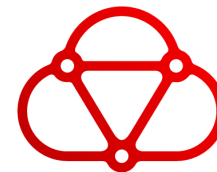


Open Science Platform: AiiDA and Materials Cloud

Giovanni Pizzi

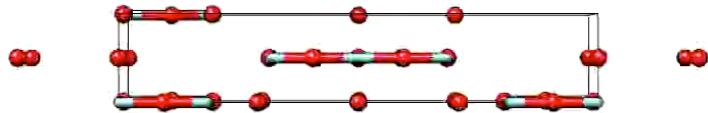
giovanni.pizzi@epfl.ch

Theory and Simulation of Materials, EPFL Lausanne



MATERIALSCLOUD

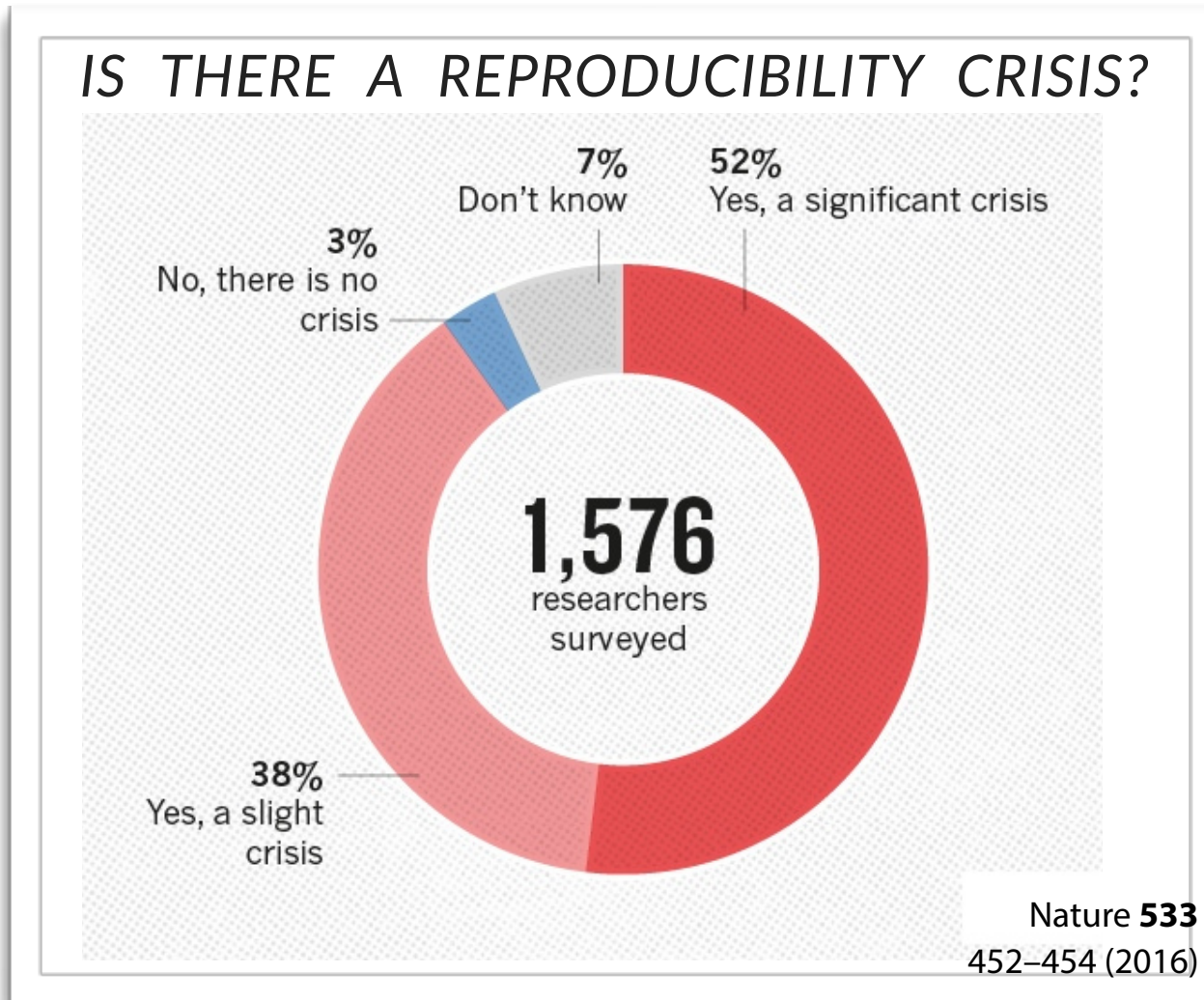
Leverage supercomputers to compute and predict materials' properties



