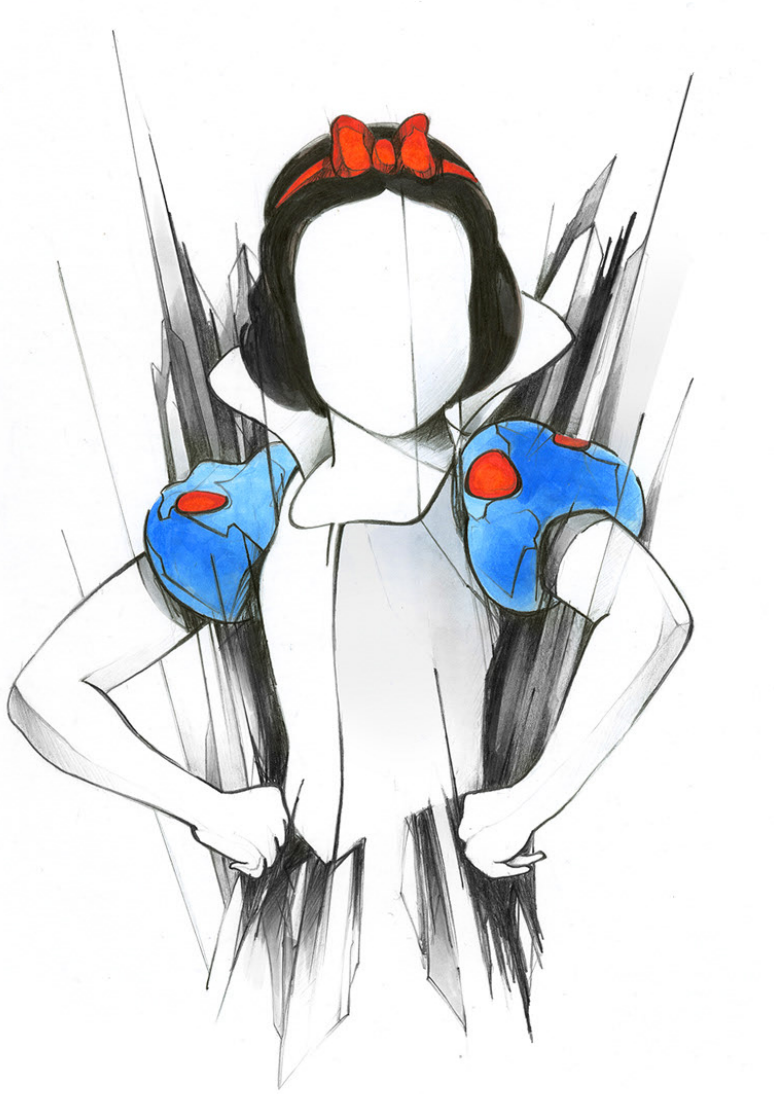


@Alexis Marcou

# PROJECT SNOW WHITE

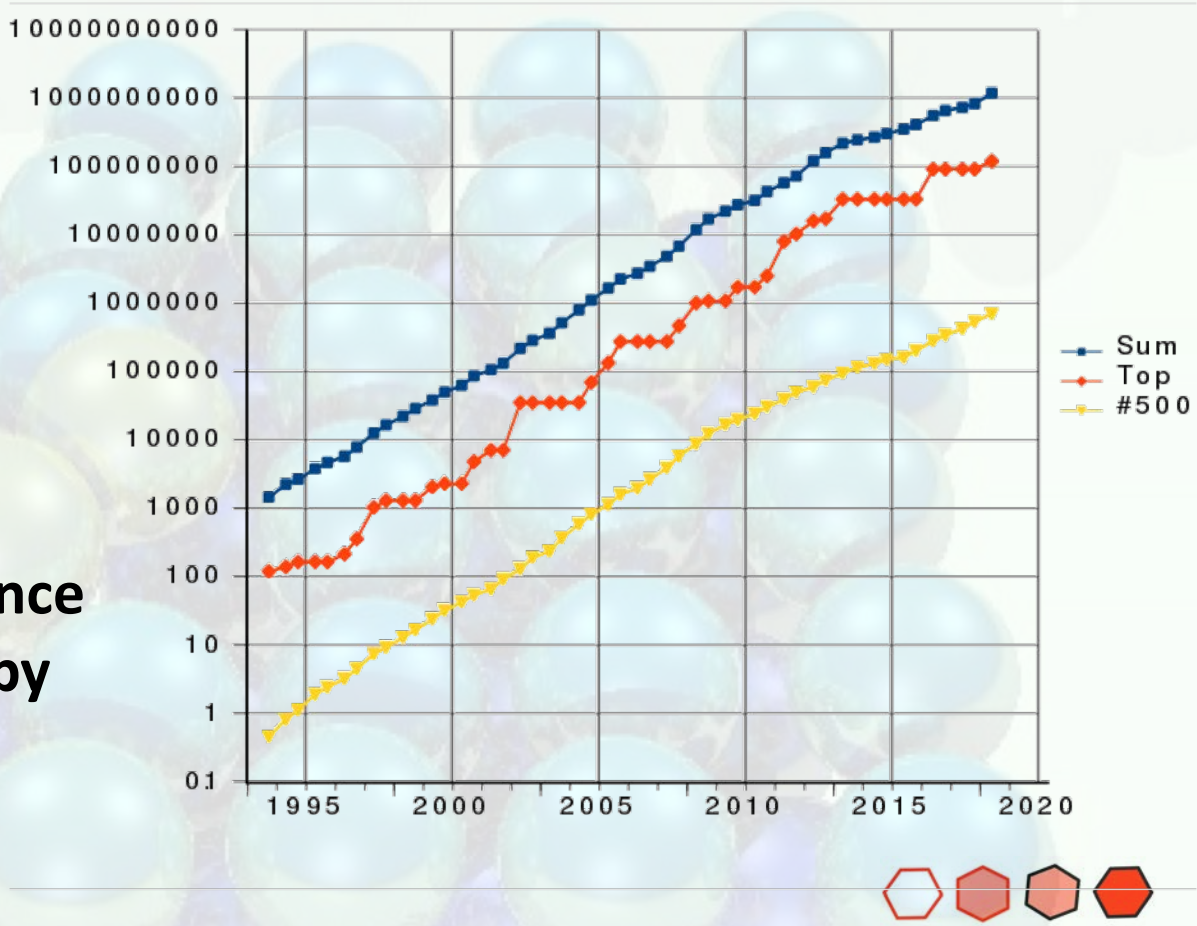
## (the FAIRest of them all)

**Nicola Marzari - EPFL**

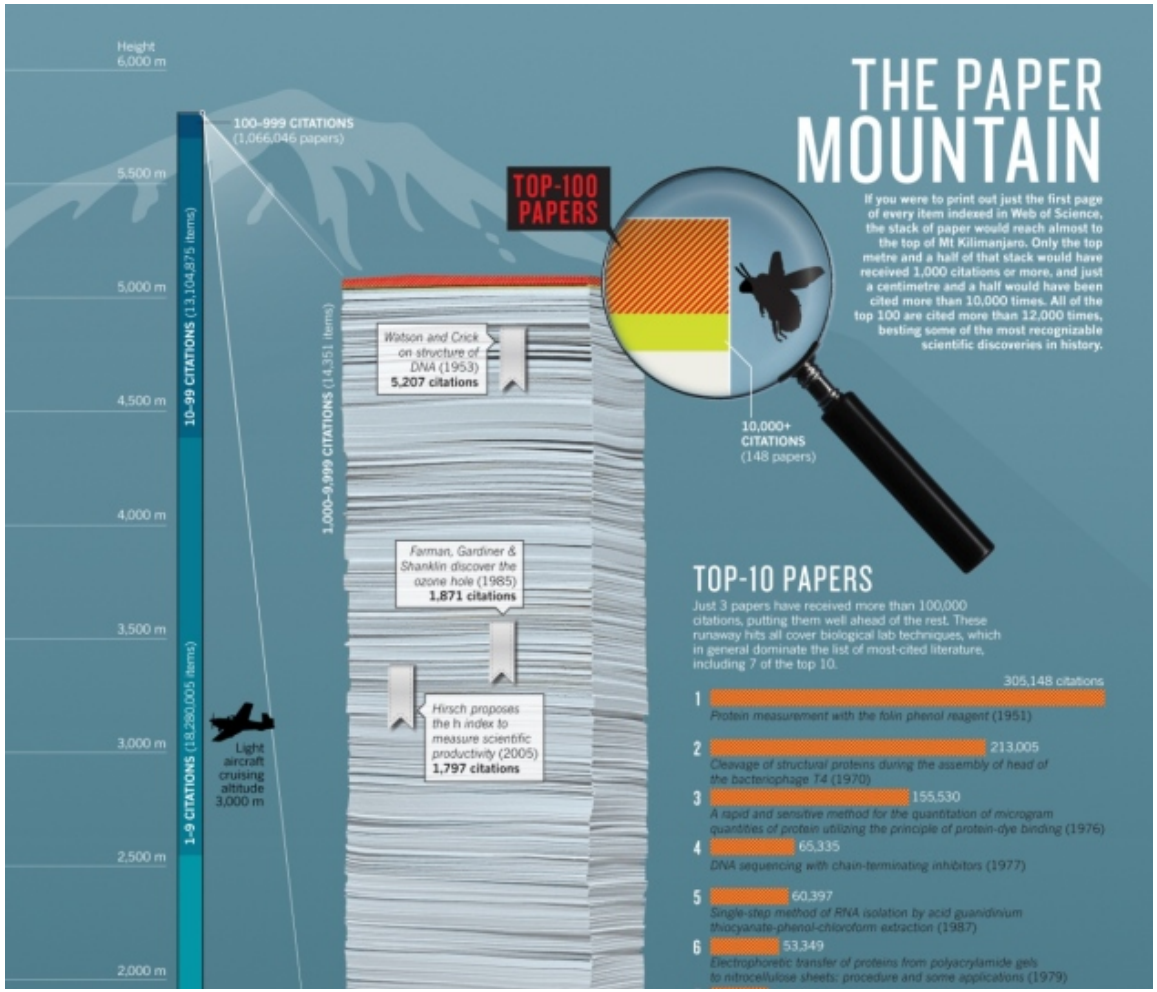
# COMPUTATIONAL SCIENCE: 100% GROWTH EVERY 14 MONTHS

