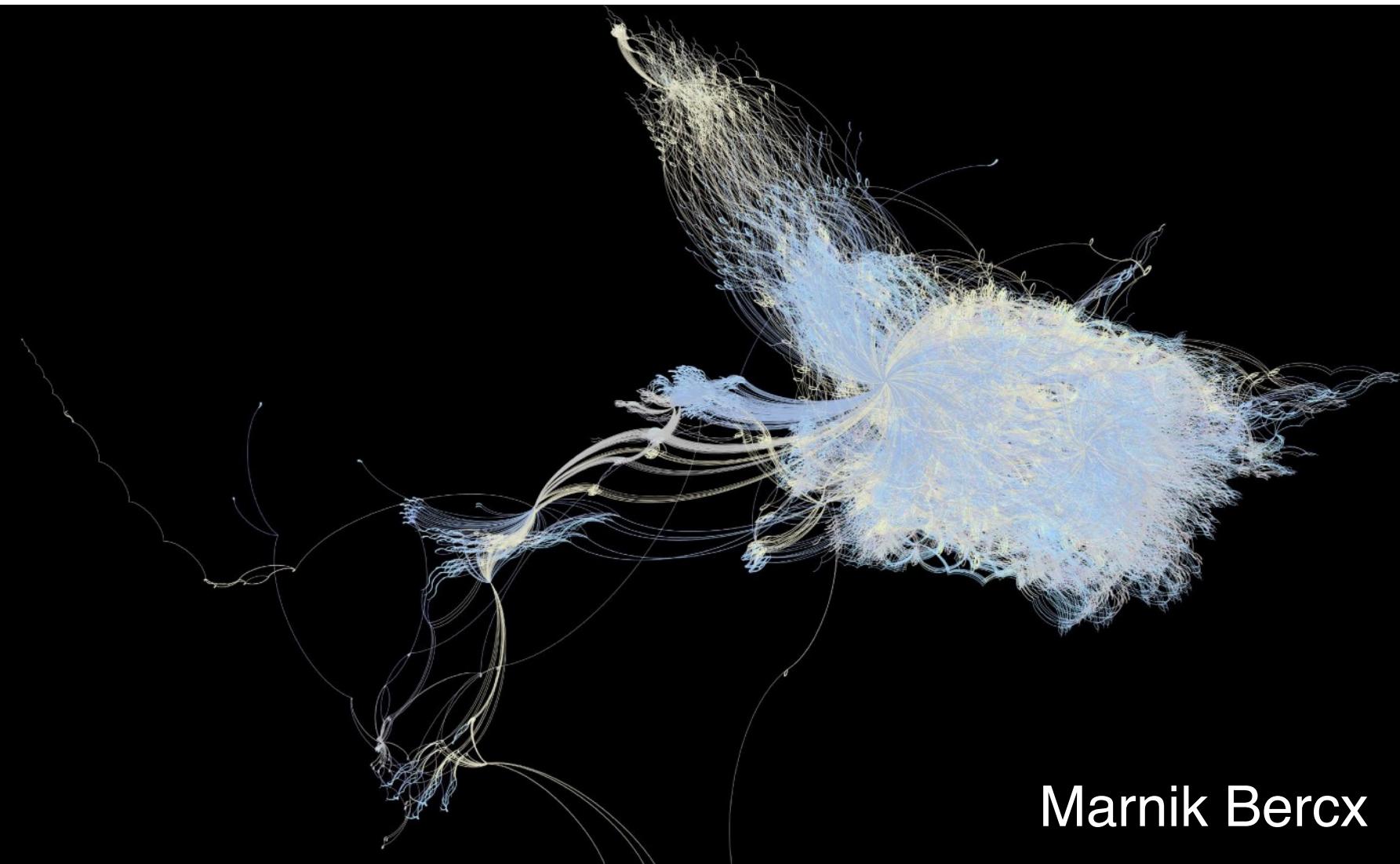


**MaX School on Advanced Materials  
and Molecular Modelling with  
Quantum ESPRESSO**



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>



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)

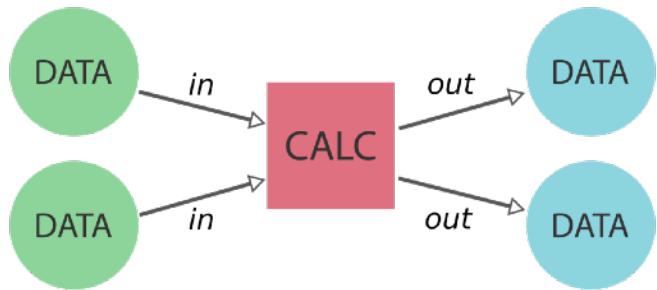
S.P. Huber et al., Scientific Data 7, 300 (2020)

