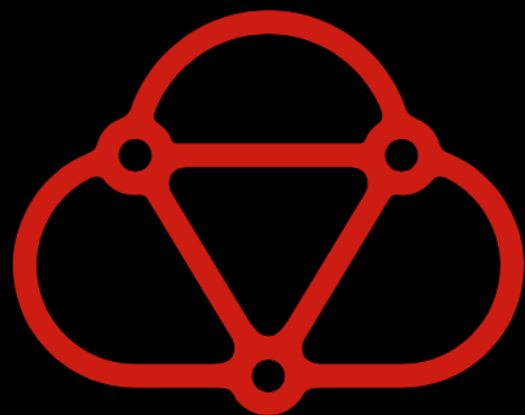
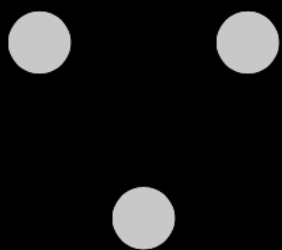




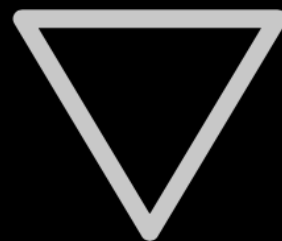
MATERIALSCLOUD



LEARN



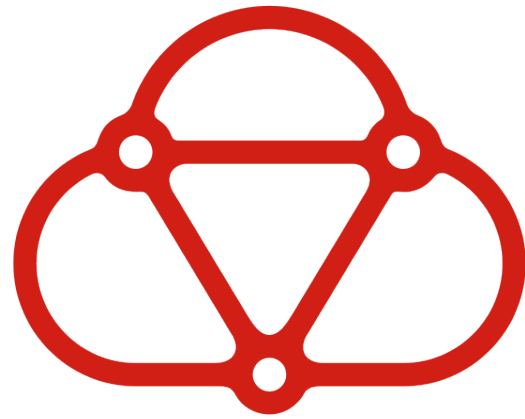
WORK



DISCOVER



EXPLORE



MATERIALSCLOUD

1. Motivation
2. AiiDA & Materials Cloud
- 3. Examples**

Leopold Talirz (EPFL)

Motivation

Computational Materials Science Challenges

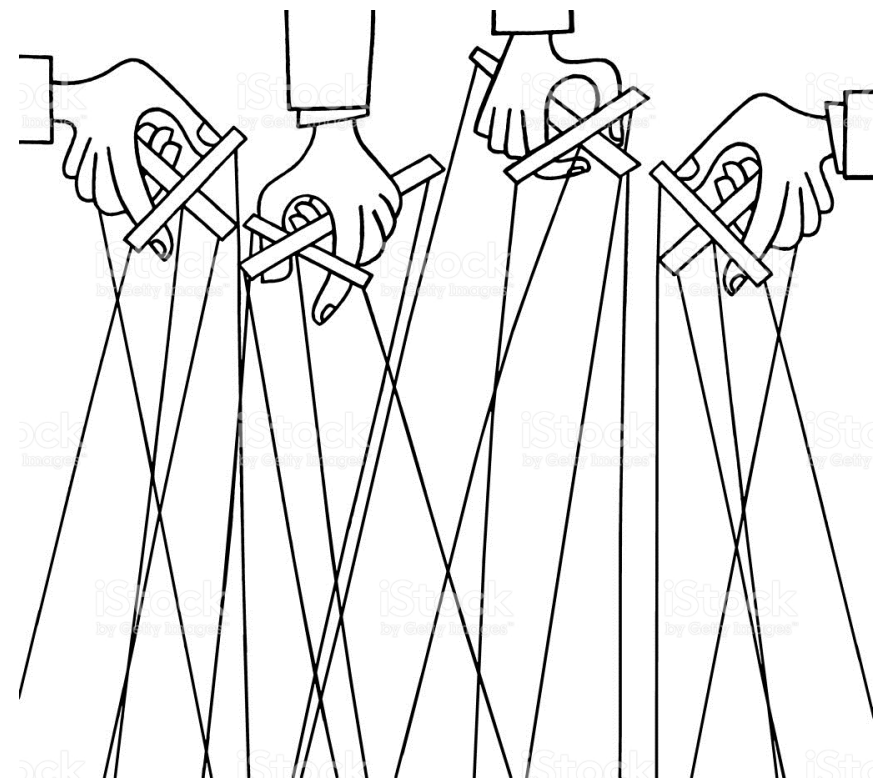
High-Throughput

"Data jungle"

Open Science

Knowledge Transfer

- Organize large numbers of calculations
- Deal with corner cases (theory, code, infrastructure)
- Many strings to pull



Source: [istockphoto.com](https://www.istockphoto.com)

Motivation

High-Throughput

"Data jungle"

Open Science

Knowledge Transfer

- Keep track of what you calculate
- Keep track of how you did it
- Within a research group:
Can Alice reproduce what Bob computed 1 year ago?



Source: academiccoachingandwriting.org

Motivation

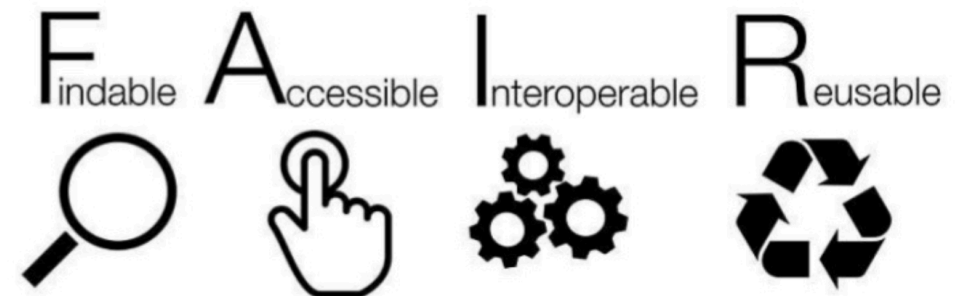
High-Throughput

"Data jungle"

Open Science

Knowledge Transfer

- Open Science
 - ~~Supporting Information~~
 - ~~Just upload everything~~
 - FAIR data
- Making data FAIR is hard, can we make it easier?



Source: Prof. Michel Dumontier

Motivation

High-Throughput

"Data jungle"

