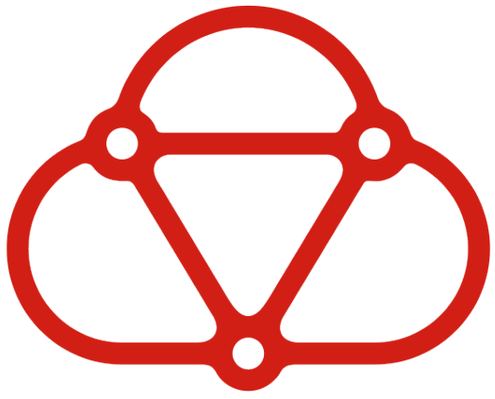
MATERIALSCLOUD

LEARN

WORK

DISCOVER

EXPLORE



MATERIALSCLOUD

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

Leopold Talirz (EPFL)

MAX

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

MARVEL

Motivation

Computational Materials Science Challenges

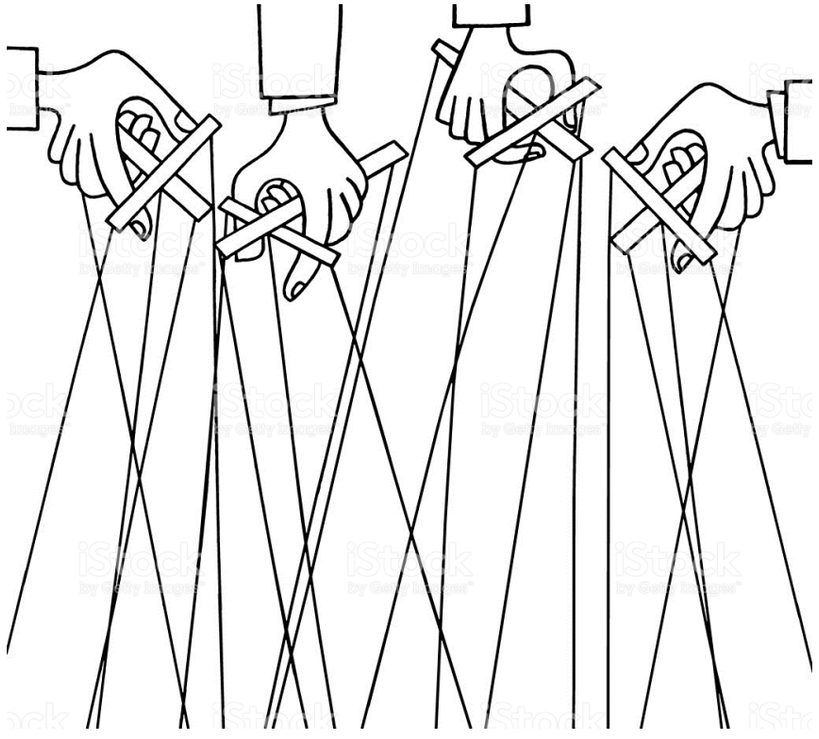
High-Throughput

"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

Motivation

Computational Materials Science Challenges

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

Computational Materials Science Challenges

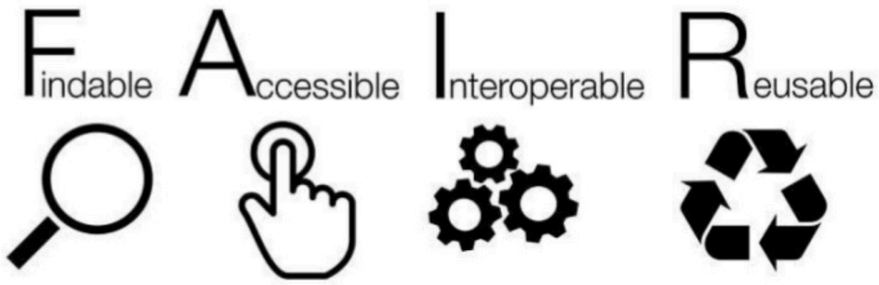
High-Throughput

"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

Computational Materials Science Challenges

High-Throughput

"Data jungle"