# 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**

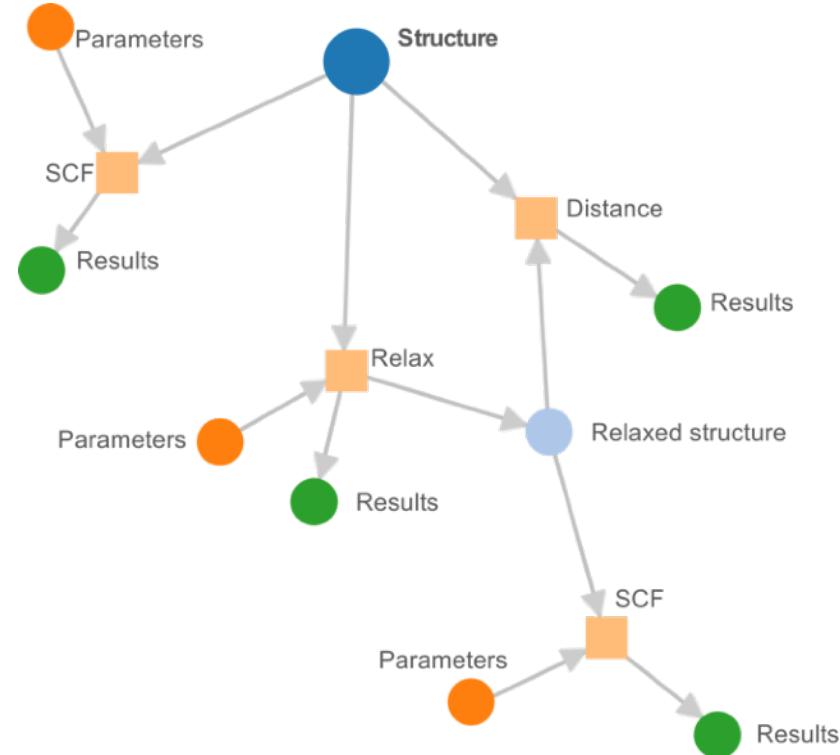


# Data provenance

---

## 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

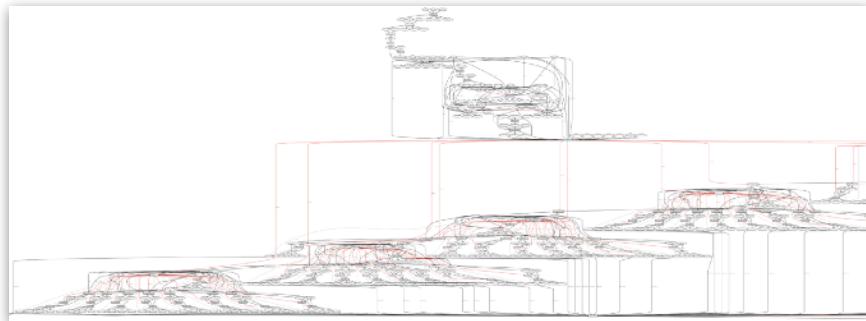
---

## Simple recipe

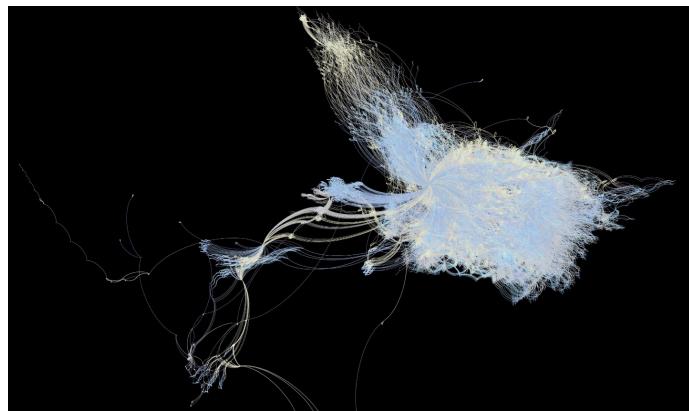
- Store data transformations or '**calculations**'
- Store its **inputs** and their metadata
- Store its **outputs** and their metadata
- Most **crucially** store the **inter-connections**

## Graph requirements

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



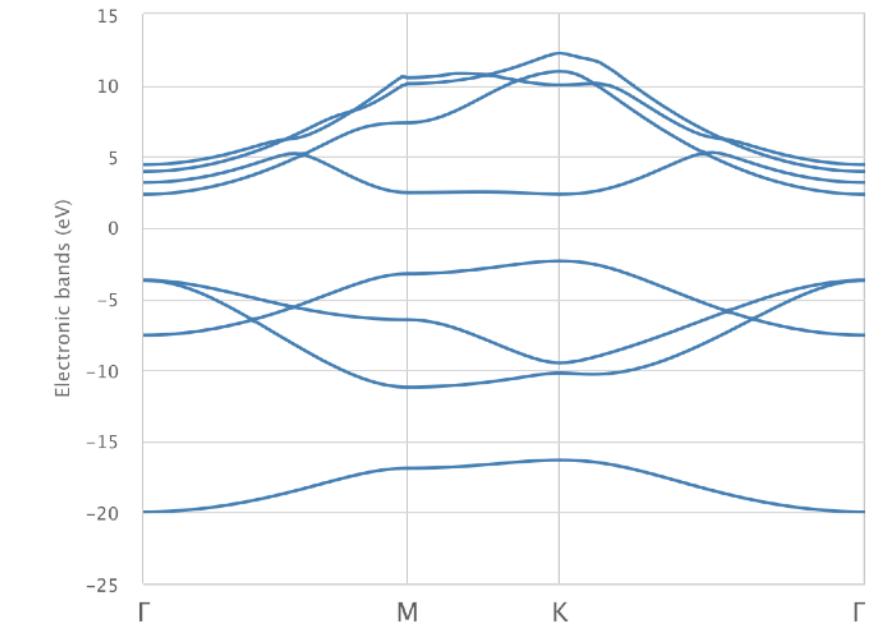
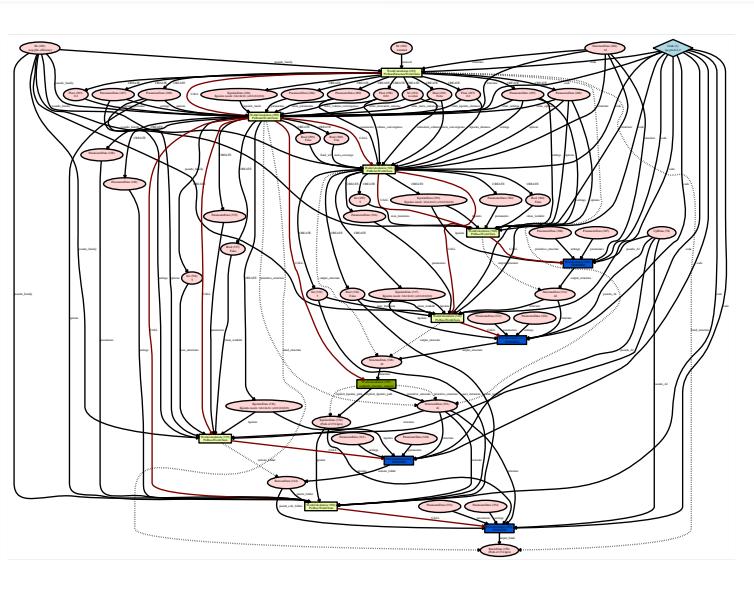
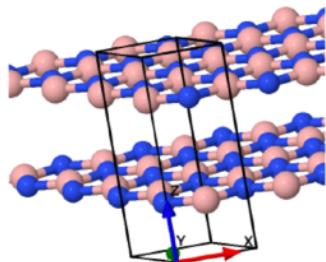
Molecular dynamics study of Lithium in a solid electrolyte.