Open Science

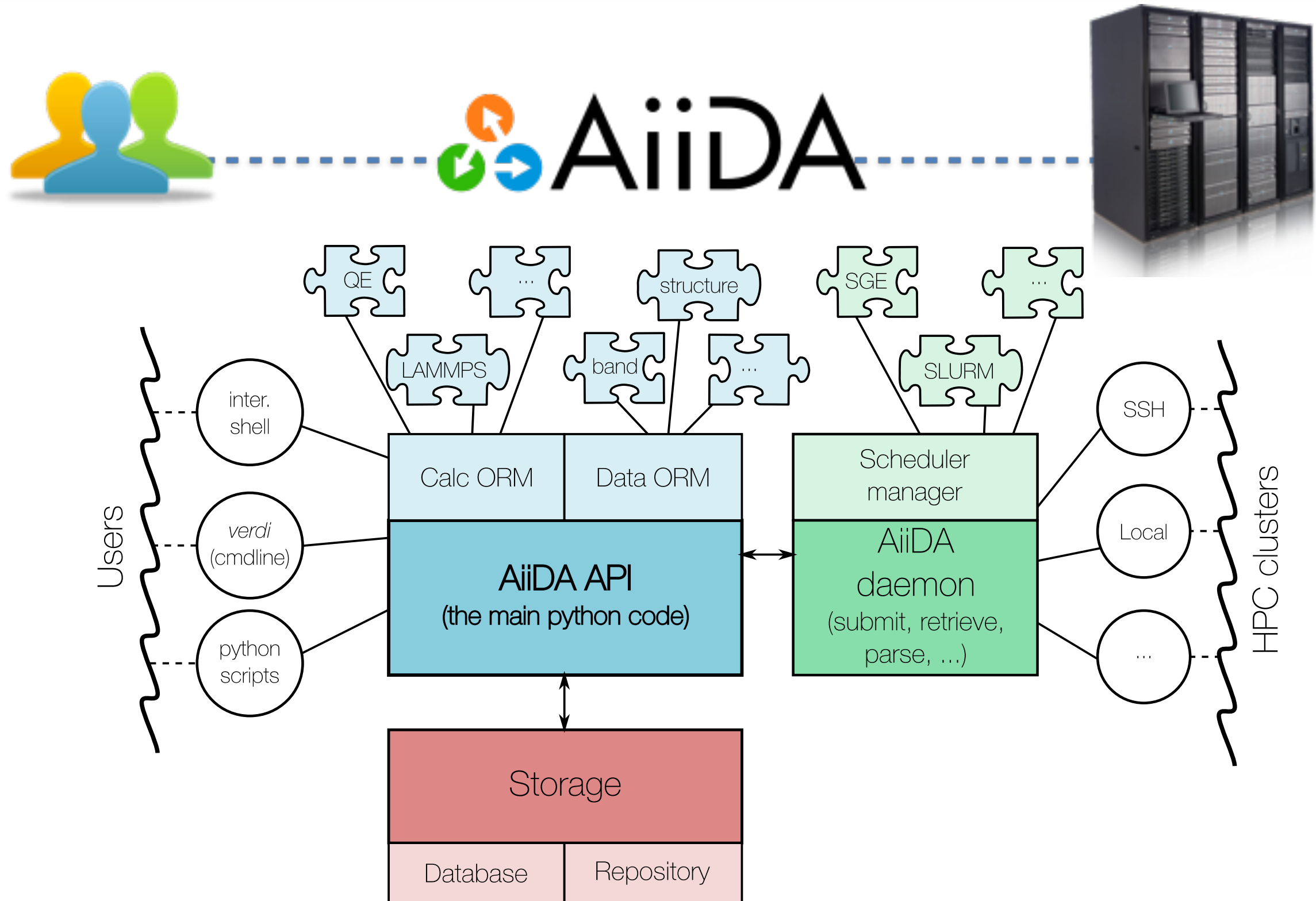
Knowledge Transfer

- How to transfer your insights & expertise, e.g.
 - reporting data sets to an experimental group
 - providing a workflow for your code to a collaborator/company
- ...



Source: quote.ucsd.edu

AiiDA – Architecture



AiiDA – Development



- **Free and open source (MIT License)**
- github.com/aiidateam/aiida_core
- 26 releases, latest version: v0.11.0
- 36 contributors since 2012

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

AiiDA plugins

ase, codtools, cp2k,
fleur, lammmps, nwchem, phonopy
quantumespresso, raspa, siesta,
vasp, wannier90, yambo
(+plugin-template)

AiiDA registry of plugins

[\[View on GitHub/register your plugin\]](#)

Available

```
"quantumespresso": {  
  "name": "aiida-quantumespresso",  
  "entry_point": "quantumespresso",  
  "state": "stable",  
  "pip_url": "git+https://github.com/aiidateam/aiida-quantumespresso",  
  "plugin_info": "https://raw.githubusercontent.com/aiidateam/aiida-quantumespresso/master/plugin_info.json",  
  "code_home": "https://github.com/aiidateam/aiida-quantumespresso",  
  "documentation_url": "http://aiida-quantumespresso.readthedocs.io/en/latest/"  
},
```

cod

The

Current state: stable

[Plugin code homepage](#) (hosted on github.com)

[Documentation: Go to plugin documentation](#)

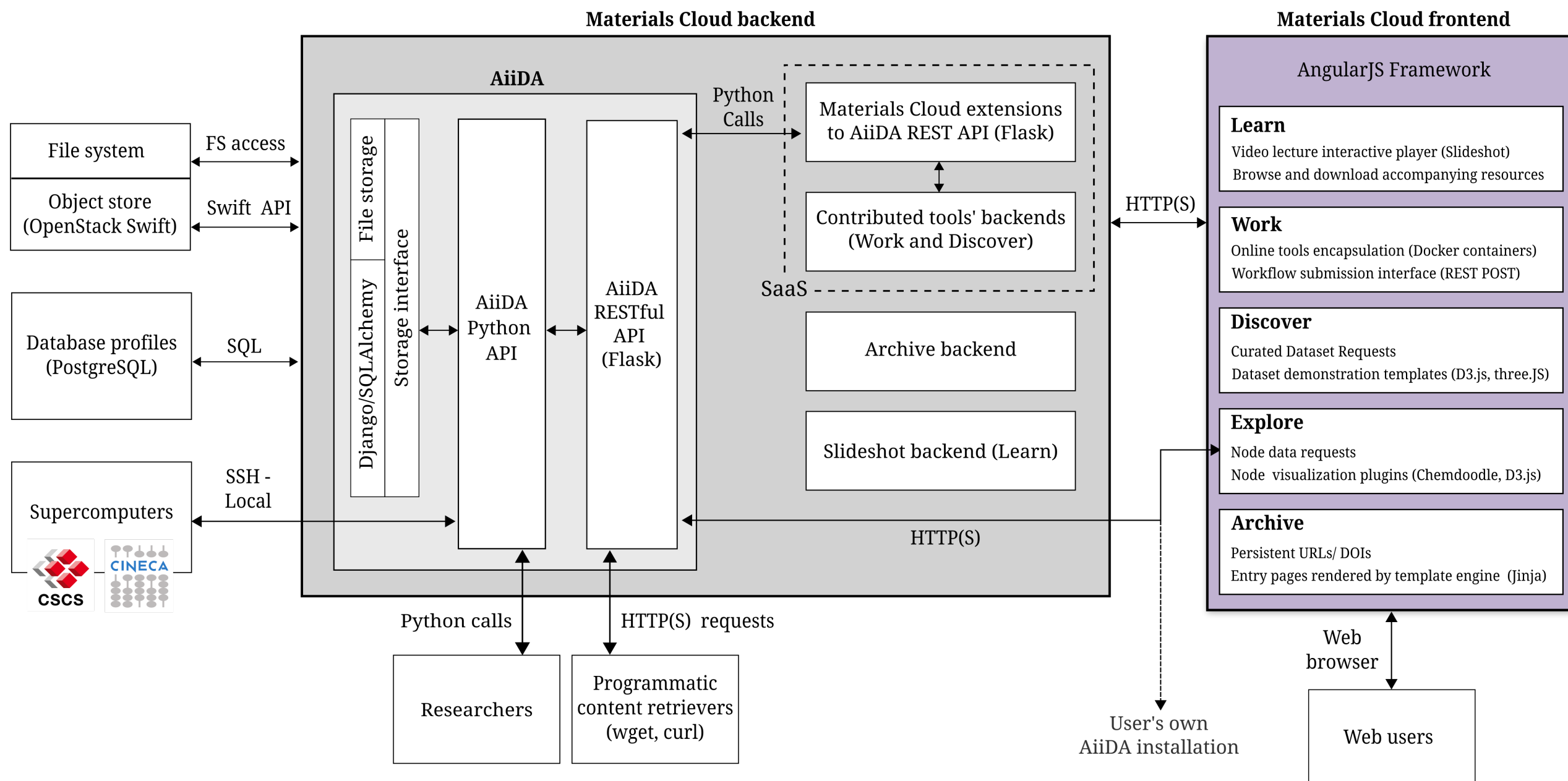
[Show plugin details](#)

