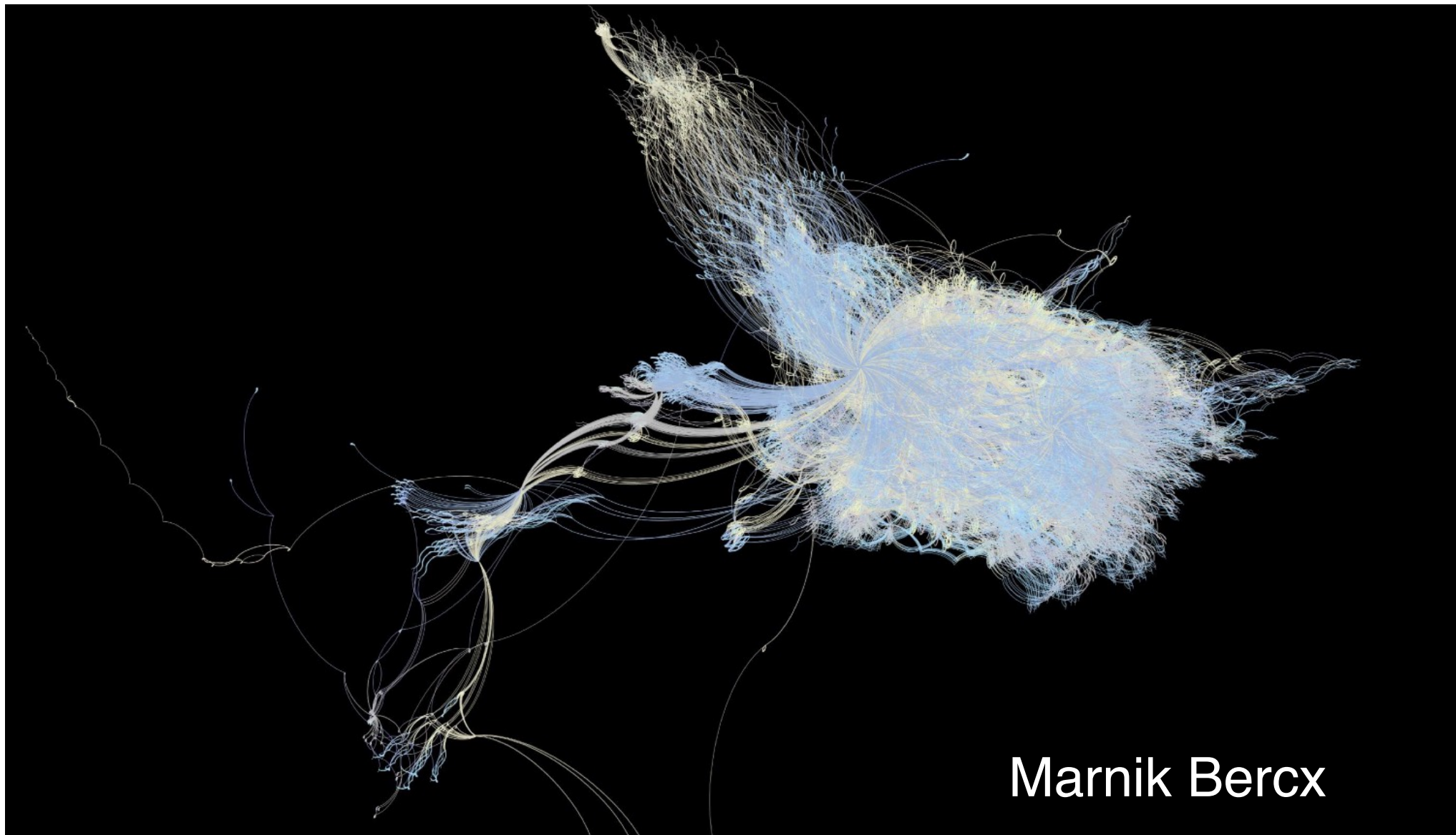


MaX School on Advanced Materials
and Molecular Modelling with
Quantum ESPRESSO



Marnik Bercx



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>



MIT LICENSED



Scalable workflow engine

Automated full data provenance



Built-in support for HPC

Flexible plugin system



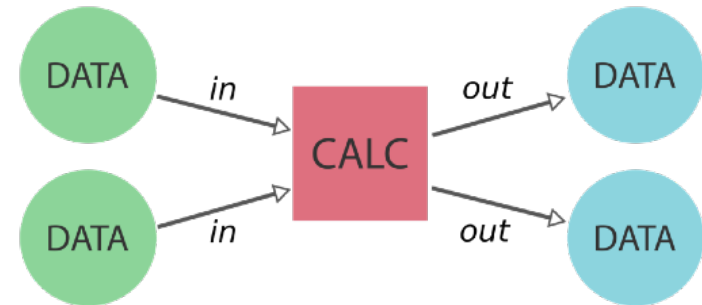
G. Pizzi et al., Comp. Mat. Sci. 111, 218-230 (2016)

