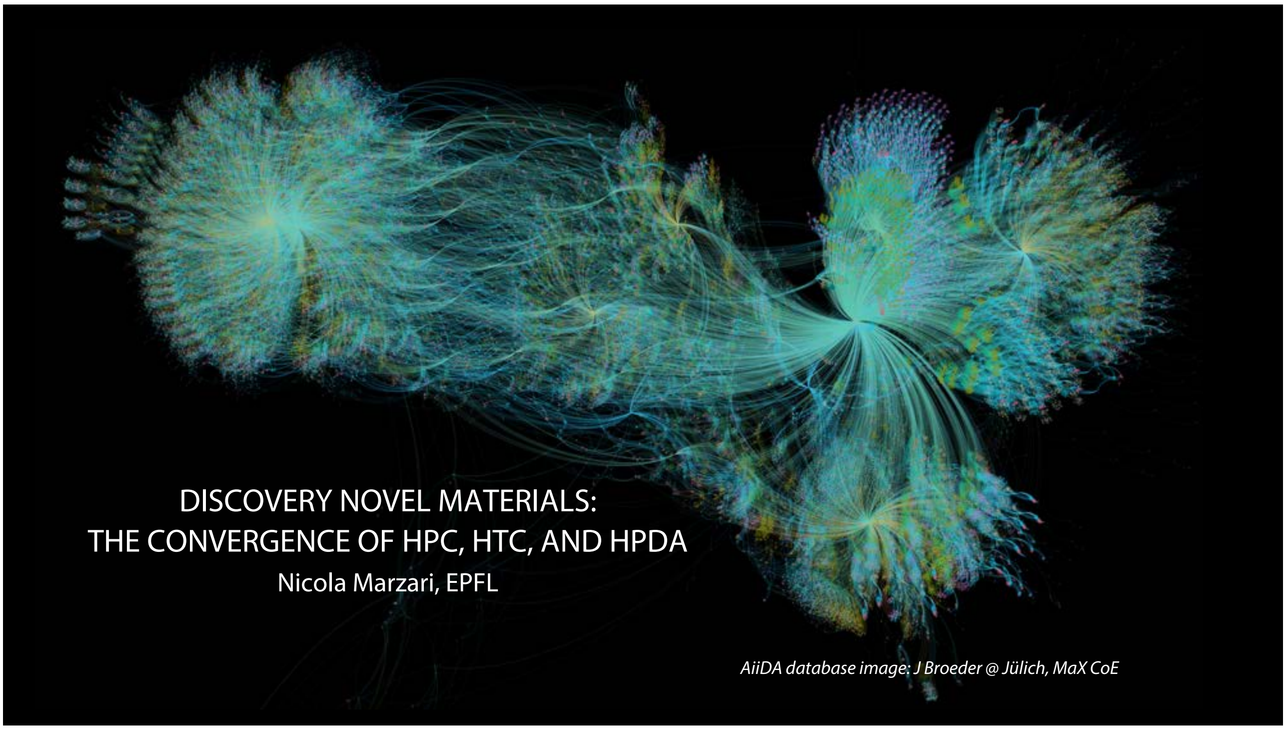
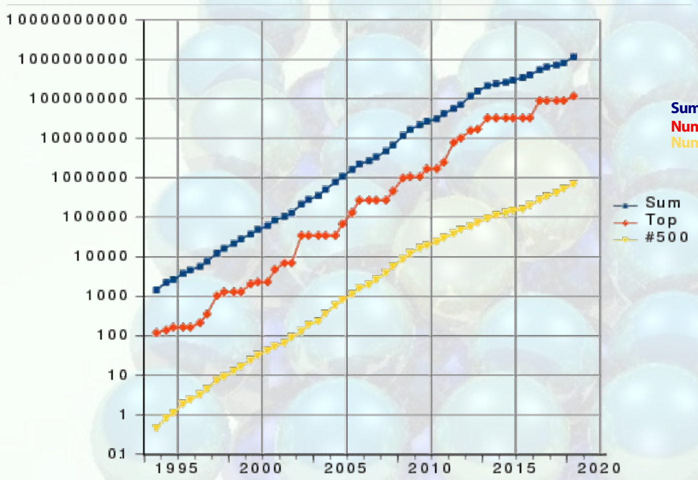