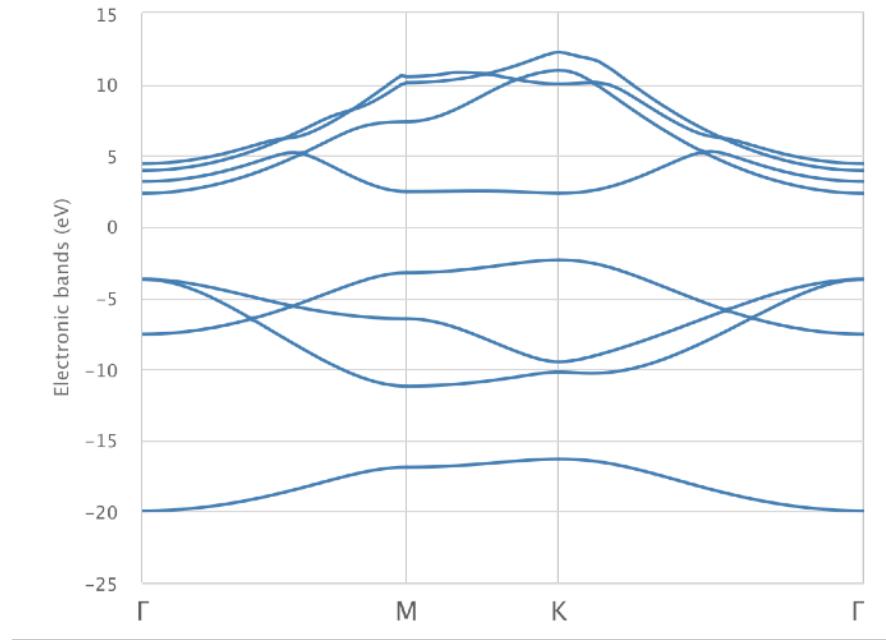
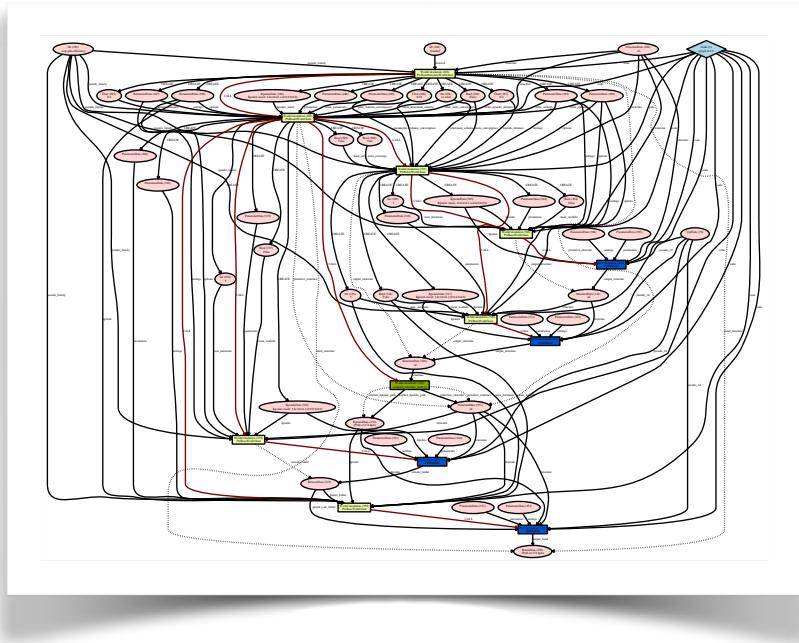
Graphical representation of actual AiiDA database