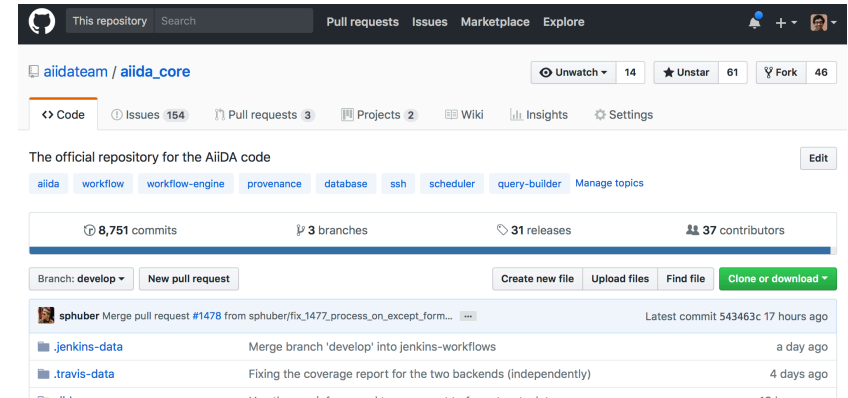
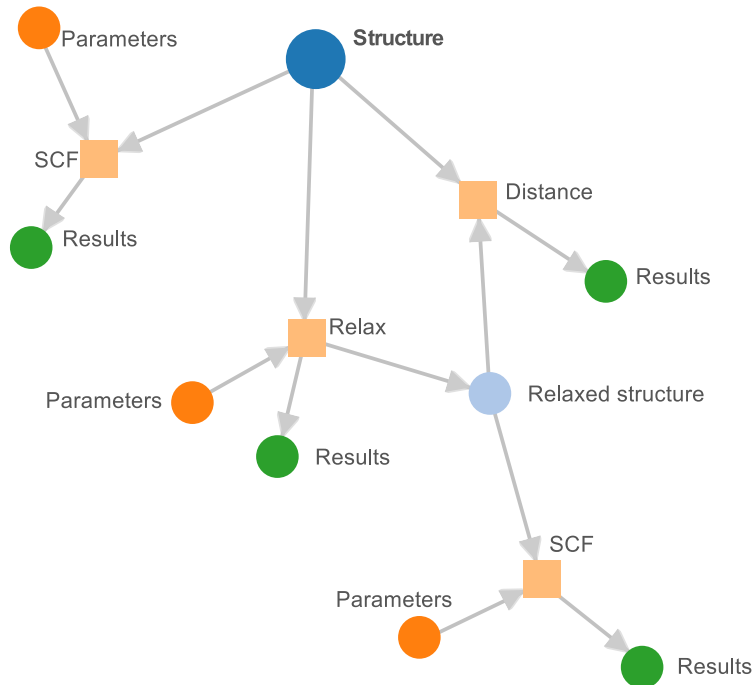
Aim: Compute properties for all of them
(and even new, invented ones)
and **discover novel functional materials**



How to manage simulations and their provenance?