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**



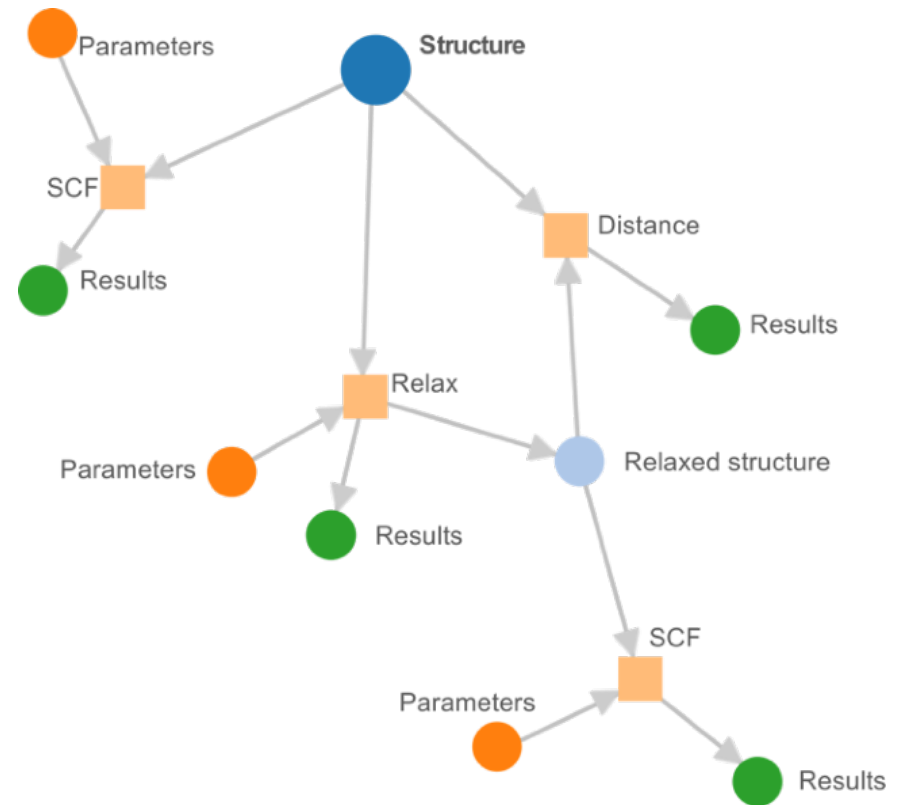
Data provenance

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



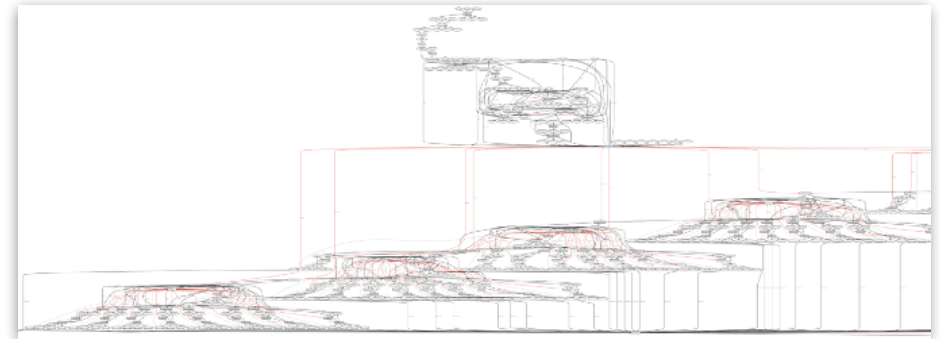
Data provenance

Simple recipe

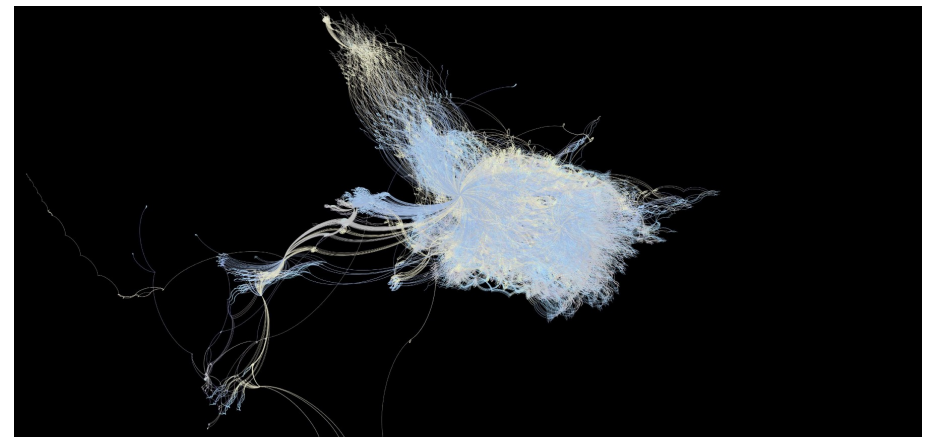
- Store data transformations or **'calculations'**
- Store its **inputs** and their metadata
- Store its **outputs** and their metadata
- Most **crucially** store the **inter-connections**

Graph requirements

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



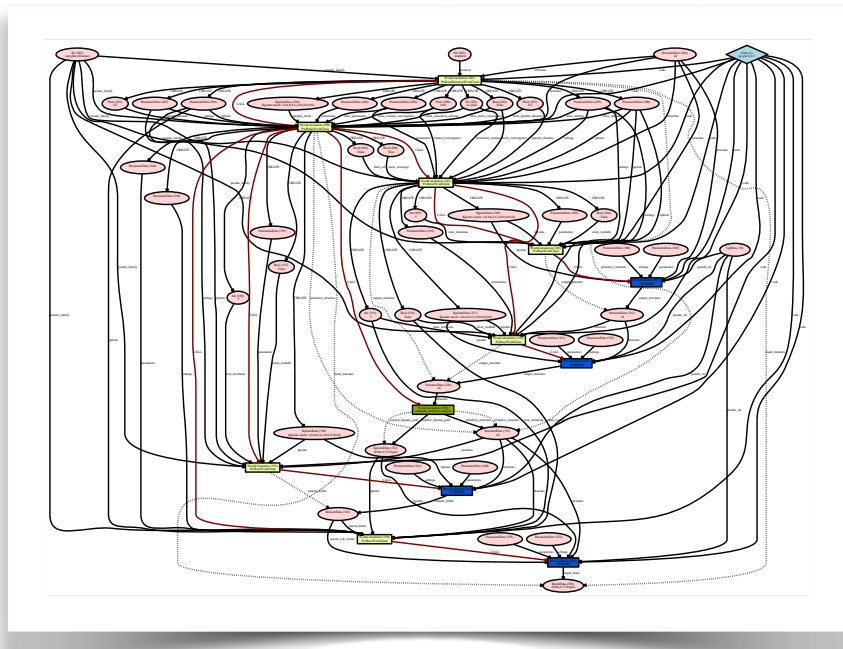
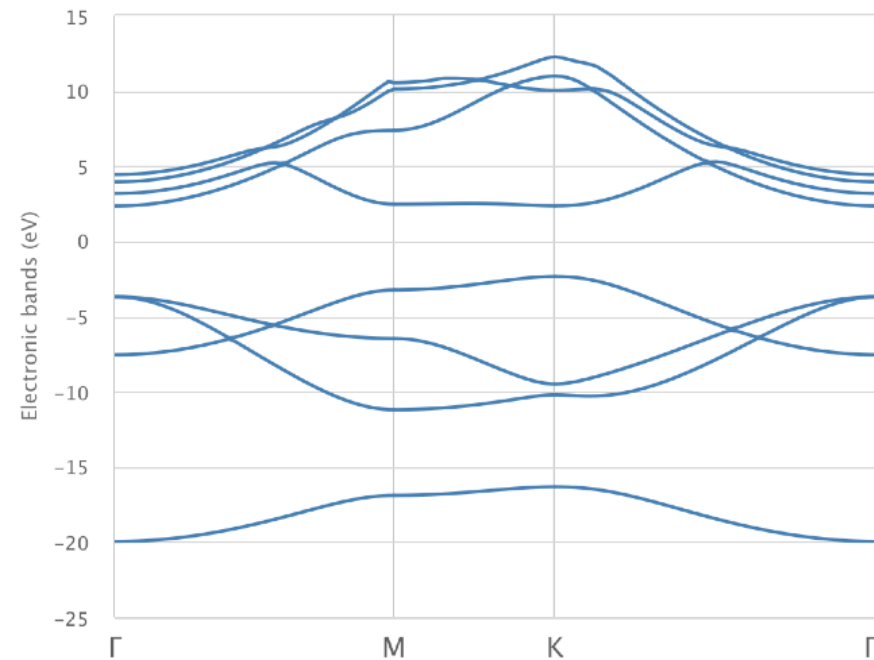
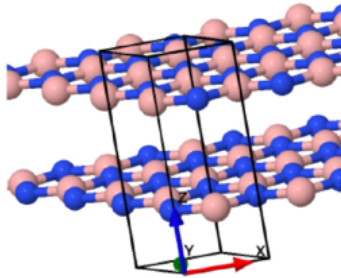
Molecular dynamics study of Lithium in a solid electrolyte.