# 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

---

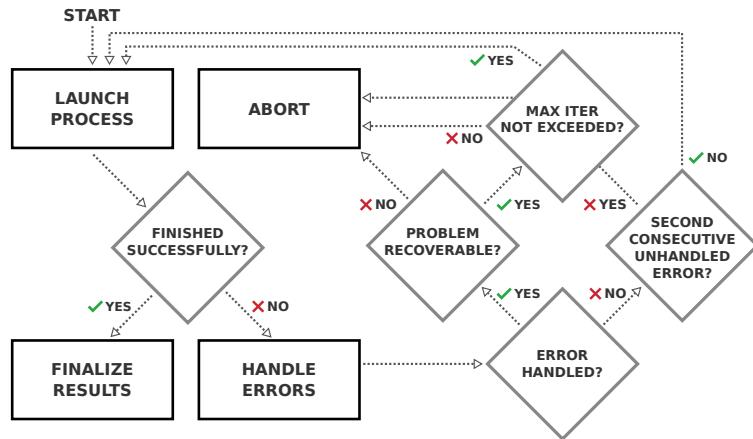
```
class BandsWorkChain(WorkChain):
    @classmethod
    def define(cls, spec):
        spec.input(
            'structure',
            valid_type=StructureData, ...)
        spec.expose_inputs(
            PwRelaxWorkChain,
            namespace='relax', ...)
        ...
        spec.outline(
            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:

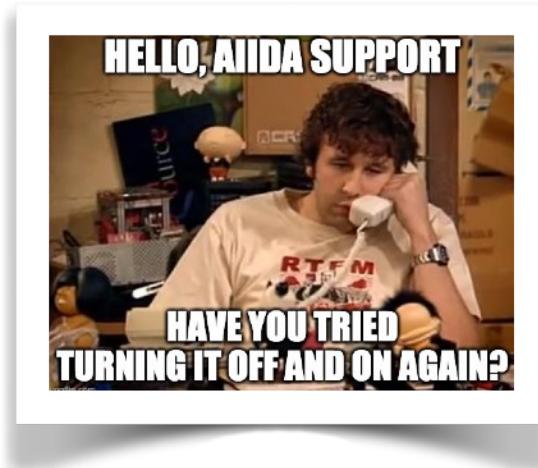
- Encode scientists' knowledge on how to calculate properties
- "Self-documenting" inputs and outputs
- Modular
- Input validation
- Robustness: error handling

# 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 image shows the AiiDA lab interface, which consists of two main windows side-by-side.

**Step 1: Select structure**

This window allows users to select a crystal structure. It includes:

- A search bar at the top with tabs for "From computer", "COD", "AIXA database", "OPTIMADE", "SMILES", and "From Examples".
- A dropdown menu showing "Silicon".
- A 3D ball-and-stick model of a silicon crystal structure.
- Selection tools: "Selection", "Appearance", "Download".
- Buttons for "Copy to clipboard", "Clear selection", and "Apply selection".
- Camera type options: "Orthographic" (selected) and "Perspective".
- Labels: "Selected atoms:" and "Selected: Si2".
- A "Confirm" button.

**Step 2: Compute bands**

This window shows the results of a calculation. It includes:

- A status bar at the top with "Previous step", "Reset", and "Next step".
- A header for "Step 2: Compute bands".
- A "Config" section.
- A "Status" section showing "Calculation sta... Waiting".
- A "Process" log window displaying the following text:

