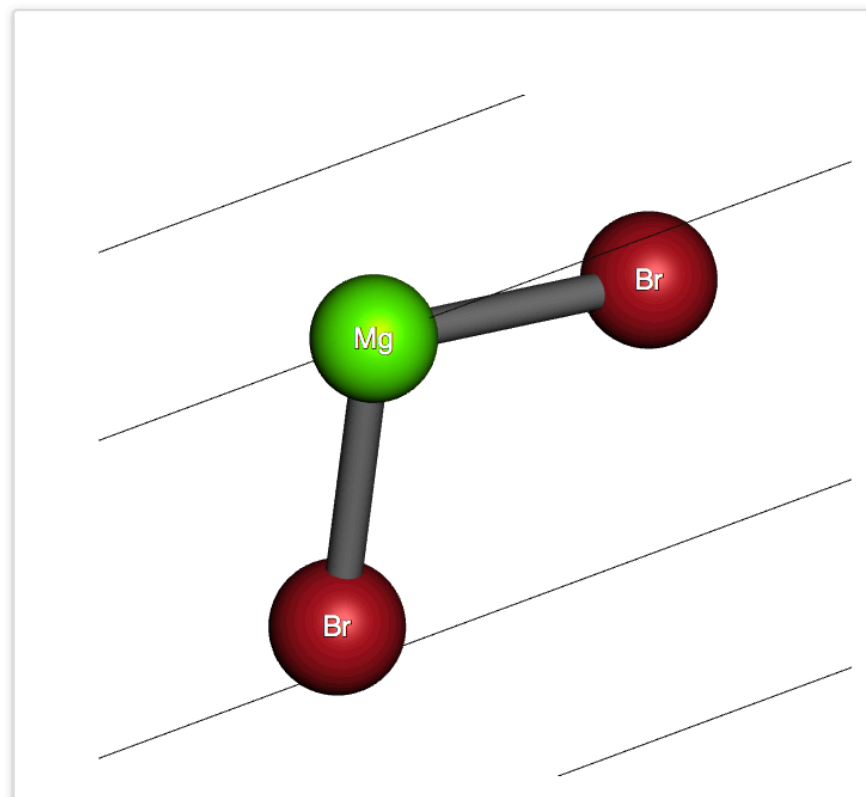
Direct links to Discover & Explore

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

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

Binding Energies:

DF2-C09 Binding energy [$\text{meV}/\text{\AA}^2$]:
(From parent COD 9009107)
rVV10 Binding energy [$\text{meV}/\text{\AA}^2$]: 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



EXPLORE

Selected Profile: 2D Structures DOI: 10.24435/materialscloud:2017.0008/v2

Grid Details Statistics

e7db98c1-9d25-4872-8236-68559c5b0702 GO

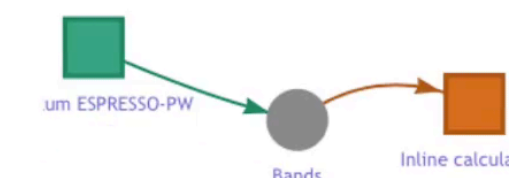
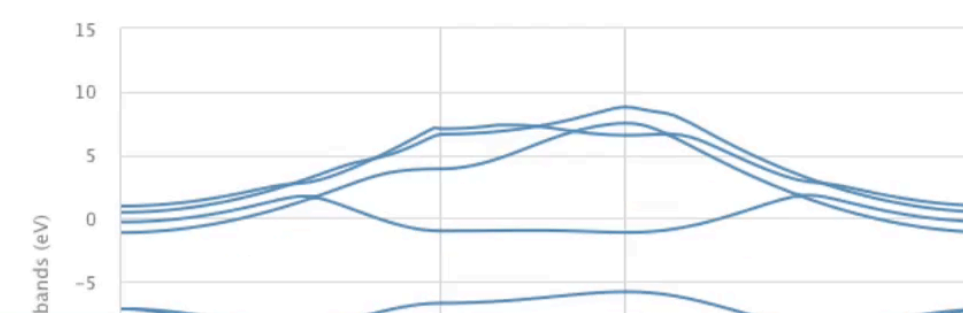
UUID: e7db98c1-9d25-4872-8236-68559c5b0702
Type: data.array.bands.BandsData
Created at 6 January 2017
Modified 8 months ago
davide_campi@epfl.ch

BandsData

AiiDA Provenance Browser

Label: Electronic bands

Selected node, Inputs, Outputs



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

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.

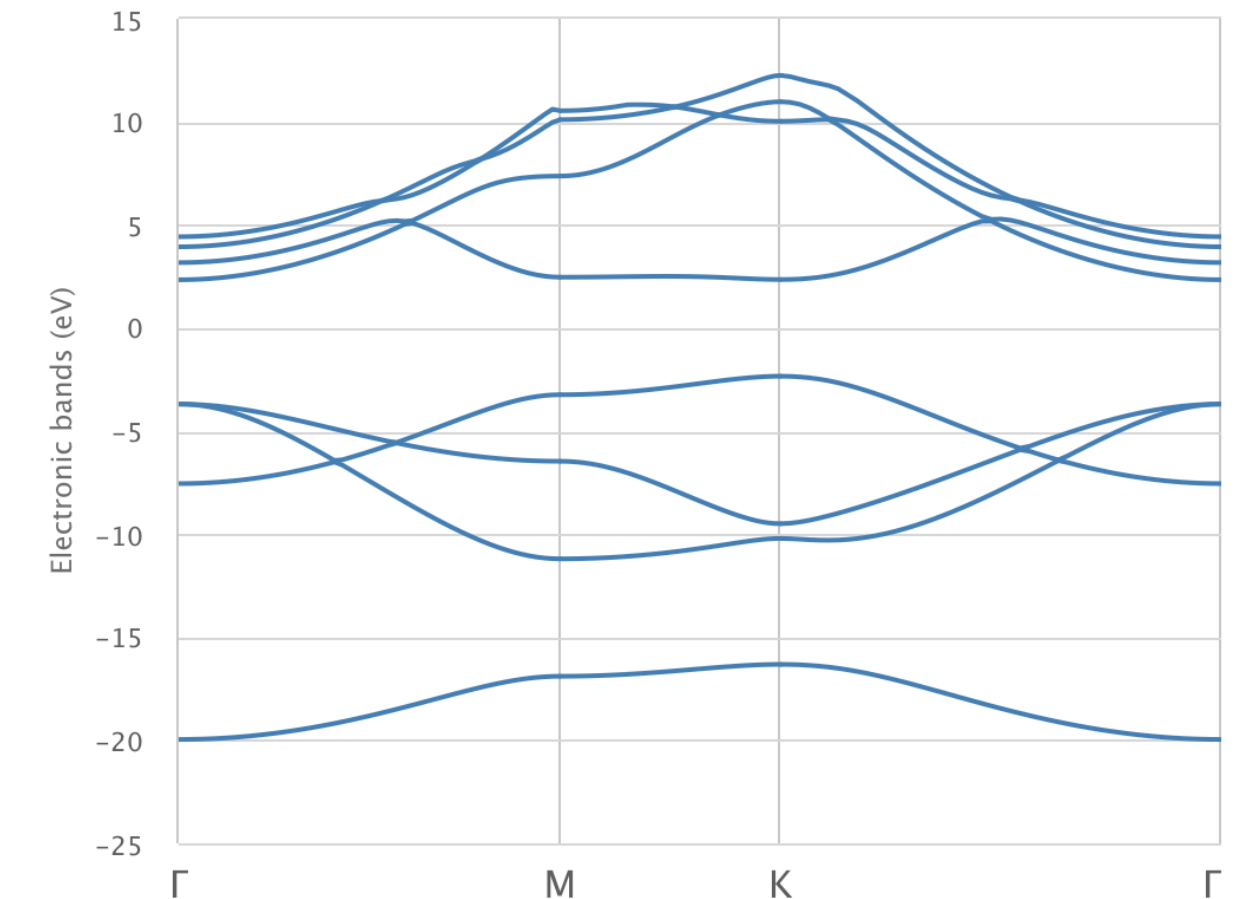
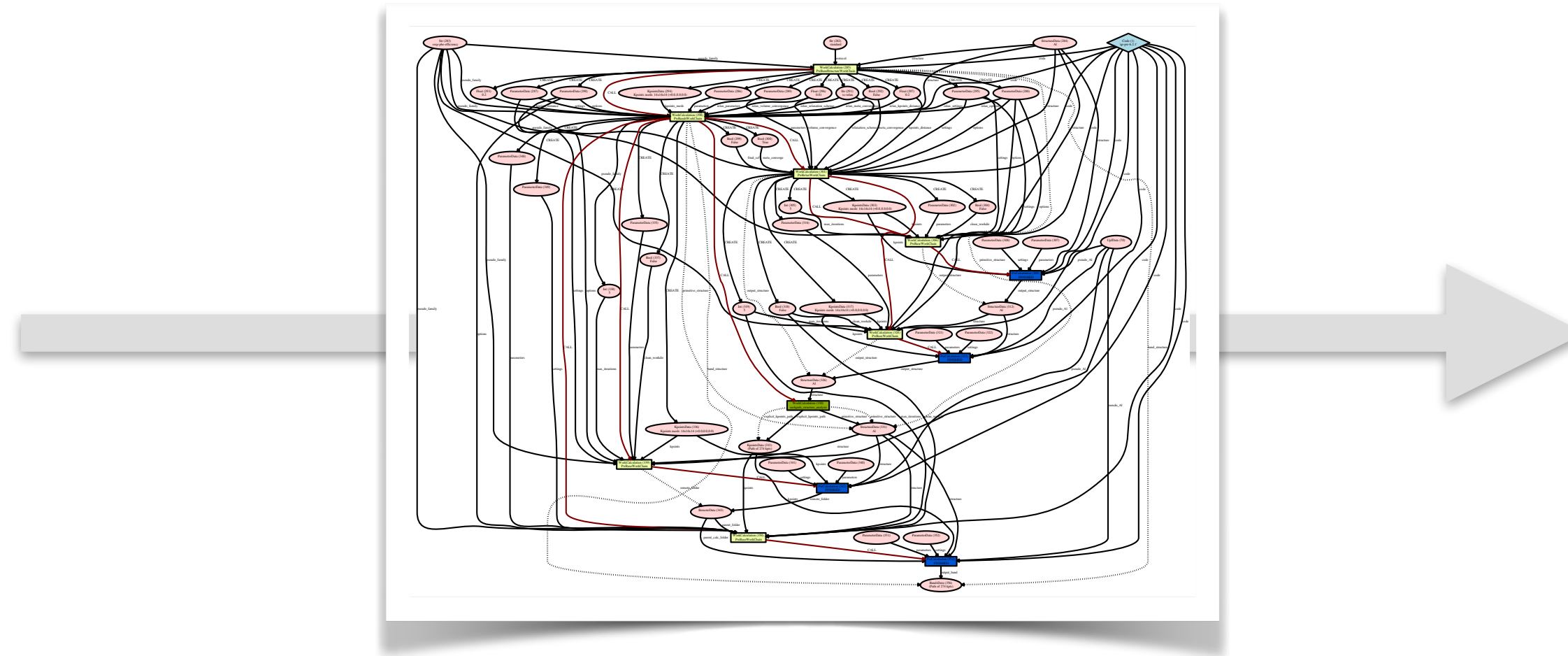
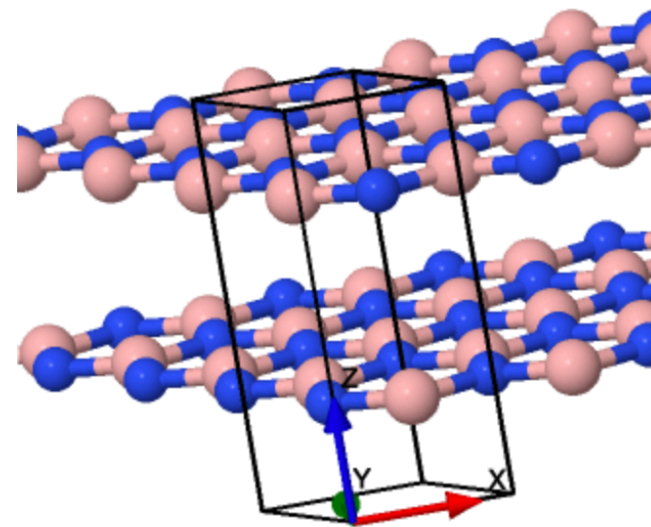
Funding Body	DMP template (using  AiiDA)	DMP template (no AiiDA)
SNF	.docx .odt .pdf	.docx .odt .pdf
H2020	.docx .odt .pdf	.docx .odt .pdf