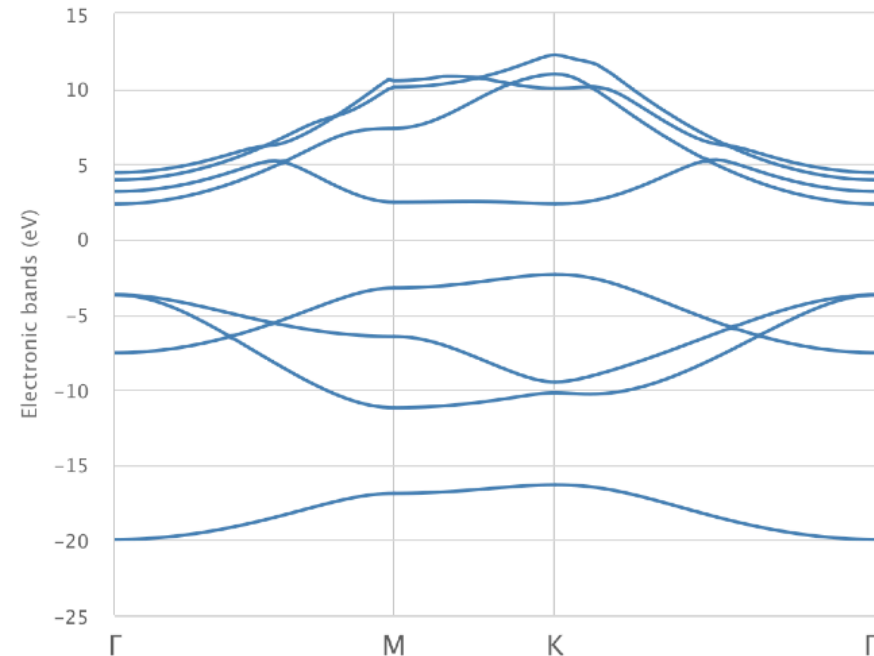
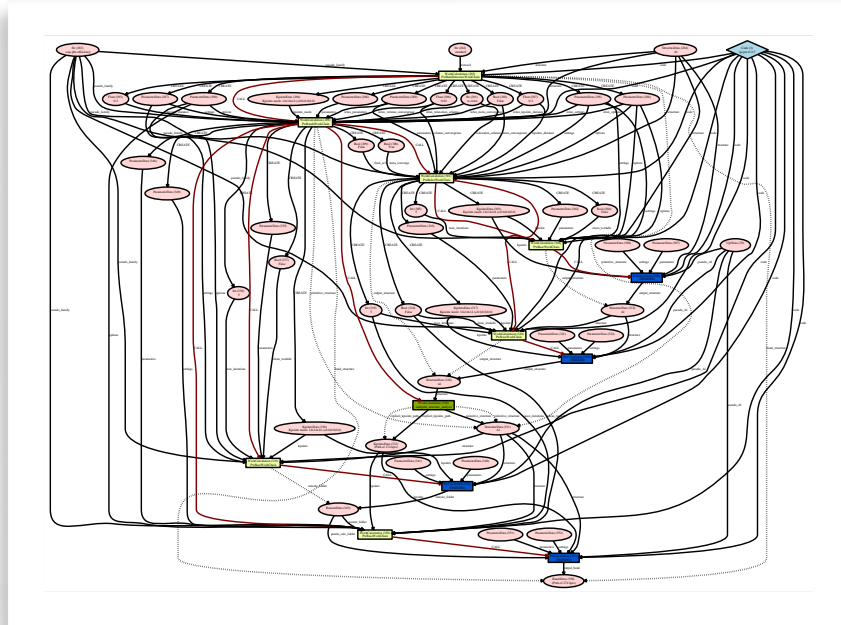
Graphical representation of actual AiiDA database

Turn-key workflows in AiiDA

- Given a material, we often need to compute advanced quantities
- These are often non-trivial and result from a complex workflow



Turn-key workflows in AiiDA



- The AiiDA provenance graph allows to know how the structure was computed and to **reproduce that single specific calculation**: *log of “what happened in the past”*
- We need also an **easy way to re-run the same calculation again** with different parameters or for a different material: **turn-key workflows**