```
Process: uuid: bc2fdac1-2871-4482-b048-e4dfff1c02e53 (plc: 203) (aiida.workflows:quantumespresso.pw.bands)
Calcjob: <latest>
Self-consistent Calculation
iteration # 1  scut= 50.00 Ry  betam=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
Davidson diagonalization with overlap
```
- A "Results" section with a "Submit" button.
- A dispersion plot showing energy (eV) on the y-axis (from -5 to 5) versus momentum path on the x-axis (GAMMA-X-U-K-GAMMA-L-W-X). The plot shows multiple red curves representing energy bands.

# Sharing in AiiDA: codes, plugins and workflows



Calculation



Data



Parsers



Transport  
and  
scheduler



Workflows



Importers &  
exporters

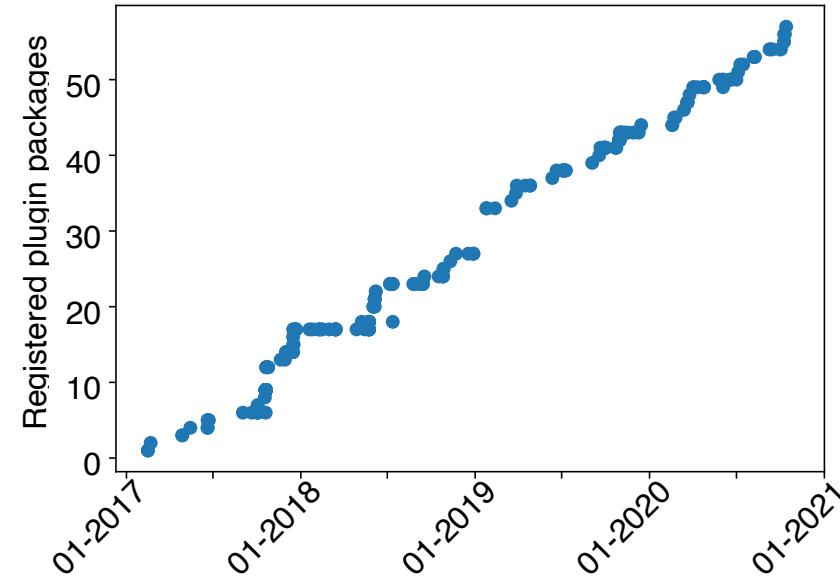


[View on GitHub/register your package]

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/>



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

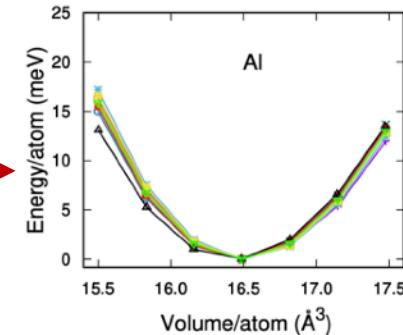
Submitted to *npj Computational Materials*

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

\$ aiida-common-workflows launch eos **siesta** --structure=Al --protocol=precise

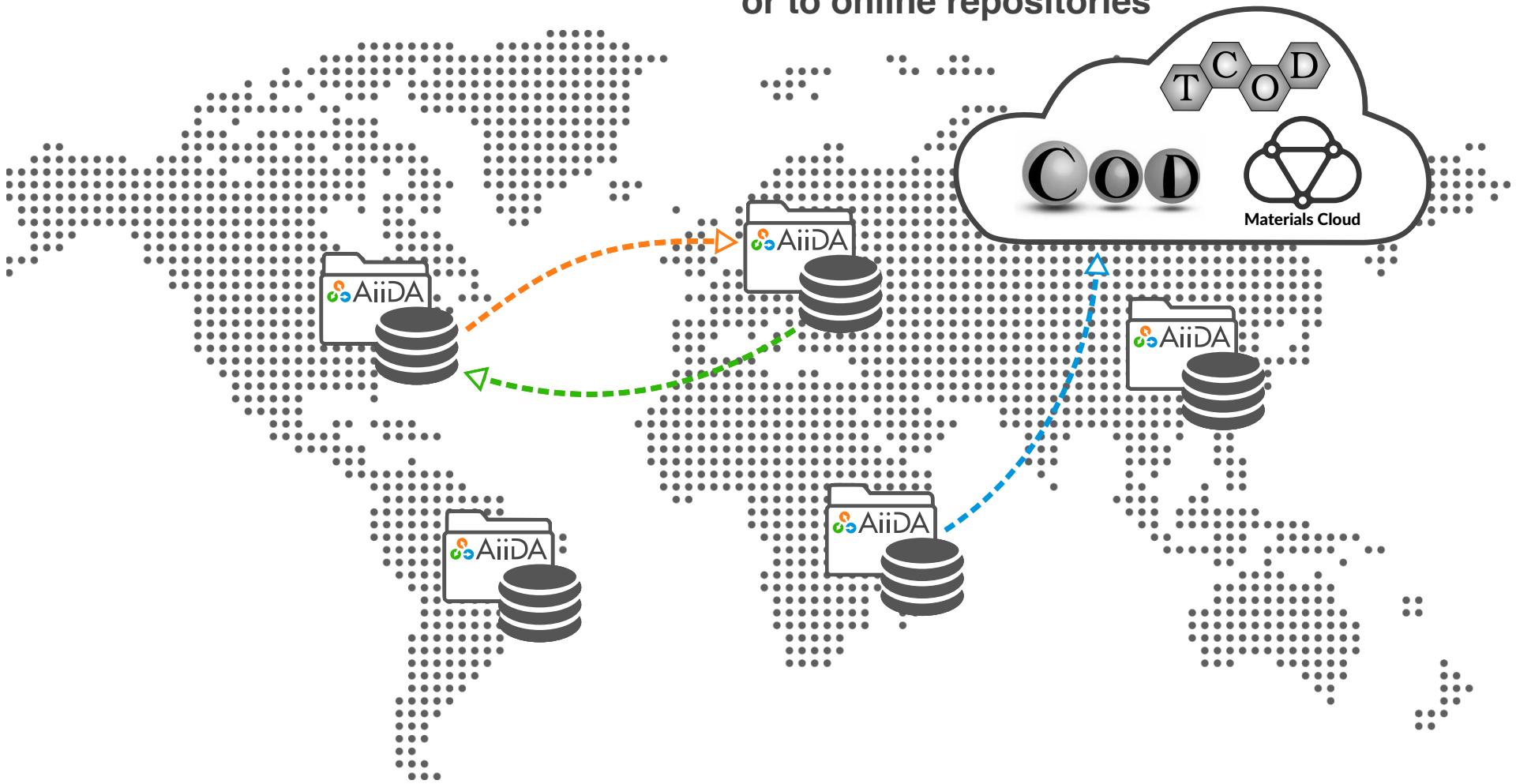
Implementations  
for 11 quantum  
codes

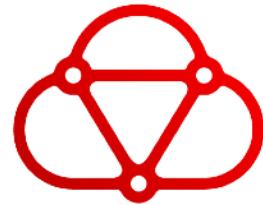
EOS only for the  
9 with PBC;  
relax and  
dissociation  
for all 11



# 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**





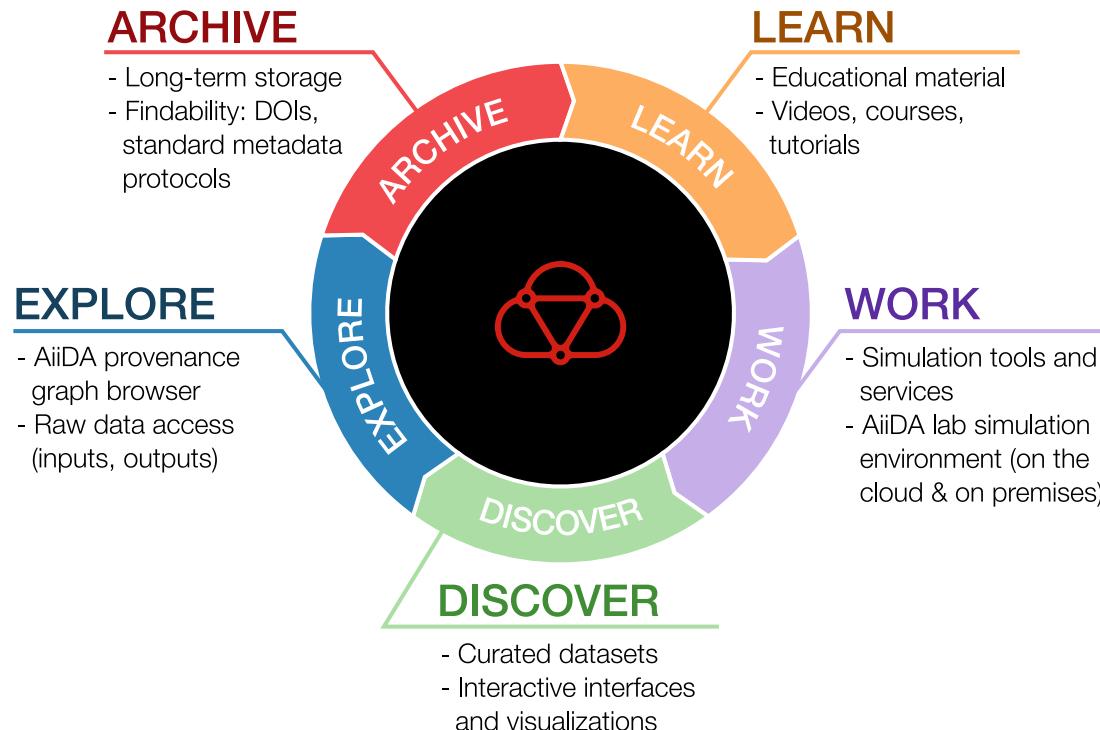
**MATERIALS**CLOUD

<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 COMPUTATION IN RESEARCH

**MARVEL events**

Video recordings of MARVEL events (Classics in molecular simulation)

**AiiDA**

**AiiDA and Materials Cloud tutorials**

Video recordings and educational material

**Quantum ESPRESSO schools**

Video recordings and educational material

**WANNIER90**

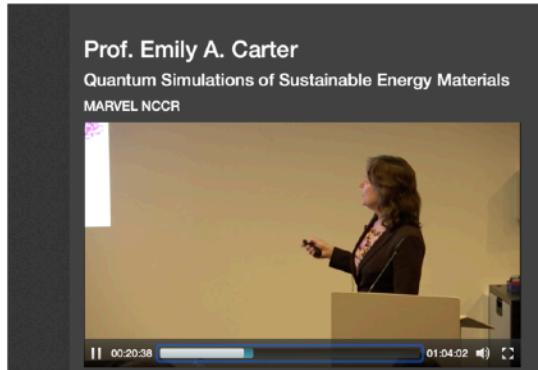
**Wannier90 schools**

Video recordings and educational material

**Quantum Simulations of Sustainable Energy Materials**  
Prof. Emily Carter

Prof. Emily A. Carter  
Quantum Simulations of Sustainable Energy Materials  
MARVEL NCCR

00:20:38 01:04:02



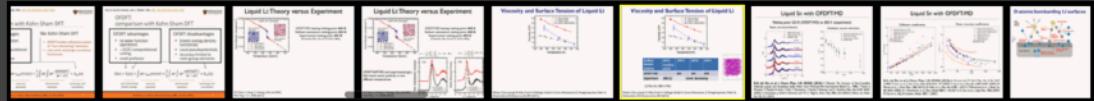
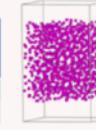
**Viscosity and Surface Tension of Liquid Li**

Viscosity (mPa) vs Temperature (K)

Temperature (K)	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, Athanassios Z. Panagiotopoulos, Pablo G. Debenedetti, AIChE Journal, **6**, 2841 (2015).



# Data generation: Materials Cloud Work

LEARN WORK DISCOVER EXPLORE ARCHIVE More ▾

The screenshot shows the Materials Cloud Work interface with a navigation bar at the top. Below the navigation bar are four service cards:

- 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 MaterialsCloud website interface. At the top, there are tabs for LEARN, WORK, DISCOVER, EXPLORE, and ARCHIVE. Below the tabs is a search bar with a magnifying glass icon and a dropdown menu for 'My records' and an email address 'marco.borelli@epfl.ch'. A 'More' button is also present. The main content area is titled 'Latest records' and displays two entries:

**Semi-local and hybrid functional DFT data for thermalised snapshots of polymorphs of benzene, succinic acid, and glycine**  
DOI: 10.24435/materialscloud:2x-7k  
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 CH<sub>3</sub>SO<sub>3</sub>H and H<sub>2</sub>O<sub>2</sub> in phenol**  
DOI: 10.24435/materialscloud:2x-7k  
Kevin Rossi, Veronika Juraskova, Raphael Wissert, Laurent Garot, Clemence Cominbeauf, Michele Coriolet  
Set of inputs to perform the calculations reported in the paper. The -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 PBEC 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 H<sub>2</sub>O<sub>2</sub> and CH<sub>3</sub>SO<sub>3</sub>H 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:2x-7t  