A calculation that took **one year in 1990** takes **one second in 2019** (33-million-fold increase).

And this is just with bits: neurons are in, and qubits on the horizon. **21st-century science and discovery will be driven by computational science.**



# WIDELY USED AND APPLIED




**THE TOP 100 PAPERS:**

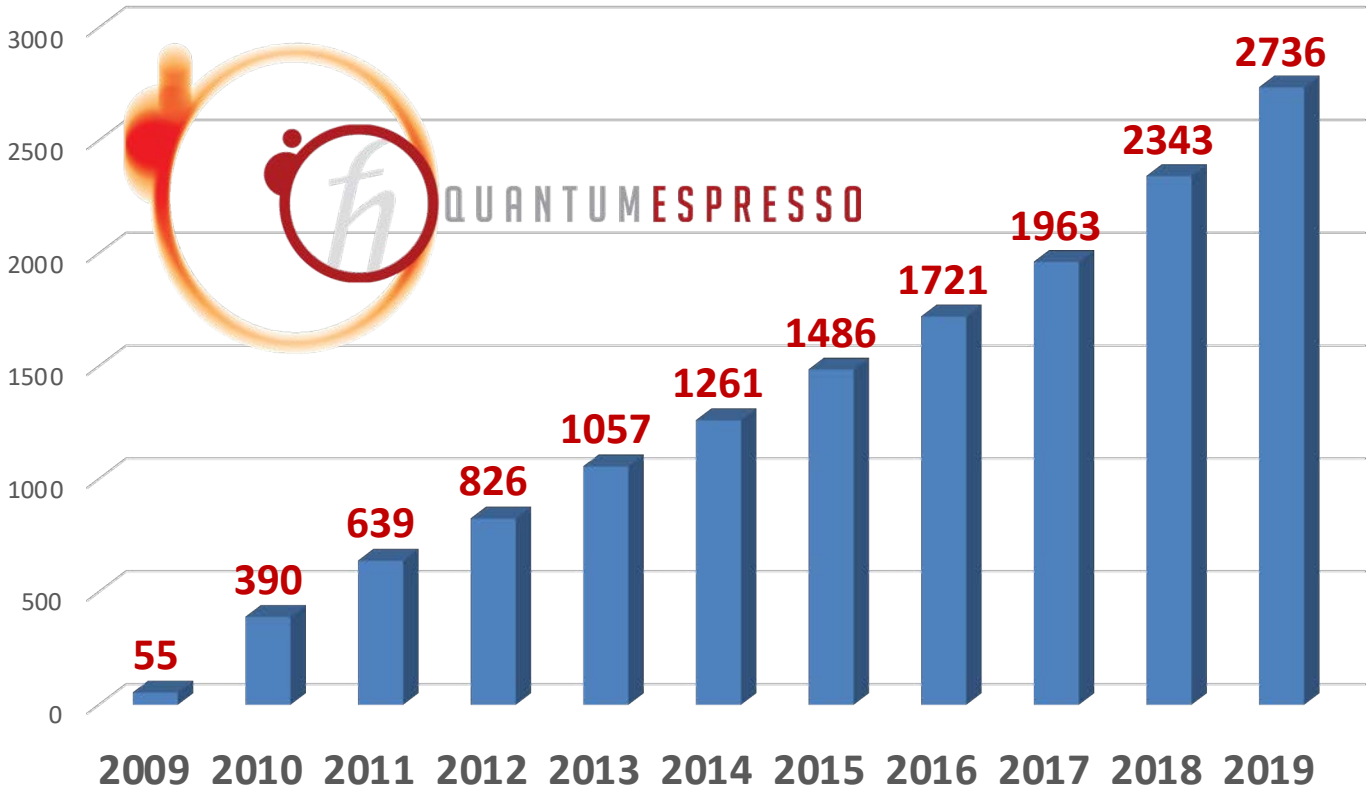
**12 papers on density-functional theory in the top-100 most cited papers in the entire scientific, medical, engineering literature, ever.**

***Nature, Oct 2014***

# SOFTWARE AS A FACILITY (PAPERS/YEAR)

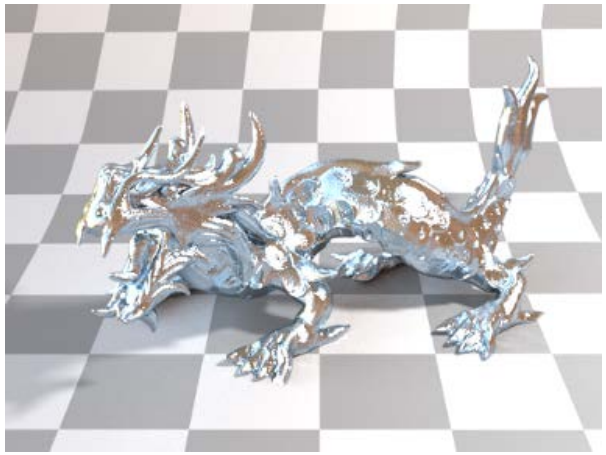
This is the most used open-source software in the world for quantum mechanical simulations.

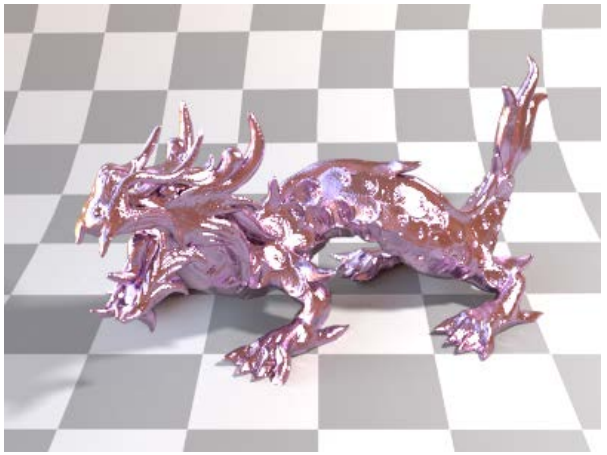
Started at EPFL in the 1980s, and still (co)-developed here.