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



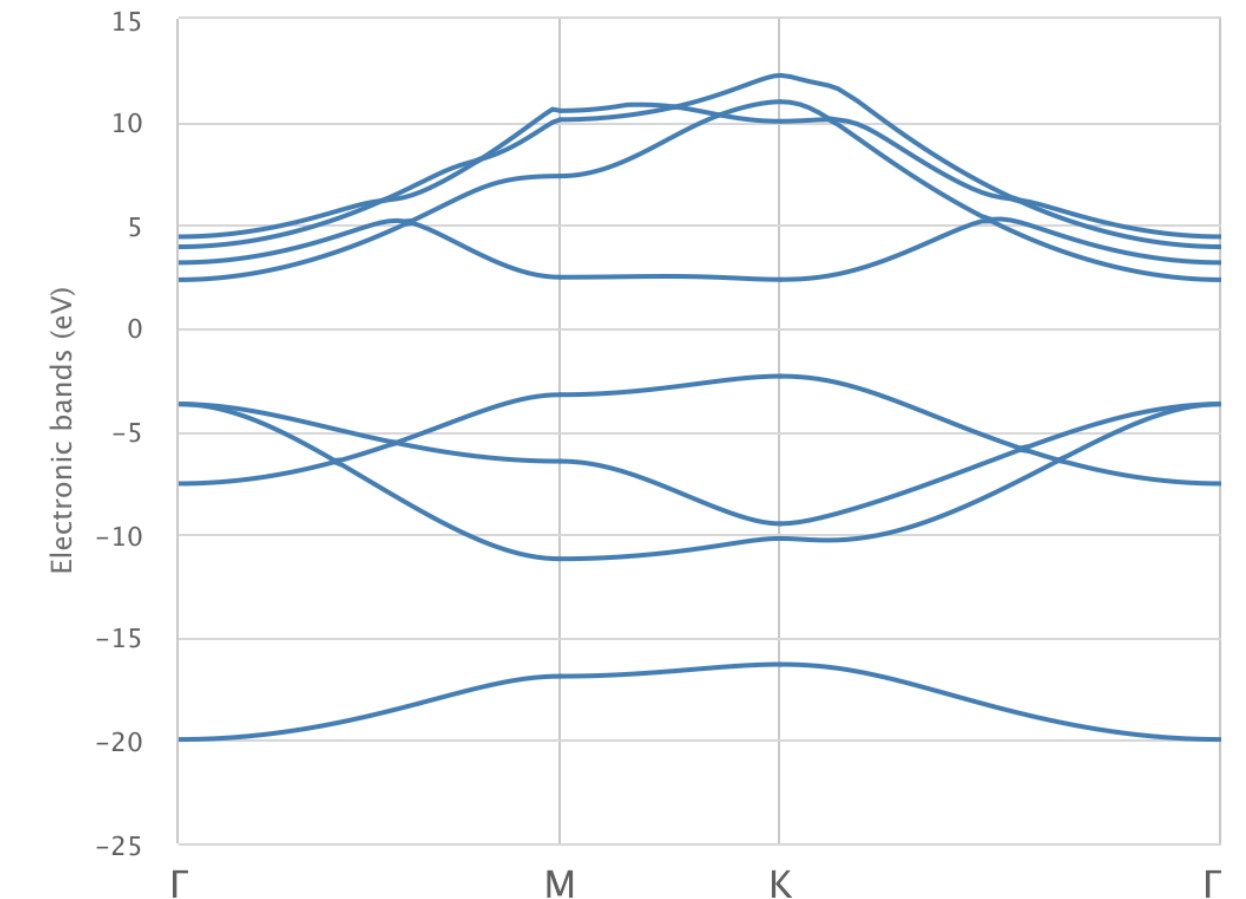
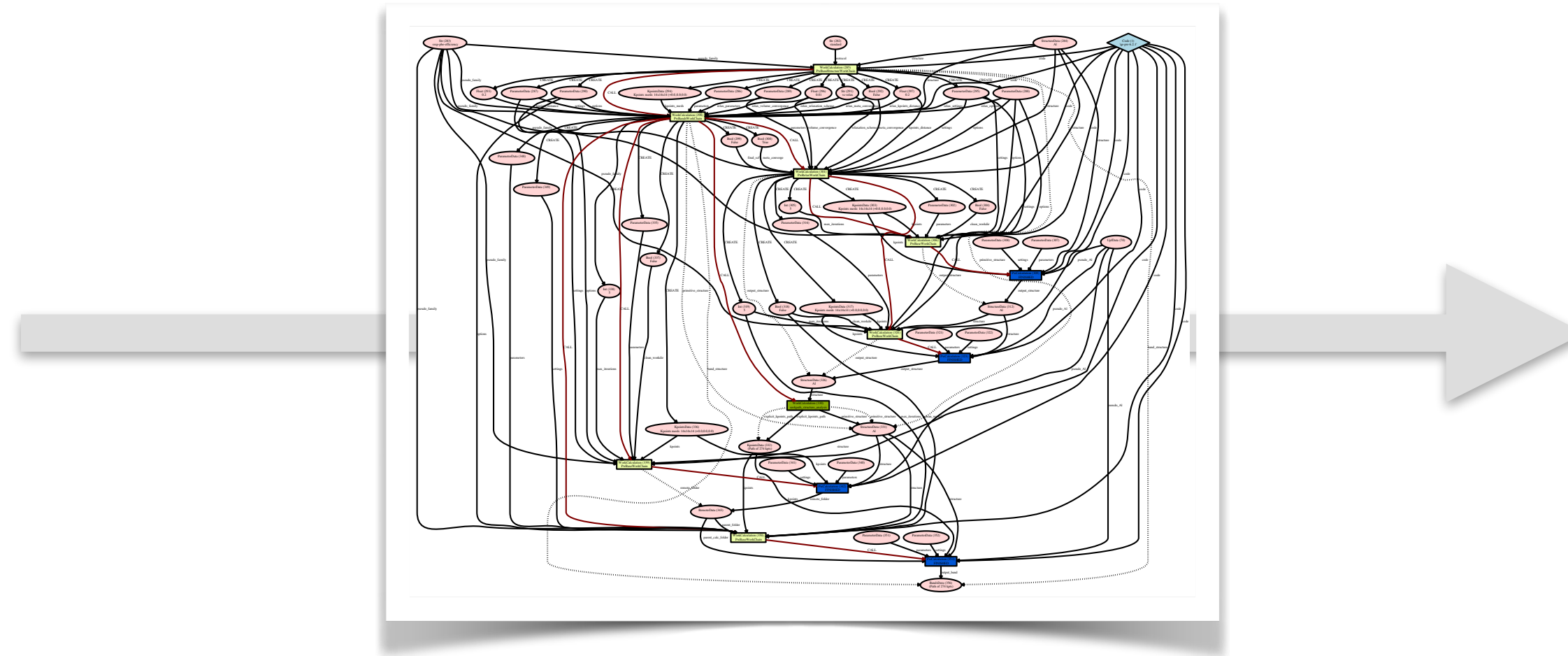
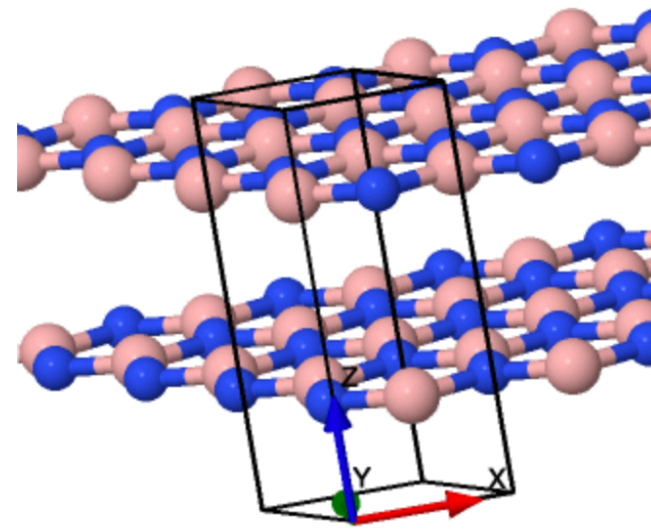
Workflows to generate data