MATERIALS ARE KEY TO SOCIETAL WELL BEING

We need novel materials for:

- **Energy harvesting, conversion, storage, efficiency**
- **Environmental protection and reparation**
- **Information and communication technologies**
- **High-tech and high-value industries**
- **Health care and biomedical engineering**
- **Pharmaceuticals** (crystallization, stability, polytypes)
- **Monitoring, provenance, and safety of foods**
- **Fundamental science (**graphene and 2D materials, topological insulators, entangled spins for quantum computing, high-T_c)
- **Experimental science** (detectors, sensors, magnets)

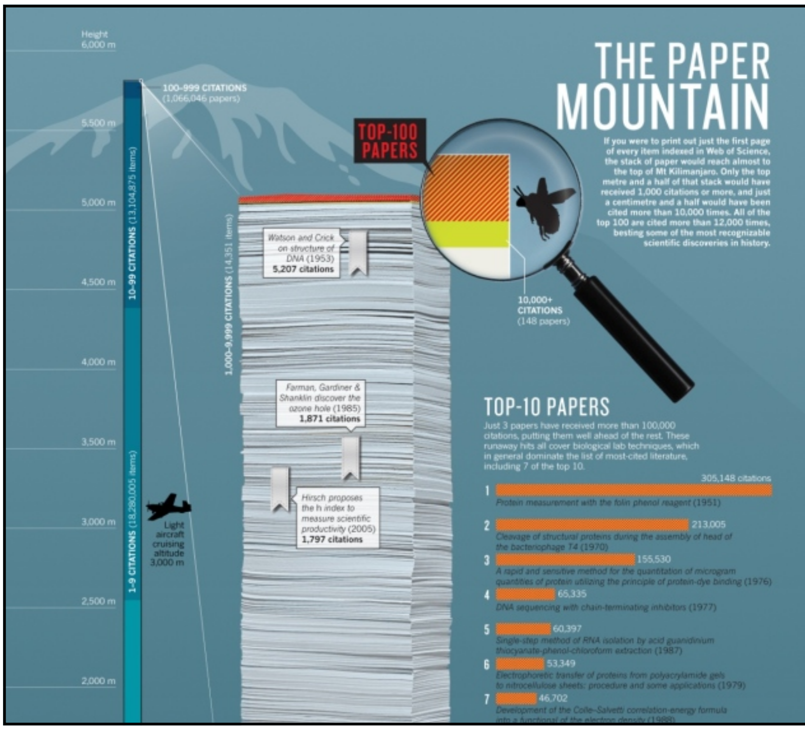
THE BUSINESS MODEL



Computing power 1993-2018

Sum of the top 500 supercomputers
Number 1
Number 500

If brick-and-mortar laboratories were to follow this pace, an experiment that took **one year in 1989** would take **one second in 2018** (30-million-fold increase)