2019 data extrapolated to the full 12 months

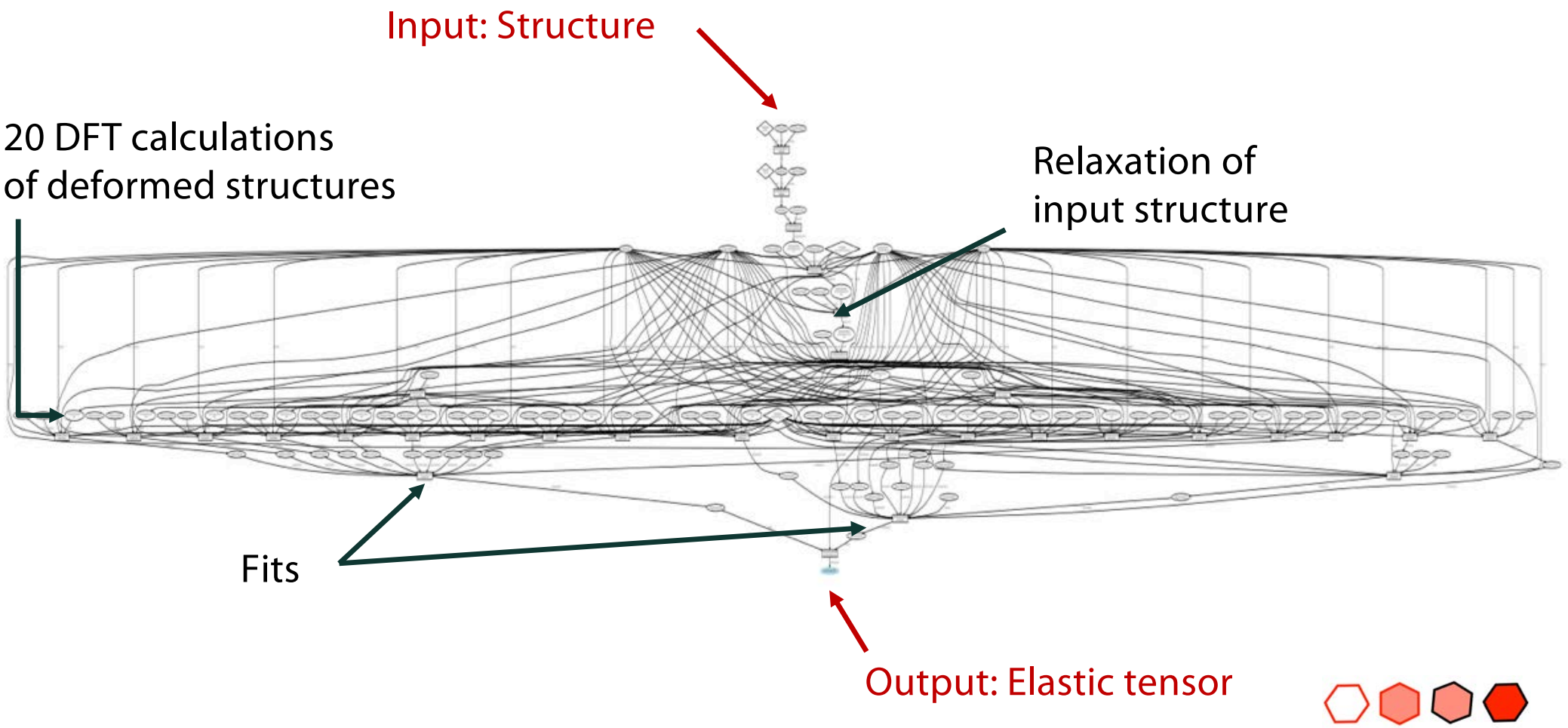
# HOW WELL CAN WE REPRODUCE THE REAL WORLD?






G. Prandini, G.M. Rignanese, and N. Marzari (2019)

# AUTOMATED, CURATED DATA ON DEMAND



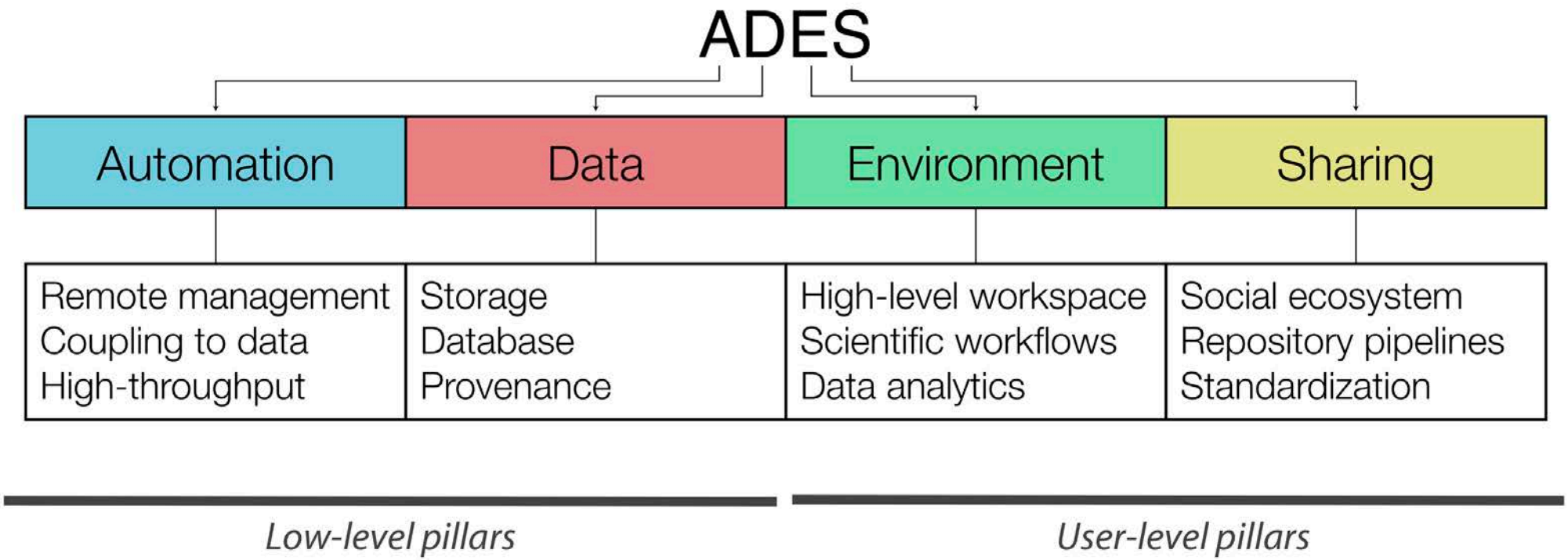
# AN OPEN SCIENCE PLATFORM, THEN

1. Widely used, **open-source community codes**

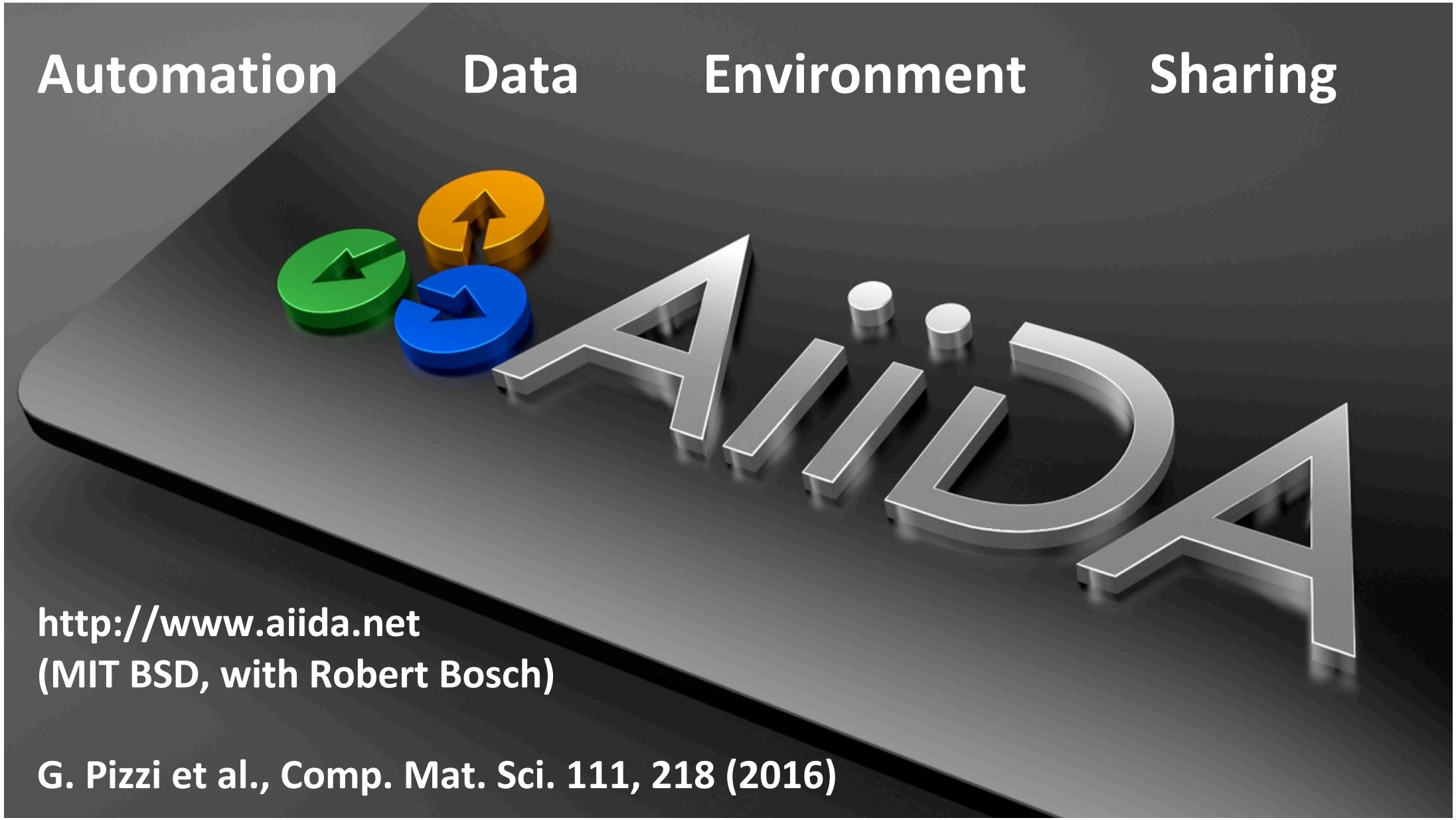

2. An **operating system** for high-throughput computational science, data provenance and reproducibility – http://aiida.net