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



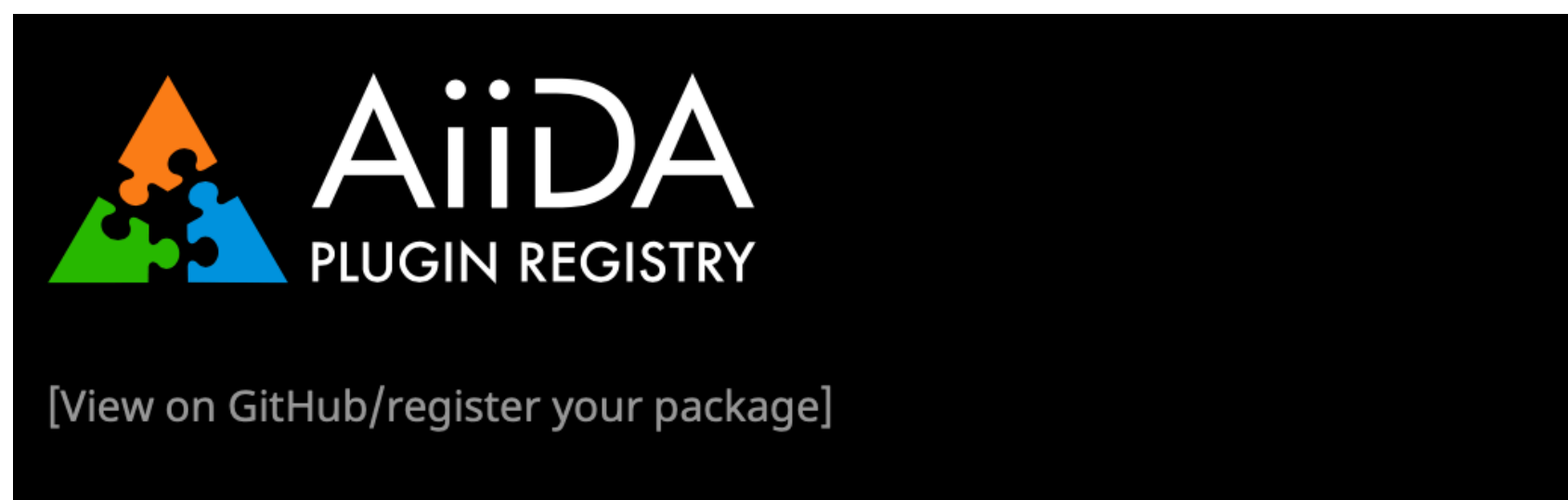
- AiiDA provenance graph: explain how the structure was computed and to **reproduce that single specific calculation**: *log of "what happened in the past"*
- AiiDA workflow engine**: Flexible python interface to encode complex scientific steps
 - Provides robustness (connection drops, ...) and allows 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



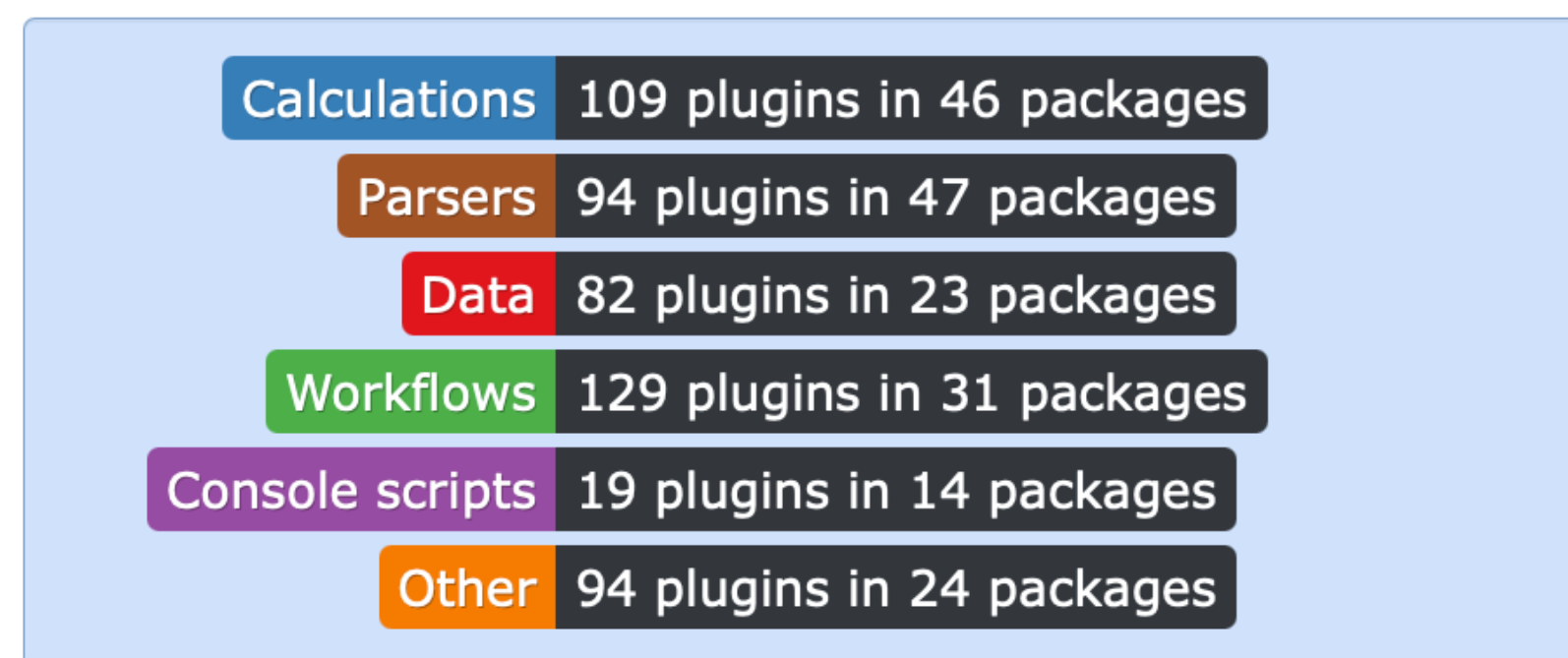
```
PwBandsWorkChain = WorkflowFactory('quantumespresso.pw.bands')
code = load_code('pw.x@daint')
structure = StructureData(ase=ase.io.read('BN.xsf'))
builder = PwBandsWorkChain.get_builder_from_protocol(code=code, structure=structure)
... # Possible overrides
workchain_node = submit(builder)
```


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

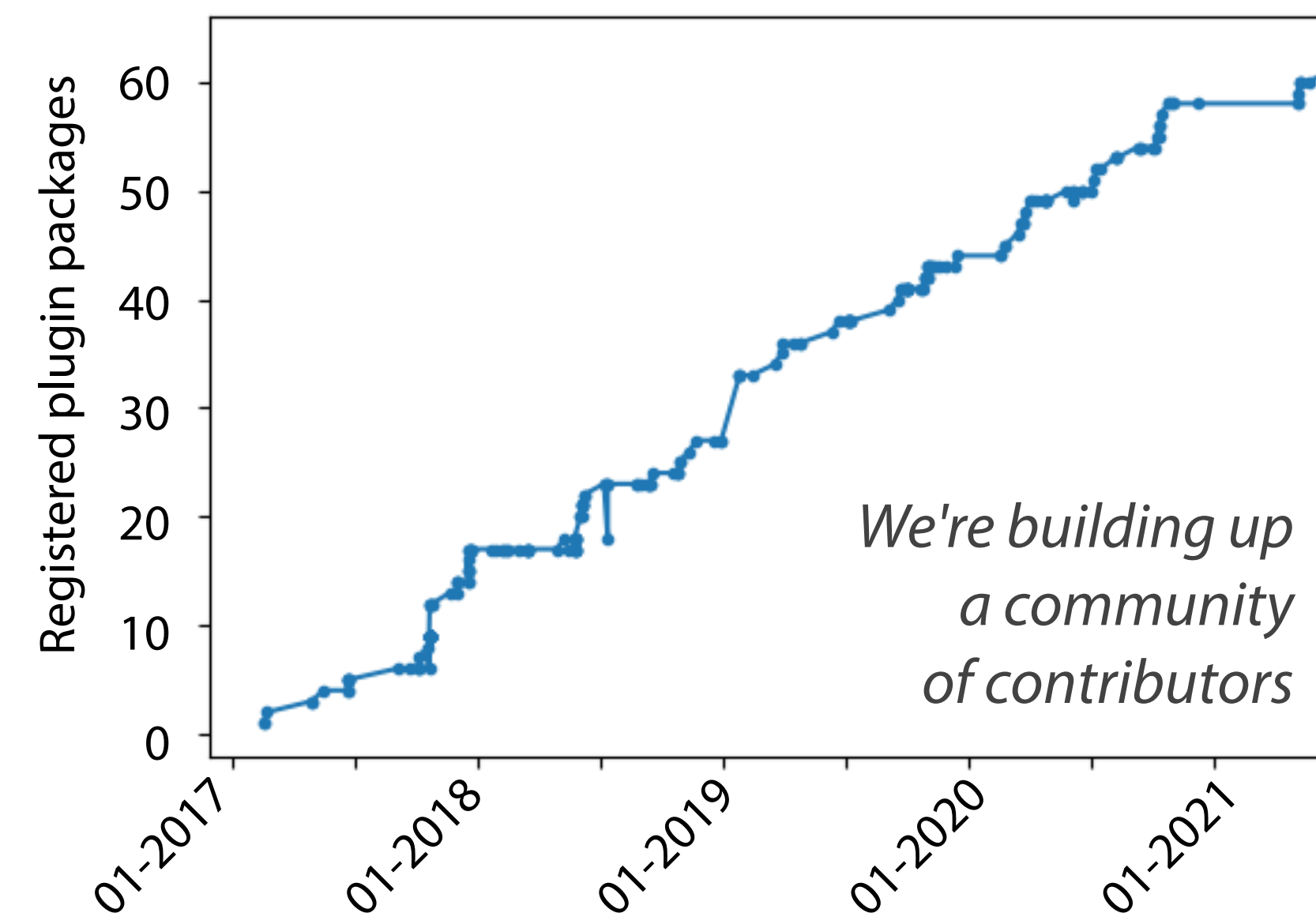


- Plugins collected in the AiiDA plugin registry
- **100+ codes currently supported**, 120+ workflows
- Many are **community-contributed**