Takeshi Suzuki, Yasushi Shirohara, Yangfan Lu, Mari Watanabe, Jadi Xu, Kenichi L. Ishikawa, Hidetaka Takegi, Minoru Nohara, Naoyuki Katsuyama, Hiroshi Sawa, Masami Fujisawa, Teruo Kanai, Jiro Itaya, Takashi Mizokawa, Shik Shin, Kozo 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)

# Open data sharing: Archive, Discover, Explore

DOIs  
assigned

materialscloud:2017.0008/v3



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

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

<sup>1</sup> 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

<sup>2</sup> Vilnius University Institute of Biotechnology, Saulėtekio al. 7, LT-10257 Vilnius, Lithuania

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

DOI: [10.24435/materialscloud:2017.0008/v3](https://doi.org/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](https://doi.org/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 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 AlIDa.

Direct links  
to Discover &  
Explore



### 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
<a href="#">2D_materials.tar.gz</a> MD5	113.0 MiB

### Description

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

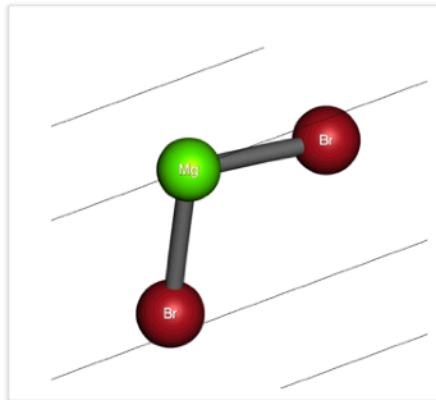
Export  
Dublin Core JSON

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

# Open data sharing: Archive, Discover, Explore

DISCOVER

Compound: MgBr<sub>2</sub>



## Info and properties

[See definitions...](#)

Formula: MgBr<sub>2</sub>

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 [meV/ $\text{\AA}^2$ ]:

(From parent COD 9009107)

rVV10 Binding energy [meV/ $\text{\AA}^2$ ]: 15

(From parent COD 9009107)

## Delta in interlayer distance (vdW vs revPBE):

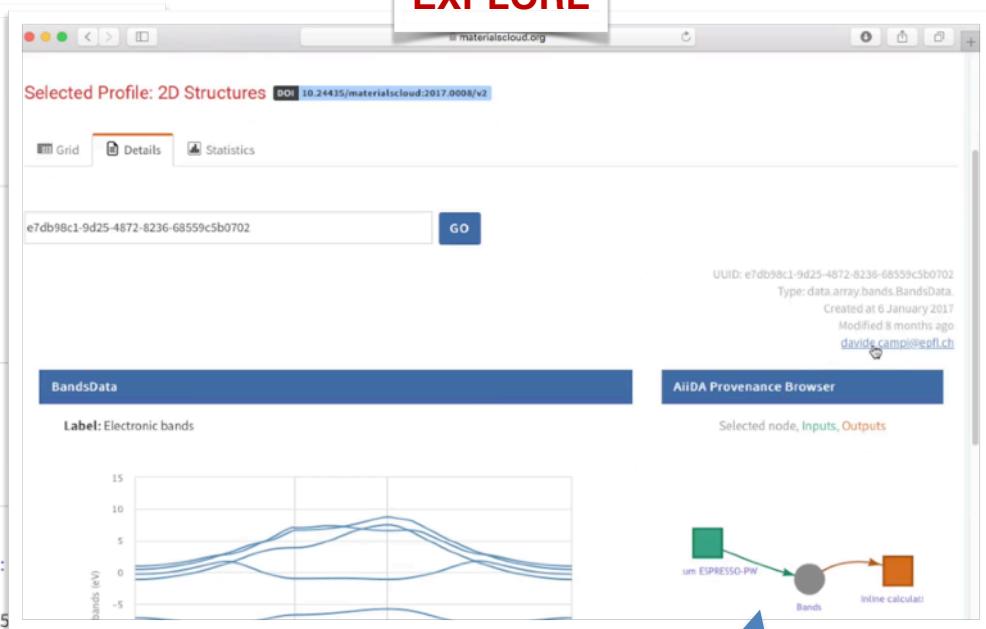
$\Delta_{\text{DF2}} [\%]$ : 17.1  (From parent COD 9009107)

$\Delta_{\text{rVV10}} [\%]$ : 18.3  (From parent COD 9009107)

Band structure

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

EXPLORE



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

# Today's tutorial: Step 1 - Log in

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

Ignore this erroneous message

The image displays three stacked panels. The top panel shows a 'Sign in' screen with an 'Invalid username or password' error message. A blue arrow points from this screen to the middle panel, which is a JupyterHub interface. The middle panel features a 'File Manager' section with a 'Quantum ESPRESSO' folder containing several files. It also includes sections for 'Codes and computers', 'Processes', and navigation links like 'Manage App' and 'URL'. The bottom panel shows a terminal window with the command 'verdi status' executed, displaying system status information.

Sign in

Invalid username or password

Username:

Password:

Sign In

jupyterhub

Files Running Clusters

Select items to perform actions on them.

Name Last Modified File size

13 uur geleden  
een paar seconden geleden  
een paar seconden geleden  
een paar seconden geleden 0 B

Logout Control Panel

File Manager Terminal Tasks App Store Help

Quantum ESPRESSO

Update available

Manage App URL

Codes and computers.

- Setup computer
- Setup code
- Dealing with codes and computers

Processes.

- Process list
- Follow a process

Manage App URL

Logout Control Panel

(base) aiida@jupyter-mbercx:~\$ verdi status

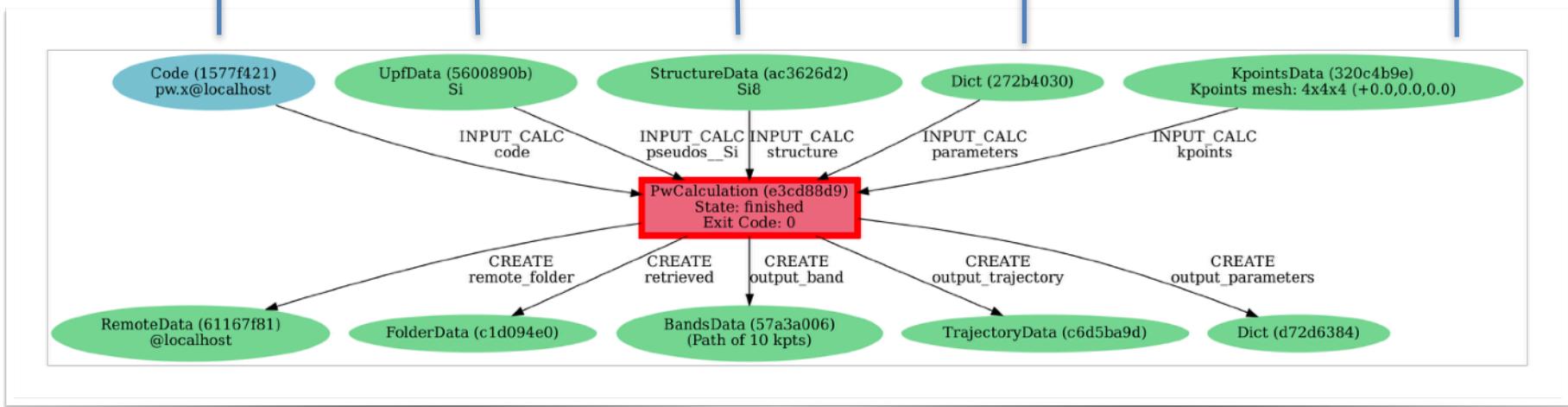
```
✓ config dir: /home/aiida/.aiida
✓ profile: On profile default
✓ repository: /home/aiida/.aiida/repository/default
✓ postgres: Connected as aiida_gs_aiida_477d3dfc78a2042156110cb00ae3618f@localhost:5432
✓ rabbitmq: Connected as amqp://guest@guest@127.0.0.1:5672?heartbeat=600
✓ daemon: Daemon is running 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:*