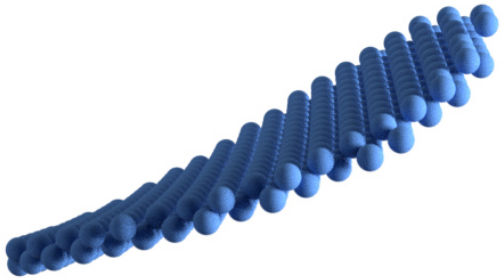

3. A **dissemination platform** for raw and curated data, simulation services, educational tools – http://materialscloud.org


# AN OPERATING SYSTEM FOR COMPUTATIONAL SCIENCE

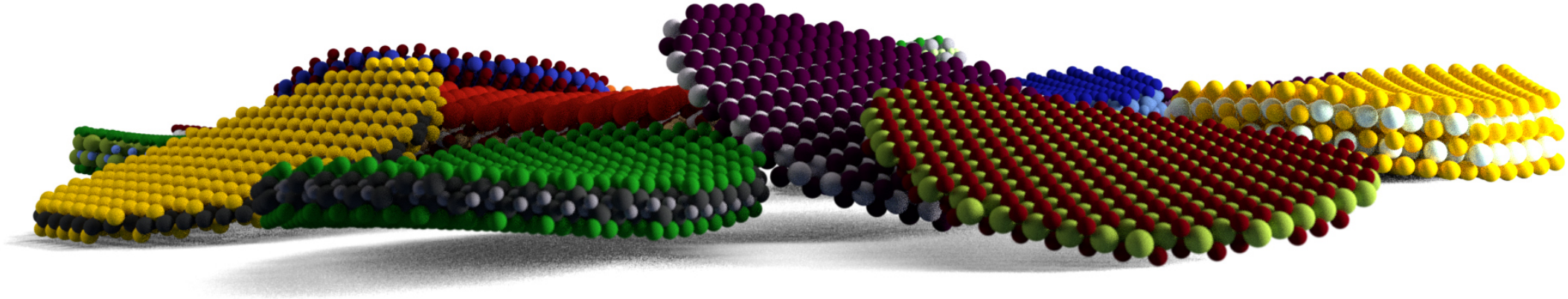



**G. Pizzi et al., Comp. Mat. Sci. 111, 218 (2016)**

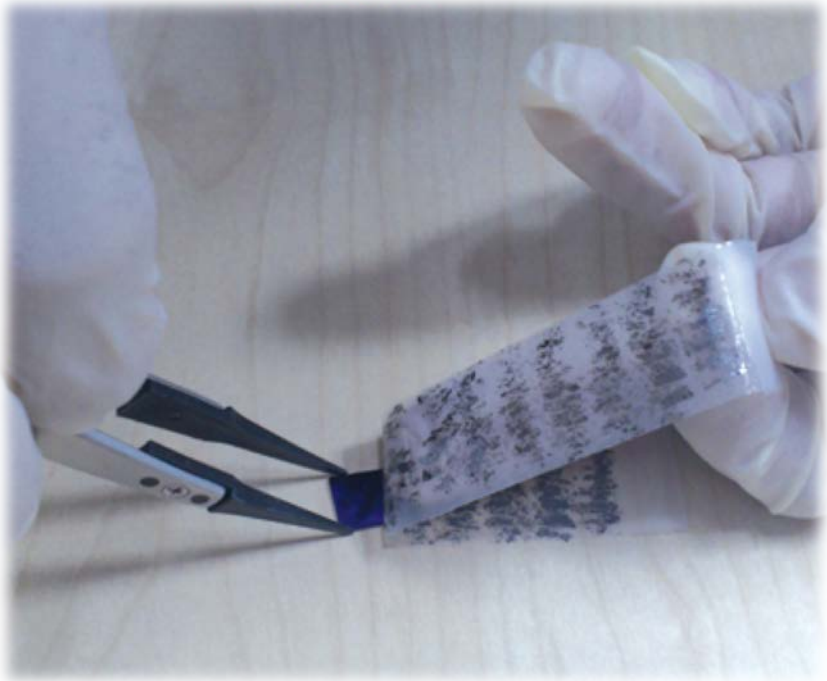

Automation
Data
Environment
Sharing
AiiDA
http://www.aiida.net
(MIT BSD, with Robert Bosch)
G. Pizzi et al., Comp. Mat. Sci. 111, 218 (2016)