Registered plugin packages: 66



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



The need for turn-key solutions



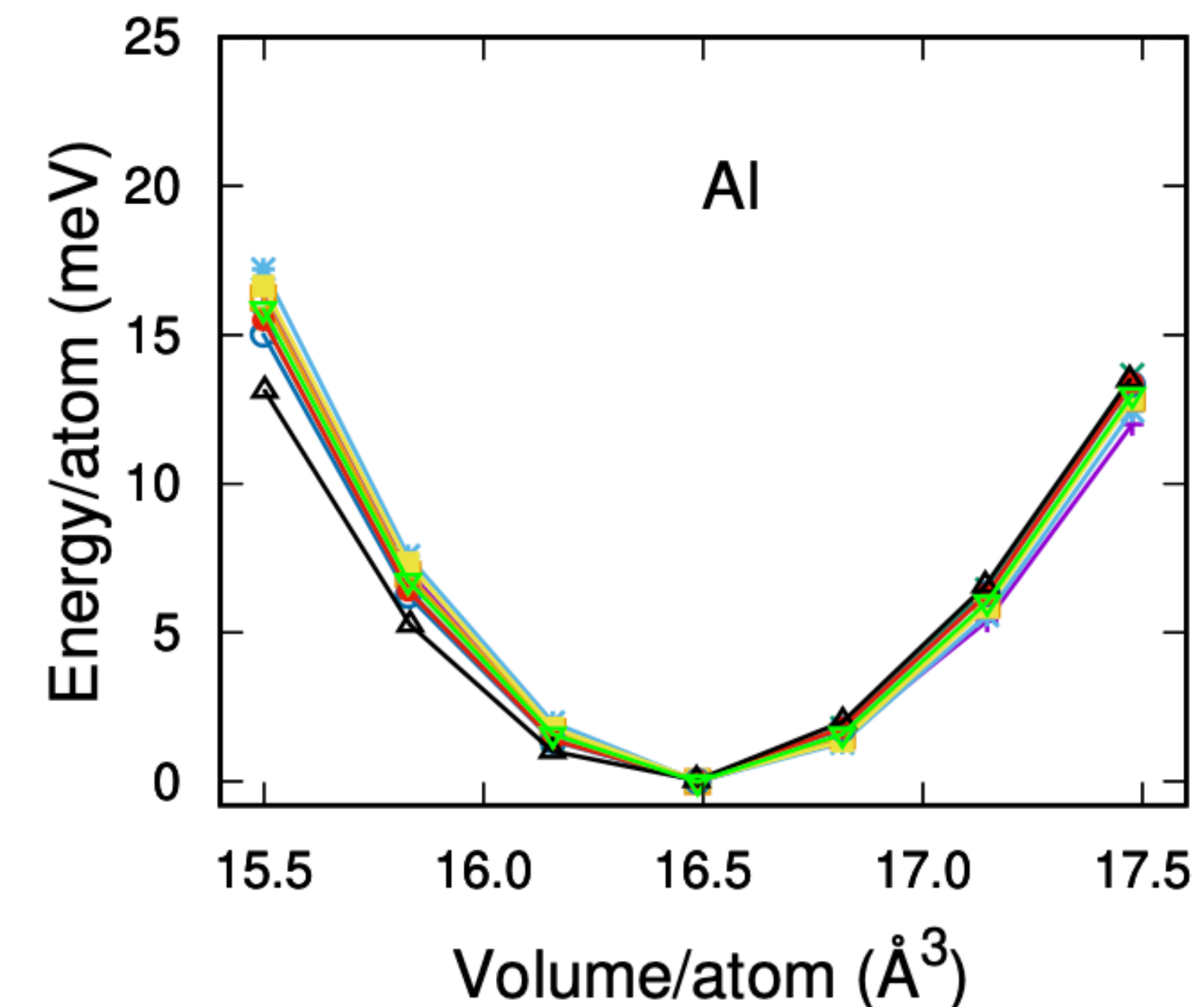
- Like in a car: many end-users, drive without need to know how the engine works
 - ▶ Engines are "robust"
 - ▶ Just turn the key and drive
- I still need a driving license, but:
 - many needs addressed by driving my own car
 - no need to learn again to drive if I change car brand

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 , Emanuele Bosoni , Marnik Bercx , Jens Bröder , Augustin Degomme , Vladimir Dikan , Kristjan Eimre , Espen Flage-Larsen , Alberto Garcia , Luigi Genovese , Dominik Gresch , Conrad Johnston , Guido Petretto , Samuel Poncé , Gian-Marco Rignanese , Christopher J. Sewell , Berend Smit , Vasily Tseplyaev , Martin Uhrin , Daniel Wortmann , Aliaksandr V. Yakutovich , Austin Zadoks , Pezhman Zarabadi-Poor , Bonan Zhu , Nicola Marzari and Giovanni Pizzi

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>



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

<https://github.com/aidataeam/aida-common-workflows/>

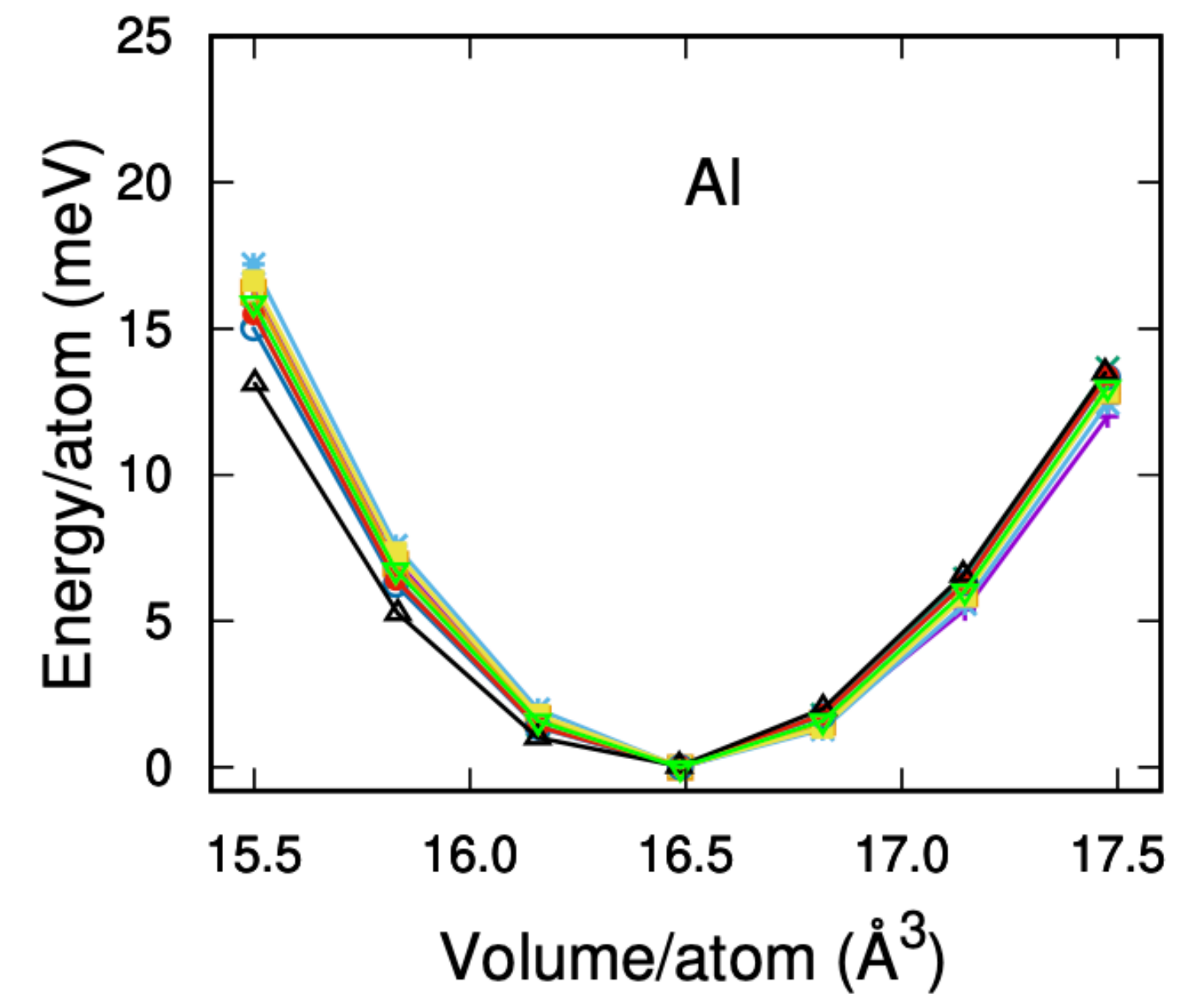
Code interoperability: common workflow interfaces

<https://github.com/aidateam/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