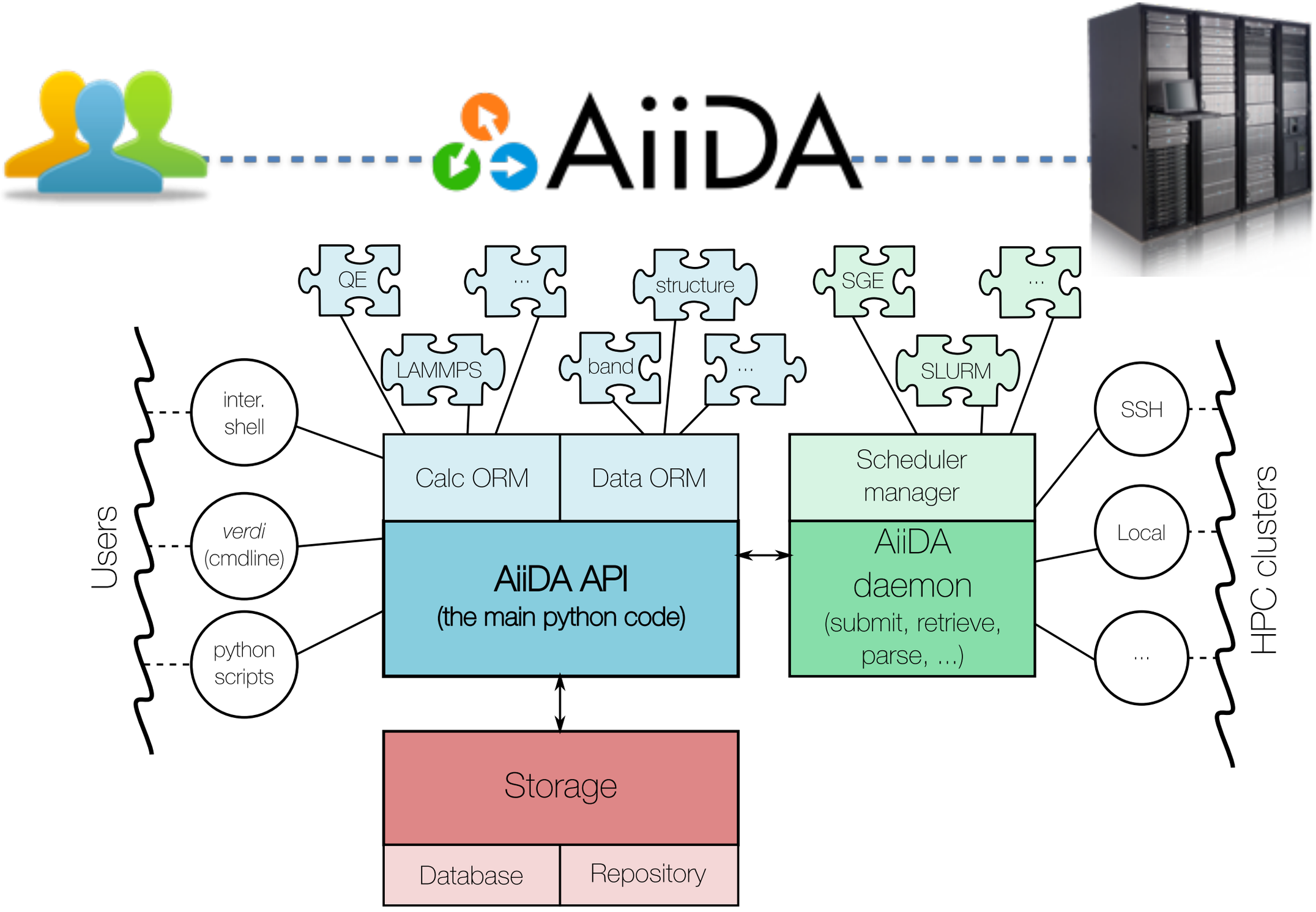
Open Science

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



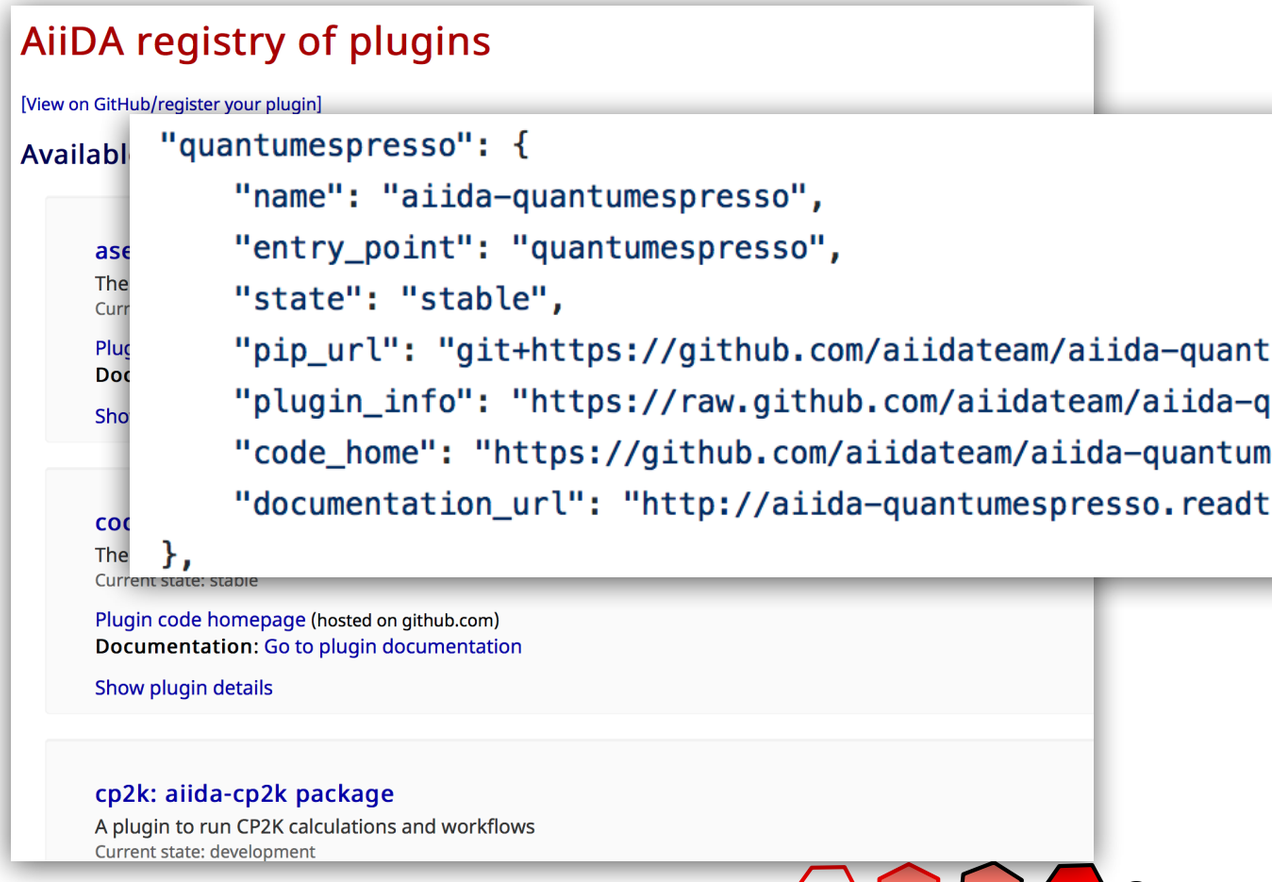
AiiDA – Development

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

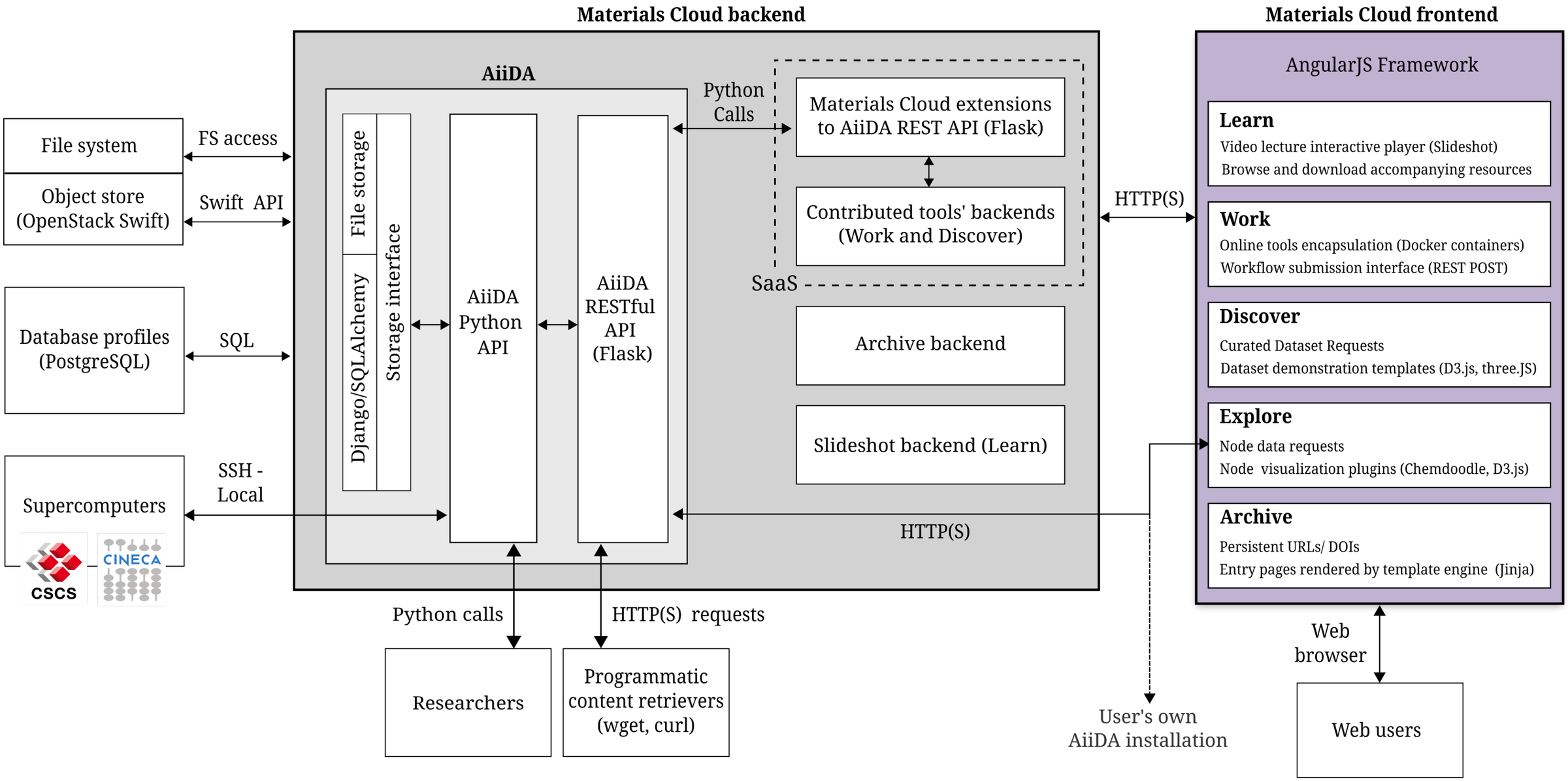
Plugin registry: aiidateam.github.io/aiida-registry

AiiDA plugins

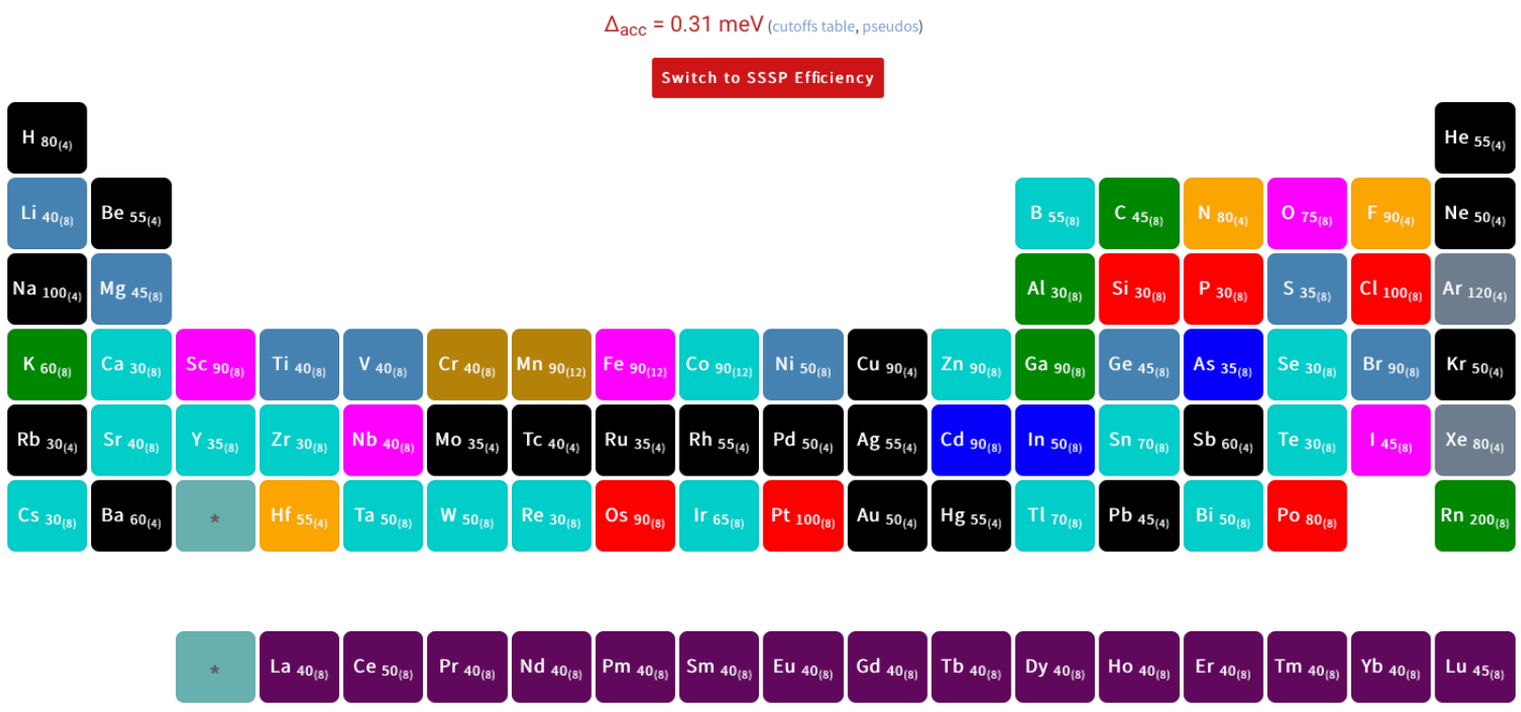
ase, codtools, cp2k,
fleur, lammps, nwchem, phonopy
quantumespresso, raspa, siesta,
vasp, wannier90, yambo
(+plugin-template)