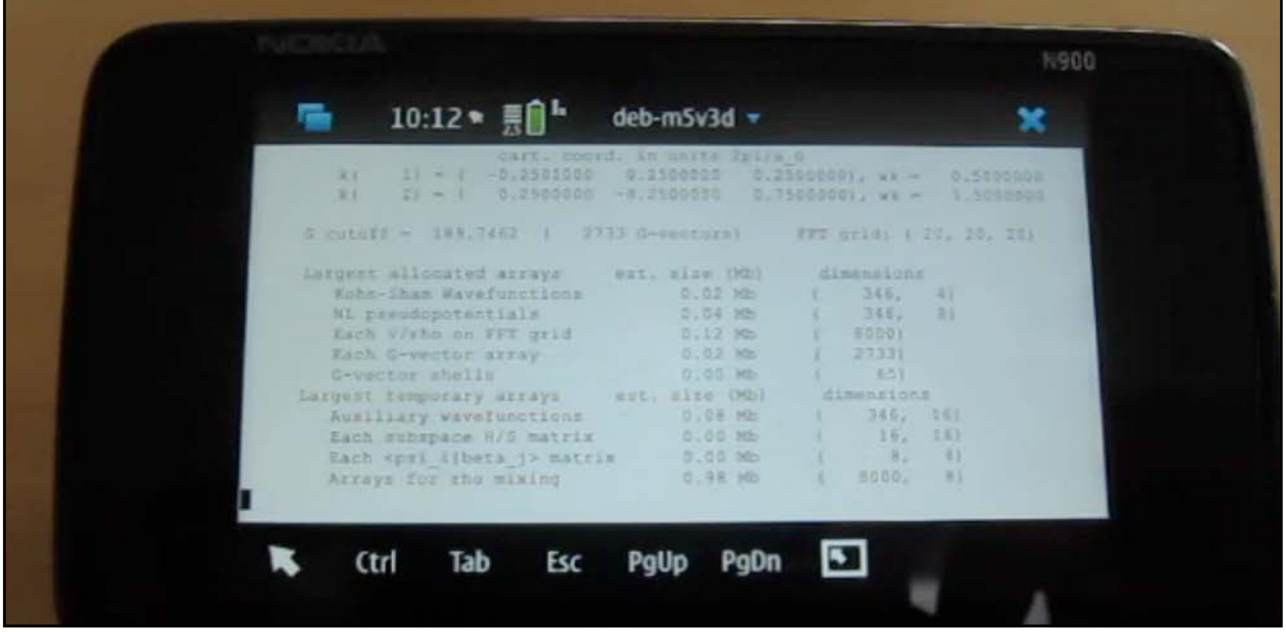


NATURE, October 2014

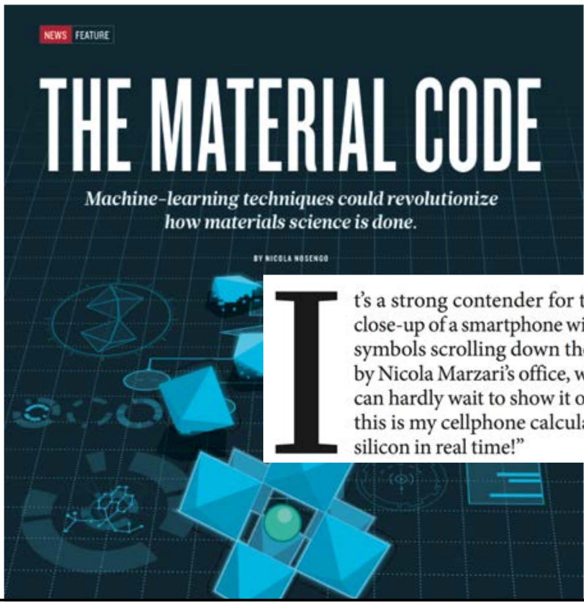
THE TOP 100 PAPERS:

12 papers on DFT in the top-100 most cited papers in the entire scientific literature, ever.

THE REAL HEROES



A SMALL STEP FOR A CELLPHONE, A GIANT LEAP FOR COMPUTERKIND


NEWS FEATURE

THE MATERIAL CODE

Machine-learning techniques could revolutionize how materials science is done.

BY NICOLA NOSENGO

It's a strong contender for the geekiest video ever made: a close-up of a smartphone with line upon line of numbers and symbols scrolling down the screen. But when visitors stop by Nicola Marzari's office, which overlooks Lake Geneva, he can hardly wait to show it off. "It's from 2010," he says, "and this is my cellphone calculating the electronic structure of silicon in real time!"