Data provenance: Directed Acyclic Graphs



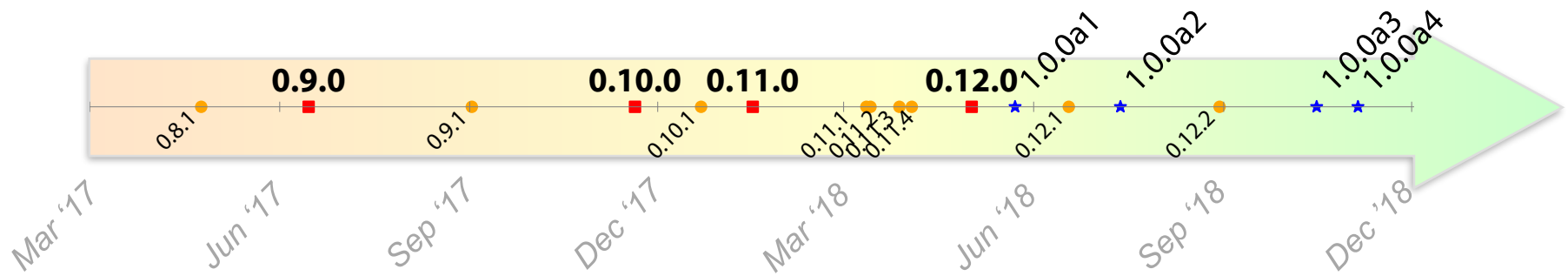
MIT license (open source)

Developed since 2013
Used in production from many
scientific research projects

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

<http://www.aiida.net>

The workflow and automation engine: AiiDA



- **AiiDA has been used in production mode for the past 3 years**
- Many development efforts ready to go in 1.0.0 (four alpha releases already out, **with 1300+ commits** w.r.t. stable 0.12.x)

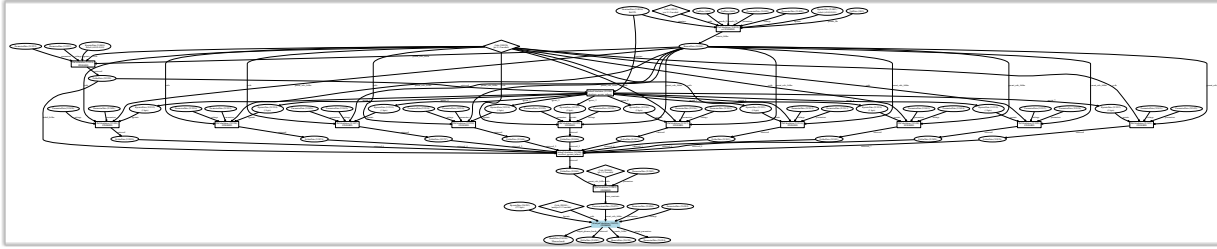
Default branch

master Updated 13 days ago by sphuber ✓ Default Change default branch

Your branches

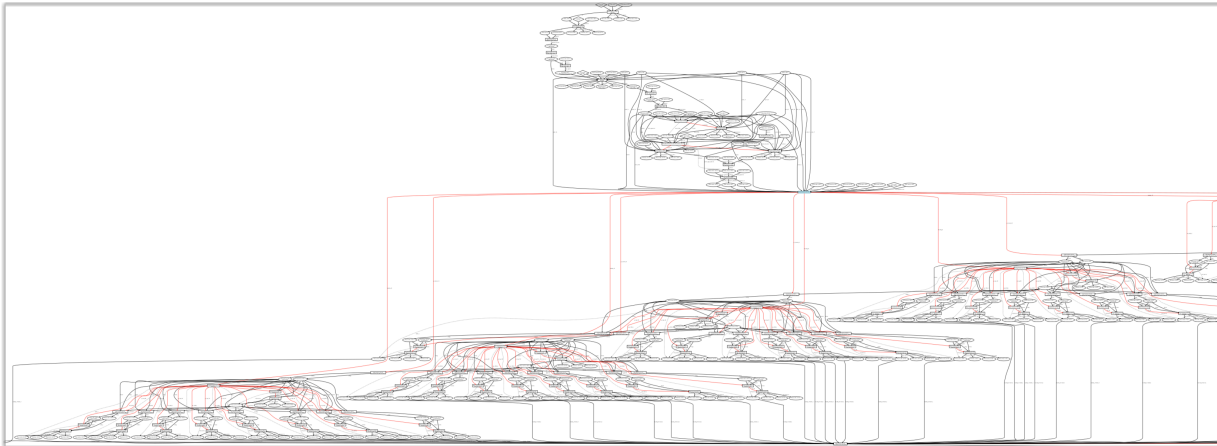
deveLop Updated a day ago by Italiz ✓ 1303 New pull request 🗑️

“Simple” graphs of workflows for a single material



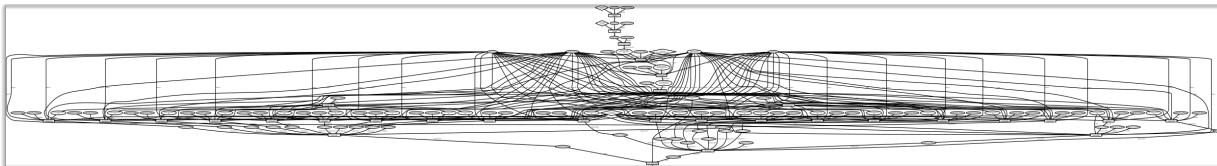
Phonon dispersion

(atom oscillations around equilibrium positions: thermal transport, electronic mobility, ...)