Materials Cloud – Architecture



Example 1 - SSSP

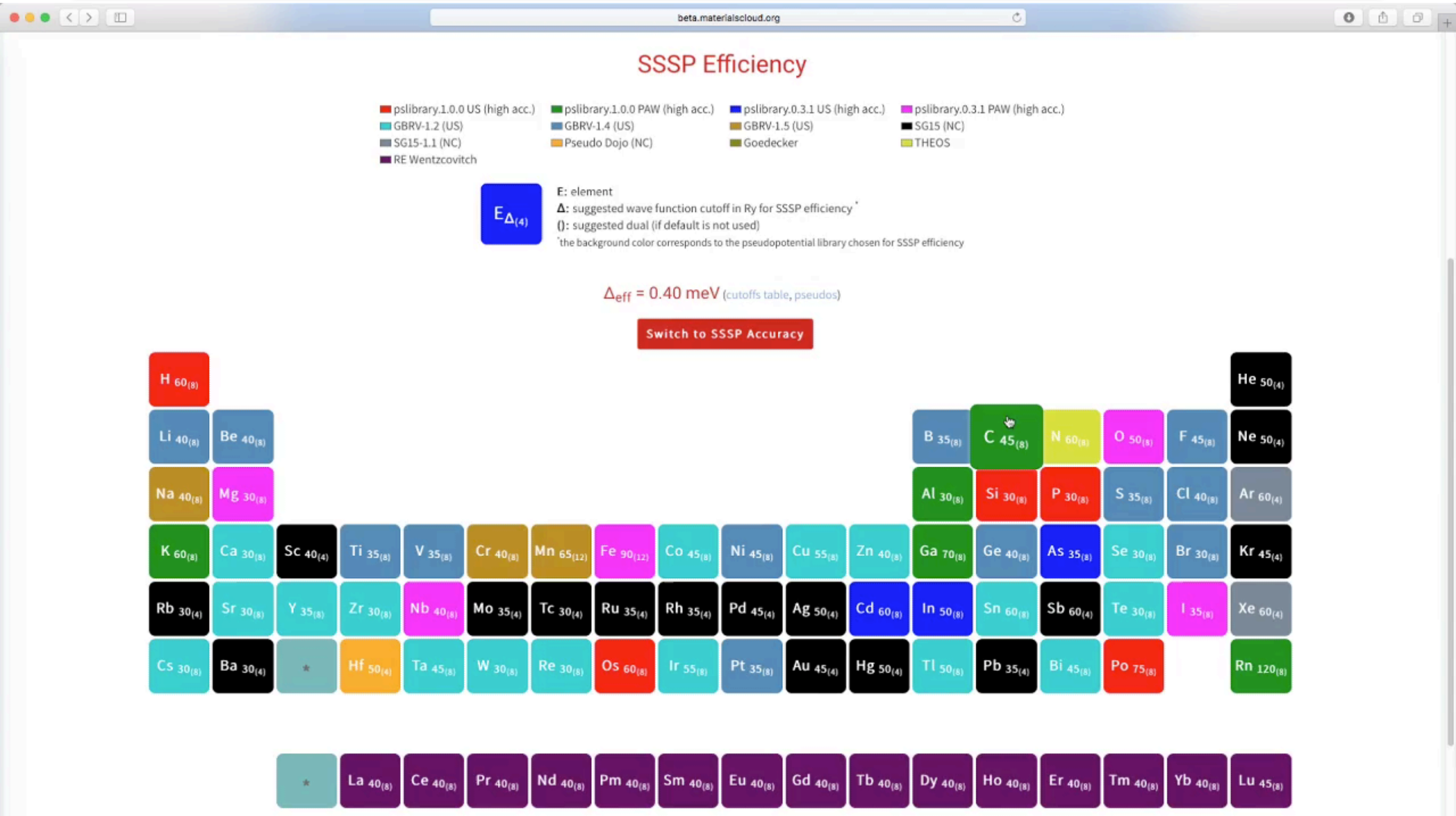


Standard Solid State Pseudo Potentials

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

SSSP - Overview

SSSP - Plots


beta.materialscloud.org
SSSP Efficiency
pslibrary.1.0.0 US (high acc.)
pslibrary.1.0.0 PAW (high acc.)
pslibrary.0.3.1 US (high acc.)
pslibrary.0.3.1 PAW (high acc.)
GBRV-1.2 (US)
GBRV-1.4 (US)
GBRV-1.5 (US)
SG15 (NC)
SG15-1.1 (NC)
Pseudo Dojo (NC)
Goedecker
THEOS
RE Wentzcovitch
$E_{\Delta_{(4)}}$
E: element
Δ: suggested wave function cutoff in Ry for SSSP efficiency *
(): suggested dual (if default is not used)
*the background color corresponds to the pseudopotential library chosen for SSSP efficiency
Δ_{eff} = 0.40 meV (cutoffs table, pseudos)
Switch to SSSP Accuracy
H 60(8)
He 50(4)
Li 40(8)
Be 40(8)
B 35(8)
C 45(8)
N 60(8)
O 50(8)
F 45(8)
Ne 50(4)
Na 40(8)
Mg 30(8)
Al 30(8)
Si 30(8)
P 30(8)
S 35(8)
Cl 40(8)
Ar 60(4)
K 60(8)
Ca 30(8)
Sc 40(4)
Ti 35(8)
V 35(8)
Cr 40(8)
Mn 65(12)
Fe 90(12)
Co 45(8)
Ni 45(8)
Cu 55(8)
Zn 40(8)
Ga 70(8)
Ge 40(8)
As 35(8)
Se 30(8)
Br 30(8)
Kr 45(4)
Rb 30(4)
Sr 30(8)
Y 35(8)
Zr 30(8)
Nb 40(8)
Mo 35(4)
Tc 30(4)
Ru 35(4)
Rh 35(4)
Pd 45(4)
Ag 50(4)
Cd 60(8)
In 50(8)
Sn 60(8)
Sb 60(4)
Te 30(8)
I 35(8)
Xe 60(4)
Cs 30(8)
Ba 30(4)
*
Hf 50(4)
Ta 45(8)
W 30(8)
Re 30(8)
Os 60(8)
Ir 55(8)
Pt 35(8)
Au 45(4)
Hg 50(4)
Tl 50(8)
Pb 35(4)
Bi 45(8)
Po 75(8)
Rn 120(8)
*
La 40(8)
Ce 40(8)
Pr 40(8)
Nd 40(8)
Pm 40(8)
Sm 40(8)
Eu 40(8)
Gd 40(8)
Tb 40(8)
Dy 40(8)
Ho 40(8)
Er 40(8)
Tm 40(8)
Yb 40(8)
Lu 45(8)