cp2k: aiida-cp2k package

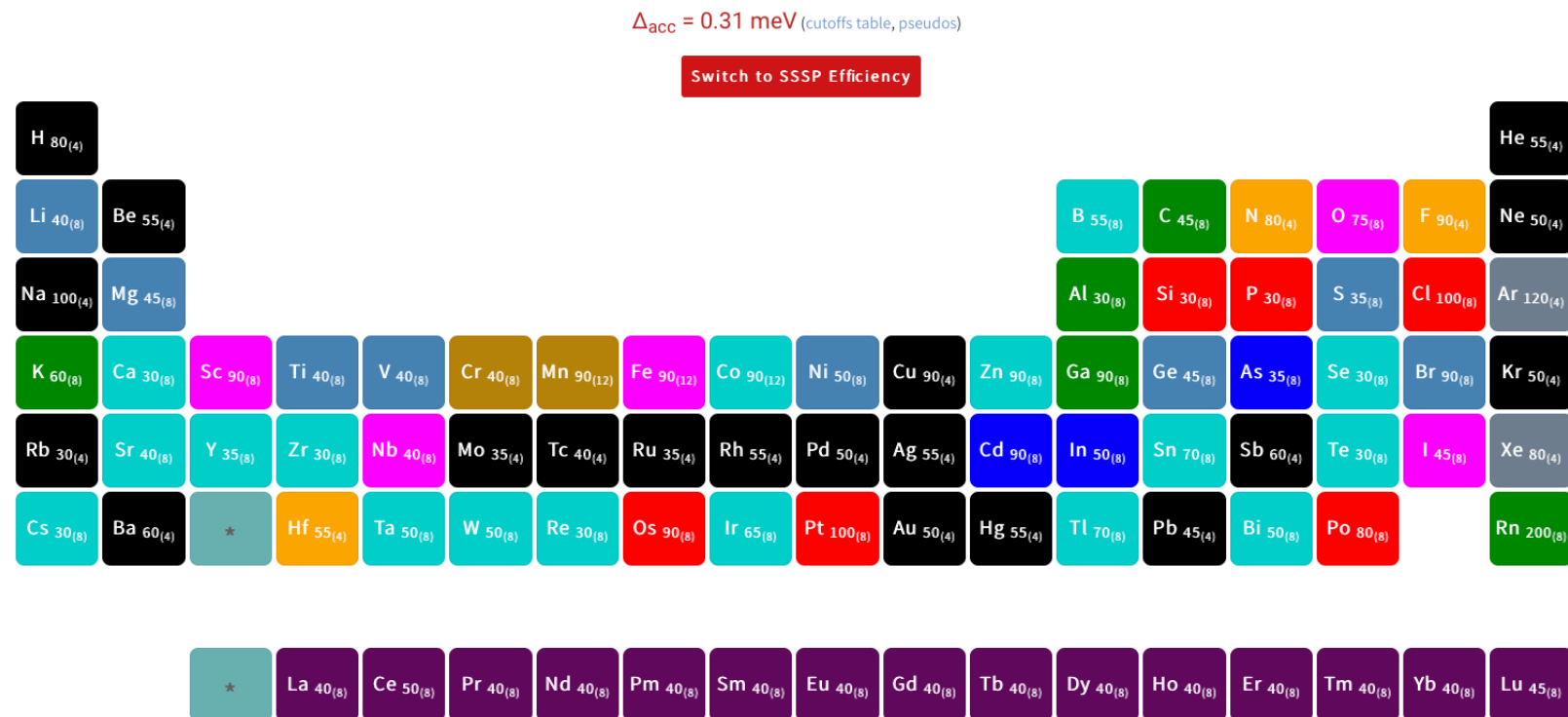
A plugin to run CP2K calculations and workflows