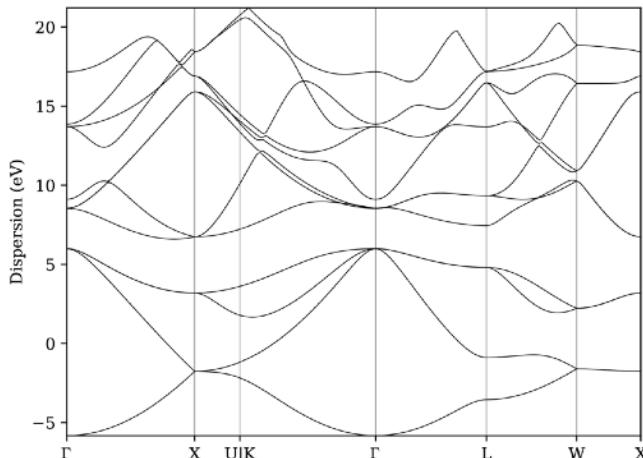
```
In [1]: PwBandsWorkChain = WorkflowFactory('quantumespresso.pw.bands')

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

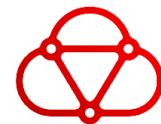
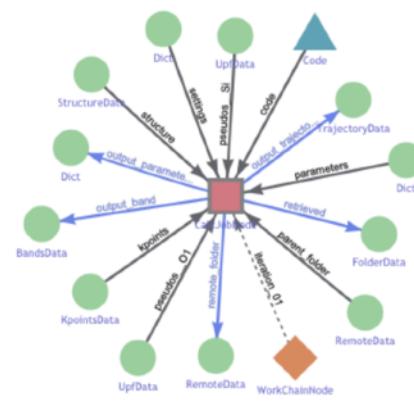
In [3]: from aiida.engine import submit

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

*Get the band structure:*



*Explore the provenance:*



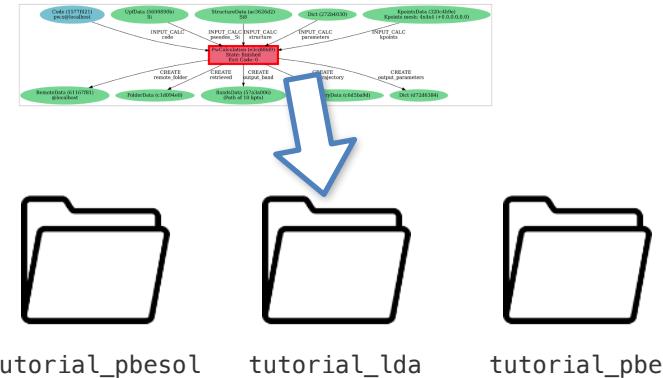
MATERIALSCLOUD

# 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_pbessol core aiida@localhost      57
      6 tutorial_lda     core aiida@localhost      57
      7 tutorial_pbe     core aiida@localhost      57
```