SSSP - Provenance

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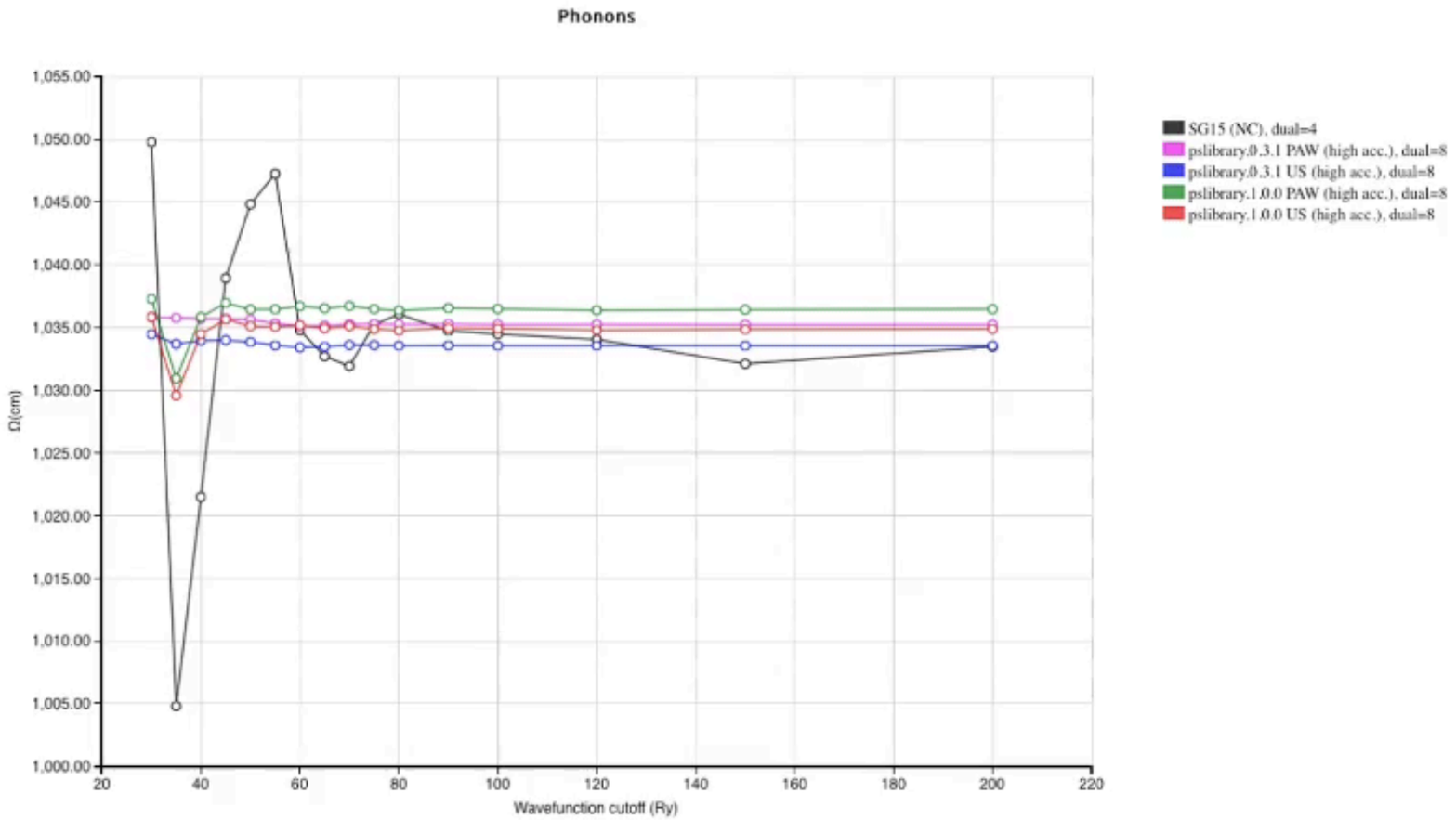
Phonons

- GBRV-1.2 (US)
  - dual=8
- Goedecker
  - dual=4
- SG15 (NC)
  - dual=4
- pslibrary.0.3.1 PAW (high acc.)
  - dual=8
- pslibrary.0.3.1 US (high acc.)
  - dual=8
- pslibrary.1.0.0 PAW (high acc.)
  - dual=8
- pslibrary.1.0.0 US (high acc.)
  - dual=8



Phonons (%)

- GBRV-1.2 (US)
  - dual=8
- Goedecker

SSSP - Provenance

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LEARN WORK DISCOVER EXPLORE ARCHIVE More

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/0f/e0/93bd-f0f7-457a-9781-c3b058bd4eeb

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

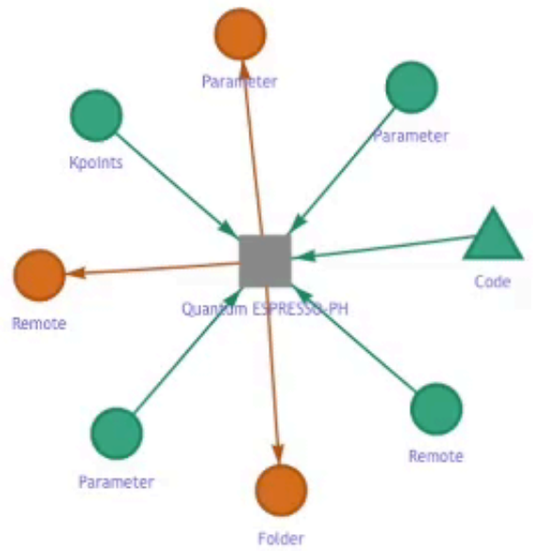
OUTPUT FILES
- aiida.out
- _scheduler-stdout.txt
- DYN_MAT/dynamical-matrix-
- _scheduler-stderr.txt

Node metadata

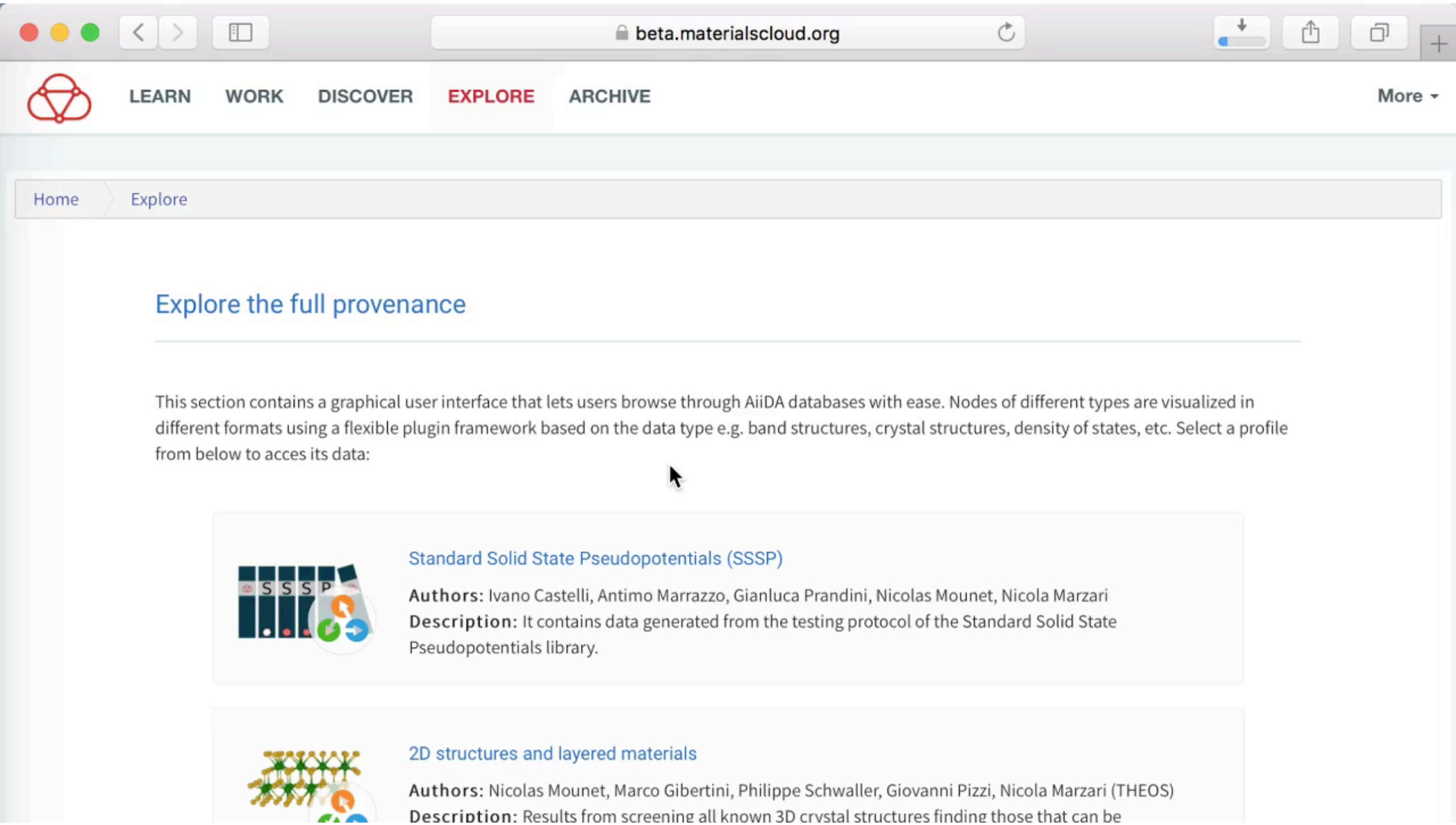
CUSTOM_SCHEDULER_COMMANDS #SBATCH -A, --account=mr0
JOBRESOURCE_PARAMS {"default_mpiprocs_per_machine":24,"num_machines":1}
LINKNAME_RETRIEVED retrieved
MAX_WALLCLOCK_SECONDS 30000
RETRIEVE_LIST ["aiida.out","DYN_MAT","./out/_ph0/aiida.phsave/tensors.xml","_scheduler-stdout.txt","_scheduler-stderr.txt"]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