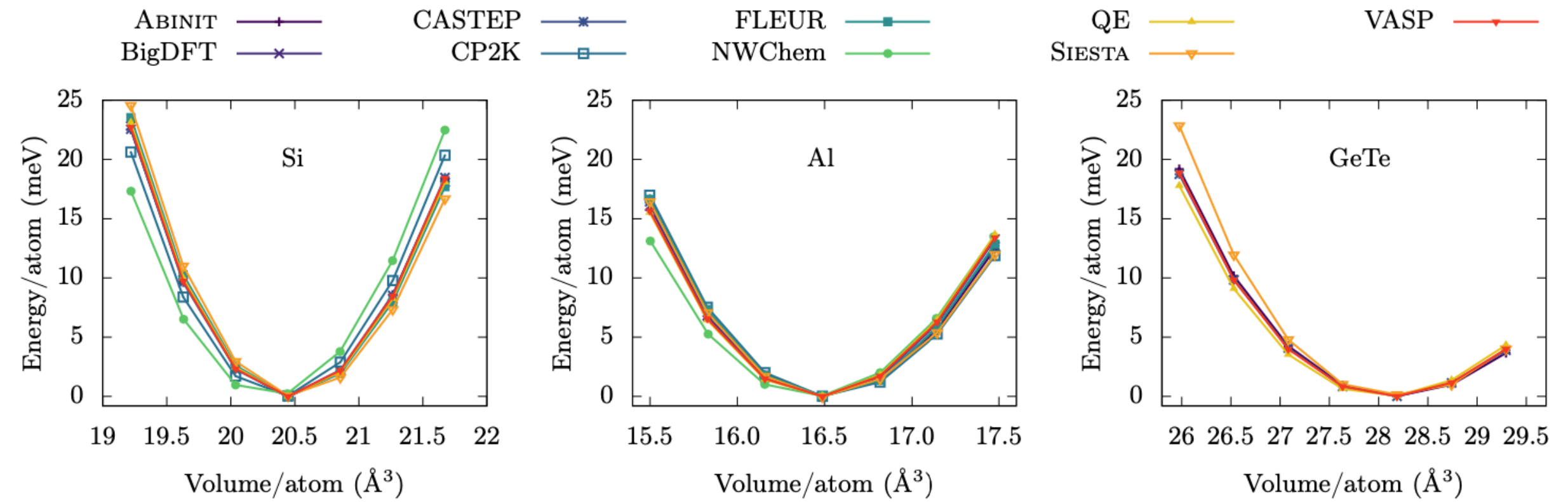
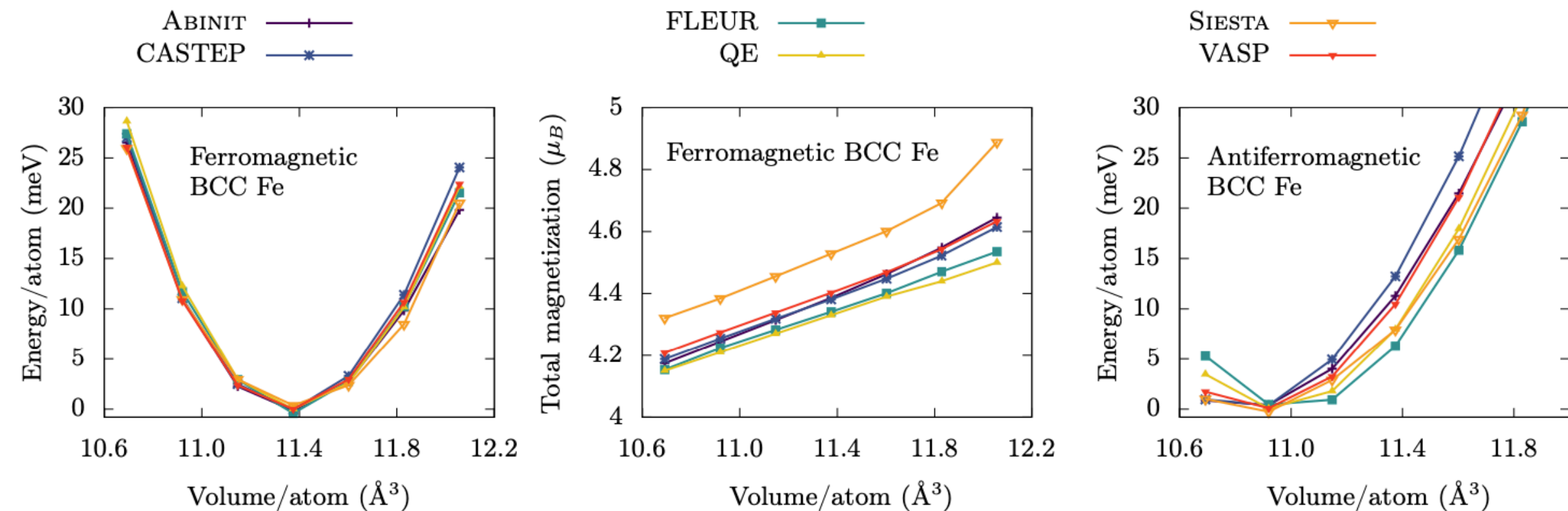
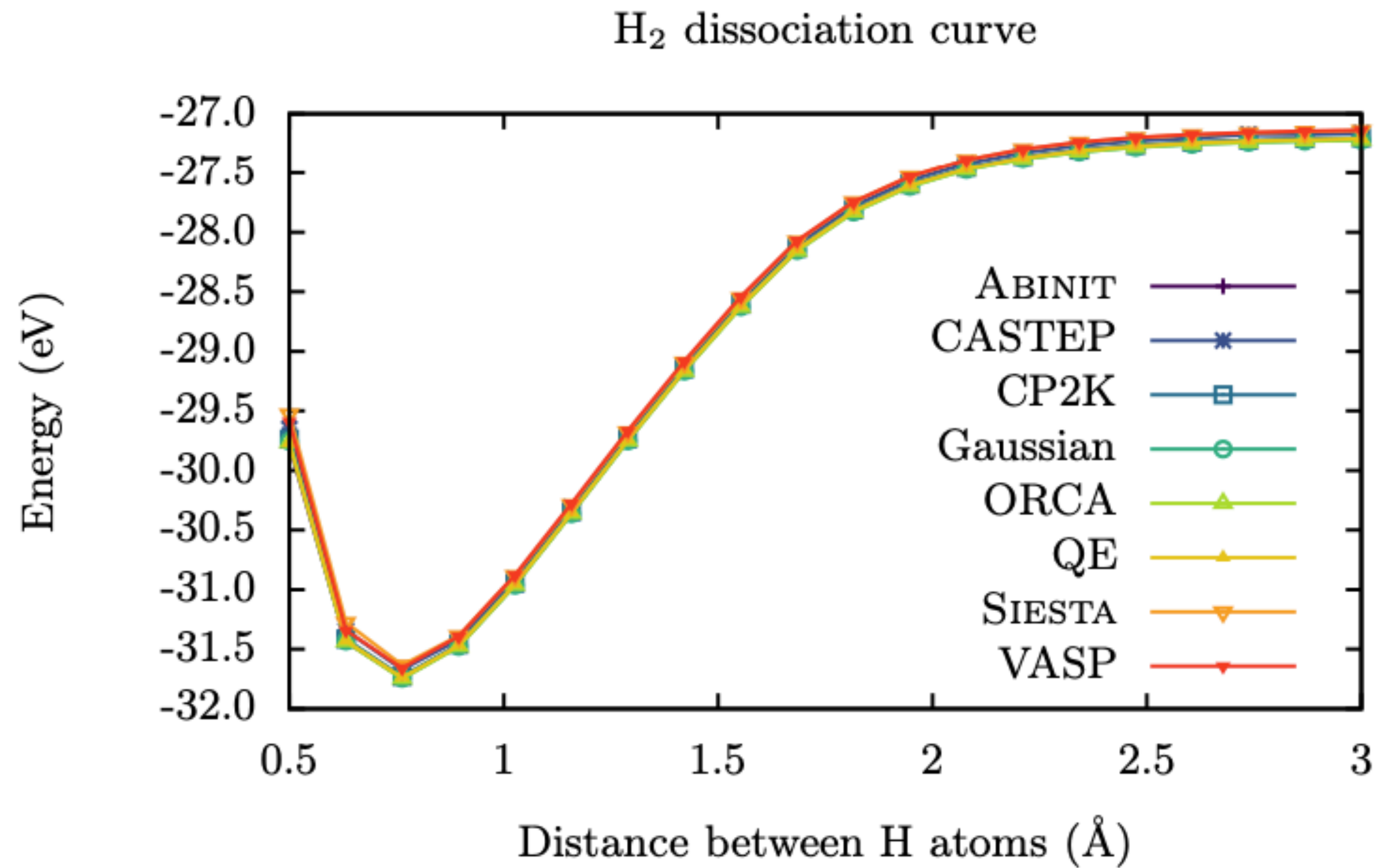


Figure 7. **EOS for Si, Al and GeTe.** Results obtained with the code-agnostic EquationOfStateWorkflow. For each code, the energy is shifted to set the minimum energy to zero. The EOS has been computed with all codes discussed in this work, except ORCA and Gaussian, which are mainly specialized for non-periodic 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

QUANTUM MOBILE
21.06.04

Search the docs ...

Quantum Mobile

Releases

USERS

Launching Quantum Mobile

Using Quantum Mobile

VirtualBox FAQ

Troubleshooting

DEVELOPERS

Customise Quantum Mobile

Build a Desktop VM

Build a Cloud VM

Build a Docker container

Create a new ansible role

MAINTAINERS

Developing Quantum Mobile

Preparing releases

Theme by the Executable Book Project

Quantum Mobile

What is Quantum Mobile

Quantum Mobile is a Virtual Machine for computational materials science.

Quantum Mobile provides a uniform environment for quantum mechanical materials simulations. Simulation codes are set up and ready to be used either directly or through the [AiiDA](#) python framework for automated workflows and provenance tracking.

Open source throughout
Based on [Ubuntu Linux](#)

Pre-built images
Available for Linux, MacOS or Windows computers, using VirtualBox. Or deploy on cloud services like OpenStack or Amazon Elastic Compute Cloud using [ansible](#).

Simulation codes pre-installed
[Abinit](#), [BigDFT](#), [CP2K](#), [Fleur](#), [Quantum ESPRESSO](#), [Siesta](#), [Wannier90](#), [Yambo](#), together with [AiiDA](#), [JupyterLab](#), and the [AiiDALab](#) Jupyter environment.

Tools pre-installed
atomistic (xcrysden, jmol, cif2cell, ase, pymatgen, seekpath, spglib, pycifrw), visualization (grace, gnuplot, matplotlib, bokeh, jupyter), simulation environment (slurm, OpenMPI, FFT/BLAS/LAPACK, gcc, gfortran, singularity).

Modular setup
with individually tested [ansible roles](#). Build your own flavour tailored to your use case.

[Wannier90](#) [Yambo](#) [AiiDA](#) [PostgreSQL](#) [RabbitMQ](#) [Slurm](#)

v: latest

- 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)



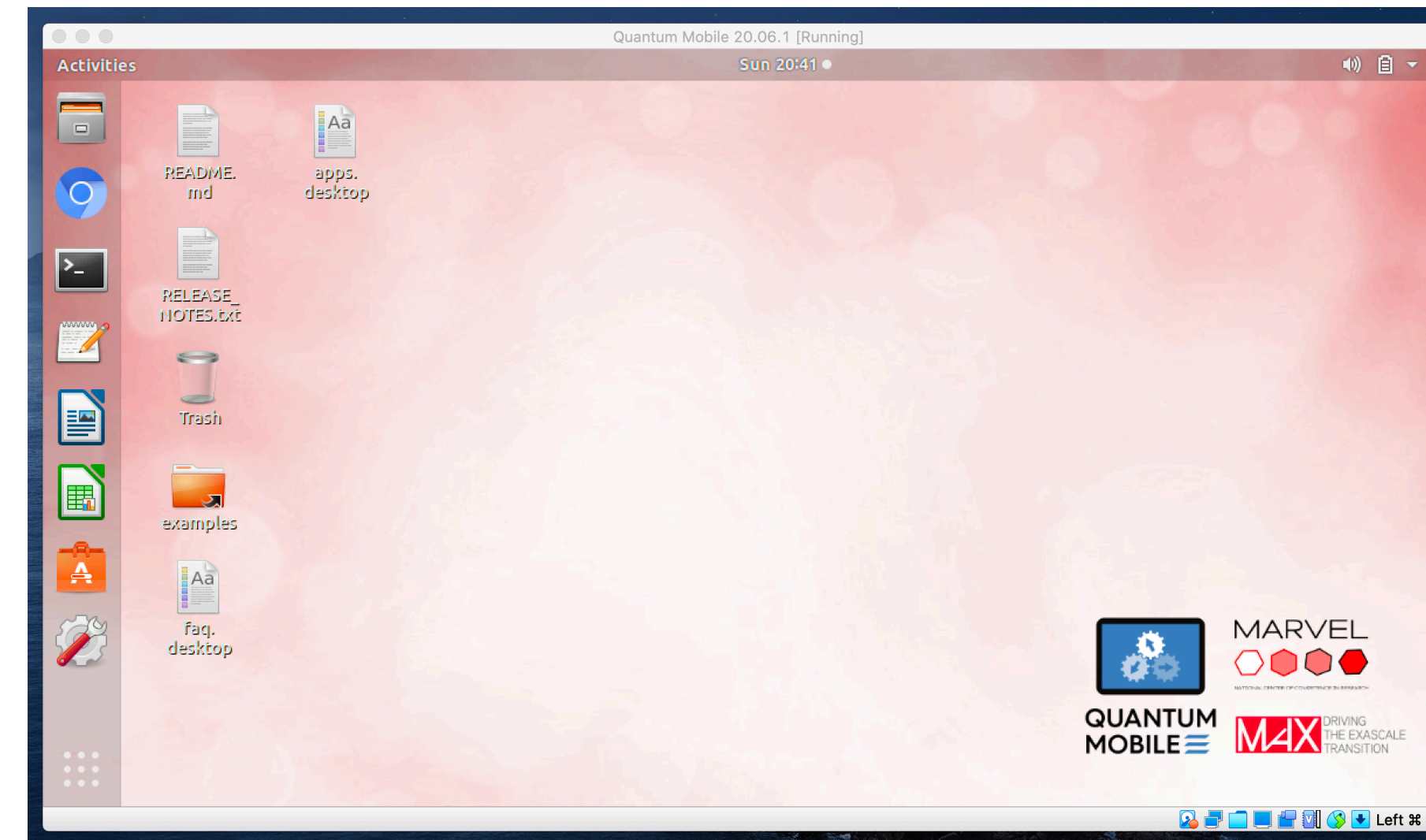
Testimonials

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

```
max@qmobile: ~  
File Edit View Search Terminal Help  
(aida) max@qmobile:~$ verdi code list  
# List of configured codes:  
# (use 'verdi code show CODEID' to see the details)  
* pk 1 - abinit-9.2.1@localhost  
* pk 2 - bigdft-1.9.1@localhost  
* pk 3 - cp2k-7.1@localhost  
* pk 4 - fleur-fleur_MPI-0.30-MaX4@localhost  
* pk 5 - fleur-inpgen-0.30-MaX4@localhost  
* pk 6 - nwchem-7.0.2@localhost  
* pk 7 - qe-pw-6.5@localhost  
* pk 8 - qe-cp-6.5@localhost  
* pk 9 - qe-pp-6.5@localhost  
* pk 10 - qe-ph-6.5@localhost  
* pk 11 - qe-neb-6.5@localhost  
* pk 12 - qe-projwfc-6.5@localhost  
* pk 13 - qe-pw2wannier90-6.5@localhost  
* pk 14 - qe-q2r-6.5@localhost  
* pk 15 - qe-dos-6.5@localhost  
* pk 16 - qe-matdyn-6.5@localhost  
* pk 17 - siesta-MaX-1.2.0@localhost  
* pk 18 - siesta-plstm-MaX-1.2.0@localhost  
* pk 19 - wannier90-wannier-3.1.0@localhost  
* pk 20 - yambo-4.5.2@localhost  
* pk 21 - yambo-p2y-4.5.2@localhost  
(aida) max@qmobile:~$ aida-common-workflows launch eos quantum_espresso --structure=Si --protocol=fast --daemon  
Submitted EquationOfStateWorkChain-2810- to the daemon  
(aida) max@qmobile:~$
```