Current state: development

Materials Cloud – Architecture



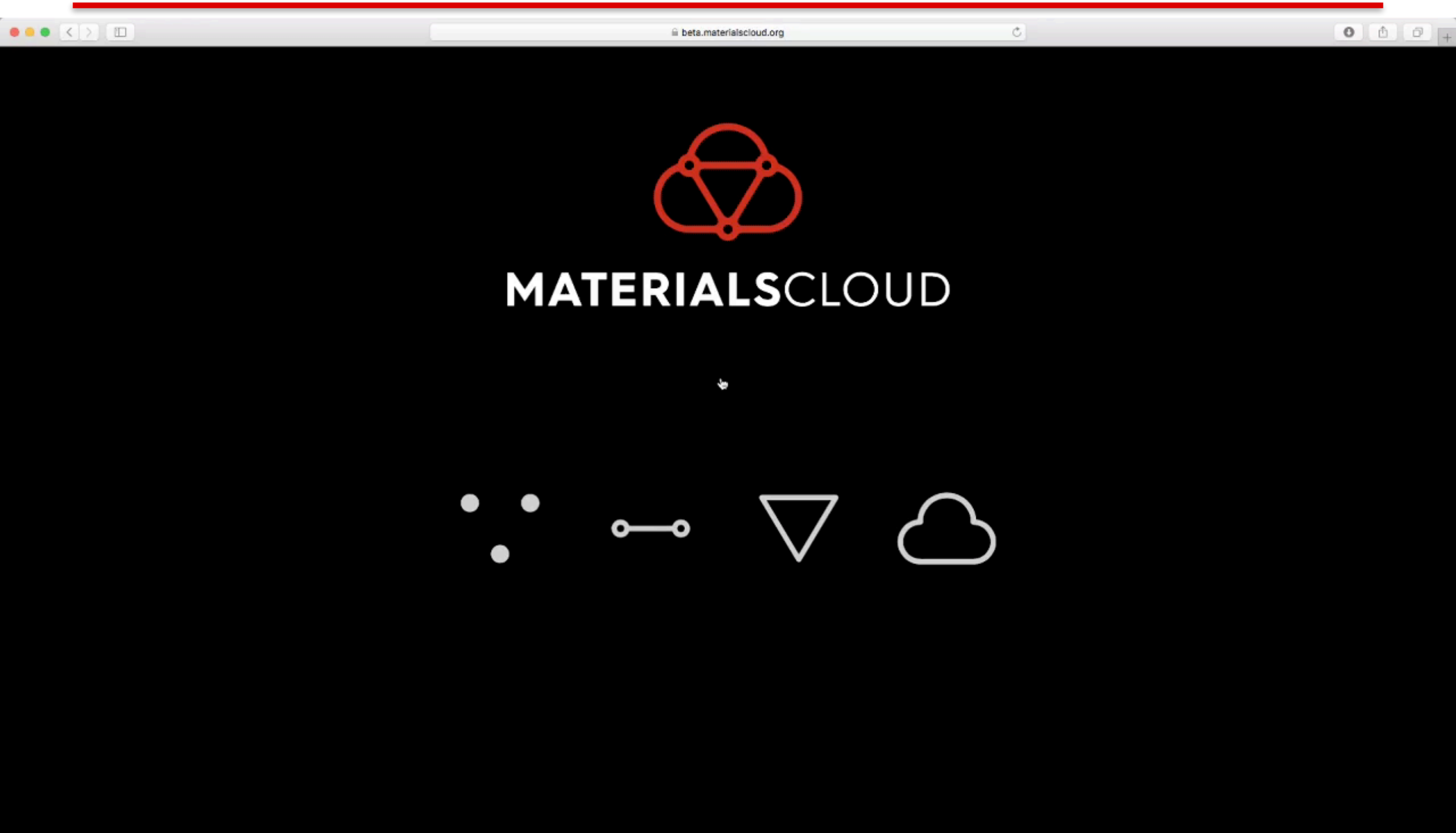
Example 1 - SSSP



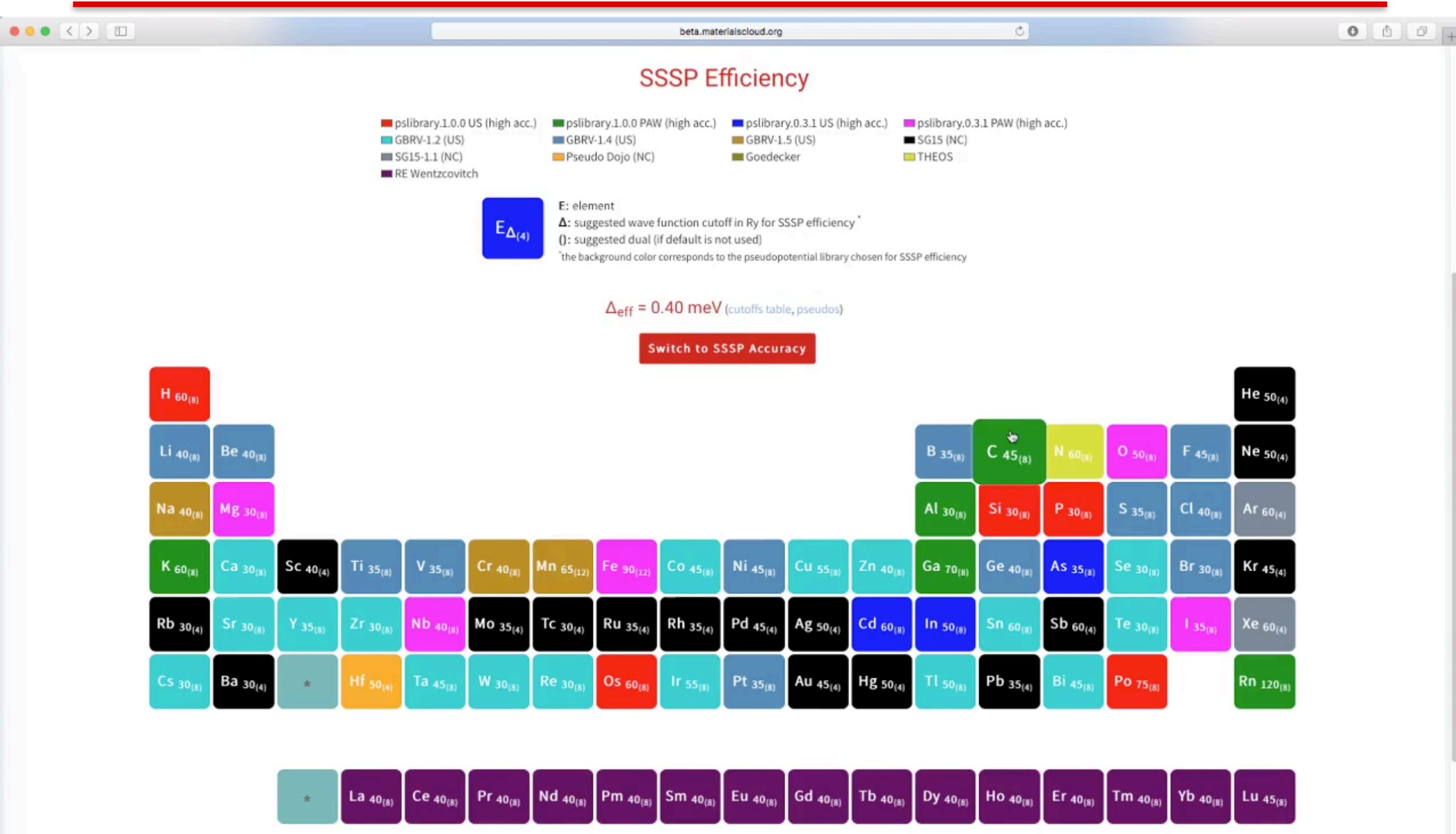
Standard Solid State Pseudo Potentials

G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet, and N. Marzari, *in preparation*

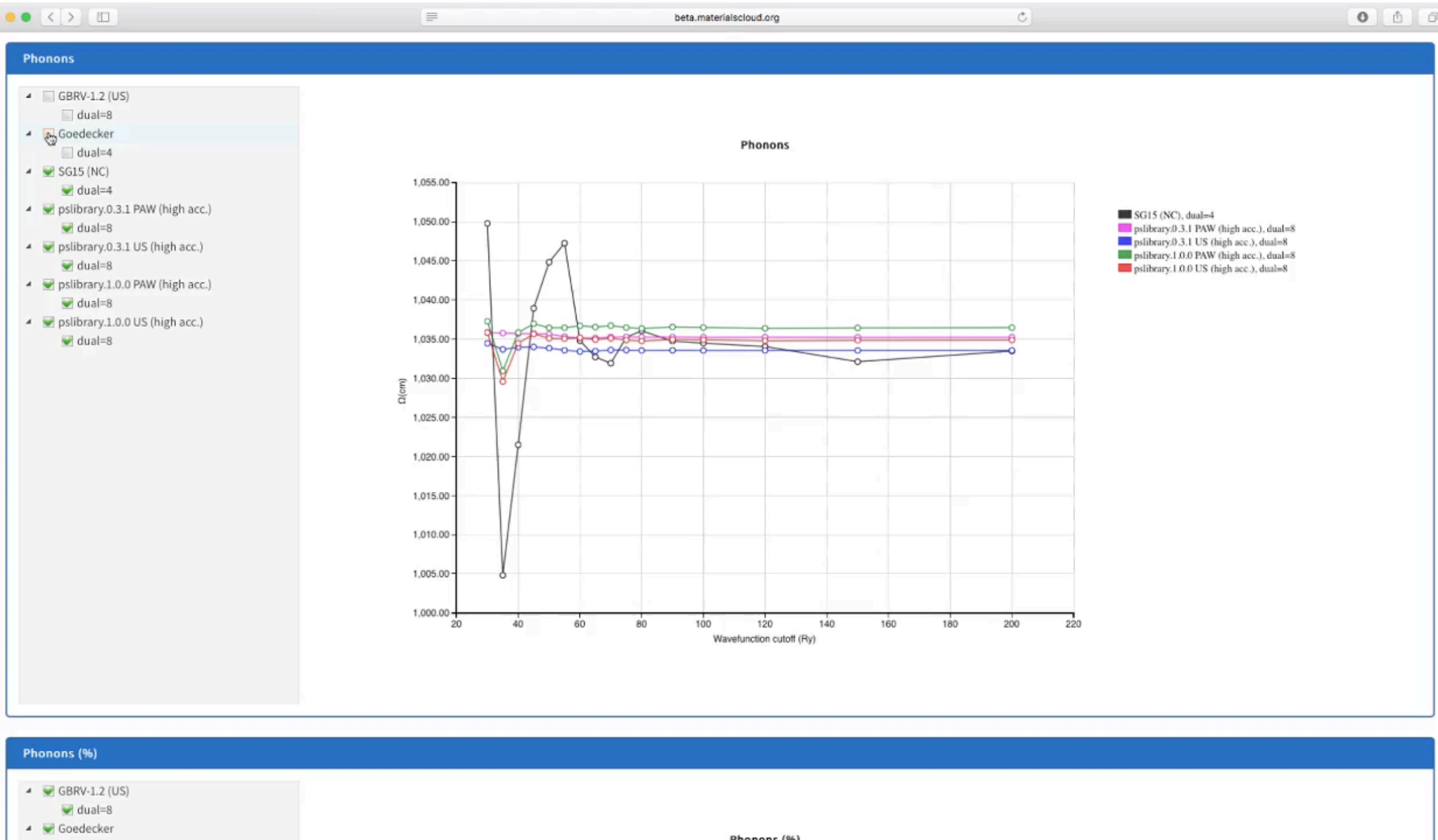
SSSP - Overview



SSSP - Plots



SSSP - Provenance



SSSP - Provenance

beta.materialscloud.org

LEARN WORK DISCOVER EXPLORE ARCHIVE

Home Explore Node details 0fe093bd-f0f7-457a-9781-c3b058bd4eeb - CALCULATION

Selected Profile: SSSP

Grid Details Statistics

0fe093bd-f0f7-457a-9781-c3b058bd4eeb GO

UUID: 0fe093bd-f0f7-457a-9781-c3b058bd4eeb
Type: calculation.job.quantumespresso.ph.PhCalculation.
Created at 19 November 2015
Modified 6 months ago
nicolas.mounet@epfl.ch

PhCalculation

JOB ID 795018
PARSER quantumespresso.ph
STATE FINISHED
SCHEDULER STATE DONE
REMOTE WORKING DIRECTORY /scratch/daint/mounet/aiida_run/0fe093bd-f0f7-457a-9781-c3b058bd4eeb

INPUT FILES

- aiida.in
- _aiidasubmit.sh
- .aiida/calcinfo.json
- .aiida/job_tmpl.json

OUTPUT FILES

- aiida.out
- _scheduler-stdout.txt
- DYN_MAT/dynamical-matrix-
- _scheduler-stderr.txt