AiiDA Provenance Browser

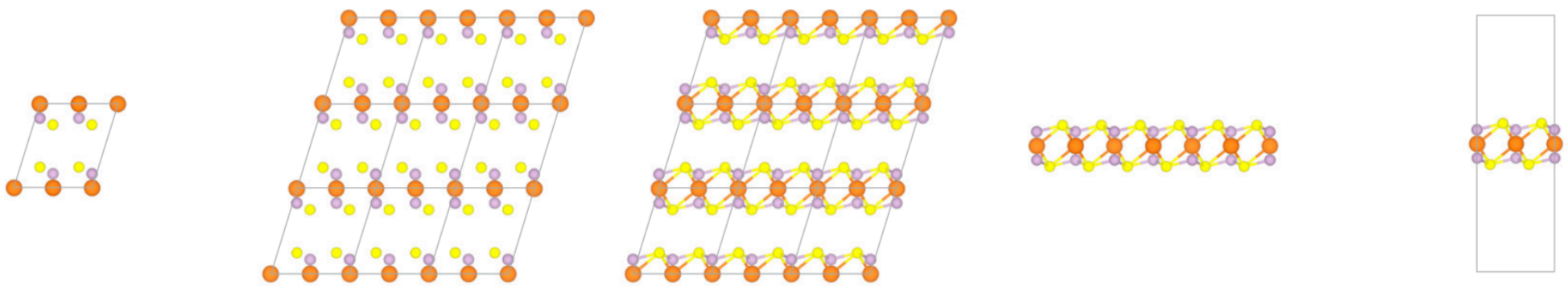
Selected node, Inputs, Outputs



SSSP - Archive



Example 2 - 2D Materials

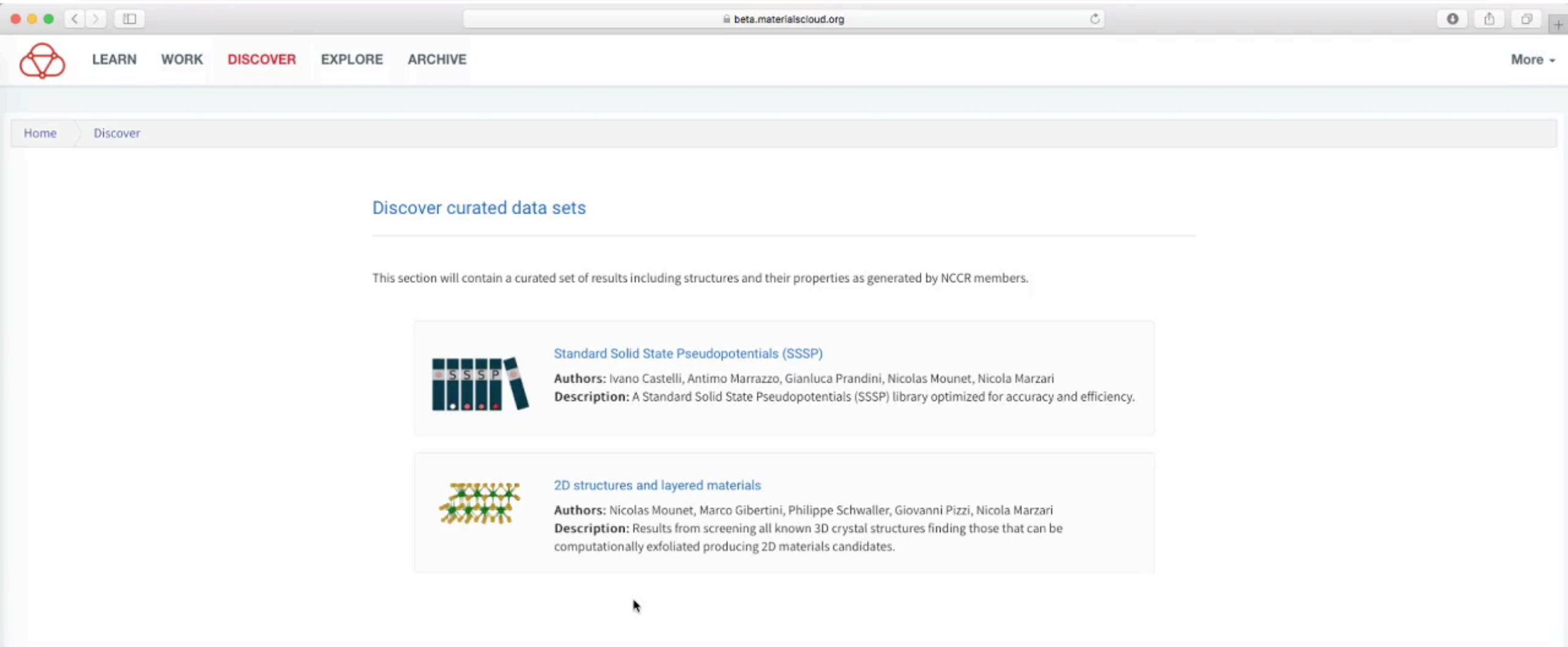


3D primitive cell → supercell → bond connectivity → 2D/1D/0D units → 2D primitive cell

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

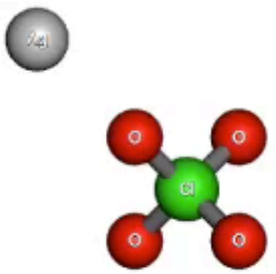
N. Mounet, M. Gibertini, P. Schwaller, A. Merkys, I. E. Castelli, A. Cepellotti, G. Pizzi & N. Marzari, arXiv:1611.05234 (2016).

2D Materials - Overview



2D Materials - Provenance

beta.materialscloud.org

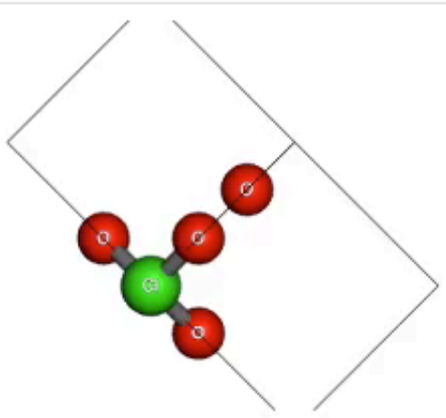


Kind	x[Å]	y[Å]	z[Å]
v_1	4.844127	0.000000	0.000000
v_2	0.000000	4.844127	0.000000
v_3	0.000000	0.000000	21.752132

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/Å^2]: 0.0191

rVV10 Binding energy [meV/Å^2]: 0.0290

3D structure atomic coordinates

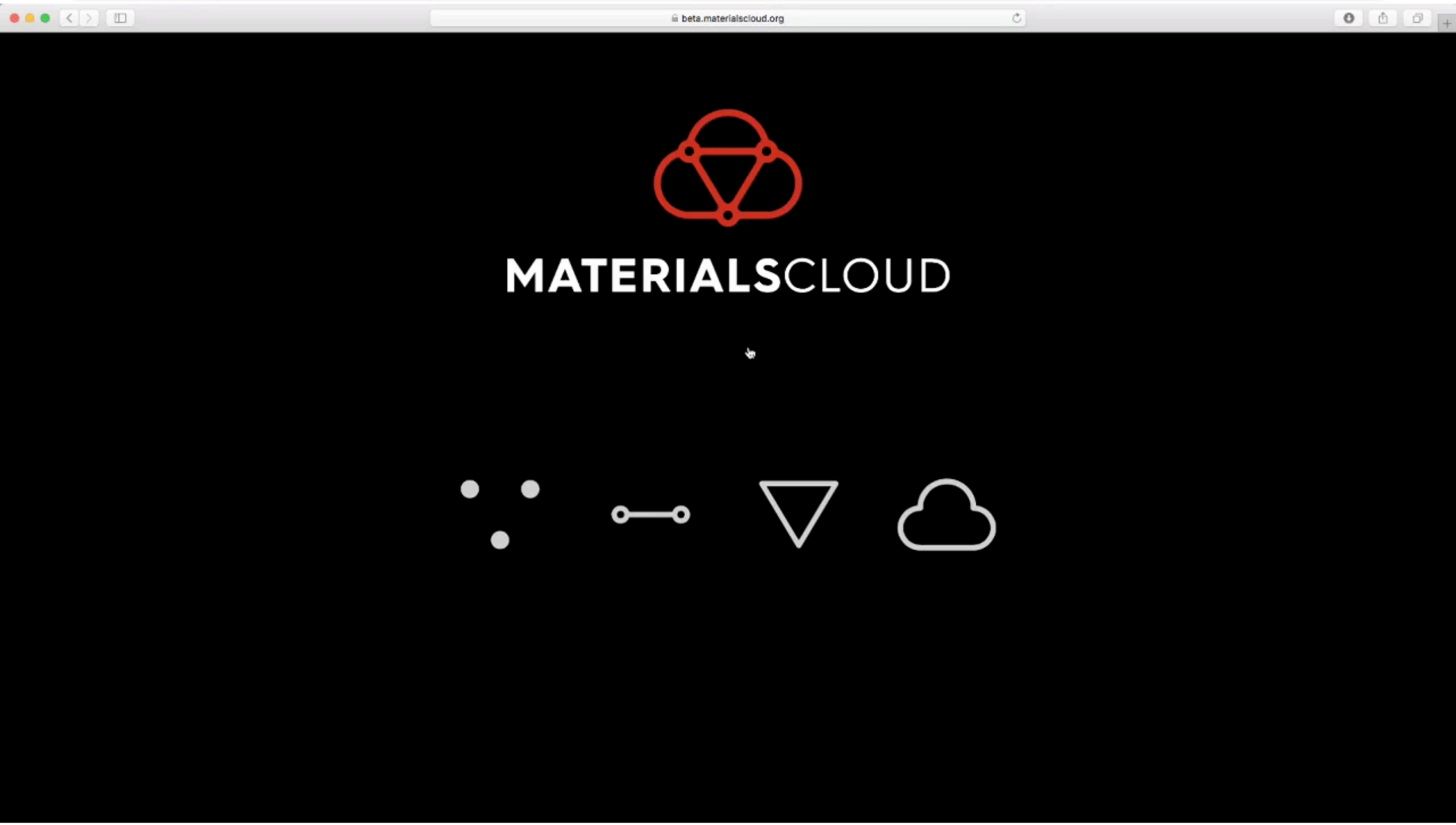
Kind label	x[Å]	y[Å]	z[Å]
Ag	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	3.373000
O	-0.822533	0.822533	2.523679
O	0.822533	-0.822533	2.523679
O	1.665467	1.665467	0.849321
O	0.822533	0.822533	4.222321