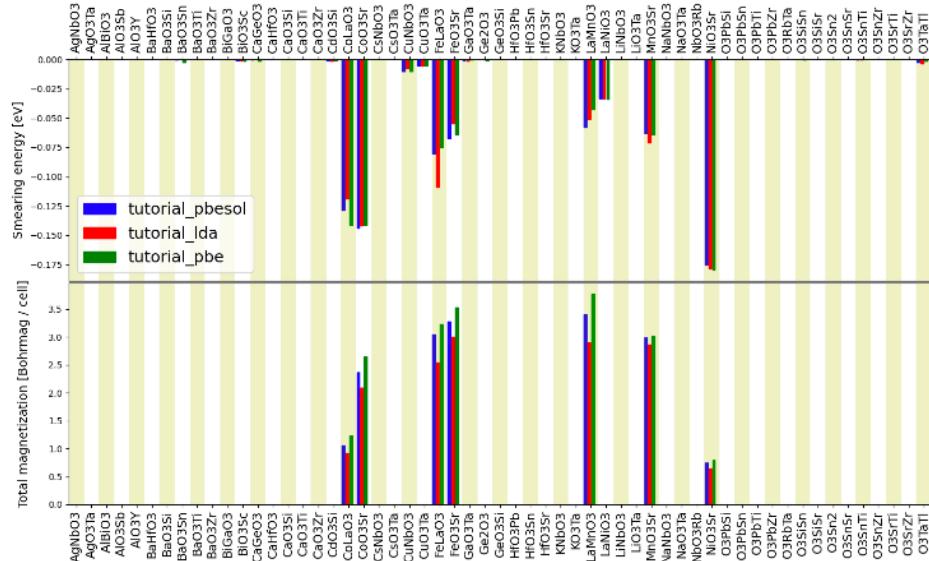


- *Using the Querybuilder*

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

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

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



# AiiDA and Materials Cloud teams

## The Materials Cloud And AiiDA teams



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

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swissuniversities

Moreover:



## H2020 Centre of Excellence “MaX”

Scaling towards exascale machines and high-throughput efficiency

## SNSF NCCR “MARVEL”

Discovery of new materials via simulations and dissemination of curated data

## Swissuniversities P-5 “Materials Cloud”

Scaling the web platform, extending to more disciplines



BIG MAP