Turn-key workflows in AiiDA

```
class BandsWorkChain(WorkChain):
    @classmethod
    def define(cls, spec):

        spec.input(
            'structure',
            valid_type=StructureData, ...)
        spec.expose_inputs(
            PwRelaxWorkChain,
            namespace='relax', ...)
        ...

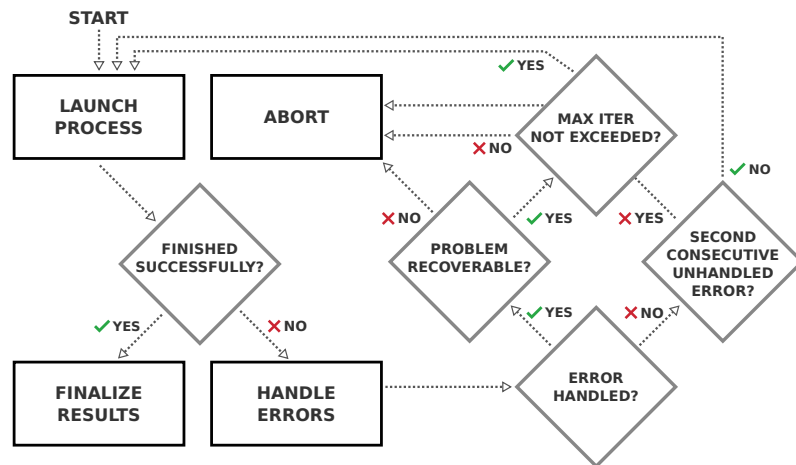
        spec.outline(
            cls.setup,
            if_(cls.should_run_relax)(
                cls.run_relax,
                cls.inspect_relax,
            ),
            if_(cls.should_run_seekpath)(
                cls.run_seekpath,
            ),
            cls.run_scf,
            cls.inspect_scf,
            ...
        )
```

Workflows:

- Encode scientists' knowledge on how to calculate properties
- "Self-documenting" inputs and outputs
- Modular
- Input validation
- Robustness: error handling

Turn-key workflows in AiiDA

Error recovery - Try to "fix" failing calculations by changing the inputs.



or...



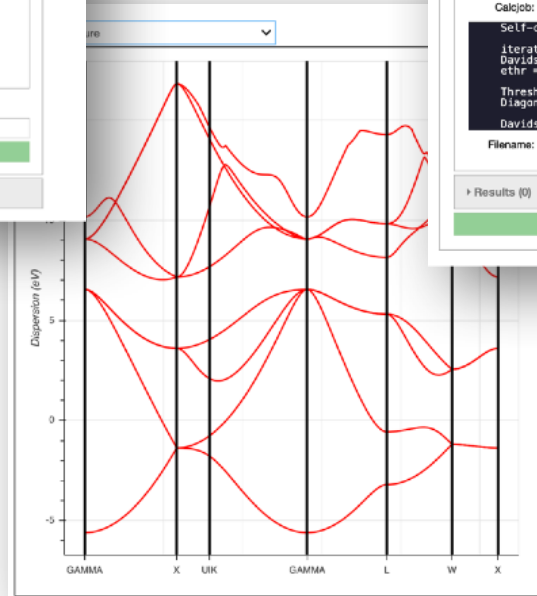
Protocols - Default computation parameters with reasonable precision.

```
In [1]: PwBandsWorkChain = WorkflowFactory('quantumespresso.pw.bands')
In [2]: builder = PwBandsWorkChain.get_builder_from_protocol(
...:     code=load_code('qe-v6.7-pw'),
...:     structure=load_node(87),
...:     protocol='fast'
...: )
In [3]: from aiida.engine import submit
In [4]: submit(builder)
Out[4]: <WorkChainNode: uuid: ... (pk: 105) (aiida.workflows:quantumespresso.pw.bands)>
```

Easy access to these simulations on the cloud

- **Easy access to these advanced HPC capabilities to everybody: AiiDA Lab**

The screenshot shows the 'Step 1: Select structure' interface. At the top, there are navigation buttons: 'Previous step', 'Reset', and 'Next step'. Below this, a section titled 'Select a structure from one of the following sources and then click "Confirm" to go to the next step.' contains tabs for 'From computer', 'COD', 'AIDA database', 'OPTIMADE', 'SMILES', and 'From Examples'. A dropdown menu under 'From Examples' shows 'Silicon'. Below the dropdown is a 3D ball-and-stick model of a silicon crystal structure. To the right of the model is a 'Selection' panel with 'Appearance' and 'Download' buttons, and a 'Selected atoms' input field. Below the model are 'Camera type' options: 'Orthographic' and 'Perspective'. At the bottom, there are fields for 'Store in AiiDA', 'Label' (containing 'Si2'), and 'Description'. A green 'Confirm' button is at the bottom right.



The screenshot shows the 'Step 2: Compute bands' interface. At the top, there are navigation buttons: 'Previous step', 'Reset', and 'Next step'. Below this, a section titled 'Specify the parameters and options for the calculation and then click on "Submit".' contains a 'Config' section. Under 'Status', there is a progress bar and a 'Calcjob' dropdown menu. The 'Calcjob' dropdown is expanded, showing a 'Self-consistent Calculation' with the following details: 'iteration # 1', 'ecut = 50.00 Ry', 'beta = 0.70', 'Davidson diagonalization with overlap', 'ethr = 1.00E-02, avg # of iterations = 3.8', 'Threshold (ethr) on eigenvalues was too large: Diagonalizing with lowered threshold', and 'Davidson diagonalization with overlap'. Below the dropdown is a 'Filename' field containing 'aiida.out' and a 'Download' button. At the bottom, there is a green 'Submit' button.