Example 3 - Phonons

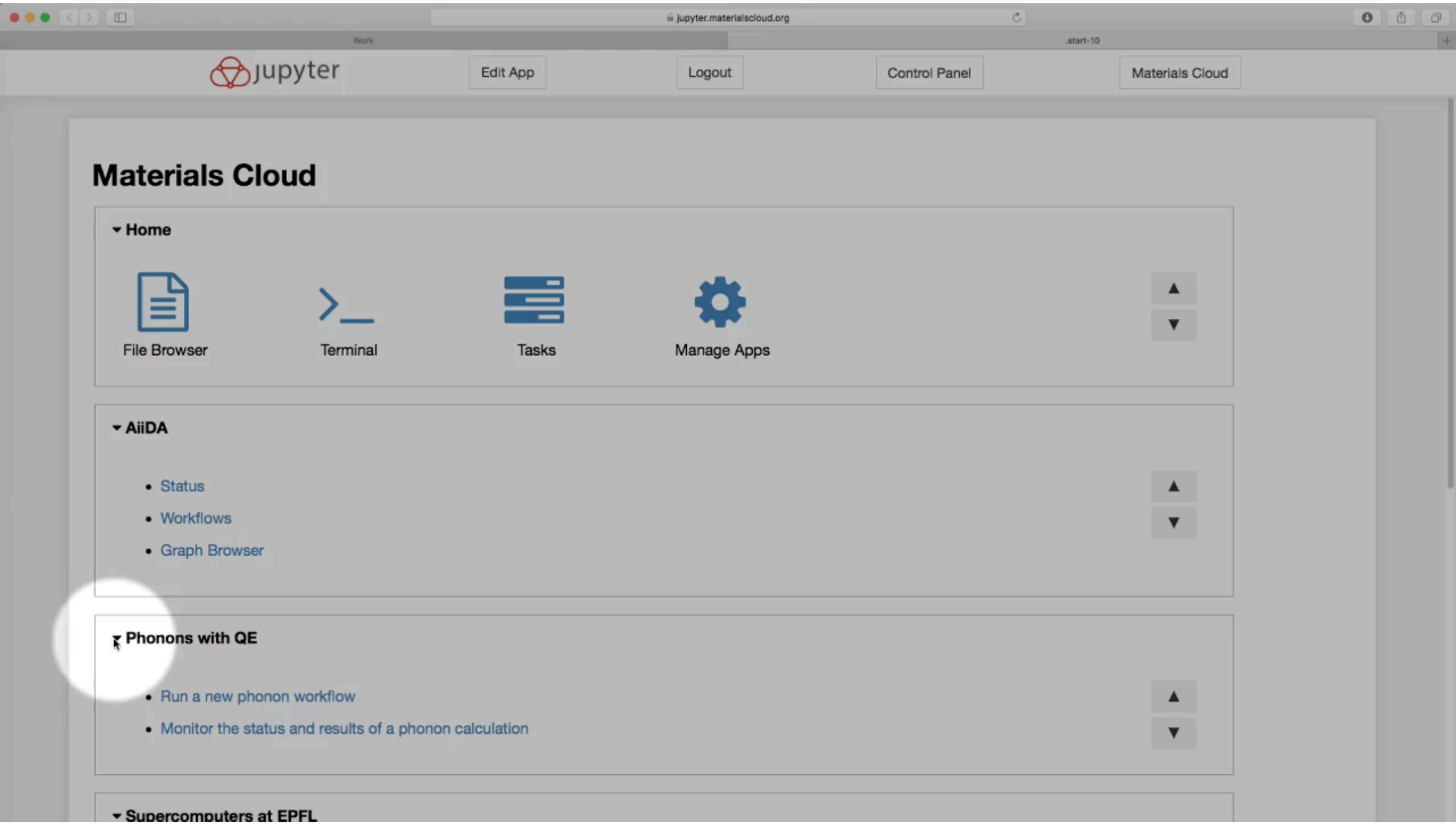
Turnkey Solution for Phonon Dispersion powered by AiiDA, QE, SSSP, Appmode