Node metadata

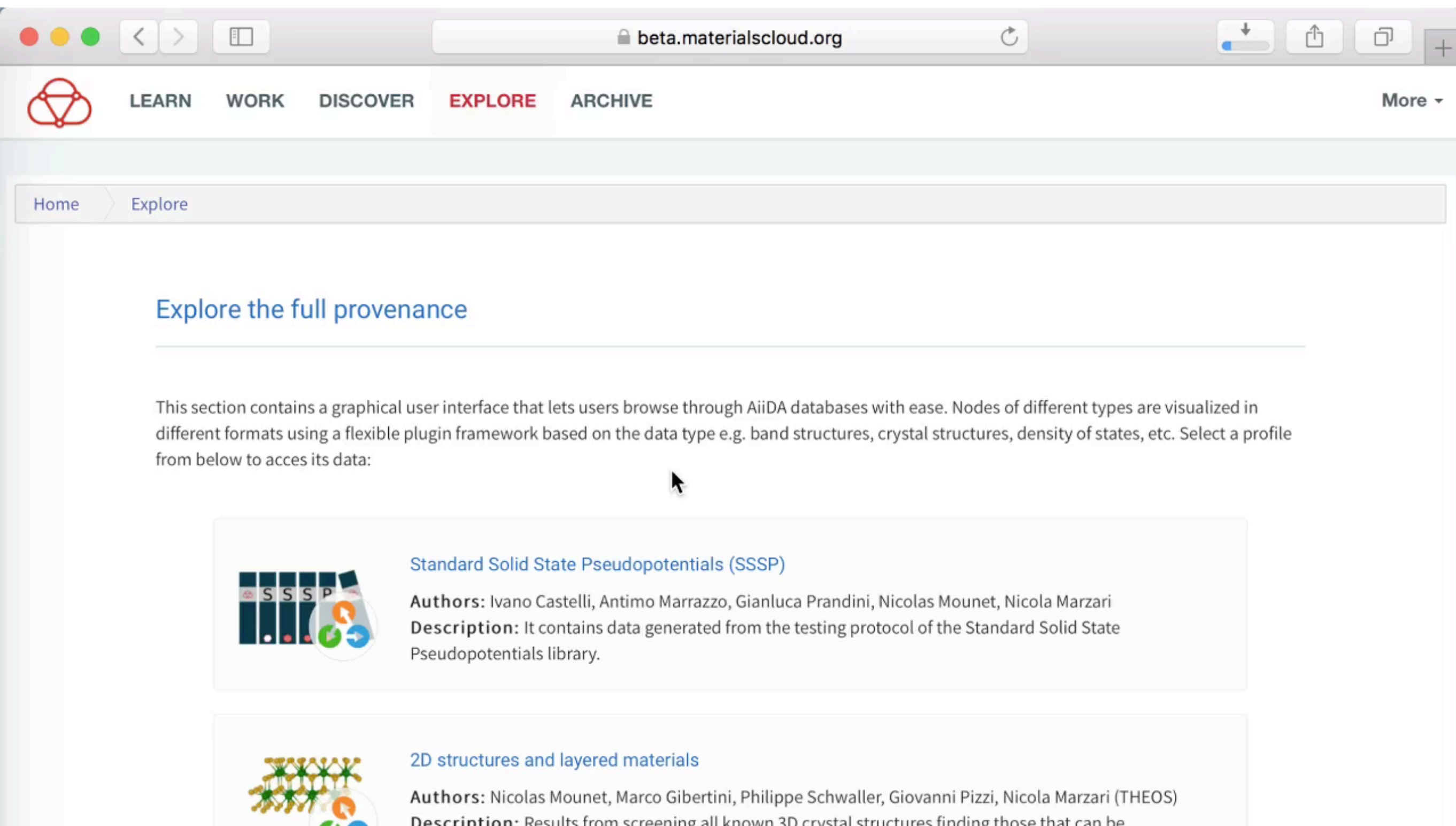
CUSTOM_SCHEDULER_COMMANDS #SBATCH -A, --account=mr0
JOBRESOURCE_PARAMS {"default_mpiproc_per_machine":24,"num_machines":1}
LINKNAME_RETRIEVED retrieved
MAX_WALLCLOCK_SECONDS 30000
RETRIEVE_LIST ["aiida.out","DYN_MAT","/out/_ph0/aiida.phsave/tensors.xml","_scheduler-stdout.txt","_scheduler-stderr.txt"]
RETRIEVE_SINGLEFILE_LIST []
SCHEDULER_LASTCHECKTIME Thu, 19 Nov 2015 00:16:37 GMT

AiiDA Provenance Browser

Selected node, Inputs, Outputs

```
graph TD; Kpoints((Kpoints)) --> QEPH[Quantum ESPRESSO-PH]; Parameter1((Parameter)) --> QEPH; Remote1((Remote)) --> QEPH; Folder((Folder)) --> QEPH; Code[Code] --> QEPH; QEPH --> Parameter2((Parameter)); QEPH --> Remote2((Remote)); QEPH --> Folder2((Folder));
```

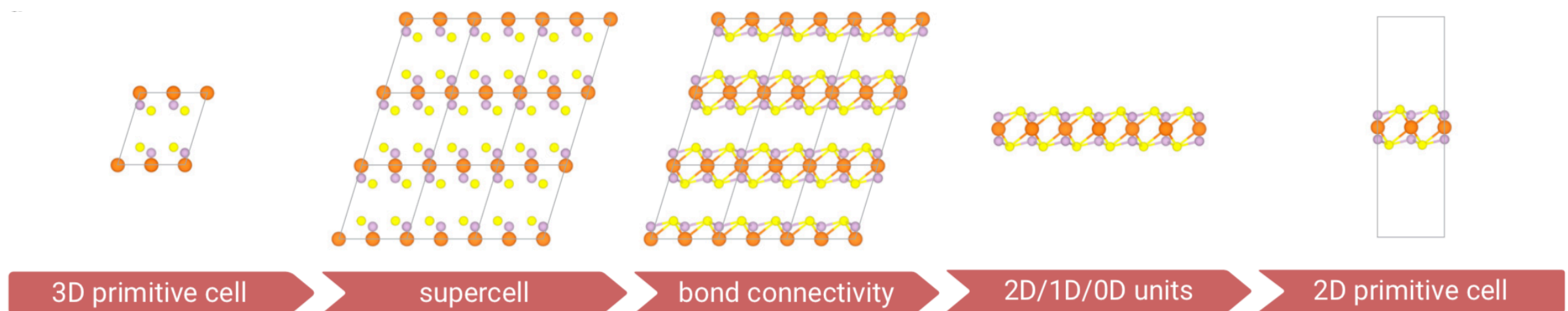
SSSP - Archive



The screenshot shows a web browser window with the address bar displaying `beta.materialscloud.org`. The website has a navigation bar with links: LEARN, WORK, DISCOVER, EXPLORE (highlighted), and ARCHIVE. Below the navigation bar, there is a sub-navigation bar with links: Home and Explore. The main content area is titled "Explore the full provenance" and contains a paragraph explaining the graphical user interface for browsing AiiDA databases. Below this, there are two featured items:

- Standard Solid State Pseudopotentials (SSSP)**
Authors: Ivano Castelli, Antimo Marrazzo, Gianluca Prandini, Nicolas Mounet, Nicola Marzari
Description: It contains data generated from the testing protocol of the Standard Solid State Pseudopotentials library.
- 2D structures and layered materials**
Authors: Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Giovanni Pizzi, Nicola Marzari (THEOS)
Description: Results from screening all known 3D crystal structures finding those that can be