Sharing in AiiDA: codes, plugins and workflows



Calculation



Data



Parsers



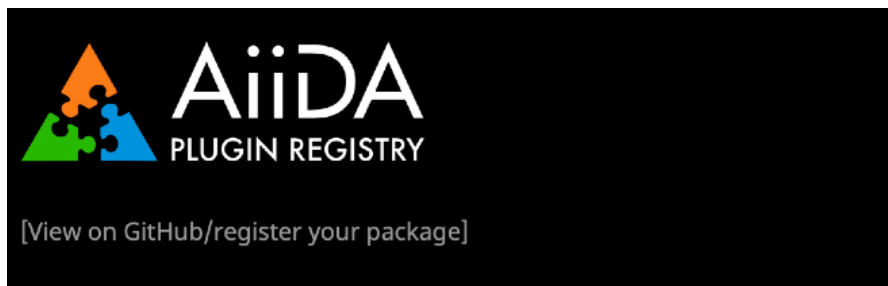
Transport
and
scheduler



Workflows



Importers &
exporters

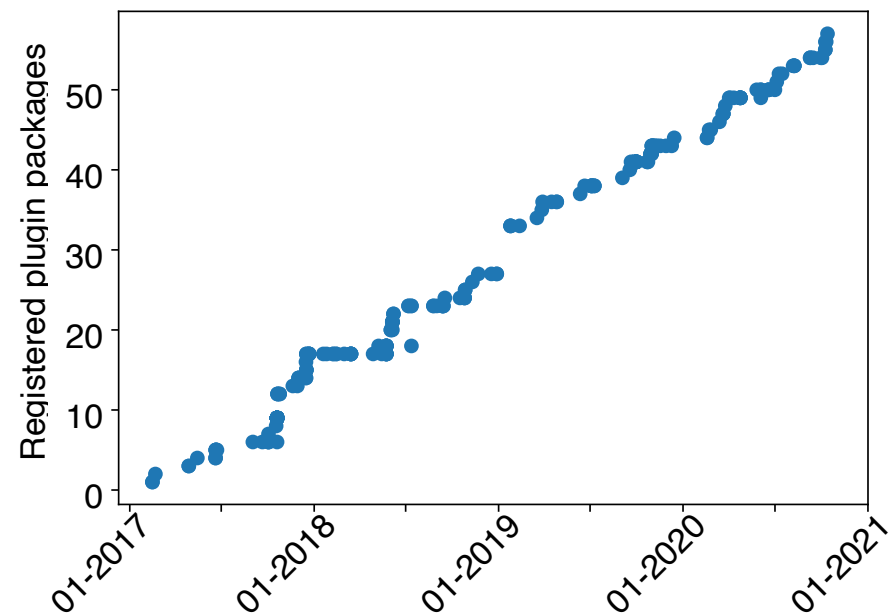


Registered plugin packages: 58

Calculations	98 plugins in 39 packages
Parsers	84 plugins in 40 packages
Data	79 plugins in 24 packages
Workflows	95 plugins in 27 packages
Console scripts	19 plugins in 14 packages
Other	95 plugins in 26 packages

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

- Plugins collected in the AiiDA plugin registry
- **Almost 100 codes currently supported, >90 workflows**
- Many are **community-contributed**



Code interoperability: common workflow interfaces

- **Long term goal:** robust, cross-validated and accessible simulations with unified interface.

Common workflows for computing materials properties using different quantum engines

Sebastiaan P. Huber,^{1,*} Emanuele Bosoni,² Marnik Bercx,¹ Jens Bröder,^{3,4} Augustin Degomme,⁵ Vladimir Dikan,² Kristjan Eimre,⁶ Espen Flage-Larsen,⁷ Alberto Garcia,² Luigi Genovese,⁵ Dominik Gresch,⁸ Conrad Johnston,⁹ Guido Petretto,¹⁰ Samuel Poncé,¹ Gian-Marco Rignanese,¹⁰ Christopher J. Sewell,¹ Vasily Tseplyaev,^{3,4} Martin Uhrin,¹ Aliaksandr V. Yakutovich,^{11,1} Austin Zadoks,¹ Pezhman Zarabadi-Poor,^{12,13} Bonan Zhu,^{14,13} Nicola Marzari,¹ and Giovanni Pizzi^{1,†}

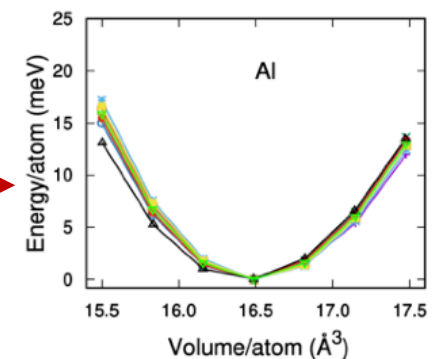
*Submitted to npj
Computational Materials*

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

```
$ aida-common-workflows launch eos siesta --structure=Al --protocol=precise
```