N. Mounet, G. Pizzi, N. Marzari

Jupyter home



Phonons - App Mode



Phonons - Live Edit

jupyter.materialscloud.org

Work | .start-10 | .phonon turnkey solution-0

jupyter | Edit App | Logout | Control Panel | Materials Cloud

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

jupyter.materialscloud.org

Work | .start-10 | .phonon turnkey solution-0

jupyter | Edit App | Logout | Control Panel | Materials Cloud

Materials Cloud

▾ Home

File Browser | Terminal | Tasks | Manage Apps

▾ AiiDA

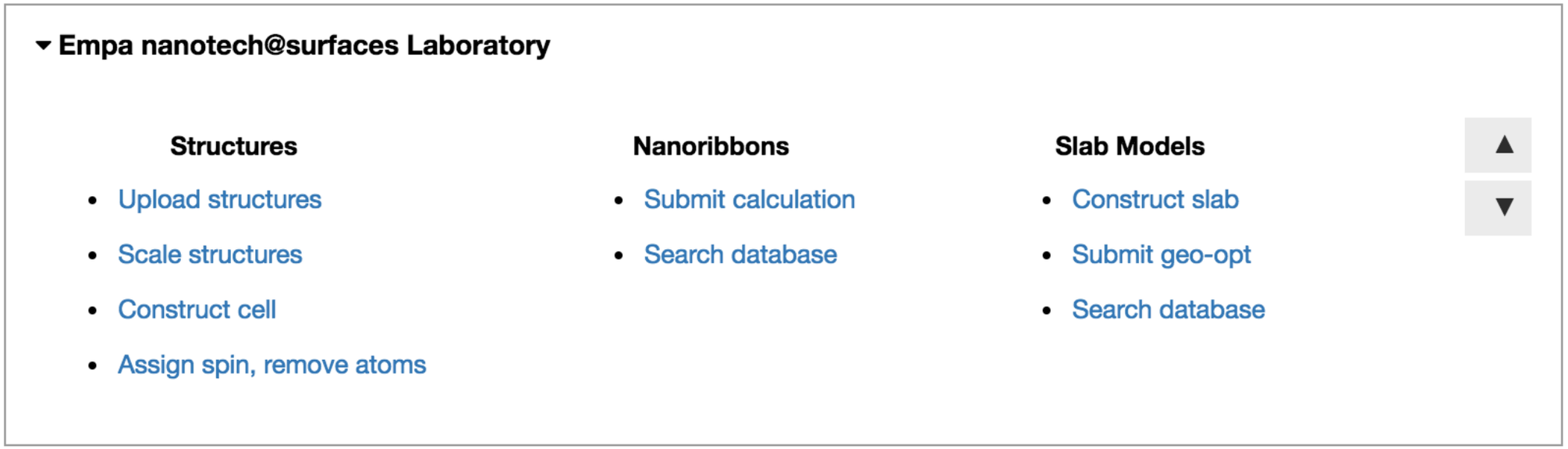
- Status
- Workflows
- Graph Browser

▾ Phonons with QE

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

▾ Supercomputers at EPFL

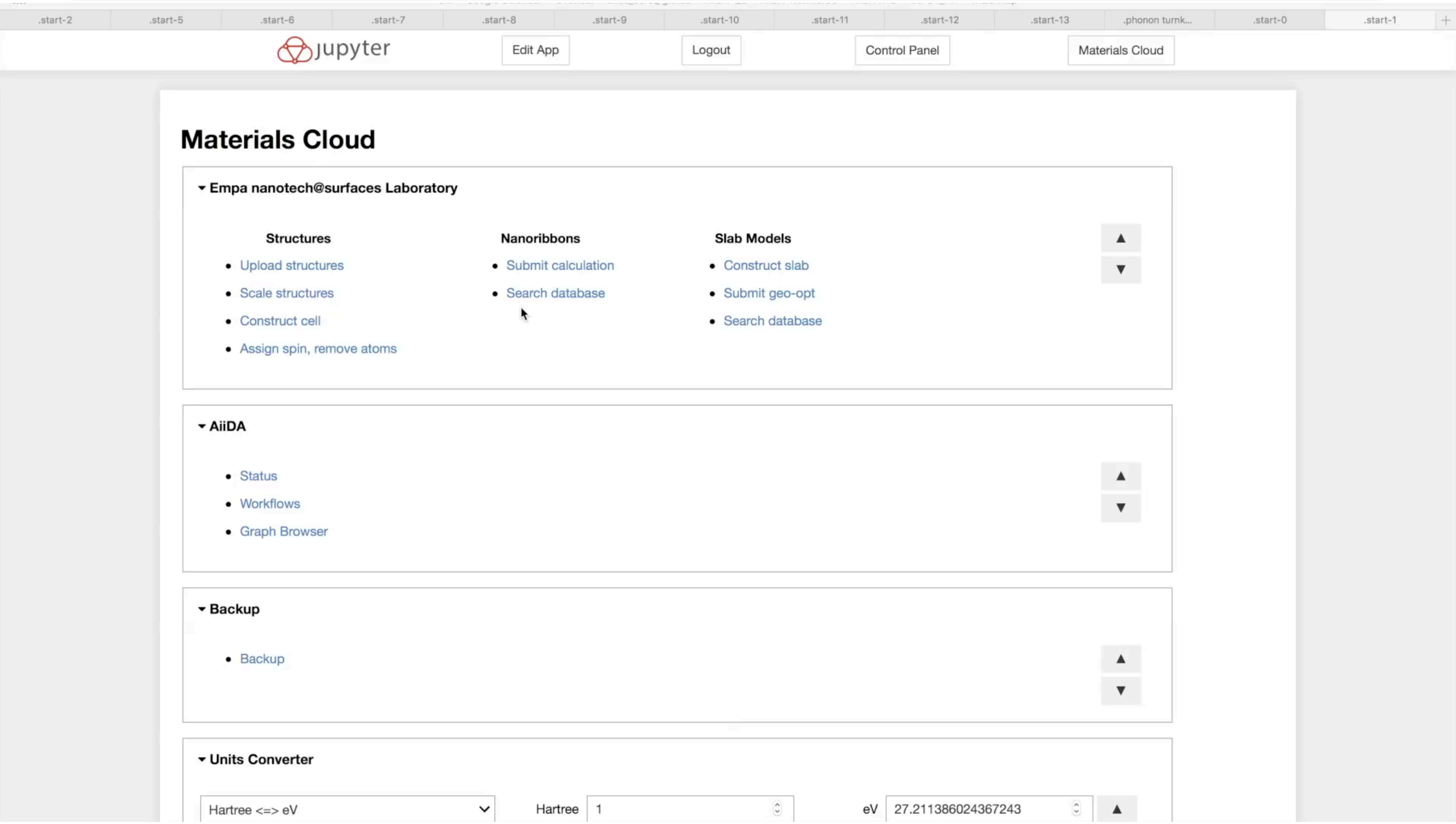
Example 4 - nanotech@surfaces



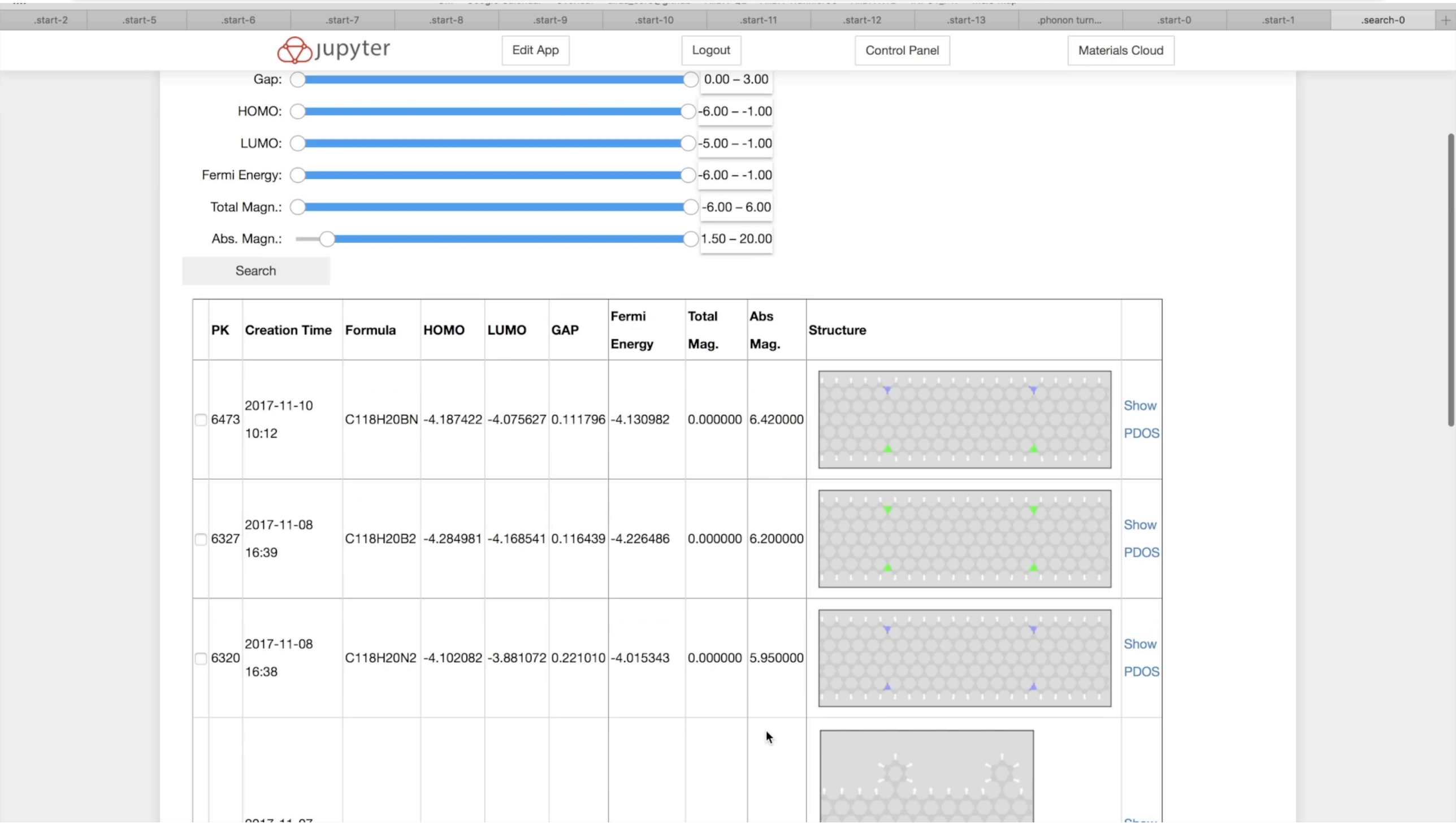
Workflows & interactive visualizations powered by AiiDA, App Mode, CP2K

Ole Schütt, Edward Ditler, Carlo Pignedoli

nanotech@surfaces - GNR database



nanotech@surfaces - Compare bands



nanotech@surfaces - PDOS

.s .s .start-6 .start-7 .start-8 .start-9 .start-10 .start-11 .start-12 .start-13 .phonon turn... .start-0 .start-1 .search-0 .show-0

jupyter Edit App Logout Control Panel Materials Cloud

Search AiiDA Database for Nanoribbons

PKs: e.g. 4062 4753 (space separated)

Formulas: e.g. C44H16 C36H4

Gap: 0.00 – 3.00

HOMO: -6.00 – -1.00

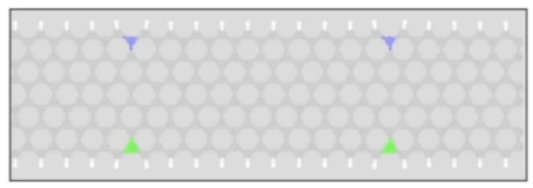
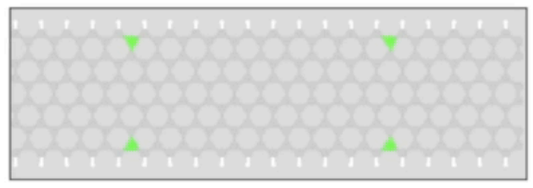
LUMO: -5.00 – -1.00