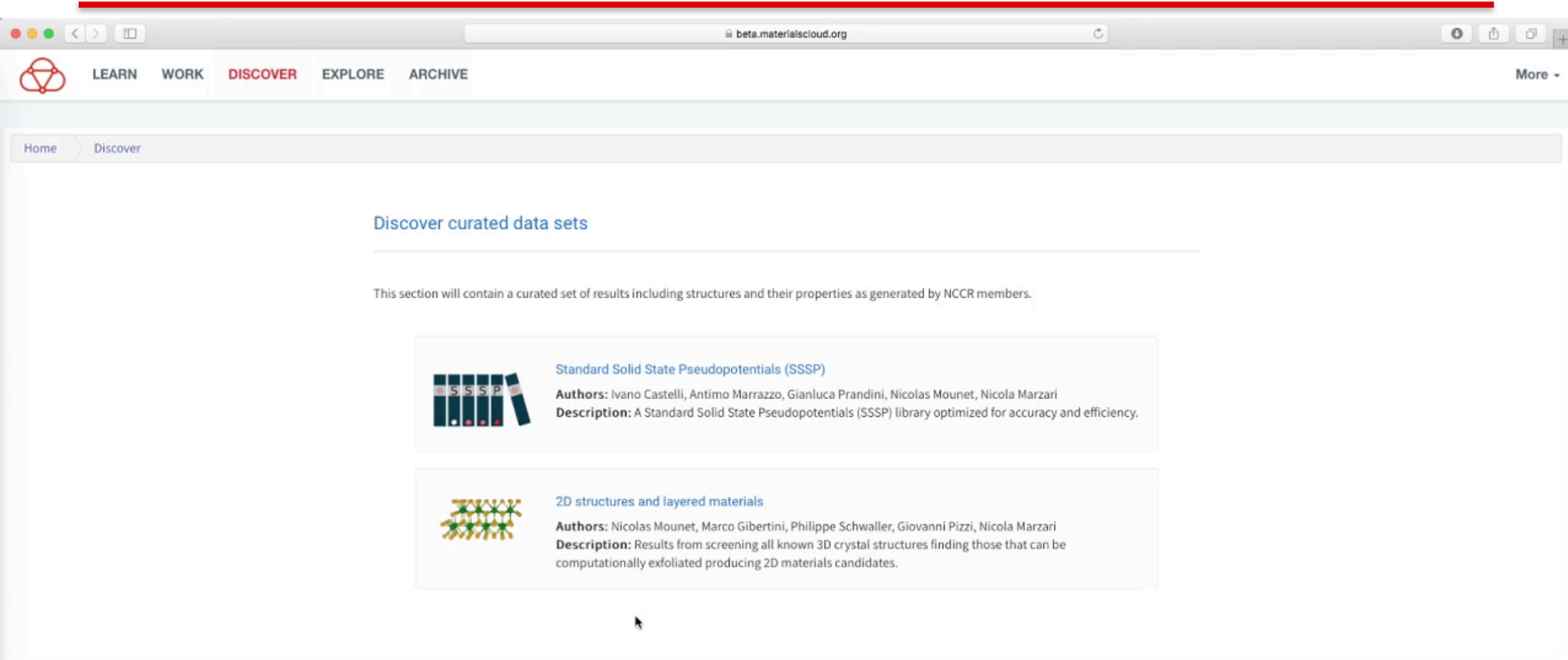
Example 2 - 2D Materials



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

N. Mounet, M. Gibertini, P. Schwaller, A. Merkys, I. E. Castelli, A. Cepellotti, G. Pizzi & N. Marzari,
[arXiv:1611.05234](https://arxiv.org/abs/1611.05234) (2016).

2D Materials - Overview

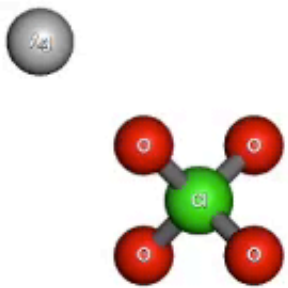


The screenshot shows a web browser window with the address bar displaying `beta.materialscloud.org`. The website has a navigation bar with links: LEARN, WORK, DISCOVER (highlighted), EXPLORE, and ARCHIVE. Below this, a breadcrumb trail shows 'Home' and 'Discover'. The main content area is titled 'Discover curated data sets' and includes a sub-header 'This section will contain a curated set of results including structures and their properties as generated by NCCR members.' Two data sets are listed:

- Standard Solid State Pseudopotentials (SSSP)**
Authors: Ivano Castelli, Antimo Marrazzo, Gianluca Prandini, Nicolas Mounet, Nicola Marzari
Description: A Standard Solid State Pseudopotentials (SSSP) library optimized for accuracy and efficiency.
- 2D structures and layered materials**
Authors: Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Giovanni Pizzi, Nicola Marzari
Description: Results from screening all known 3D crystal structures finding those that can be computationally exfoliated producing 2D materials candidates.

2D Materials - Provenance

beta.materialscloud.org

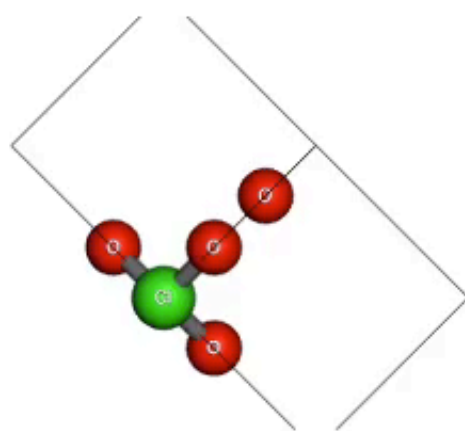


Kind	x[Å]	y[Å]	z[Å]
v ₁	4.844127	0.000000	0.000000
v ₂	0.000000	4.844127	0.000000
v ₃	0.000000	0.000000	21.752132

Kind label	x[Å]	y[Å]	z[Å]
Cl [?]	2.422063	2.422063	10.876066
O [?]	3.262352	1.581775	11.745996
O [?]	1.581775	3.262352	11.745996
O [?]	3.262352	3.262352	10.006136
Ag [?]	0.000000	4.844127	10.876066
O [?]	1.581775	1.581775	10.006136

Select 3D parent: AgO4Cl - I-42m (COD - 9008281)

3D parent structure



3D structure cell

Kind	x[Å]	y[Å]	z[Å]
v ₁	-2.488000	2.488000	3.373000
v ₂	2.488000	-2.488000	3.373000
v ₃	2.488000	2.488000	-3.373000

DF2-C09 Binding energy [meV/Å²]: 0.0191

rVV10 Binding energy [meV/Å²]: 0.0290

3D structure atomic coordinates

Kind label	x[Å]	y[Å]	z[Å]
Ag [?]	0.000000	0.000000	0.000000
Cl [?]	0.000000	0.000000	3.373000
O [?]	-0.822533	0.822533	2.523679
O [?]	0.822533	-0.822533	2.523679
O [?]	1.665467	1.665467	0.849321
O [?]	0.822533	0.822533	4.222321