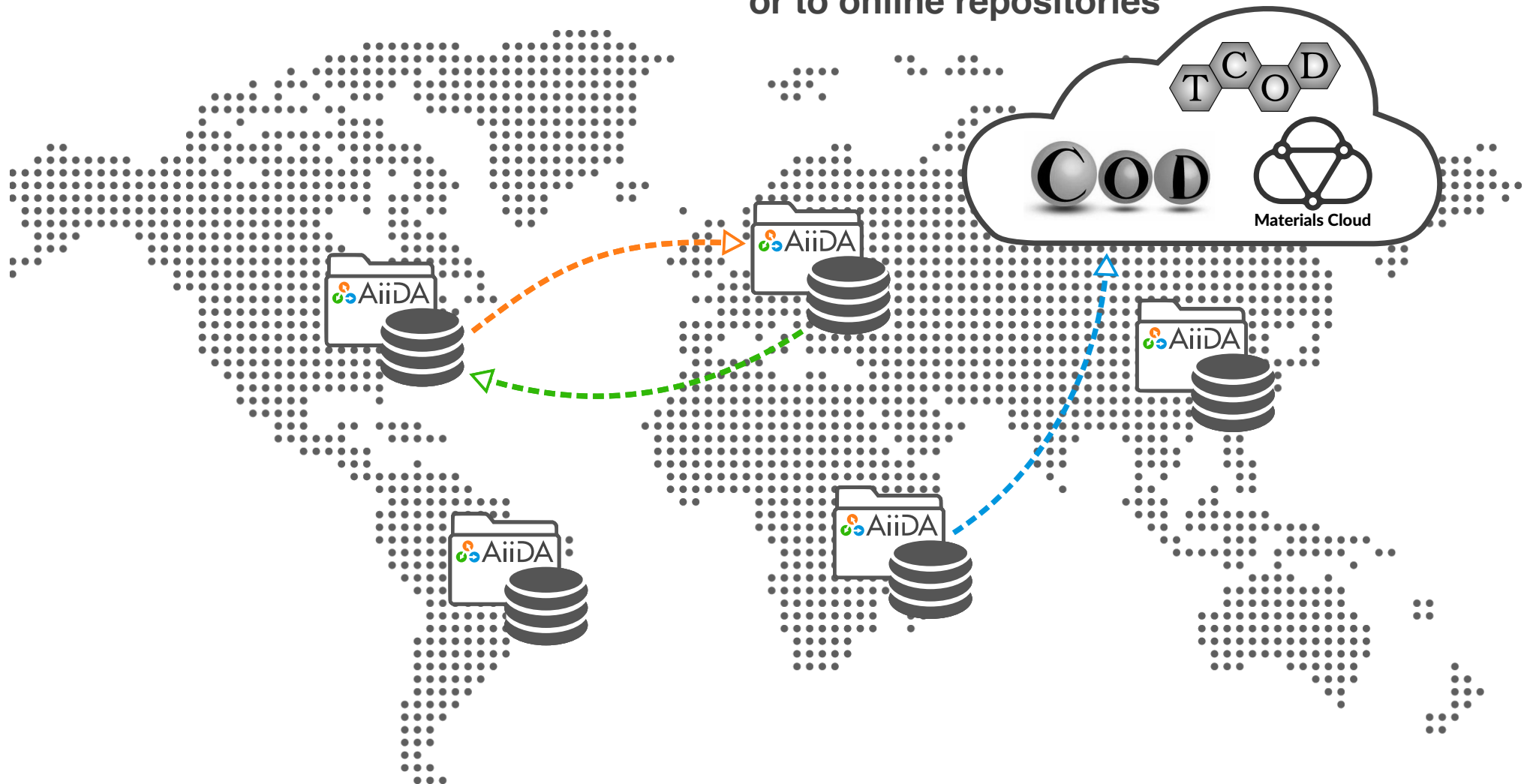
Implementations
for 11 quantum
codes

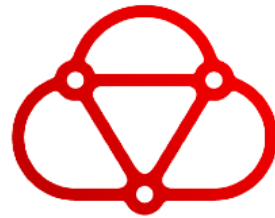
EOS only for the
9 with PBC;
relax and
dissociation
for all 11



Sharing in AiiDA: data and graphs

- *Private* AiiDA instances
- UUIDs to uniquely identify nodes
- Data can be shared to other AiiDA repositories or to online repositories





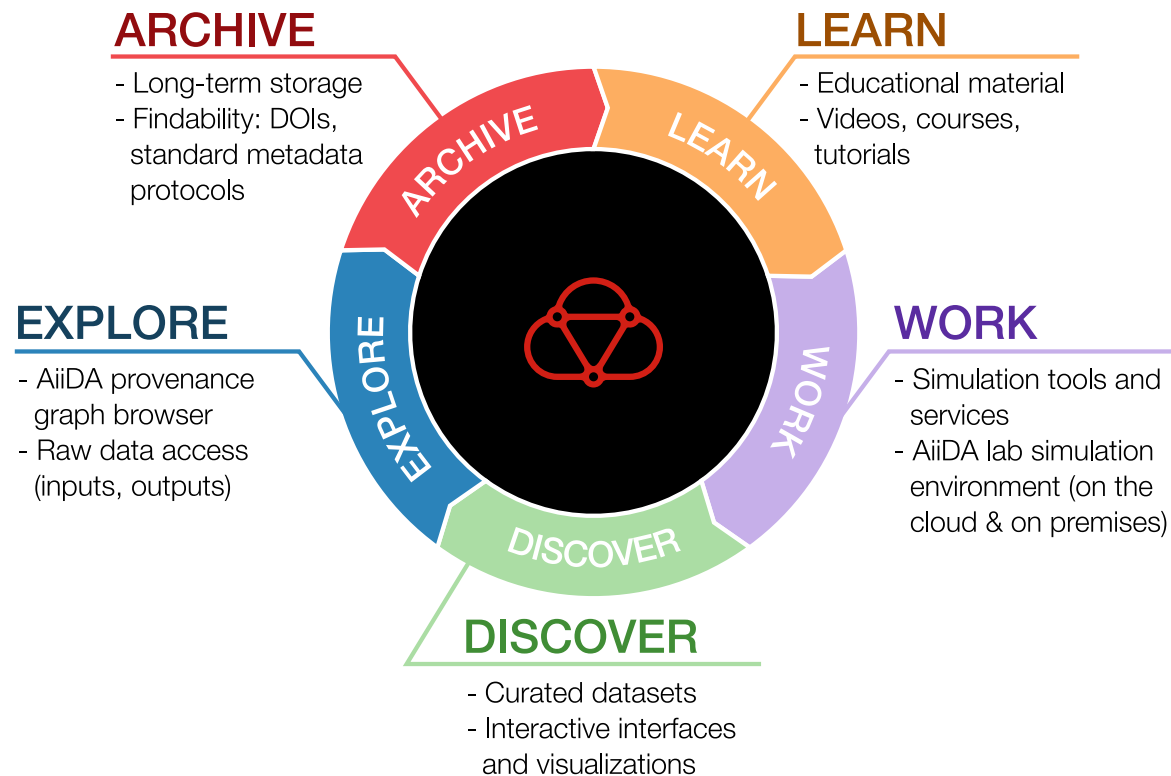
MATERIALSCLOUD

<https://www.materialscloud.org>

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

Materials Cloud

- **AiiDA** is the ‘engine’, like **Git** - used in production *since 2015*
- **Materials Cloud** is the dissemination platform (like **GitHub**) and more (cloud computing and data generation platform) - online since *Dec 2017*



Materials Cloud Learn: Educational platform

Learn with videos and slides

Add new video

Lecture recordings and tutorial videos on computational materials science topics for students and experts alike.

You can find more videos on the [Materials Cloud Youtube channel](#).

MARVEL



NATIONAL CENTRE OF COMPUTATIONAL RESEARCH

MARVEL events

Video recordings of MARVEL events (Classics in molecular



AiiDA and Materials Cloud tu
Video recordings and educat



Quantum ESPRESSO schoo
Video recordings and educat

WANNIER90

Wannier90 schools

Video recordings and educat

Quantum Simulations of Sustainable Energy Materials

Prof. Emily Carter

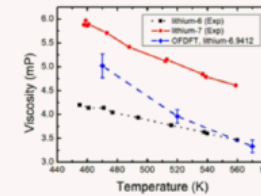
Prof. Emily A. Carter

Quantum Simulations of Sustainable Energy Materials

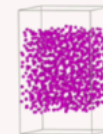
MARVEL NCCR



Viscosity and Surface Tension of Liquid Li

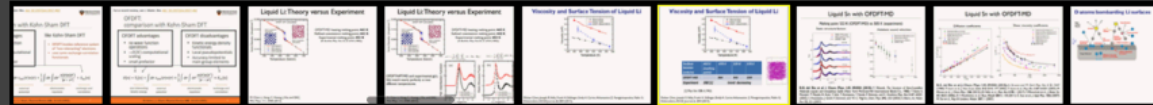


Surface tension (mN/m)	453 K (melting point)	470 K	520 K	570 K
OFDFT-MD		364	345	339
Experiment	398 [1]			trend: decreasing



[1] Phys. Rev. **128**, 6 (1962)

Mohan Chen, Joseph R. Vella, Frank H. Stillinger, Emily A. Carter, Athanasios Z. Panagiotopoulos, Pablo G. Debenedetti, AIChE Journal, **6**, 2841 (2015).