QUANTUM
MOBILE





NATIONAL CENTRE OF COMPETENCE IN RESEARCH



Running in Quantum Mobile

```
max@qmobile: ~  
File Edit View Search Terminal Help  
(aida) max@qmobile:~$ verdi  
# List of configured codes:  
# (use 'verdi code show CODEID')  
* pk 1 - abinit-9.2.1@localho  
* pk 2 - bigdft-1.9.1@localho  
* pk 3 - cp2k-7.1@localhost  
* pk 4 - fleur-fleur_MPI-0.30  
* pk 5 - fleur-inpge-0.30-Ma  
* pk 6 - nwchem-7.0.2@localho  
* pk 7 - qe-pw-6.5@localhost  
* pk 8 - qe-cp-6.5@localhost  
* pk 9 - qe-pp-6.5@localhost  
* pk 10 - qe-ph-6.5@localhost  
* pk 11 - qe-neb-6.5@localhos  
* pk 12 - qe-projwfc-6.5@loca  
* pk 13 - qe-pw2wannier90-6.5  
* pk 14 - qe-q2r-6.5@localhos  
* 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@lo  
(aida) max@qmobile:~$ aida-  
Submitted EquationOfStateWork  
(aida) max@qmobile:~$
```

```
max@qmobile: ~  
File Edit View Search Terminal Help  
(aida) max@qmobile:~$ verdi process list  
PK Created Process label Process State Process status  
-----  
-----  
2819 1m ago EquationOfStateWorkChain [Waiting] Waiting for child processes: 2882, 2895, 2909,  
2923, 2940, 2957  
2882 37s ago QuantumEspressoCommonRelaxWorkChain [Waiting] Waiting for child processes: 2898  
2895 35s ago QuantumEspressoCommonRelaxWorkChain [Waiting] Waiting for child processes: 2912  
2898 35s ago PwRelaxWorkChain [Waiting] Waiting for child processes: 2928  
2909 34s ago QuantumEspressoCommonRelaxWorkChain [Waiting] Waiting for child processes: 2929  
2912 32s ago PwRelaxWorkChain [Waiting] Waiting for child processes: 2945  
2923 31s ago QuantumEspressoCommonRelaxWorkChain [Waiting] Waiting for child processes: 2946  
2928 29s ago PwBaseWorkChain [Waiting] Waiting for child processes: 2960  
2929 27s ago PwRelaxWorkChain [Waiting] Waiting for child processes: 2963  
2940 26s ago QuantumEspressoCommonRelaxWorkChain [Waiting] Waiting for child processes: 2964  
2945 25s ago PwBaseWorkChain [Waiting] Waiting for child processes: 2967  
2946 24s ago PwRelaxWorkChain [Waiting] Waiting for child processes: 2970  
2957 23s ago QuantumEspressoCommonRelaxWorkChain [Waiting] Waiting for child processes: 2971  
2960 22s ago PwCalculation [Waiting] Monitoring scheduler: job state RUNNING  
2963 21s ago PwBaseWorkChain [Waiting] Waiting for child processes: 2974  
2964 21s ago PwRelaxWorkChain [Waiting] Waiting for child processes: 2977  
2967 19s ago PwCalculation [Waiting] Monitoring scheduler: job state QUEUED  
2970 18s ago PwBaseWorkChain [Waiting] Waiting for child processes: 2980  
2971 18s ago PwRelaxWorkChain [Waiting] Waiting for child processes: 2983  
2974 17s ago PwCalculation [Waiting] Monitoring scheduler: job state QUEUED  
2977 16s ago PwBaseWorkChain [Waiting] Waiting for child processes: 2986  
2980 15s ago PwCalculation [Waiting] Monitoring scheduler: job state QUEUED  
2983 15s ago PwBaseWorkChain [Waiting] Waiting for child processes: 2989  
2986 14s ago PwCalculation [Waiting] Monitoring scheduler: job state QUEUED  
2989 13s ago PwCalculation [Waiting] Monitoring scheduler: job state QUEUED  
  
Total results: 25  
  
Info: last time an entry changed state: 10s ago (at 21:11:33 on 2021-07-26)  
(aida) max@qmobile:~$
```



Running in Quantum Mobile

The image shows a terminal window with the following content:

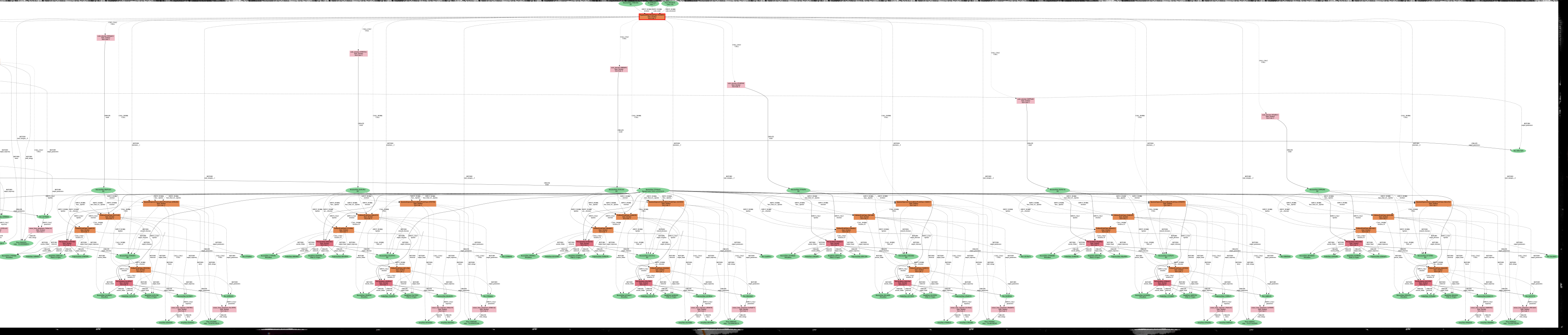
```
(aida) max@qmobile:~$ verdi code show CODEID
# List of configured codes:
# (use 'verdi code show CODEID' to show details)
* pk 1 - abinit-9.2.1@localhost
* pk 2 - bigdft-1.9.1@localhost
* pk 3 - cp2k-7.1@localhost
* pk 4 - fleur-fleur_MPI-0.30@localhost
* pk 5 - fleur-inpgen-0.30-Max@localhost
* pk 6 - nwchem-7.0.2@localhost
* pk 7 - qe-pw-6.5@localhost
* pk 8 - qe-cp-6.5@localhost
* pk 9 - qe-pp-6.5@localhost
* pk 10 - qe-ph-6.5@localhost
* pk 11 - qe-neb-6.5@localhost
* pk 12 - qe-projwfc-6.5@localhost
* pk 13 - qe-pw2wannier90-6.5@localhost
* pk 14 - qe-q2r-6.5@localhost
* pk 15 - qe-dos-6.5@localhost
* pk 16 - qe-matdyn-6.5@localhost
* pk 17 - siesta-MaX-1.2.0@localhost
* pk 18 - siesta-plstm-MaX-1.2.0@localhost
* pk 19 - wannier90-wannier-3.0@localhost
* pk 20 - yambo-4.5.2@localhost
* pk 21 - yambo-p2y-4.5.2@localhost
(aida) max@qmobile:~$ verdi process list
PK Created Process label
-----
2819 1m ago EquationOfStateWorkChain
2923, 2940, 2957
2882 37s ago QuantumEspressoCommonRelaxW
2895 35s ago QuantumEspressoCommonRelaxW
2898 35s ago PwRelaxWorkChain
2909 34s ago QuantumEspressoCommonRelaxW
2912 32s ago PwRelaxWorkChain
2923 31s ago QuantumEspressoCommonRelaxW
2928 29s ago PwBaseWorkChain
2929 27s ago PwRelaxWorkChain
2940 26s ago QuantumEspressoCommonRelaxW
2945 25s ago PwBaseWorkChain
2946 24s ago PwRelaxWorkChain
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
(aida) max@qmobile:~$
```

The plot window, titled "Figure 1", shows Energy [eV] vs Volume [Å³]. The y-axis ranges from -0.09 to -0.04, and the x-axis ranges from 39 to 43. The plot shows a parabolic curve with a minimum at approximately 41 Å³ and -0.09 eV. A value of -3.1060000000e2 is displayed at the top of the plot area.

