PROJECT SNOW WHITE
(the FAIRest of them all)

Nicola Marzari - EPFL

@Alexis Marcou
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.
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.

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

Input: Structure

20 DFT calculations of deformed structures

Relaxation of input structure

Fits

Output: Elastic tensor
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](http://aiida.net)

3. A **dissemination platform** for raw and curated data, simulation services, educational tools – [http://materialscloud.org](http://materialscloud.org)
AN OPERATING SYSTEM FOR COMPUTATIONAL SCIENCE

ADES

Automation
- Remote management
- Coupling to data
- High-throughput

Data
- Storage
- Database
- Provenance

Environment
- High-level workspace
- Scientific workflows
- Data analytics

Sharing
- Social ecosystem
- Repository pipelines
- Standardization

Low-level pillars

User-level pillars

G. Pizzi et al., Comp. Mat. Sci. 111, 218 (2016)
Automation  Data  Environment  Sharing

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

Individual DFT calculations

Lowdimfinder on relaxed structure

Quantum ESPRESSO Workflow
FROM DATABASE TO CALCULATION

Electronic &
Magnetic
Workflow
RELAXING ATOMS, GEOMETRY

Phonon calculation
Stabilization procedure

Displace atoms along unstable eigenvectors
Final atomic/cell relaxation
LET THE COMPUTER DO THE WORK FOR YOU 😊
Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

Authors: Nicolas Maouet1, Marco Gibernini2, Philippe Schwaller1, Davide Campi3, Andrius Merkys2,3, Antino Marruzzo2, Thibaut Sekier3, Ivan E. Castelli1, Andrea Cepollotti1, Giovanni Pizzi1,2, Nicola Marzari1

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How to cite this entry

Description
Two-dimensional (2D) materials have emerged as promising candidates for next generation electronic and optoelectronic applications. Yet, only a few dozen 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 1619 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 3313 compounds that are either easily or potentially exfoliable. In particular, a subset of 1364 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 2318 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 20 materials (structural parameters, bond 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
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Direct links to Discover & Explore
- 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 curated data sets

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

**Standard solid-state pseudopotentials (SSSP)**

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**

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).
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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://nccr-marvel.ch

http://max-centre.eu

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H2020 Marketplace
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H2020 EPFL Fellows
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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.”