Example 3 - Phonons

▼ Phonons with QE

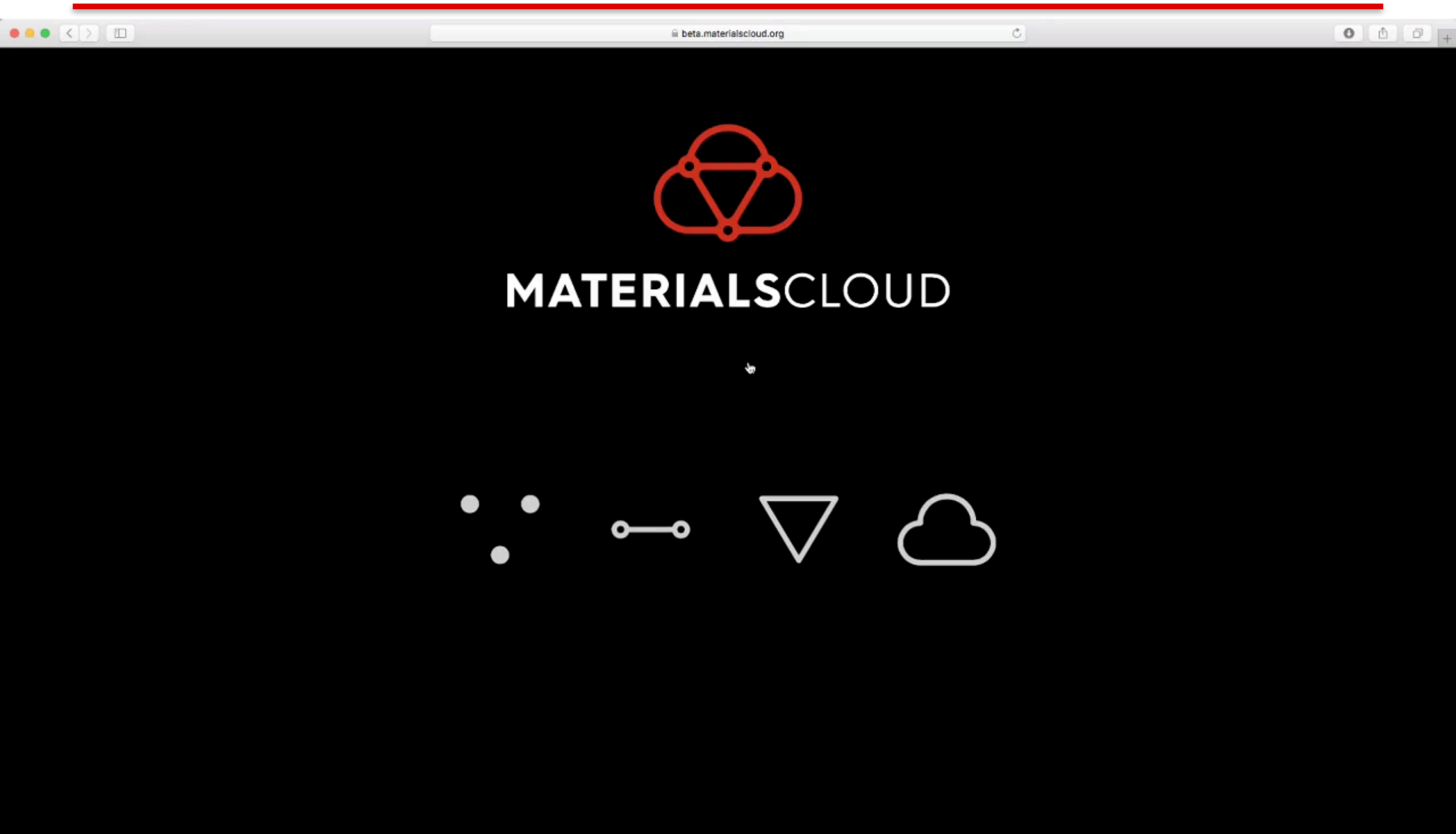
- [Run a new phonon workflow](#)
- [Monitor the status and results of a phonon calculation](#)



Turnkey Solution for Phonon Dispersion
powered by AiiDA, QE, SSSP, Appmode

N. Mounet, G. Pizzi, N. Marzari

Jupyter home



Phonons - App Mode

jupyter

Edit App Logout Control Panel Materials Cloud

Materials Cloud

▼ Home

File Browser Terminal Tasks Manage Apps

▼ AiiDA

- Status
- Workflows
- Graph Browser

▼ Phonons with QE

- Run a new phonon workflow
- Monitor the status and results of a phonon calculation

▼ Supercomputers at EPFL

Phonons - Live Edit

The screenshot shows a JupyterLab environment with a browser window at the top displaying the URL `jupyter.materialscloud.org`. Below the browser, the JupyterLab header includes the Jupyter logo and buttons for "Edit App", "Logout", "Control Panel", and "Materials Cloud". The main content area is titled "Phonon turn-key solution" and lists the authors as "Nicolas Mounet, Giovanni Pizzi (THEOS, EPFL)". It describes the workflow as an automatic process for computing phonon dispersion, powered by Quantum ESPRESSO, AiiDA, SSSP, and custom workflows. A list of dependencies is provided: Quantum ESPRESSO, AiiDA, SSSP, custom workflows for AiiDA, and AppMode for Jupyter. A citation prompt is shown: "If you use this tool in your research, please cite [INSERT CITATION HERE]". The interface features two main input sections: "Crystal structure" with an "Upload Structure" button, a checkbox for "Use an example structure", and a dropdown menu currently set to "Diamond"; and "Main input" with radio buttons for "Structure relaxation" (options: no relaxation, relax only atoms, relax cell and atoms) and a checkbox for "Use magnetism".

Phonon turn-key solution

Authors: Nicolas Mounet, Giovanni Pizzi (THEOS, EPFL)

This automatic workflow allows to compute the phonon dispersion of a material with a minimal set of input parameters. It is powered by:

- [Quantum ESPRESSO](#) as the quantum engine
- [AiiDA](#) as the automation platform
- [SSSP](#) as the curated pseudopotential family
- Custom-made workflows for AiiDA to manage the selection of parameters, the error handling, ...
- [AppMode for Jupyter](#) to create a simple UI

If you use this tool in your research, please cite [INSERT CITATION HERE]

Crystal structure

Upload Structure

☐ Use an example structure

Diamond

Main input

Structure relaxation: ☐ no relaxation
☐ relax only atoms
☒ relax cell and atoms

☐ Use magnetism

Phonons - Results

The screenshot shows the Materials Cloud Jupyter interface. At the top, there's a navigation bar with the Jupyter logo, 'Edit App', 'Logout', 'Control Panel', and 'Materials Cloud' buttons. Below this, the 'Materials Cloud' header is followed by a 'Home' section with icons for 'File Browser', 'Terminal', 'Tasks', and 'Manage Apps'. The 'AiiDA' section contains links for 'Status', 'Workflows', and 'Graph Browser'. The 'Phonons with QE' section, which is highlighted, contains two links: 'Run a new phonon workflow' and 'Monitor the status and results of a phonon calculation'. The 'Supercomputers at EPFL' section is partially visible at the bottom.

Materials Cloud

▼ Home

File Browser Terminal Tasks Manage Apps

▼ AiiDA

- Status
- Workflows
- Graph Browser

▼ Phonons with QE

- Run a new phonon workflow
- Monitor the status and results of a phonon calculation

▼ Supercomputers at EPFL

Example 4 - nanotech@surfaces

▼ Empa nanotech@surfaces Laboratory

Structures

- [Upload structures](#)
- [Scale structures](#)
- [Construct cell](#)
- [Assign spin, remove atoms](#)

Nanoribbons

- [Submit calculation](#)
- [Search database](#)

Slab Models

- [Construct slab](#)
- [Submit geo-opt](#)
- [Search database](#)

▲

▼

Workflows & interactive visualizations
powered by AiiDA, App Mode, CP2K

Ole Schütt, Edward Ditle, Carlo Pignedoli

nanotech@surfaces - GNR database

.start-2 .start-5 .start-6 .start-7 .start-8 .start-9 .start-10 .start-11 .start-12 .start-13 .phonon turnk... .start-0 .start-1 +

jupyter Edit App Logout Control Panel Materials Cloud

Materials Cloud

▼ Empa nanotech@surfaces Laboratory

Structures	Nanoribbons	Slab Models
• Upload structures • Scale structures • Construct cell • Assign spin, remove atoms	• Submit calculation • Search database	• Construct slab • Submit geo-opt • Search database

▼ AiiDA

- Status
- Workflows
- Graph Browser

▼ Backup

- Backup

▼ Units Converter

Hartree <=> eV Hartree 1 eV 27.211386024367243

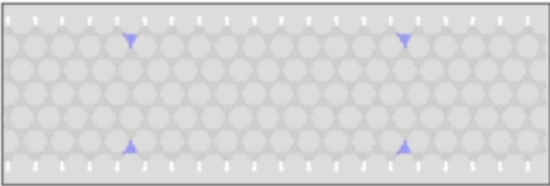
nanotech@surfaces - Compare bands

Top navigation: .start-2, .start-5, .start-6, .start-7, .start-8, .start-9, .start-10, .start-11, .start-12, .start-13, .phonon turn..., .start-0, .start-1, .search-0