Nature, 5 May 2016

GREAT ENTHUSIASM FOR MATERIALS DISCOVERY

MAJOR EFFORTS WORLDWIDE

2011 – US: the Materials Genome Initiative
Materials Project (Berkeley), SUNCAT (Stanford), AFLOW (Duke), CHiMaD (NIST)
2014 – 2026 CH: 18 MCHF MARVEL (Computational Design and Discovery of Novel Materials)
2015 – UK: 8.6 MGBP, Materials Computational Discovery Centre, U. Liverpool
2015 – H2020: 14 M€, Centres of Excellence on materials' simulations:
MaX – Materials Design at the Exascale (renewed for 2018-21); NoMaD – Novel Materials Discovery, E-CAM – Simulation and Modelling

2015 - US DOE: 60 M$, 5 Centers on Comp. Materials Science, 4-years renewable: U. Chicago, UC Berkeley, Rutgers, ORNL, USC

2016 – DK: 22 M$, Villum Centre for the Science of Sustainable Fuels and Chemicals (DTU Lyngby and Stanford)

2016 – US NSF: 35 M$, 2 Institutes on Scientific Software, 5 years: MolSSI (Stony Brook), Molecular Sciences Software Institute; SGCI (US San Diego) Science Gateways Community Institute

2017 - US Simons Foundation, 15 M$/year, Center on Computational Quantum Physics

2017 - US Toyota Research Institutes, 35 M$, Predictive Battery Performance news & views

MATERIALS MODELLING

The frontiers and the challenges

Materials simulations have become a dominant force in the world of science and technology. The intellectual challenges lying ahead to sustain such a paradigm shift are discussed.

Nicola Marzari

1) **PREDICTIVE ACCURACY**

2) **REALISTIC COMPLEXITY**

3) **MATERIALS' INFORMATICS**

NATURE MATERIALS | VOL 15 | APRIL 2016 | www.nature.com/naturematerials 381

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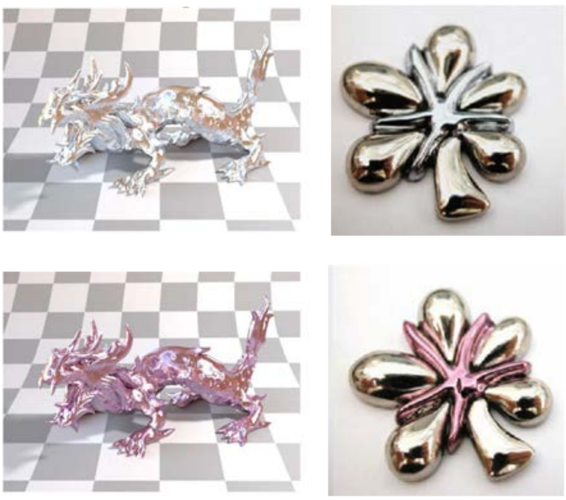
HOW WELL CAN WE REPRODUCE THE REAL WORLD?



with Gianluca Prandini (EPFL) and Gian-Marco Rignanese (UC Louvain)

ELECTRICAL RESISTIVITY (TEMP, DOPING)

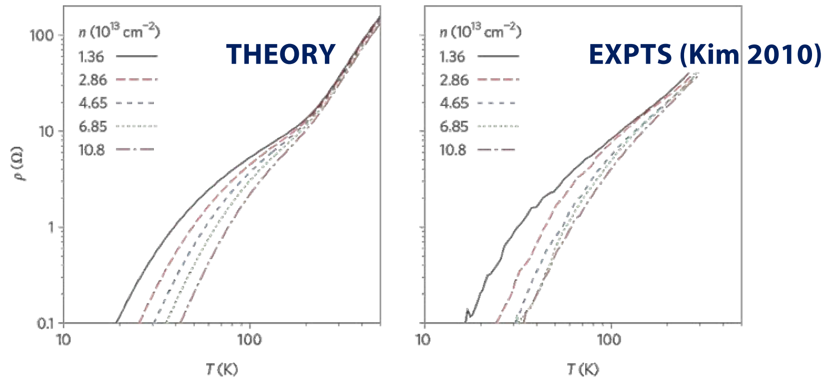
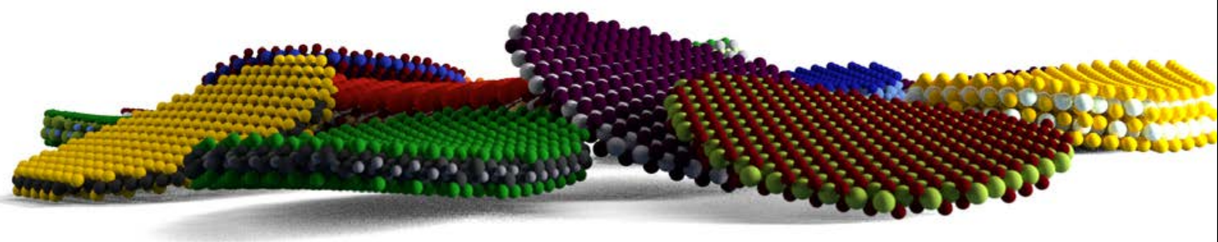