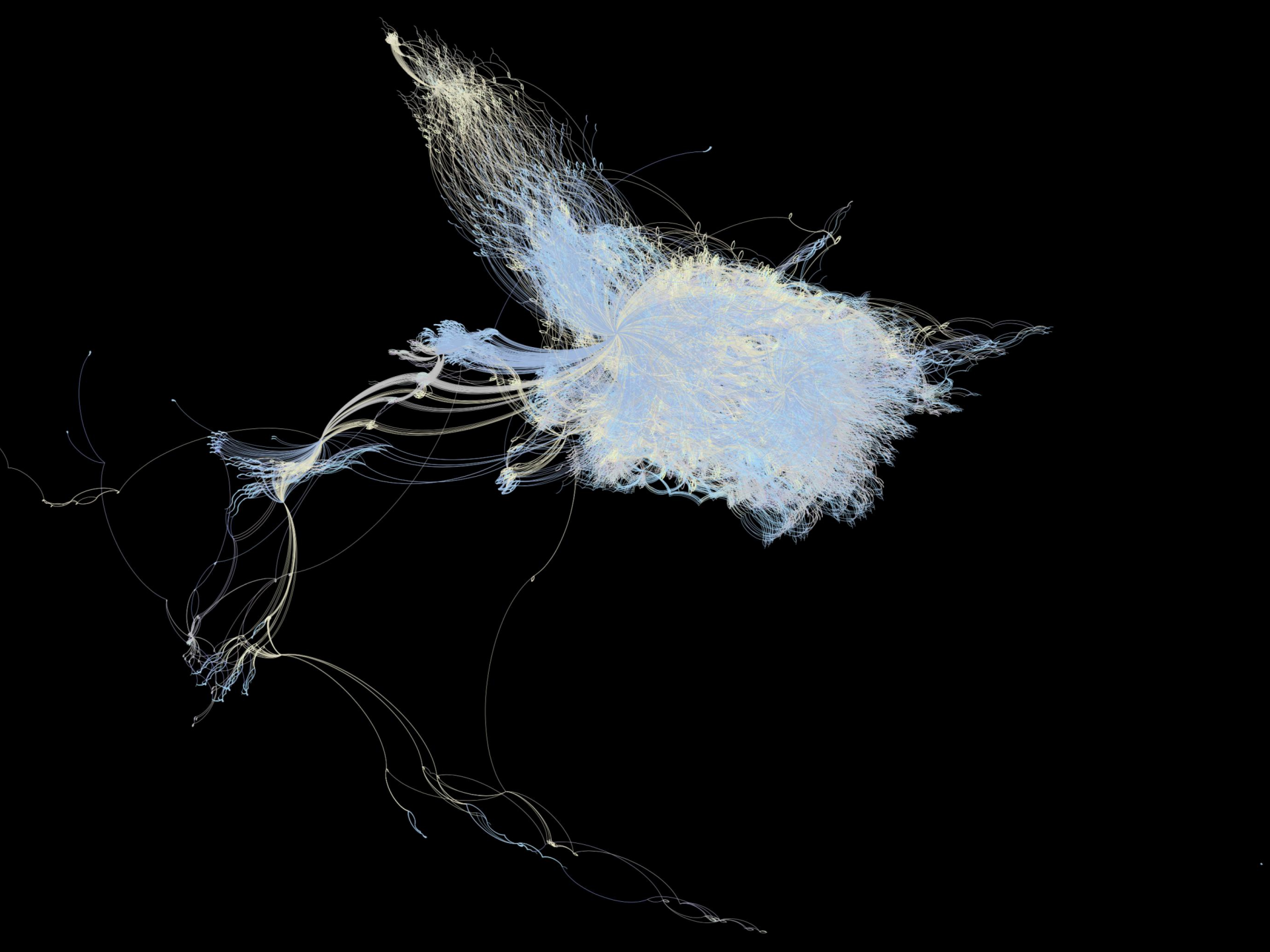
Molecular dynamics of Lithium in a solid electrolyte