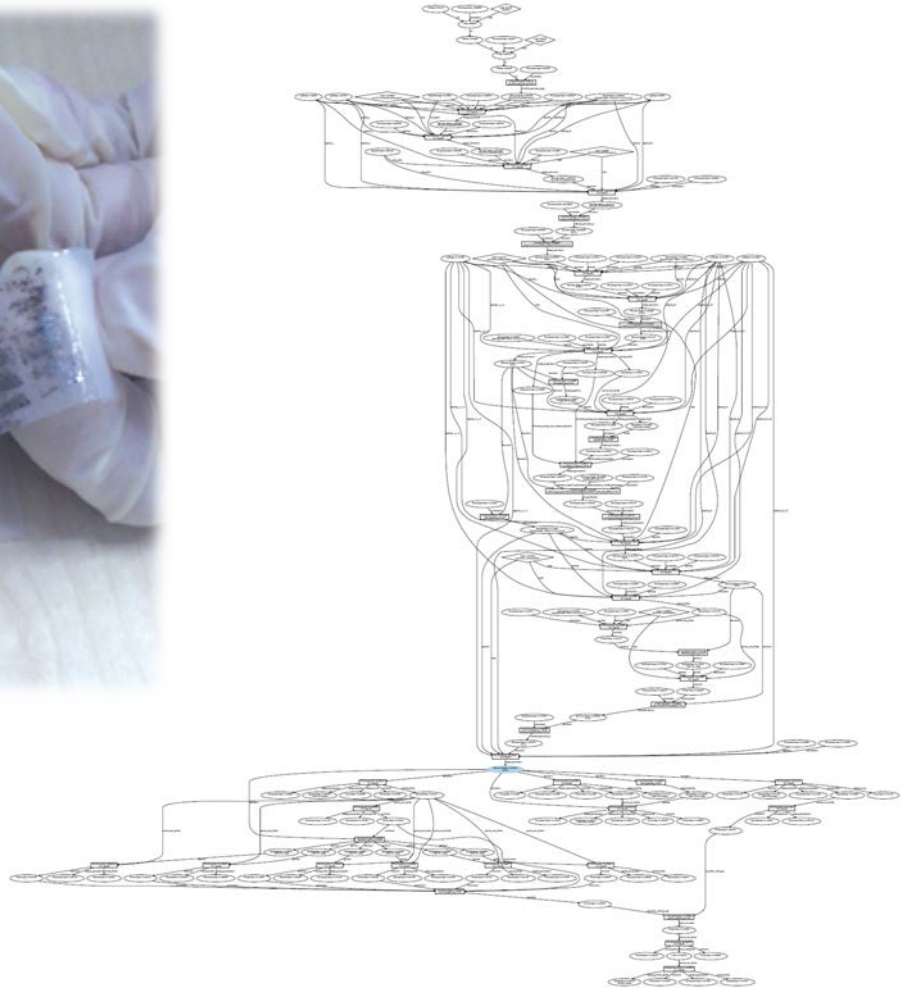
# COMPUTATIONAL EXFOLIATION OF ALL KNOWN INORGANIC MATERIALS



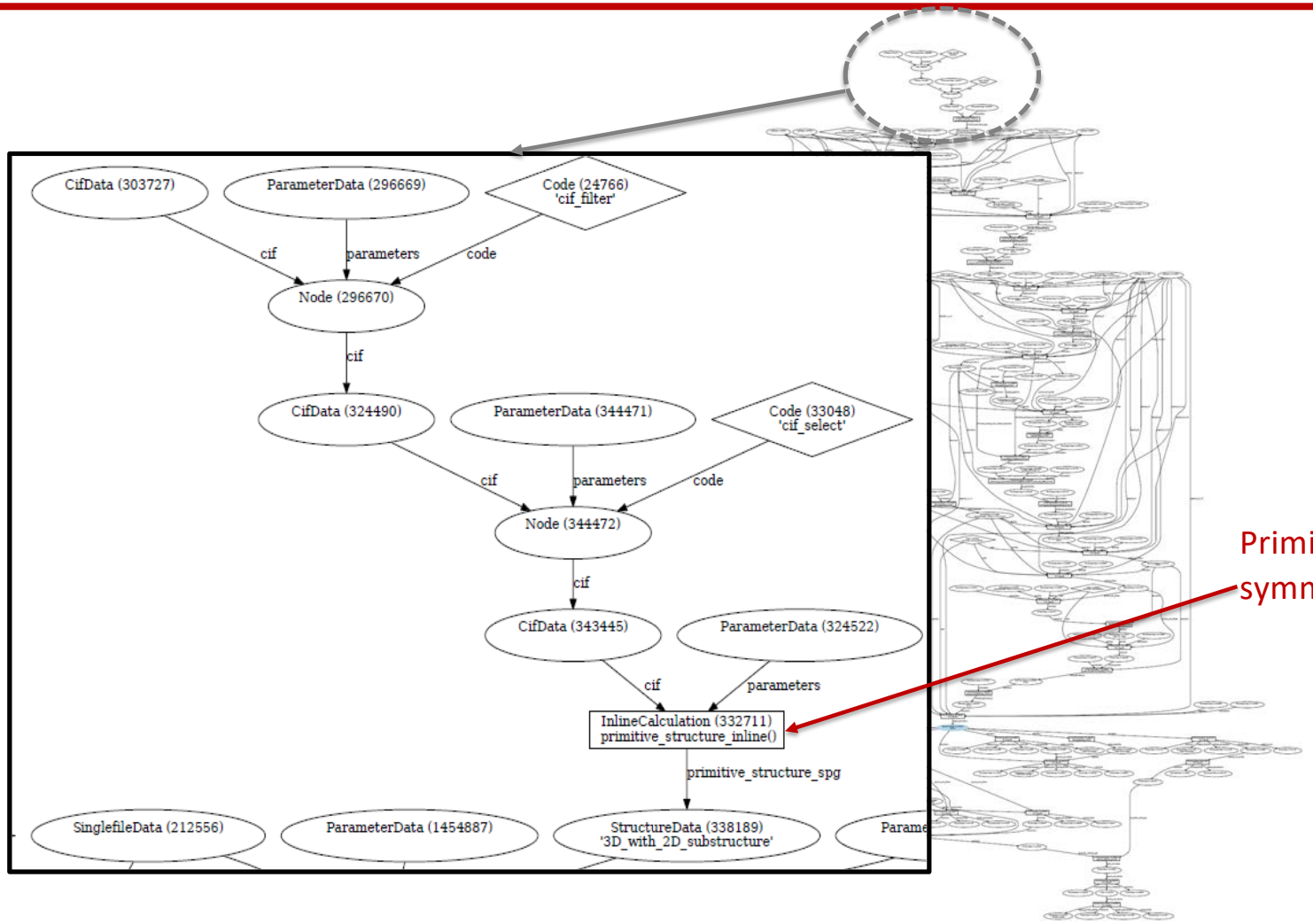
# LET’S START FROM ONE MATERIALS (BUT WE HAVE 1 MILLION!)