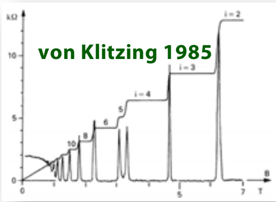
Figure 1 | Electrical resistivity of graphene as a function of temperature and doping (ρ, electrical resistivity; T, temperature; n, carrier density). Left panel: first-principles results obtained using a combination of density-functional perturbation theory, many-body perturbation theory and Wannier interpolations to solve the Boltzmann transport equation. Right panel: experimental data. Adapted from ref. 4, American Chemical Society.

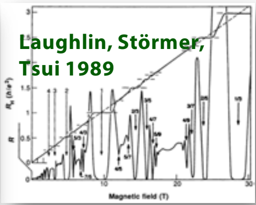
C.-H. Park *et al.*, Nano Letters (2014)
T. Y. Kim, C.-H. Park, and N. Marzari, Nano Letters (2016)

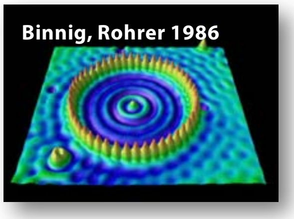
COMPUTATIONAL EXFOLIATION OF ALL KNOWN INORGANIC MATERIALS

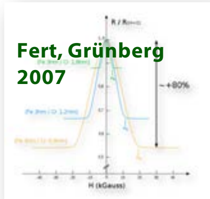


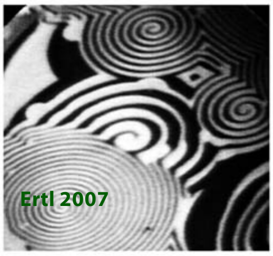
PHYSICS AND CHEMISTRY IN LOW DIMENSIONS

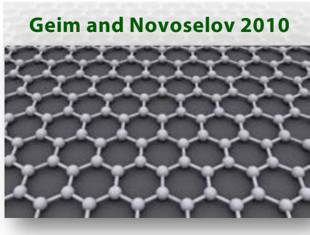




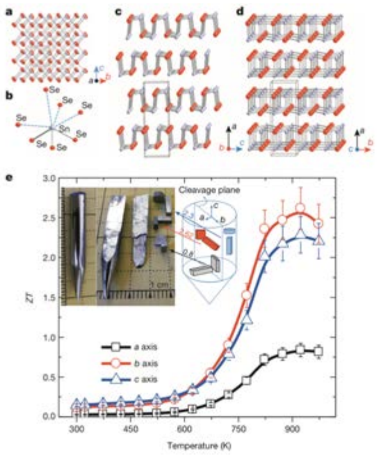


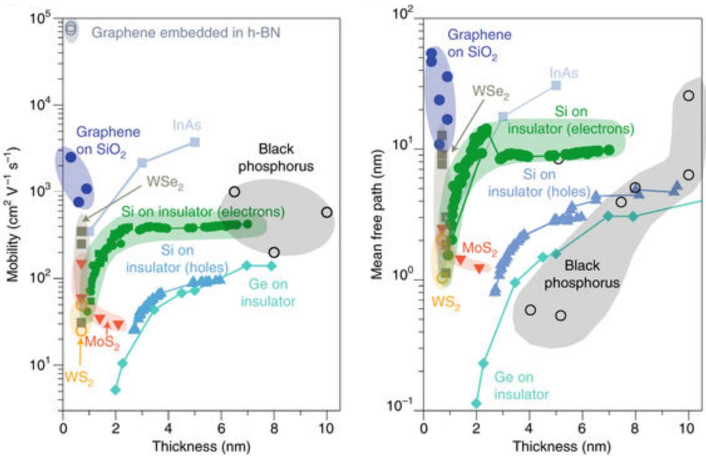






WHY LAYERED OR LOW-DIMENSIONAL MATERIALS?

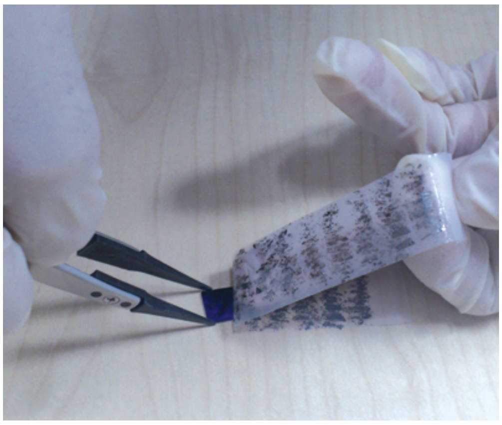




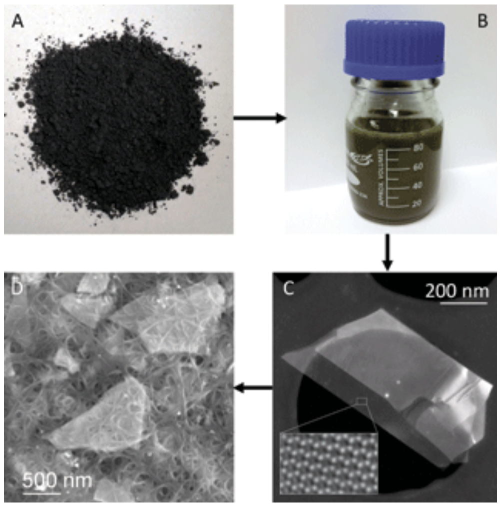
M. Kanatzidis, nature 13184 (2014)

G. Iannaccone *et al.*, Nature Nano (2018)

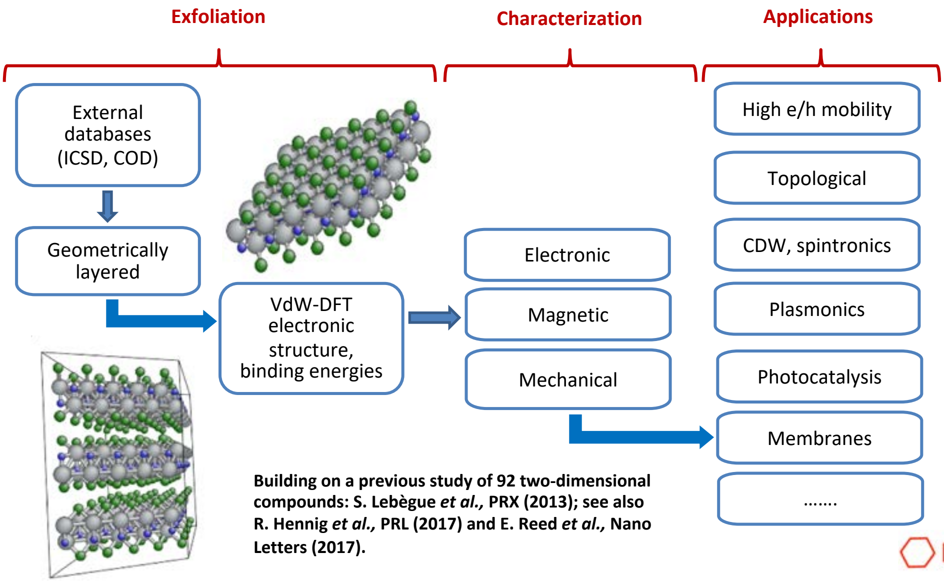
HOW DO WE PRODUCE 2D MATERIALS?