(Discover novel, safe and efficient electrolytes for Li-batteries)

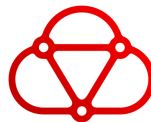


Elastic constants

(response of materials to stresses and deformations)



Open Science Platform: AiiDA + Materials Cloud

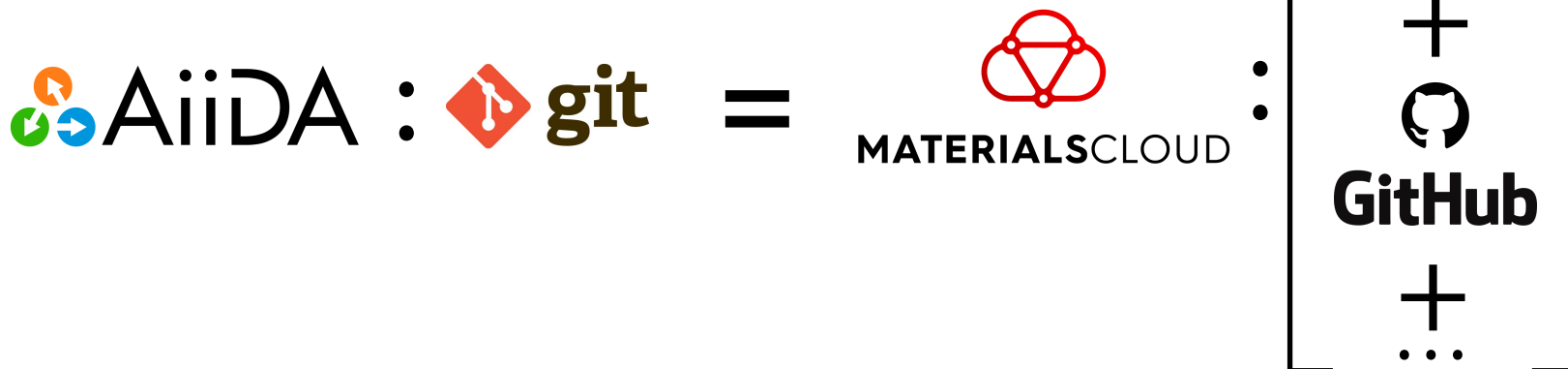


MATERIALSCLOUD

<https://www.materialscloud.org>

Online since February 2018

**Cloud dissemination platform for FAIR data sharing
and more (cloud simulation and data generation platform)**



Open and FAIR data sharing: Archive, Discover, Explore

materialscloud:2017.0008

SCIENTIFIC DATA

re3data.org
REPOSITORY OF RESEARCH DATA (R3) IDENTIFIERS
http://doi.org/10.17616/R3.225W
Materials Cloud



FAIRsharing.org
standards, databases, policies

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

Authors: 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*}

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DOI: [10.24435/materialscloud:2017.0008/v2](https://doi.org/10.24435/materialscloud:2017.0008/v2) (version v2, submitted on 21 March 2018)

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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, etc.) 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

DOIs assigned

[FAIRsharing.org](https://www.fairsharing.org)
re3data.org

+

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

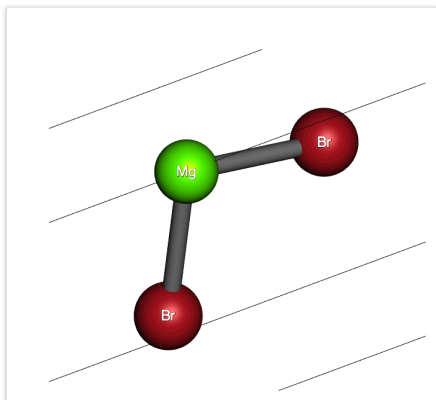
Direct links to Discover & Explore



DISCOVER (CURATED DATA) & EXPLORE (RAW DATA)