@ Nature/NUS

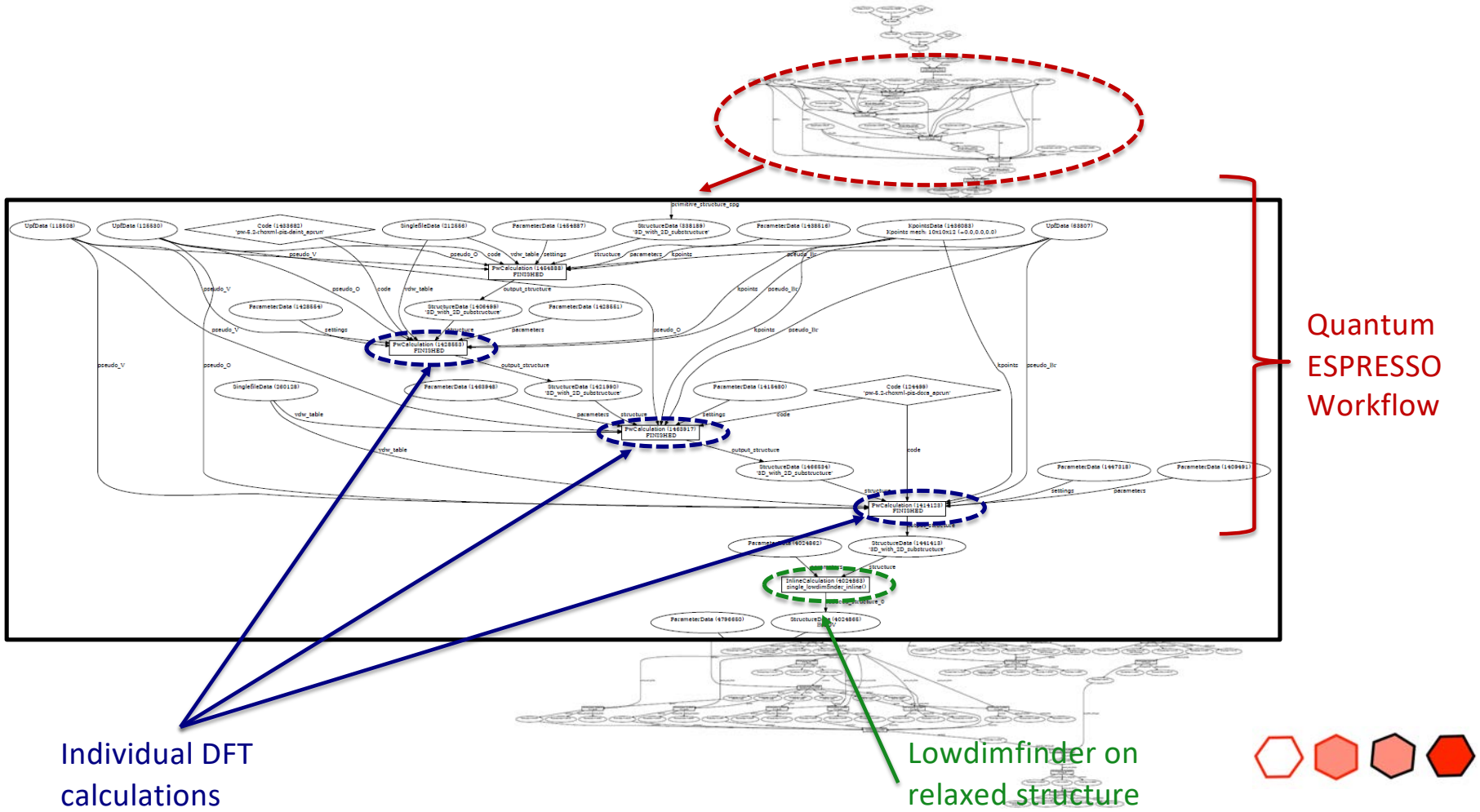


# FROM DATABASE TO CALCULATION

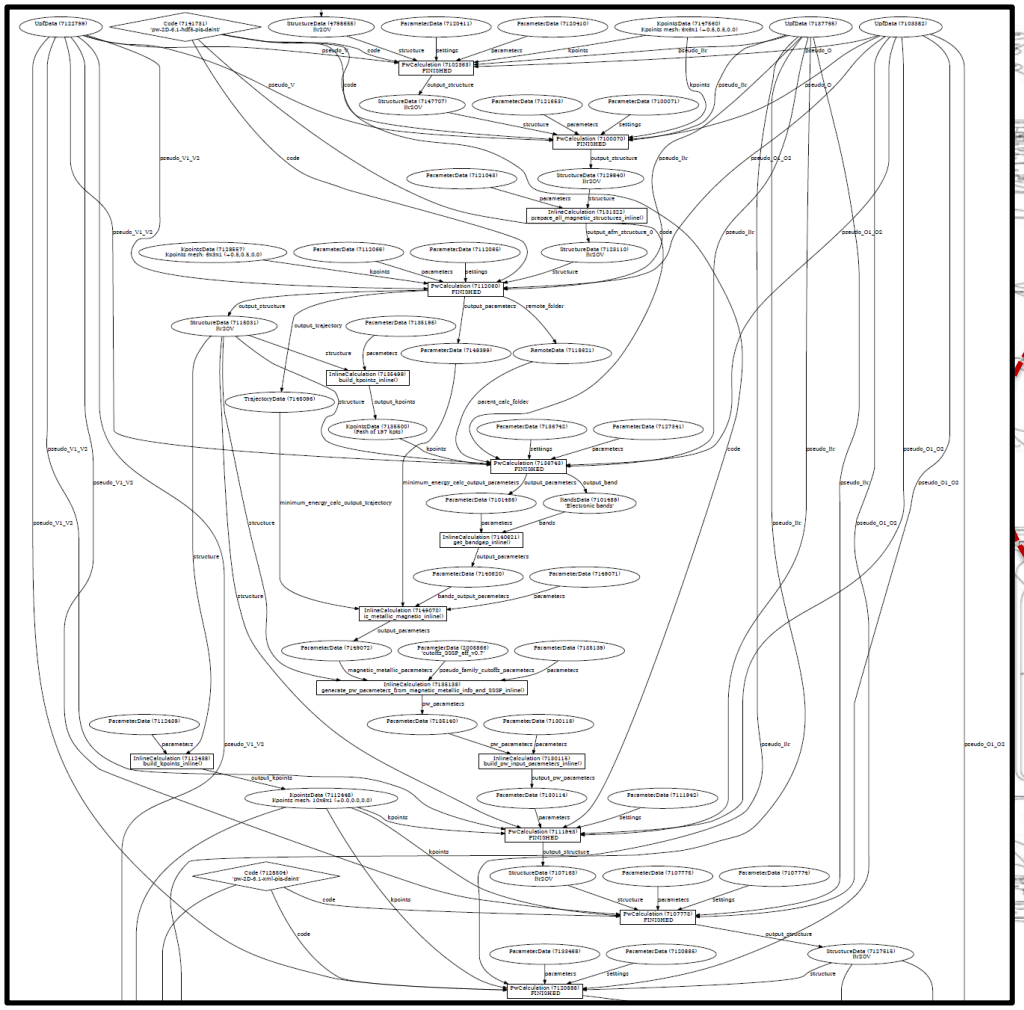


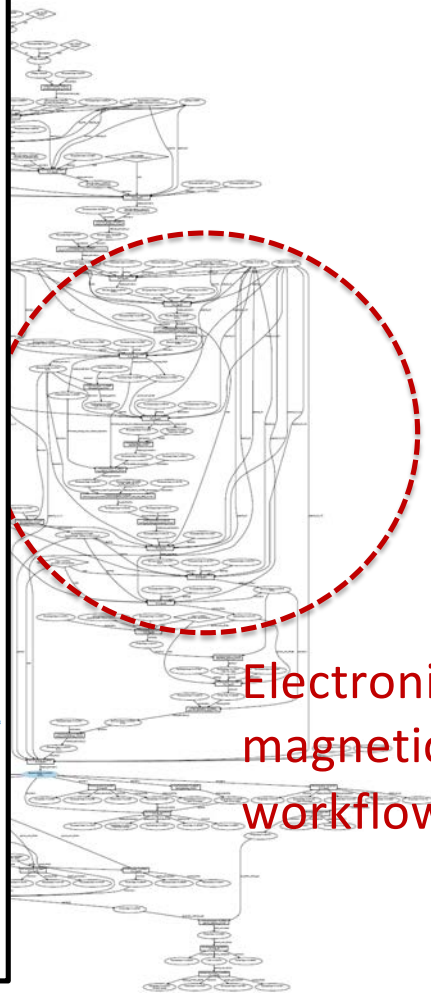

Primitive cell & structure symmetry refinement

# FINDING THE ELECTRONIC GROUND STATE



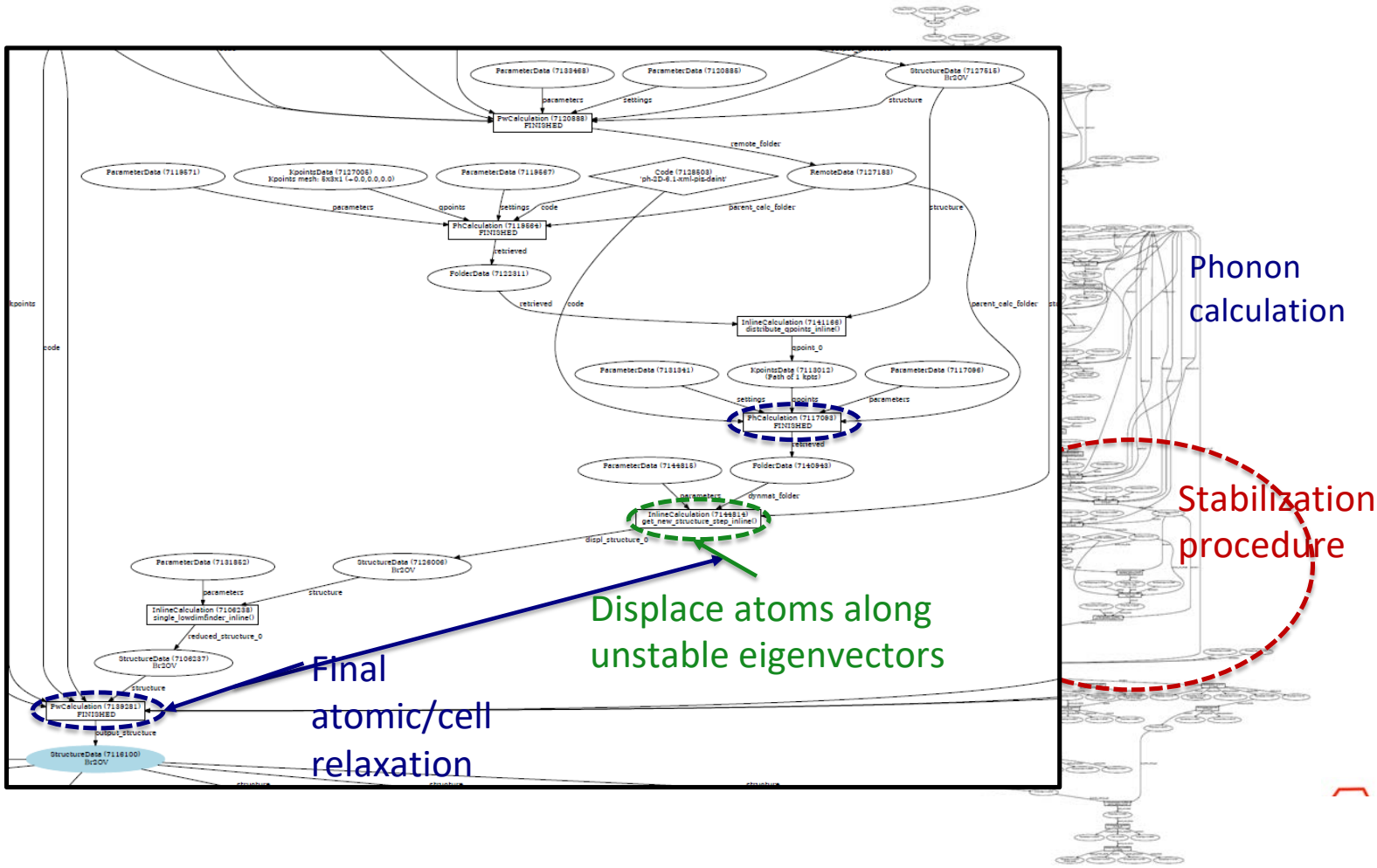
# FROM DATABASE TO CALCULATION



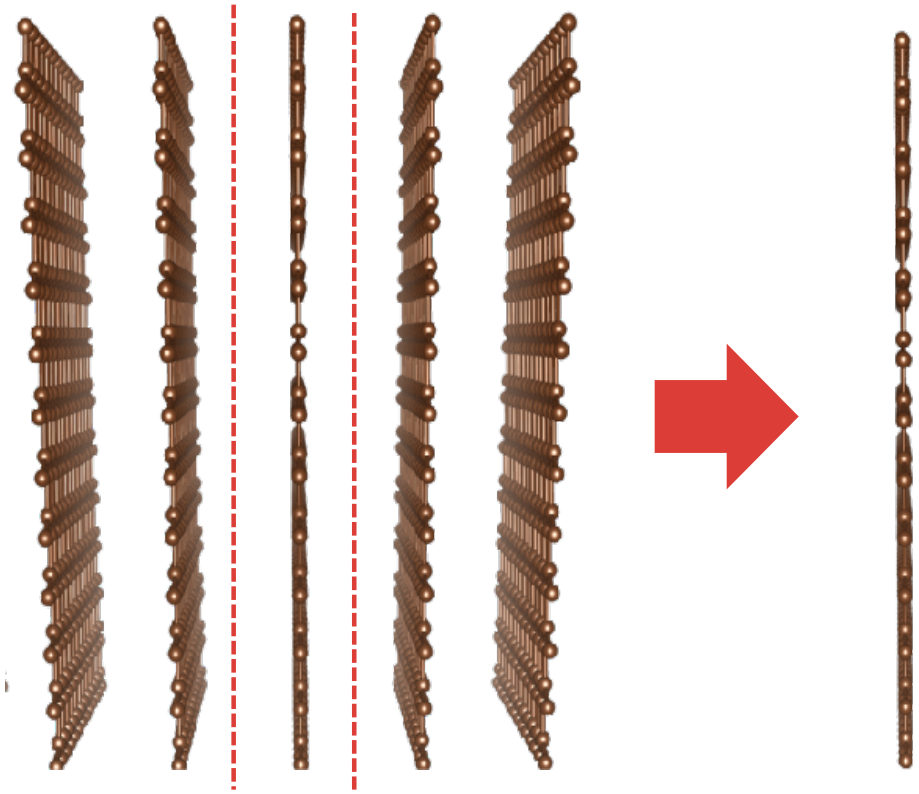


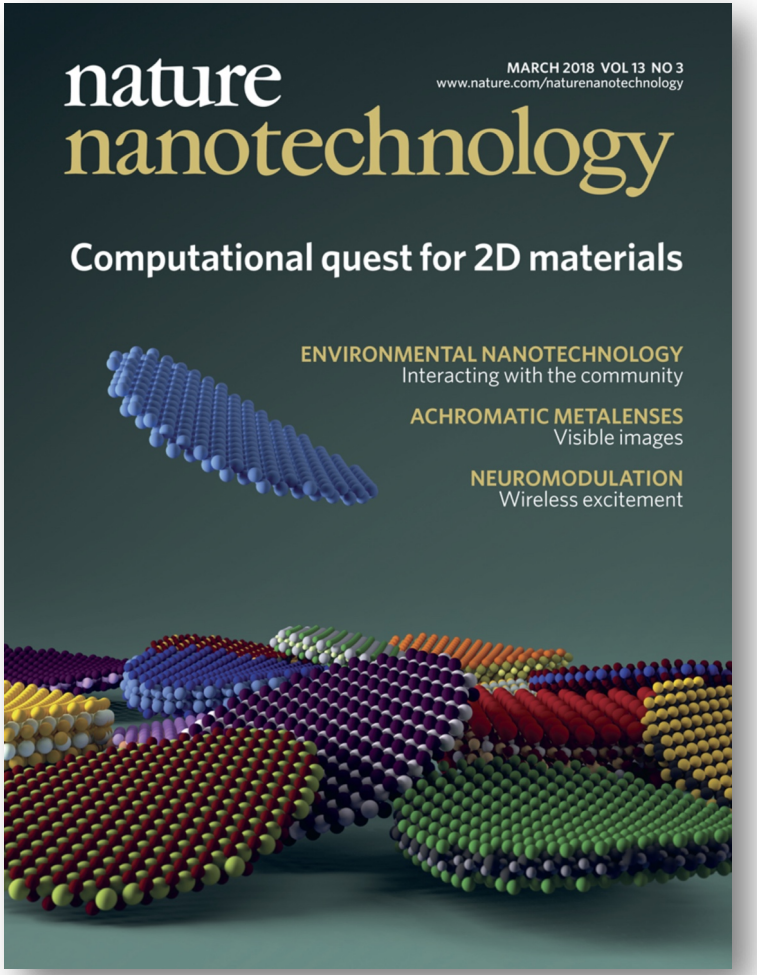
Electronic & magnetic workflow

# RELAXING ATOMS, GEOMETRY



# LET THE COMPUTER DO THE WORK FOR YOU ☺

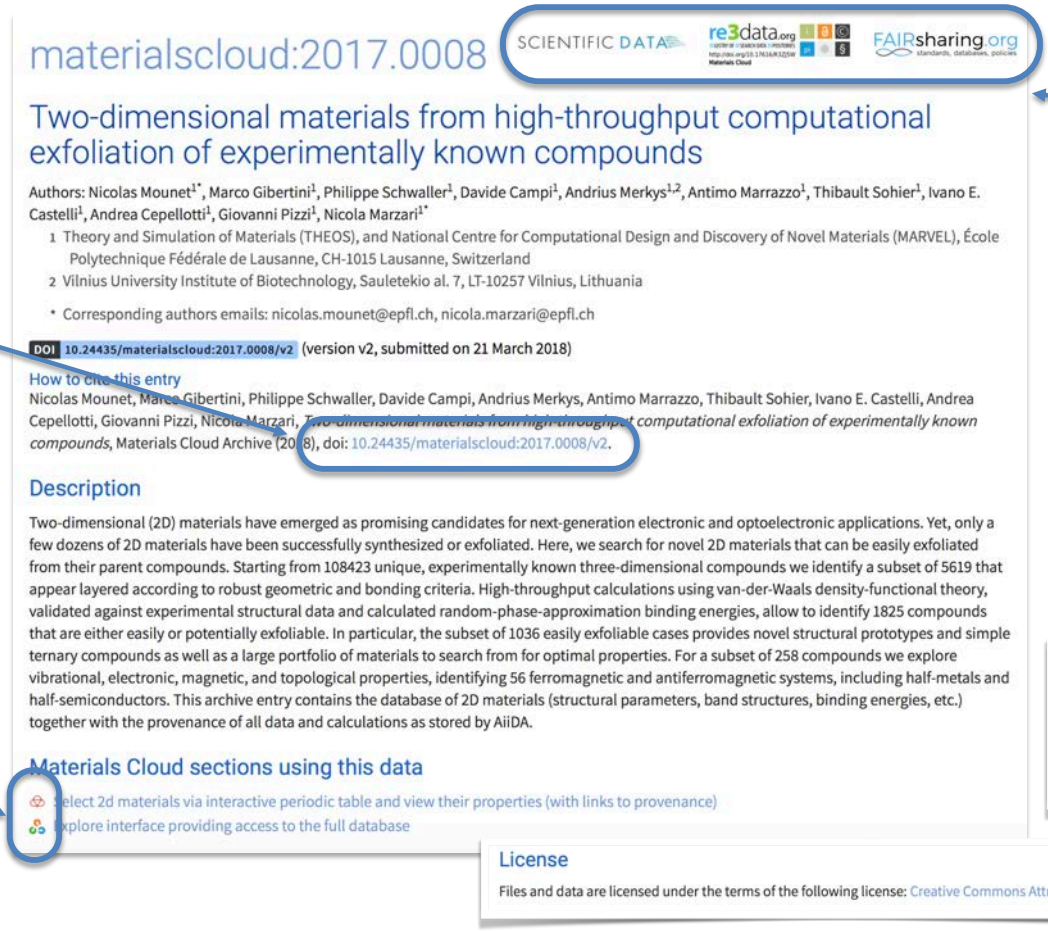




# *ARCHIVE, EXPLORE, DISCOVER* ON THE MATERIALS CLOUD

DOIs assigned

Direct links to Discover & Explore



materialscloud:2017.0008

SCIENTIFIC DATA re3data.org FAIRsharing.org

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

Authors: Nicolas Mounet[1*], Marco Gibertini[1], Philippe Schwaller[1], Davide Campi[1], Andrius Merkys[1,2], Antimo Marrazzo[1], Thibault Sohier[1], Ivano E. Castelli[1], Andrea Cepellotti[1], Giovanni Pizzi[1], 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/v2 (version v2, submitted on 21 March 2018)

How to cite this entry

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 (2018), doi: 10.24435/materialscloud:2017.0008/v2.

### 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

### License



FAIRsharing.org

+

re3data.org

+

Recommended data repository by Nature's journal Scientific Data

+

Indexed by Google Dataset Search

+

Registered on EUDAT/EOSC's B2FIND

Exposes data in JSON and XML via standardised machine-readable protocols, like OAI-PMH and Dublin Core

Discover

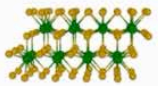
## Discover curated data sets

Add DISCOVER section

This section will contain a curated set of results including structures and their properties as generated by NCCR members.

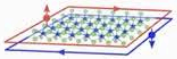

### Standard solid-state pseudopotentials (SSSP) DOI 10.24435/materialscloud:2018.0001/v3

**Authors:** Gianluca Prandini, Antimo Marrazzo, Ivano E. Castelli, Nicolas Mounet & Nicola Marzari
**Description:** A Standard Solid State Pseudopotentials (SSSP) library optimized for precision and efficiency.