Data generation: Materials Cloud **Work**



LEARN

WORK

DISCOVER

EXPLORE

ARCHIVE

More ▾



Tools

Computational tools to work
with your data online



Quantum Mobile

Quantum simulation codes +
AiiDA in a virtual machine



AiiDA lab

Run your own simulations
using AiiDA on the cloud



AiiDA registry

The official registry of AiiDA
plugins

Quantum Mobile

- **Downloadable VM** with preinstalled **AiiDA and codes** like QE, Yambo, Fleur, Siesta, CP2K, ...
- Includes **same AiiDA lab apps environment** as on Materials Cloud
- Ideal for **education** (courses, tutorials, ...)

Open data sharing: Archive, Discover, Explore

The screenshot shows the EPFL Open Data Archive website. At the top, there is a navigation bar with the EPFL logo and menu items: LEARN, WORK, DISCOVER, EXPLORE, and ARCHIVE. Below the navigation bar is a search bar with a magnifying glass icon and a search button. To the right of the search bar are links for 'About | Submission instructions | FAQs', an 'Upload a record' button, a 'My records' button, and a user profile dropdown menu showing 'marco.borelli@epfl.ch'. Below the navigation bar, there is a section titled 'Latest records' with a grid of logos for Scientific Data, Google Dataset Search, re3data.org, EUDAT, FAIR, and FAIRsharing.org. Three record entries are listed below the logos:

Latest records

Semi-local and hybrid functional DFT data for thermalised snapshots of polymorphs of benzene, succinic acid, and glycine
DOI: [10.24438/materialscloud:vpj1](https://doi.org/10.24438/materialscloud:vpj1)
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: [10.24438/materialscloud:2x-7x](https://doi.org/10.24438/materialscloud:2x-7x)
Kevin Fossi, Veronika Jurešková, Raphael Wischert, Laurent Garol, Clemence Gominboouf, Michele Geriotti
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: [10.24438/materialscloud:zqqt](https://doi.org/10.24438/materialscloud:zqqt)
Takeshi Suzuki, Yasushi Shinohara, Yangfan Lu, Mari Watanabe, Jiali Xu, Konichi L. Ishikawa, Hideo Takegaki, Minoru Nohara, Naoyuki Katayama, Hiroshi Sawo, Masami Fujisawa, Teruto Kanai, Jiro Itatani, Takashi Mizokawa, Shik Shin, Kozo Okuzaki

Recommended data repository
by Nature's journal **Scientific Data**

Indexed by **Google Dataset Search**
and by EUDAT/EOSC's **B2FIND**

Registered on [FAIRsharing.org](https://www.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)

Open data sharing: Archive, Discover, Explore



Export
Dublin Core JSON

materialscloud:2017.0008/v3

DOIs assigned

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

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

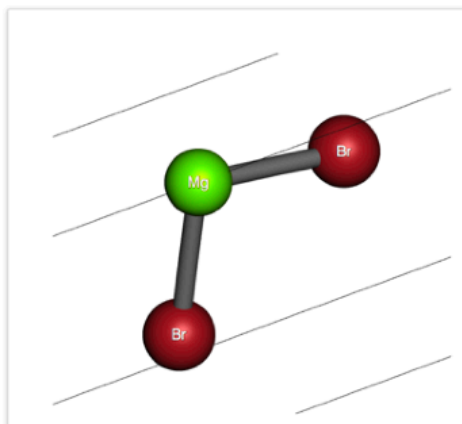
Direct links to Discover & Explore

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: Cdl2
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
 Δ_{rVV10} [%]: 18.3

Band structure



EXPLORE

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

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

Today's tutorial: Step 1 - Log in

<https://qe-school.aiida-tutorials.net/>

Ignore this erroneous message

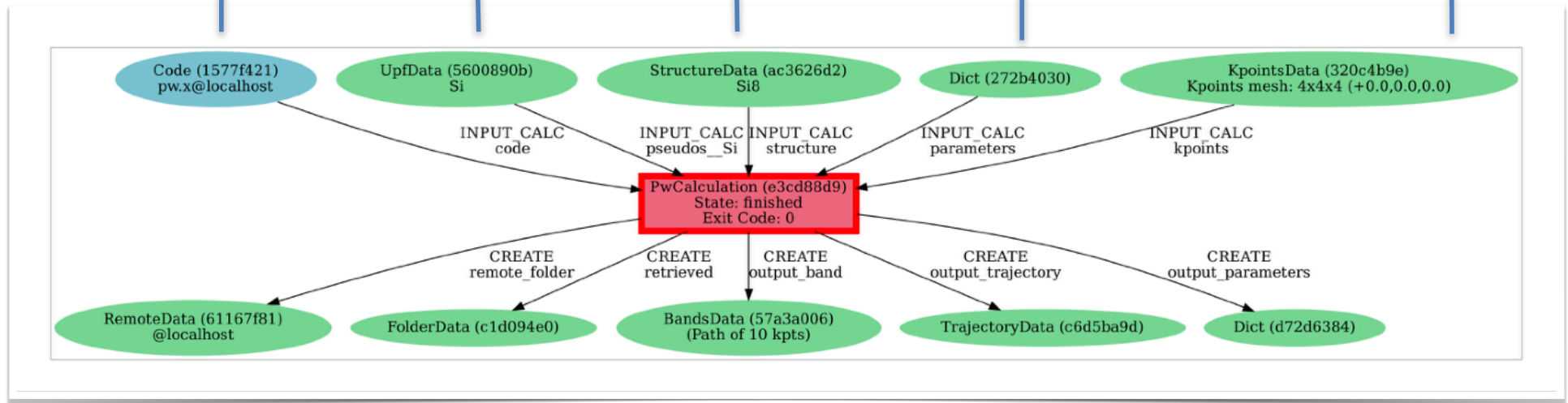
The image illustrates the initial steps of logging into the JupyterHub interface. It shows a 'Sign in' form with an 'Invalid username or password' error message. A blue arrow points from this error message to the 'Terminal' and 'Codes and computers' sections of the interface. The 'Terminal' section shows the 'Quantum ESPRESSO' application, and the 'Codes and computers' section shows the 'Setup computer' and 'Setup code' options. A terminal window at the bottom shows the output of the 'verdi status' command.

```
(base) aiida@jupyter-mbercx:~$ verdi status
✓ config dir: /home/aiida/.aiida
✓ profile: On profile default
✓ repository: /home/aiida/.aiida/repository/default
✓ postgres: Connected as aiida_qs_aiida_477d3dfc78a2042156110cb00ae3618f@localhost:5432
✓ rabbitmq: Connected as amqp://guest:guest@127.0.0.1:5672?heartbeat=600
✓ daemon: Daemon is running as PID 970 since 2021-05-27 06:56:18
(base) aiida@jupyter-mbercx:~$
```

Today's tutorial: Step 2 - Calculations

We'll start by running a simple `pw.x` calculation through AiiDA and learn:

- *Importing a structure*
- *Installing pseudos*
- *Setting up a code*
- *Specifying the k-point mesh*
- *Setting up input parameters*



- *Generate a provenance graph for the `pw.x` calculation*
- *Analyse the outputs*

Today's tutorial: Step 3 - Workflows

Next we'll run the `PwBandsWorkChain` to calculate the band structure.