DISCOVER

Compound: MgBr_2



Info and properties
[See definitions...](#)

Formula: MgBr_2
Spacegroup: P-3m1
Pointgroup: -3m
Prototype: CdI2
Band gap [eV]: 4.8

Magnetic properties:
Magnetic State: non-magnetic
Tot. Magnetization [$\mu\text{B}/\text{cell}$]: -
Abs. Magnetization [$\mu\text{B}/\text{cell}$]: -

Binding Energies:
DF2-C09 Binding energy [$\text{meV}/\text{\AA}^2$]:
(From parent COD 9009107)
rVV10 Binding energy [$\text{meV}/\text{\AA}^2$]: 15
(From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):
 Δ_{DF2} [%]: 17.1 (From parent COD 9009107)
 Δ_{rVV10} [%]: 18.3 (From parent COD 9009107)

Band structure



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

EXPLORE

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

WORK: AiiDA Lab (submission)

- Our **cloud data generation platform** and **data analysis platform**
- Strongly based on AiiDA + Jupyter + App Mode

The screenshot displays the AiiDA Lab Materials Cloud interface. At the top, the AiiDA Lab logo is on the left, and navigation buttons for 'Edit App', 'Logout', 'Control Panel', and 'Materials Cloud' are on the right. The main content area is titled 'Materials Cloud' and is organized into three sections:

- Home:** Contains four icons: 'File Browser' (document icon), 'Terminal' (code icon), 'Tasks' (list icon), and 'Manage Apps' (gear icon). A vertical scrollbar is on the right.
- Calculation examples:** Features the text 'Please choose the code:' followed by two logos: 'CP2K' (orange block letters) and 'QUANTUMESPRESSO' (red and white circular logo). A vertical scrollbar is on the right.
- Empa nanotech@surfaces Laboratory - Scanning Probe Microscopy:** Lists four categories: 'General', 'STM', 'PDOS', and 'AFM'. A vertical scrollbar is on the right.

WORK: AiiDA Lab

Jupyter Edit App Logout Control Panel Materials Cloud

pk

Load pk

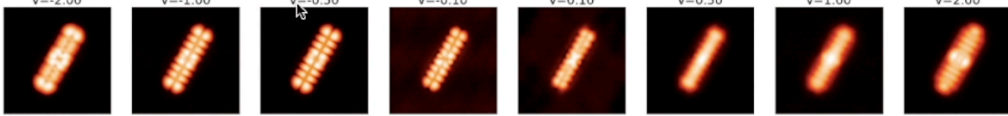
Scanning tunneling microscopy

STM series

add series

clear

V=-2.00 V=-1.00 V=-0.50 V=-0.10 V=0.10 V=0.50 V=1.00 V=2.00

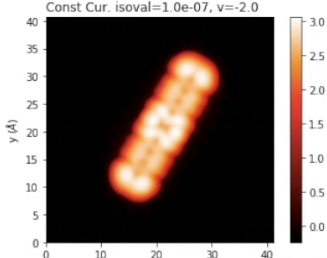


STM single

series

bias

Const Cur. isoval=1.0e-07, v=-2.0



Possible integration/collaboration points

- **Development and integration plans:**
 - **AiiDA Lab**
 - Deployment with kubernetes for autoscaling
 - Integration fo Authentication and Authorization with B2ACCESS
 - *Registration of AiiDA Lab as a service on EOSC?*
 - Development and deployment of “turn-key” workflows for the materials science community as the “services”
 - **Archive**
 - Migration of Archive to Invenio v3 or EUDAT’s B2SHARE (based on Invenio) [deciding now, 2 developers participating in the Invenio Boot Camp in March; is B2SHARE still supported?]
 - Integration in EUDAT’s B2FIND

Technical requirements for kubernetes@EOSC

AiiDA lab

- helm support
- storageclass for persistent volumes with dynamic provisioning (uid: 1000, gid: 1000)
- authentication: to decide between B2ACCESS / EGI check-in

Feature requirements for B2SHARE (Materials Cloud Archive)

- Review stage for deposits: moderators can request changes & approve
- Create new versions existing deposits
- Embargo period: publish x months after deposition
- Reserve DOI for deposit prior to publishing