### 2D structures and layered materials DOI 10.24435/materialscloud:2017.0008/v2

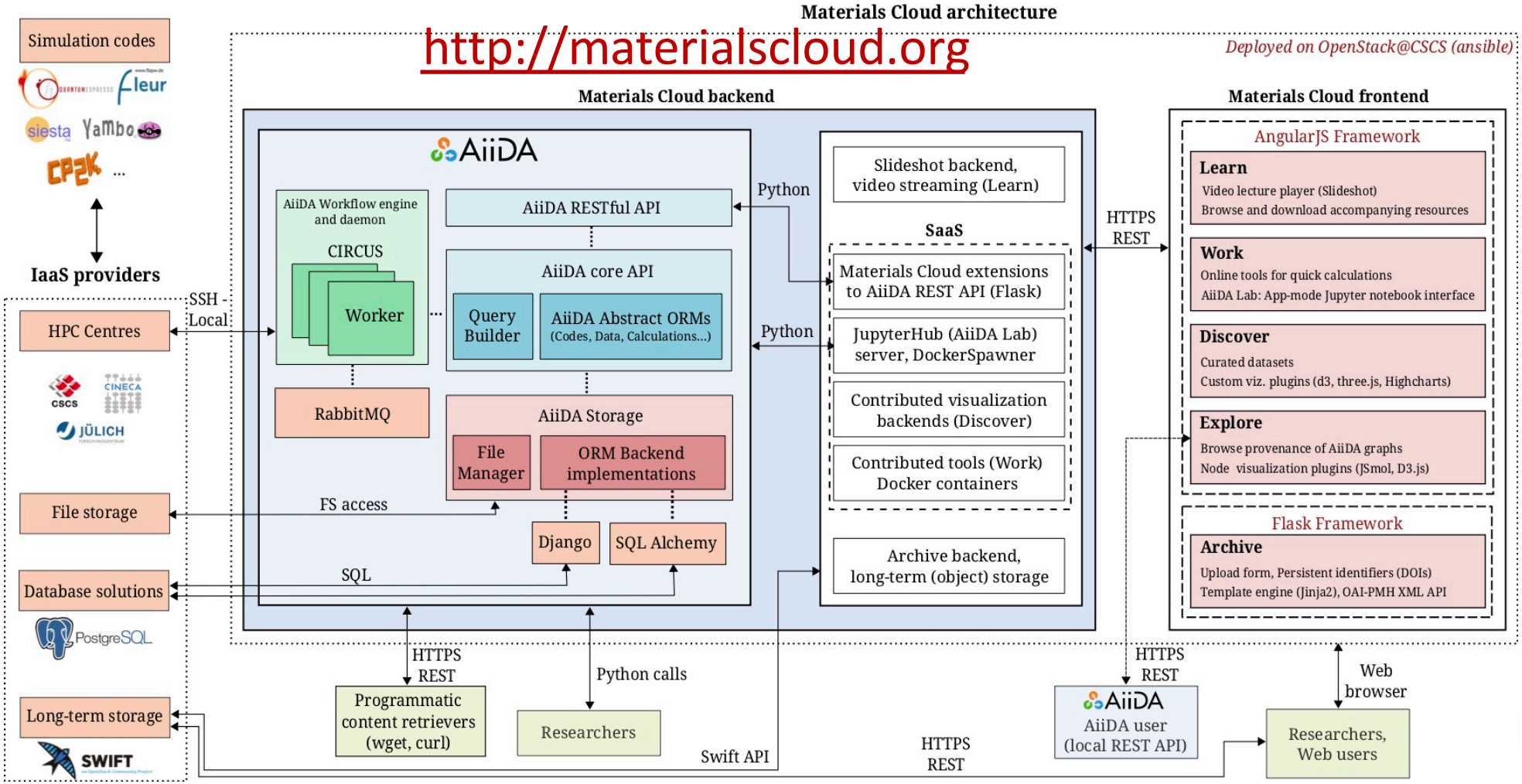
**Authors:** Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Davide Campi, Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano E. Castelli, Andrea Cepellotti, Giovanni Pizzi & Nicola Marzari
**Description:** Results from screening known 3D crystal structures finding those that can be computationally exfoliated, producing 2D materials candidates. If you use this work please cite N. Mounet et al, Nat. Nanotech., doi:10.1038/s41565-017-0035-5 (2018).

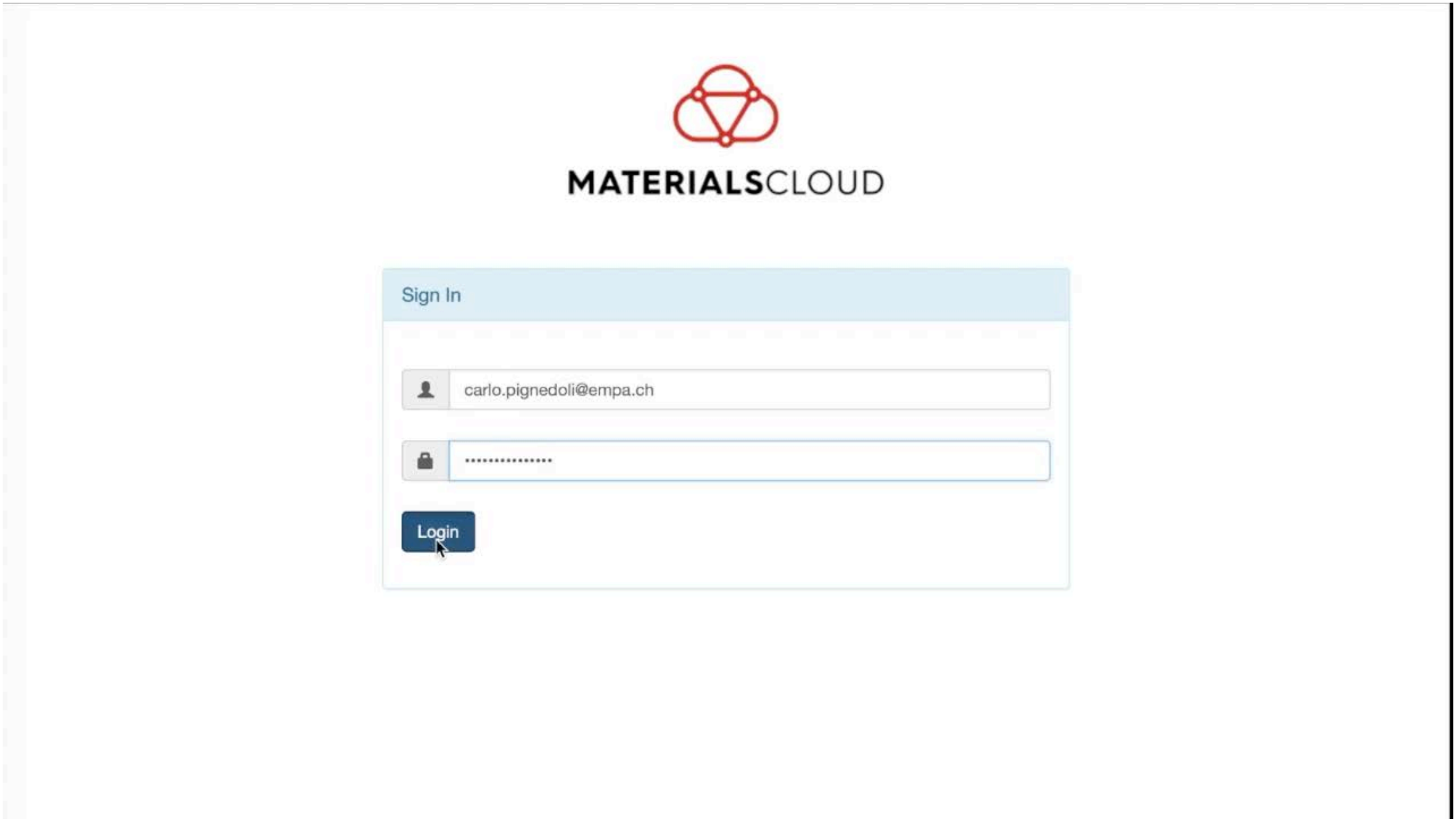


### 2D topological insulators

**Authors:** Antimo Marrazzo, Marco Gibertini, Davide Campi, Nicolas Mounet & Nicola Marzari
**Description:** Results from screening exfoliable materials for 2D topological insulators (Quantum Spin Hall Insulators).

# SOFTWARE, DATA, AND SERVICES INSTALLATION




MATERIALSCLOUD
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carlo.pignedoli@empa.ch
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CONCLUDING THOUGHTS: HARDWARE…

# ...vs SOFTWARE

- We do not have the hardware that brought us to the Moon
- But we do have the software

```
# Filename:     STABLE_ORBIT.agc
# Purpose:      Part of the source code for Colossus 2A, AKA Comanche 055.
#               It is part of the source code for the Command Module's (CM)
#               Apollo Guidance Computer (AGC), for Apollo 11.

P38     TC    AVFLAGA          # THIS VEHICLE ACTIVE
        TC    +2
P78     TC    AVFLAGP          # OTHER VEHICLE ACTIVE
        TC    P20FLGON         # SET UPDATFLG, TRACKFLG
        CAF   V06N33SR         # DISPLAY TIG
        TC    VNDSPLY
        CAF   V06N55SR         # DISPLAY CENTANG
        TCR   BANKCALL
        CADR  GOFLASHR
        TCF   GOTOP00H         # TERMINATE
```


Margaret Hamilton @ MIT

# CONCLUSIONS

1) Computational science will be a driver for the decades to come, with a unique scaling with respect to other resources
2) It is naturally free, open science, replicated everywhere in the world at the flick of a switch
3) We are building the infrastructural tools to disseminate it with persistent, reproducible data (raw and curated)
4) **As a scientific society, we have development models for scientific hardware, but not for scientific software – long-term careers and recognition.**

# SUPPORT FROM


http://epfl.ch

Open Science Fund (2019-21)





SWISS NATIONAL SCIENCE FOUNDATION










http://nccr-marvel.ch

Swiss National Centre for Computational Design and Discovery of Novel Materials (2014-18, 2018-22, 2022-26)

http://max-centre.eu

H2020 Centre of Excellence MaX: Materials Design at the Exascale (2015-18, 2018-21)

H2020 Nanoscience Foundries and Fine Analysis
H2020 European Materials Modelling Council
H2020 Graphene Flagship
H2020 Marketplace
H2020 Intersect
H2020 EPFL Fellows
H2020 EPFL Innovators
H2020 Marie Curie
PASC
PRACE
IBM
Constellium
Innosuisse
Solvay
Varinor
Samsung

*"Things were done very differently on the farm when I was your age, Kenny."*