Fermi Energy: -6.00 – -1.00

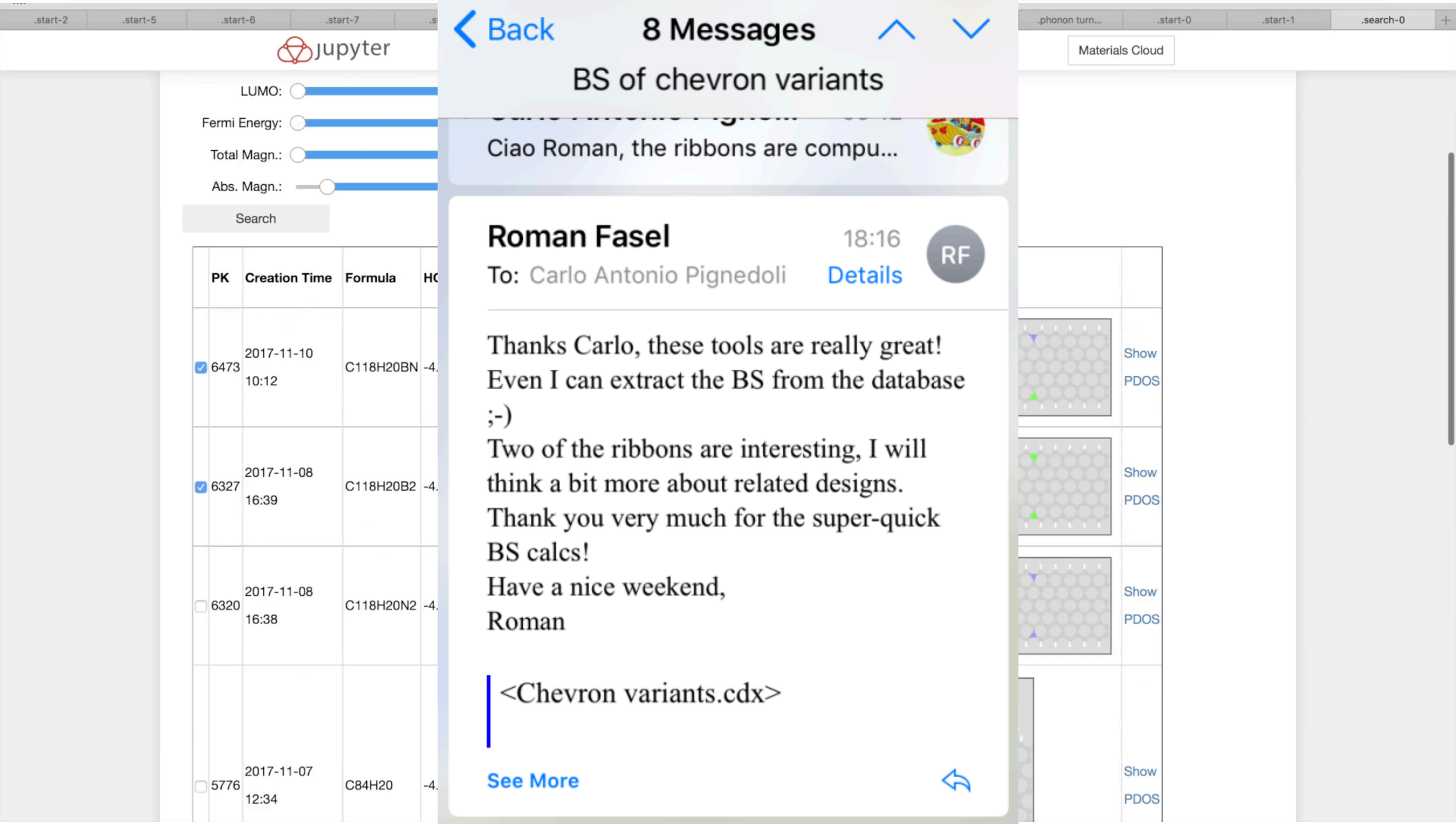
Total Magn.: -6.00 – 6.00

Abs. Magn.: 1.50 – 20.00

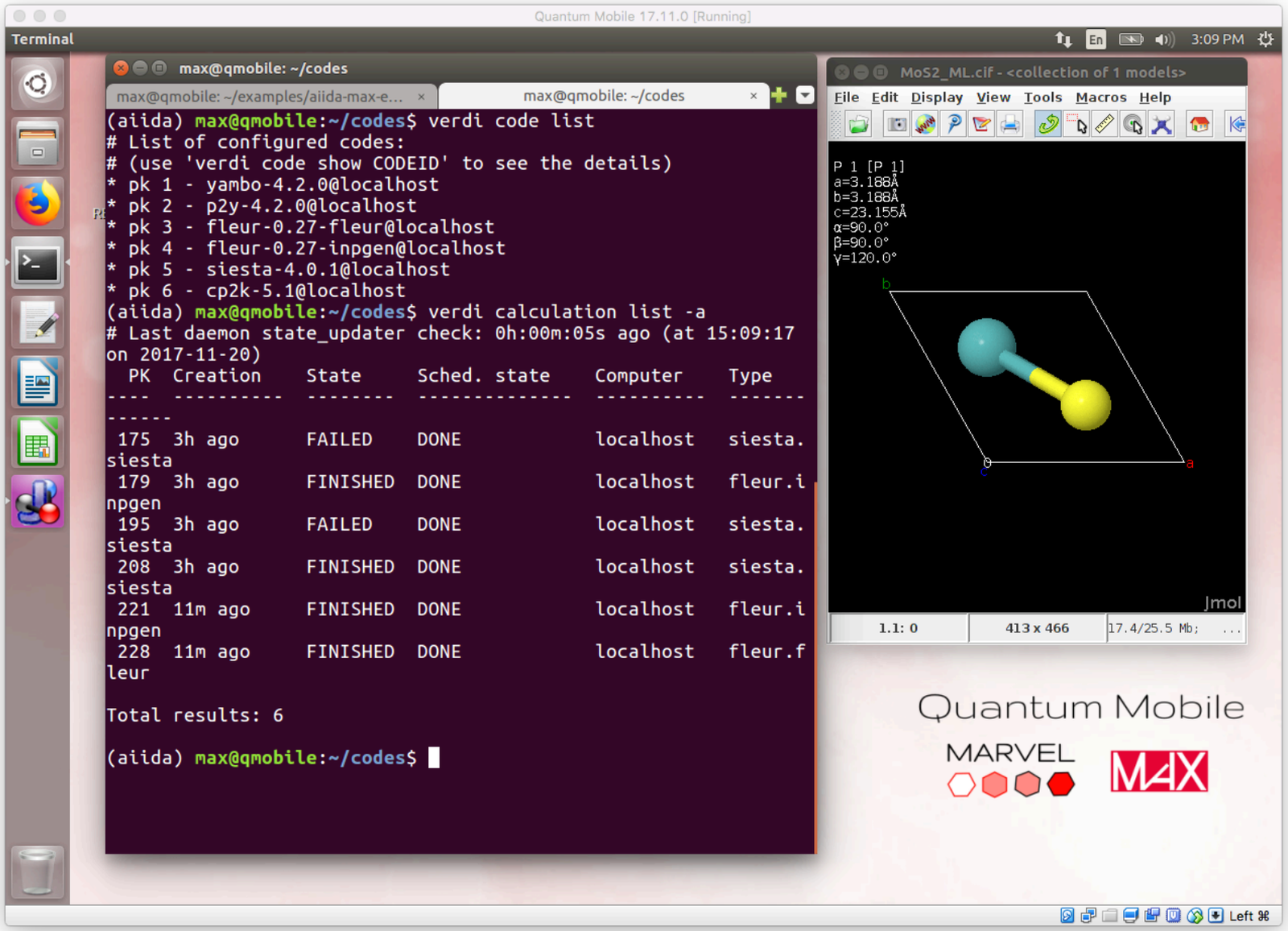
Search

	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 - LDOS & Spin density



Quantum Mobile Virtual Machine



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

Runs on Linux, MacOS and Windows hosts using VirtualBox

Download: http://bit.do/quantum-mobile

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, ...

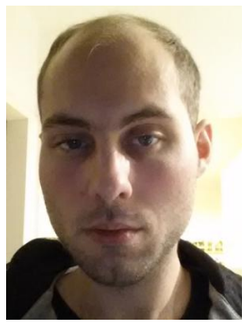
- Easy to write
- Run where you like
  - on your machine (your machine, your setup)
  - on Quantum Mobile (your machine, our setup)
  - on Materials Cloud (our machine, our setup)

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)

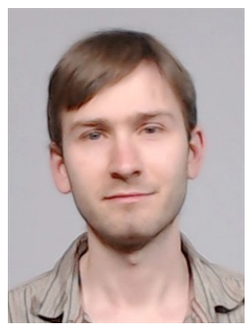

Elsa Passaro (EPFL)


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