Jupyter interface controls: Edit App, Logout, Control Panel, Materials Cloud

Sliders and Search:

- Gap: 0.00 – 3.00
- HOMO: -6.00 – -1.00
- LUMO: -5.00 – -1.00
- Fermi Energy: -6.00 – -1.00
- Total Magn.: -6.00 – 6.00
- Abs. Magn.: 1.50 – 20.00
- Search

PK	Creation Time	Formula	HOMO	LUMO	GAP	Fermi Energy	Total Mag.	Abs Mag.	Structure	
☐ 6473	2017-11-10 10:12	C118H20BN	-4.187422	-4.075627	0.111796	-4.130982	0.000000	6.420000		Show PDOS
☐ 6327	2017-11-08 16:39	C118H20B2	-4.284981	-4.168541	0.116439	-4.226486	0.000000	6.200000		Show PDOS
☐ 6320	2017-11-08 16:38	C118H20N2	-4.102082	-3.881072	0.221010	-4.015343	0.000000	5.950000		Show PDOS
										

nanotech@surfaces - PDOS

Search AiiDA Database for Nanoribbons

PKs:

Formulas:

Gap: 0.00 – 3.00

HOMO: -6.00 – -1.00

LUMO: -5.00 – -1.00

Fermi Energy: -6.00 – -1.00

Total Magn.: -6.00 – 6.00

Abs. Magn.: 1.50 – 20.00

	PK	Creation Time	Formula	HOMO	LUMO	GAP	Fermi Energy	Total Mag.	Abs Mag.	Structure	
☒	6473	2017-11-10 10:12	C118H20BN	-4.187422	-4.075627	0.111796	-4.130982	0.000000	6.420000		Show PDOS
☒	6327	2017-11-08 16:39	C118H20B2	-4.284981	-4.168541	0.116439	-4.226486	0.000000	6.200000		Show PDOS
☐	6320	2017-11-08 16:38	C118H20N2	-4.102082	-3.881072	0.221010	-4.015343	0.000000	5.950000		Show PDOS

nanotech@surfaces - I DOS & Spin density

The image is a horizontal collage of three distinct digital interfaces. On the left, a portion of a JupyterLab web application is visible, featuring a top navigation bar with tabs labeled '.start-2' through '.start-7'. Below this are four interactive sliders for 'LUMO:', 'Fermi Energy:', 'Total Magn.:', and 'Abs. Magn.:'. A search bar is positioned below the sliders. The main area contains a table with columns 'PK', 'Creation Time', 'Formula', and 'HOMO-LUMO Gap (eV)'. Four rows are shown, with the first two checked. The middle section displays a screenshot of an iPhone's Messages app. The conversation header shows '8 Messages' and the contact name 'Roman Fasel'. The message body contains a thank-you note from Roman to Carlo Antonio Pignedoli regarding band structure (BS) calculations and a file named '<Chevron variants.cdx>'. The rightmost section shows the Materials Cloud website, specifically the 'Materials Search' page. It includes a search bar at the top and a table of results. Each result row features a small thumbnail image of a material's crystal structure and a link labeled 'Show PDOS'.

Quantum Mobile Virtual Machine

Terminal window output:

```
(aiida) max@qmobile: ~/codes$ verdi code list
# List of configured codes:
# (use 'verdi code show CODEID' to see the details)
* pk 1 - yambo-4.2.0@localhost
* pk 2 - p2y-4.2.0@localhost
* pk 3 - fleur-0.27-fleur@localhost
* pk 4 - fleur-0.27-inpgen@localhost
* pk 5 - siesta-4.0.1@localhost
* pk 6 - cp2k-5.1@localhost
(aiida) max@qmobile: ~/codes$ verdi calculation list -a
# Last daemon state_updater check: 0h:00m:05s ago (at 15:09:17 on 2017-11-20)
PK  Creation      State      Sched. state  Computer  Type
-----
175  3h ago         FAILED     DONE         localhost siesta.
siesta
179  3h ago         FINISHED   DONE         localhost fleur.i
npgen
195  3h ago         FAILED     DONE         localhost siesta.
siesta
208  3h ago         FINISHED   DONE         localhost siesta.
siesta
221  11m ago        FINISHED   DONE         localhost fleur.i
npgen
228  11m ago        FINISHED   DONE         localhost fleur.f
leur
Total results: 6
(aiida) max@qmobile: ~/codes$
```

Jmol window output:

```
MoS2_ML.cif - <collection of 1 models>
P 1 [P 1]
a=3.188Å
b=3.188Å
c=23.155Å
α=90.0°
β=90.0°
γ=120.0°
```

Quantum Mobile
MARVEL MAX

- Ubuntu 16.04
- **AiiDA, jupyter**
- **QE, Siesta, fleur, yambo, cp2k + AiiDA plugins**
- Visualization tools (xcrysden, ...)
- ready to use for tutorials, lectures, exercise, ...
- **Modular setup: roll your own**

Runs on Linux, MacOS and Windows hosts using VirtualBox

Conclusions



- Workflows & Daemon help with automation
- AiiDA graph = map of the data jungle
- Your calculations are ready for Open Science



- Public Beta, give it a try!
- Archive: accepting submissions from MARVEL, EPFL, **MaX**, NFFA, ...



- Easy to write
- Run where you like
 - on your machine (your machine, your setup)
 - on Quantum Mobile (your machine, our setup)
 - on Materials Cloud (our machine, our setup)

AiiDA & Materials Cloud Teams



Marco
Borelli
(EPFL)



Andrea Cepellotti
(EPFL)



Fernando
Gargiulo
(EPFL)



Rico
Häuselmann
(EPFL)



Sebastiaan
P. Huber
(EPFL)



Boris Kozinsky
(BOSCH)



Snehal P.
Kumbhar
(EPFL)



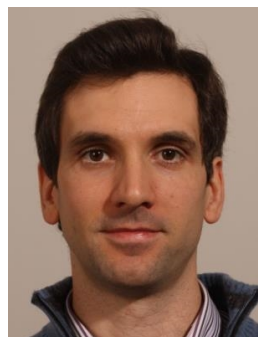
Leonid
Kahle
(EPFL)



Nicola Marzari
(EPFL)



Andrius
Merkys
(Vilnius)



Nicolas Mounet
(EPFL)



Elsa
Passaro
(EPFL)



Giovanni Pizzi
(EPFL)



Thomas
Schulthess
(ETHZ,CSCS)



Ole
Schütt
(EMPA)



Leopold
Talirz
(EPFL)



Martin
Uhrin
(EPFL)



Joost
VandeVondele
(ETHZ,CSCS)



Aliaksandr
Yakutovich
(EPFL)



Spyros
Zoupanos
(EPFL)

20+ plugin contributors for [Quantum ESPRESSO](#), [Wannier90](#), [CP2K](#), [FLEUR](#), [Exciting](#), [YAMBO](#), [SIESTA](#), [VASP](#), ...

Contributors to `aiida_core` and former AiiDA team members — Valentin Bersier, Jocelyn Boullier, Jens Broeder, Christoph Koch, Dominik Gresch, Eric Hontz, Tiziano Müller, Riccardo Sabatini, Phillippe Schwaller

The CSCS support teams

AiiDA Tutorial @Cineca

Date: 30th May - 1 June 2018

Location: Cineca, Bologna, Italy

Slots: 40 students/postdocs/researchers



Audience: know Linux, **interest in high-throughput**

Cost: Free, for grants see web site

<https://events.prace-ri.eu/event/709/>

Contacts and info



Website: aiida.net

Docs: aiida-core.readthedocs.io

Git repo: github.com/aiidateam/aiida_core/

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



<https://www.facebook.com/aiidateam>



@aiidateam



Materials Cloud: beta.materialscloud.org

- **Jupyter:** jupyter.materialscloud.org

- **Archive:** archive.materialscloud.org

- **Apps:** github.com/materialscloud-org

Quantum Mobile: <http://bit.do/quantum-mobile>