Use the protocol:

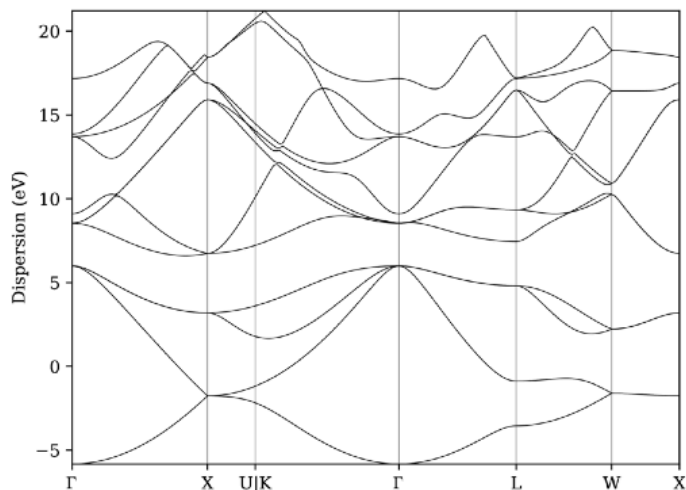
```
In [1]: PwBandsWorkChain = WorkflowFactory('quantumespresso.pw.bands')

In [2]: builder = PwBandsWorkChain.get_builder_from_protocol(
...:     code=load_code('qe-v6.7-pw'),
...:     structure=load_node(87),
...:     protocol='fast'
...: )

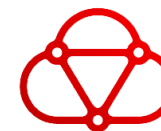
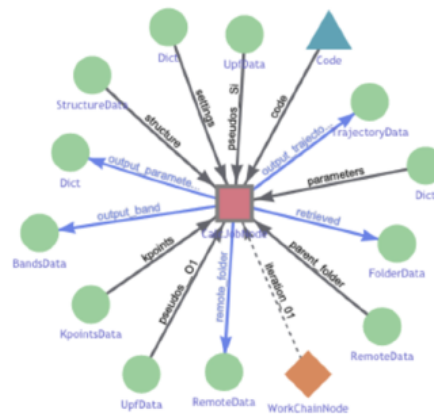
In [3]: from aiida.engine import submit

In [4]: submit(builder)
Out[4]: <WorkChainNode: uuid: ... (pk: 105) (aiida.workflows:quantumespresso.pw.bands)>
```

Get the band structure:



Explore the provenance:



MATERIALSCLOUD

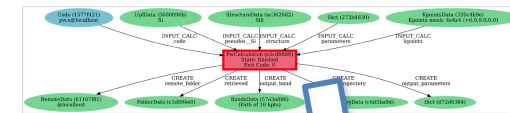
Today's tutorial: Step 4 - Managing data

Finally we'll learn how to manage and query our data!

- *Importing data*
- *Organising your data with groups*

```
$ verdi group list --count
Info: to show groups of all types, use the '-a/--all' option.
```

PK	Label	Type string	User	Node count
5	tutorial_pbesol	core	aiida@localhost	57
6	tutorial_lda	core	aiida@localhost	57
7	tutorial_pbe	core	aiida@localhost	57

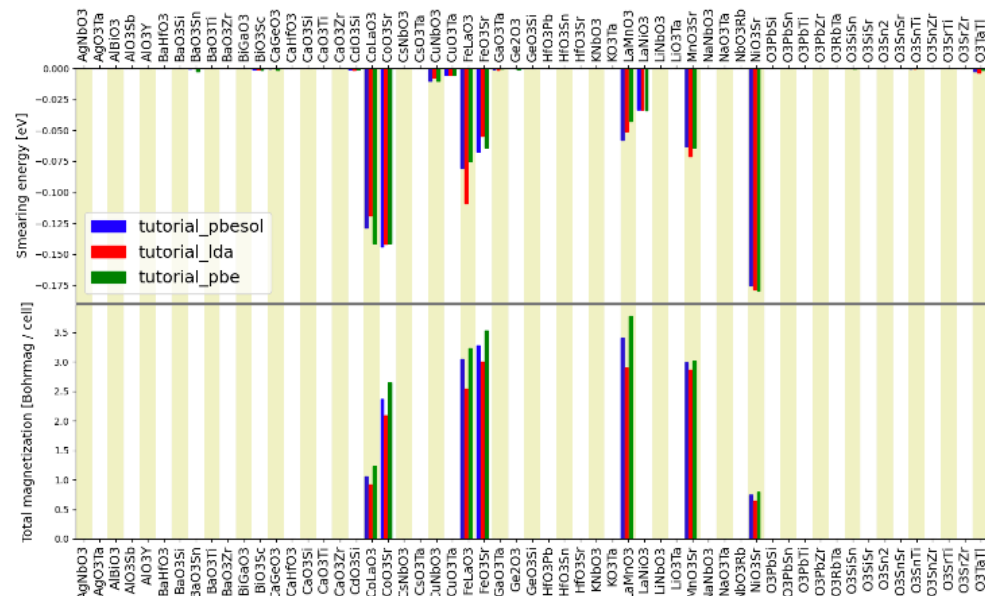


- *Using the Querybuilder*

```
In [1]: qb = QueryBuilder()
```

```
In [2]: qb.append(
...:     Group,
...:     filters={'label': 'tutorial_pbesol'},
...:     tag='group'
...: )
```

```
In [3]: ...
```



AiiDA and Materials Cloud teams

The Materials Cloud And AiiDA teams



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Discovery of new materials via simulations and dissemination of curated data

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Swissuniversities P-5 “Materials Cloud”

Scaling the web platform, extending to more disciplines

Moreover:



BIG MAP