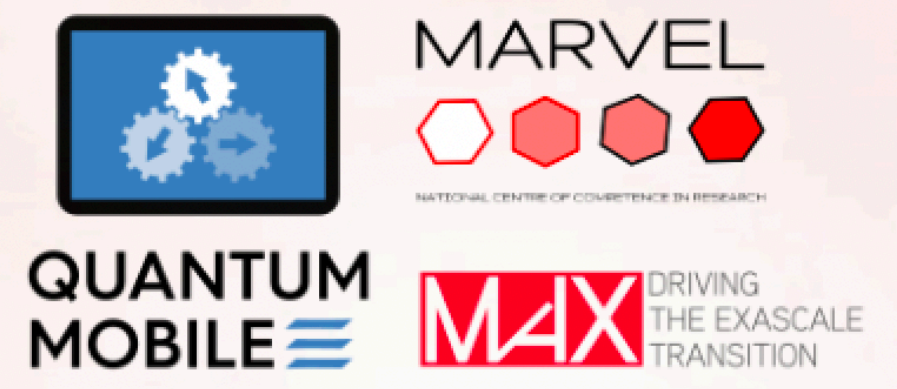
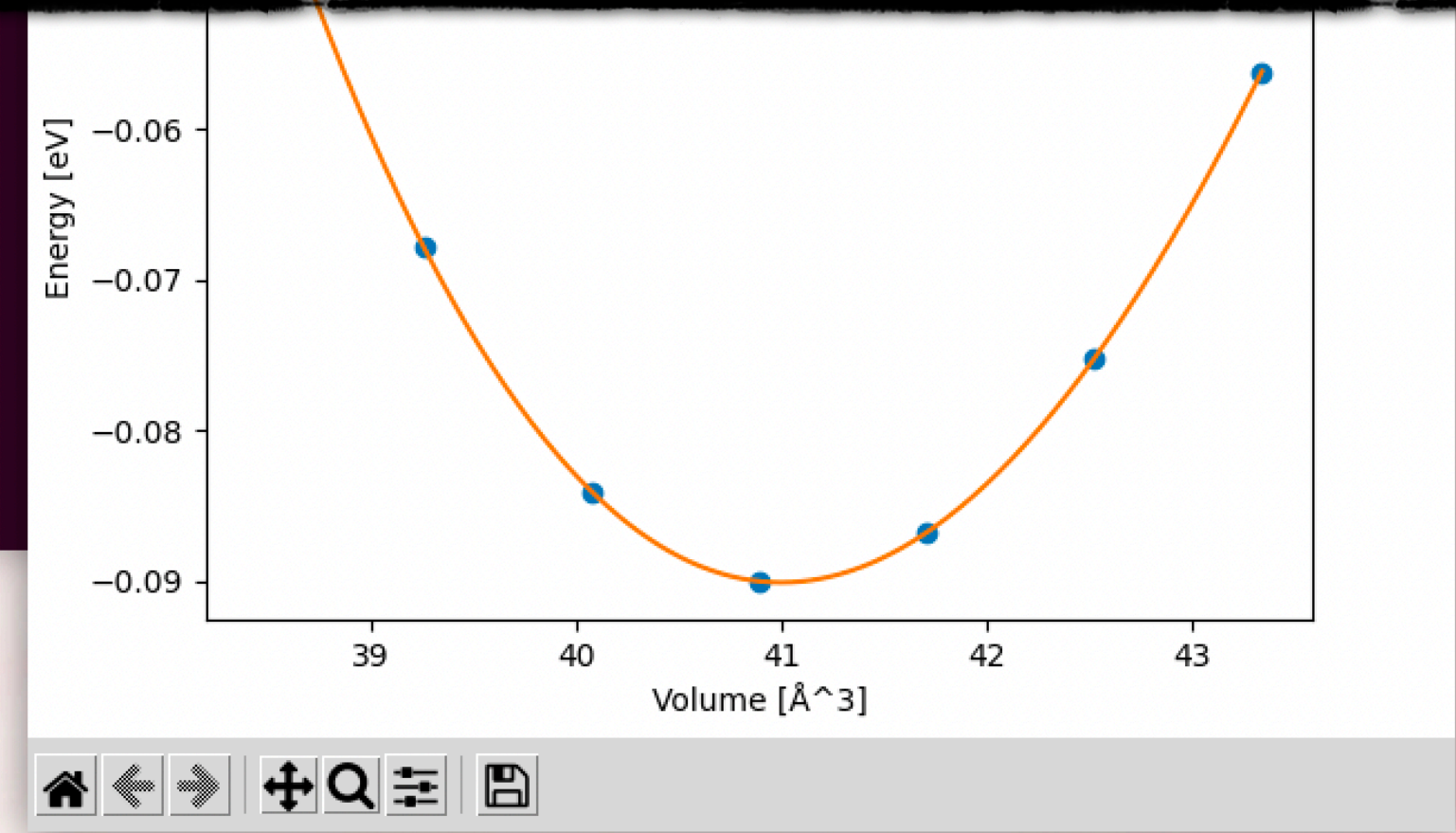
Running in Quantum Mobile

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



```
2940 29s ago PwRelaxWorkChain
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:~$
```



All data is available and reproducible!

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materialscloud:2021.73

Common workflows for computing material properties using different quantum engines

Sebastiaan P. Huber^{1*}, Emanuele Bosoni², Marnik Bercx¹, Jens Bröder^{3,4}, Augustin Degomme⁵, Vladimir Dikan², Kristjan Eimre⁶, Espen Flage-Larsen^{7,8}, Alberto Garcia², Luigi Genovese⁵, Dominik Gresch⁹, Conrad Johnston¹⁰, Guido Petretto¹¹, Samuel Poncé¹, Gian-Marco Rignanese¹¹, Christopher J. Sewell¹, Berend Smit¹², Vasily Tseplyaev^{3,4}, Martin Uhrin¹, Daniel Wortmann³, Aliaksandr V. Yakutovich^{12,1}, Austin Zadoks¹, Pezhman Zarabadi-Poor^{13,14}, Bonan Zhu^{15,14}, Nicola Marzari¹, Giovanni Pizzi^{1*}

1 Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
2 Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Campus UAB, 08193 Bellaterra, Spain
3 Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany
4 Department of Physics, University of Jülich, D-52425 Jülich, Germany
5 Univ. Grenoble Alpes, CNRS, SIMONS, UMR 5175, PHEAS, 38000 Grenoble, France
6 nanotech@surf, Swiss National Superconducting Cyclotron Laboratory, CH-5170 Villigen, Switzerland
7 SINTEF Industry, NO-4893 Trondheim, Norway

Files

File name	Size	Description
README.md MD5	7.6 KiB	A file describing the contents of the `archive.zip` file and instructions on how to reproduce the data
archive.zip MD5	1.2 GiB	A zip file that contains all the data and scripts necessary to reproduce the curated data from the provided AiiDA archive and reproduce the plots from that curated data

License

Files and data are licensed under the terms of the following license: [Creative Commons Attribution 4.0 International](#). Metadata, except for email addresses, are licensed under the [Creative Commons Attribution Share-Alike 4.0 International](#) license.

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

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: 198)
# 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
```

File: aiida.fdf

SIESTA

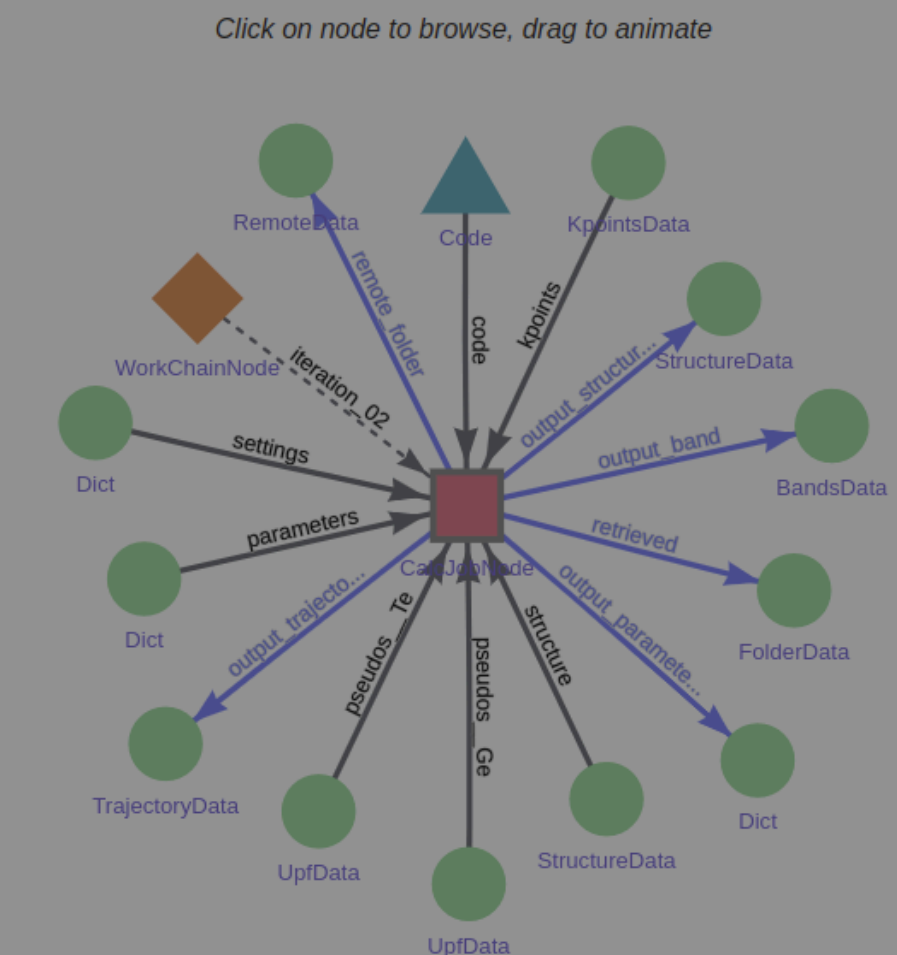
```
atomiccoordinatesformat Ang
electronictemperature 25 meV
geometrymustconverge T
latticeconstant 1.0 Ang
maxscfiterations 100
maxwalltime 36000
mdconstantvolume True
mdmaxforcetol 0.005 eV/Ang
mdmaxstresstol 0.7 GPa
mdnumcgsteps 100
mdtypeofrun cg
mdvariablecell True
meshsizes [48 48 48]
numberofatoms 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
```

File: aiida.in

Quantum ESPRESSO

```
&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
```

AiiDA Provenance Browser



License

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

Current plans: second phase of collaboration

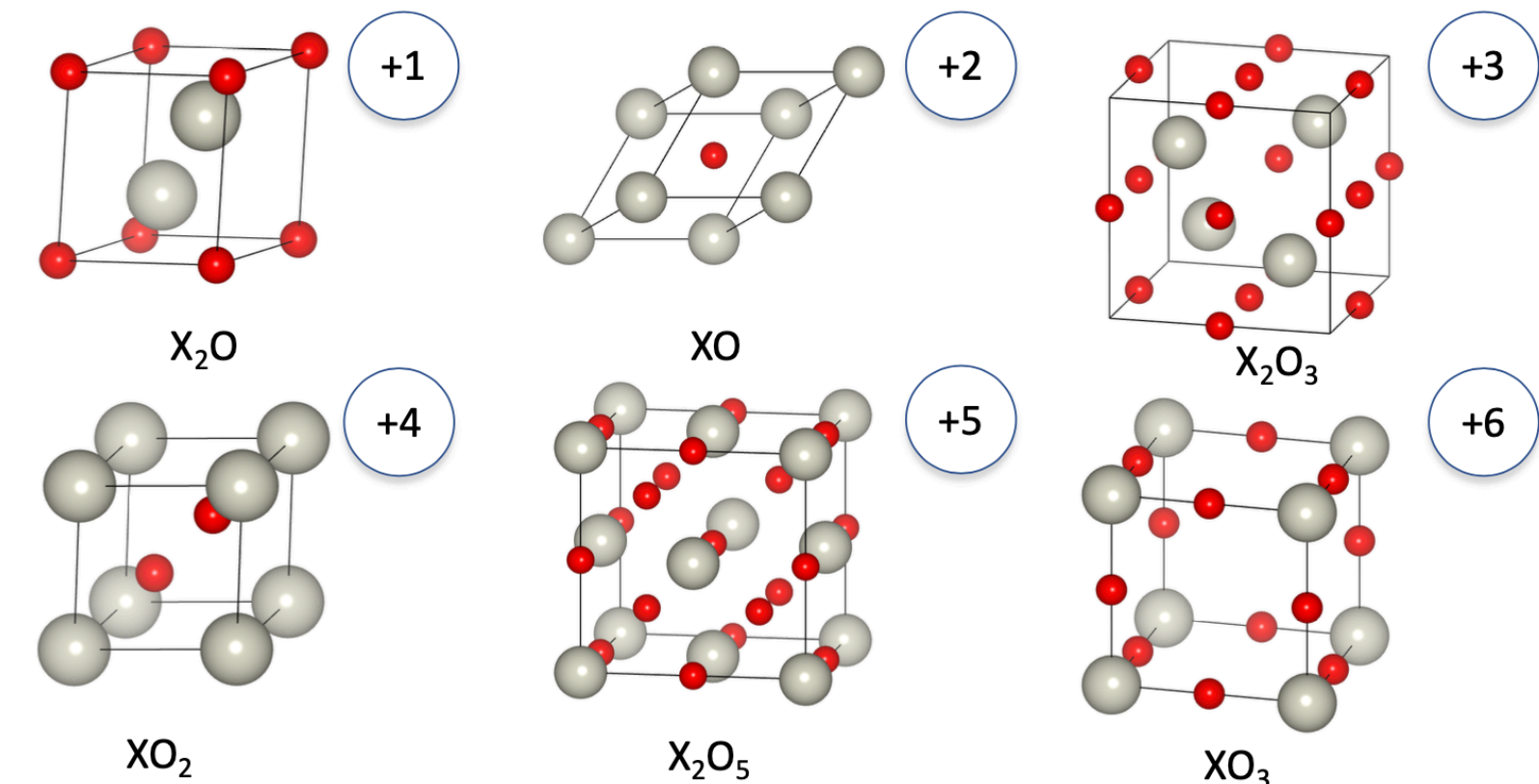
Project now continuing with an even larger group of collaborators

- 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

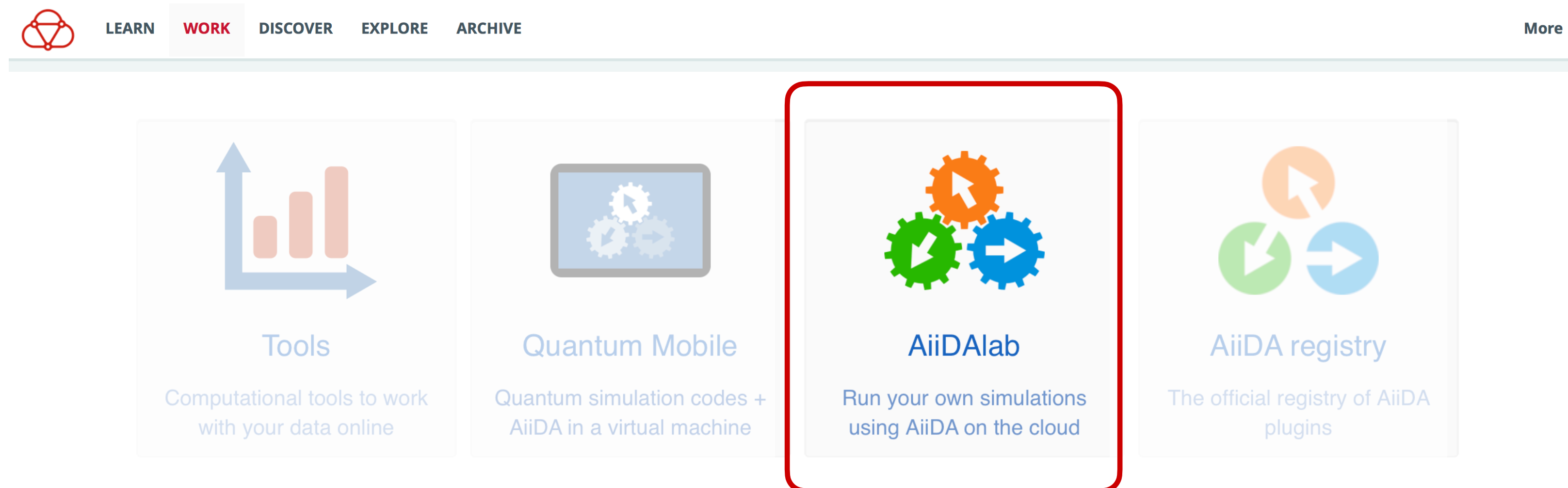
- AiiDAlab GUI

- ...



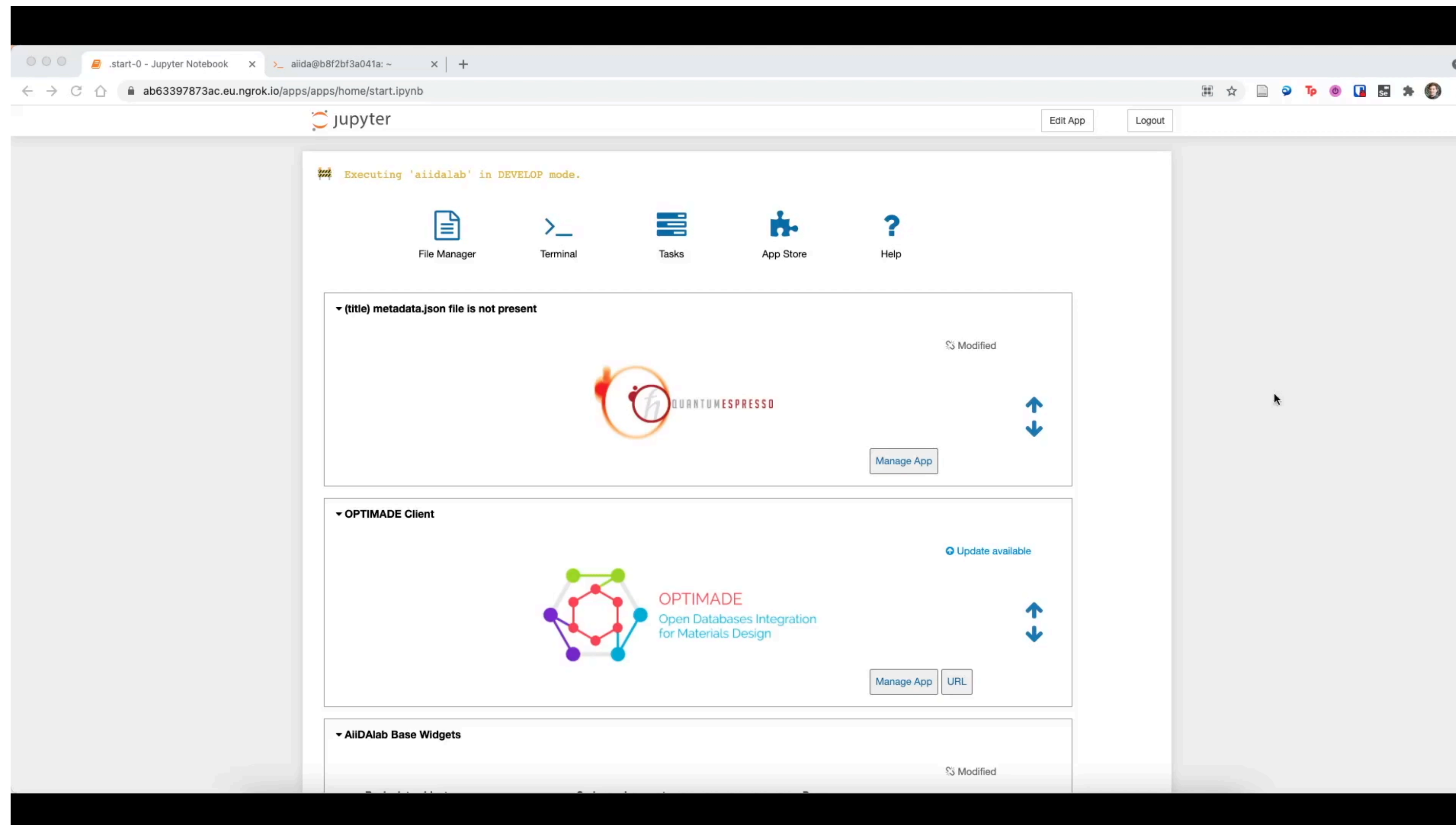
Follow-up of the work of S. Cottenier (see talk of yesterday), comparing of various oxide configurations across all codes involved
Not only testing accuracy, but also releasing automated recipes to run with that accuracy!

Data generation: Materials Cloud Work



AiiDA lab

- 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



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

Making simulations accessible: AiiDAlab experience at EMPA (CH)

Making simulations accessible
with



<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)



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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 aiiida-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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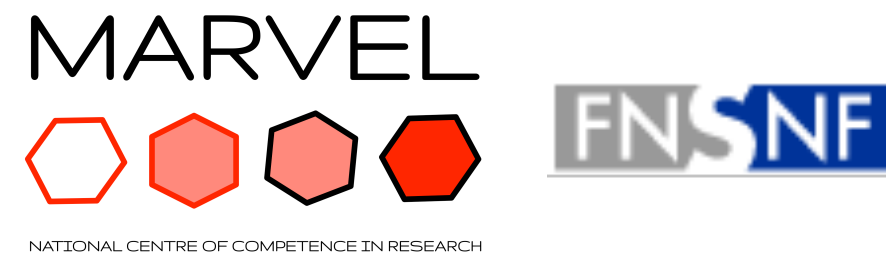
Check for updates

Common workflows for computing material properties using different quantum engines

Sebastiaan P. Huber¹✉, Emanuele Bosoni², Marnik Bercx¹, Jens Bröder^{3,4}, Augustin Degomme⁵, Vladimir Dikan², Kristjan Eimre⁶, Espen Flage-Larsen^{7,8}, Alberto Garcia², Luigi Genovese⁵, Dominik Gresch⁹, Conrad Johnston¹⁰, Guido Petretto¹¹, Samuel Poncé¹, Gian-Marco Rignanese¹¹, Christopher J. Sewell¹, Berend Smit¹², Vasily Tseplyaev^{3,4}, Martin Uhrin¹, Daniel Wortmann³, Aliaksandr V. Yakutovich^{1,12}, Austin Zadoks¹, Pezhman Zarabadi-Poor^{13,14}, Bonan Zhu^{14,15}, Nicola Marzari¹ and Giovanni Pizzi¹✉

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

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SNSF NCCR "MARVEL"

Discovery of new materials via simulations and dissemination of curated data



H2020 Centre of Excellence "MaX"

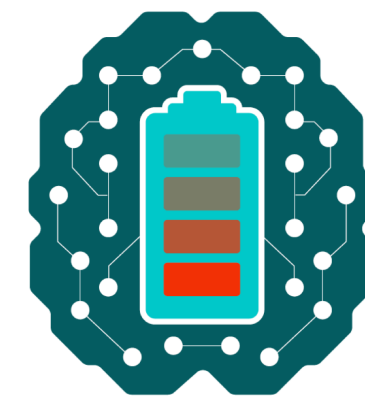
Scaling towards exascale machines and high-throughput efficiency

swissuniversities

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