Mechanical (e.g. Geim/Novoselov, fig. from Nature/NUS) **or liquid exfoliation** (e.g. Nicolosi/Coleman, fig. from Science). Also, bottom-up: **CVD and wet chemical synthesis.**

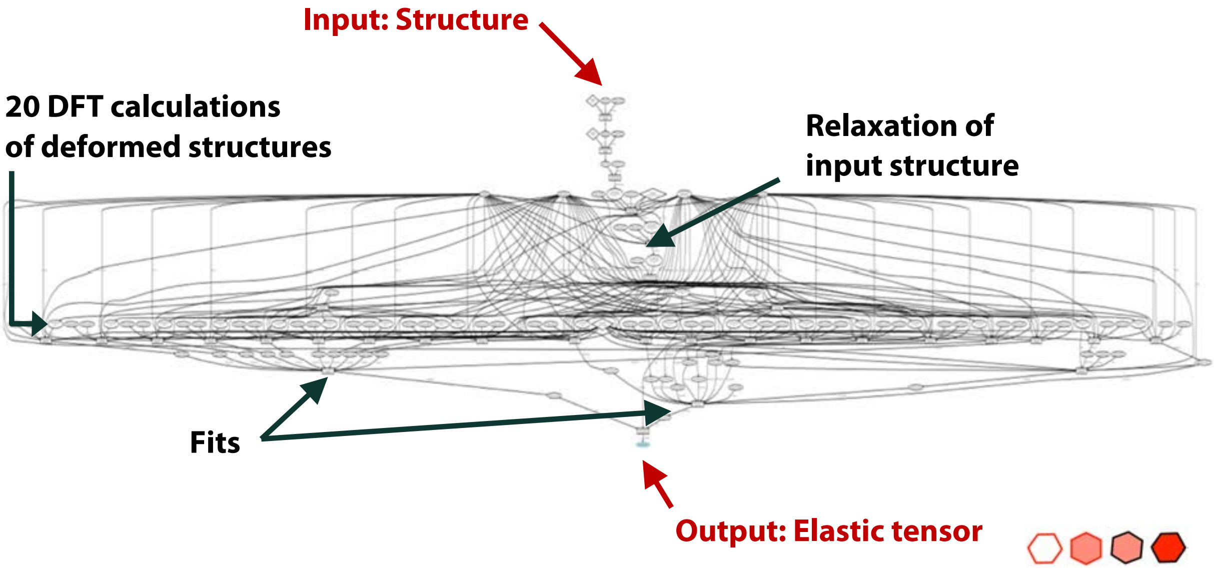


HIGH-THROUGHPUT COMPUTATIONAL EXFOLIATION



Building on a previous study of 92 two-dimensional compounds: S. Lebègue *et al.*, PRX (2013); see also R. Hennig *et al.*, PRL (2017) and E. Reed *et al.*, Nano Letters (2017).

AUTOMATIC WORKFLOWS: FROM STRUCTURE TO PROPERTY



COMPUTATIONAL SCIENCE AS A MIDDLE-AGES WORKSHOP

COMPUTATIONAL SCIENCE SHOULD BE…

reproducible
often not possible from the data reported in papers

searchable
find existing calculations, reuse them and data-mine

reliable
results persisted in repositories, automated procedures to reduce errors and verify results

shareable
community to share results, cross-validate them, and boost scientific discovery

OPEN SCIENCE PLATFORM FOR MATERIALS DISCOVERY

AiiDA

MATERIALS CLOUD

http://aiida.net

http://materialscloud.org

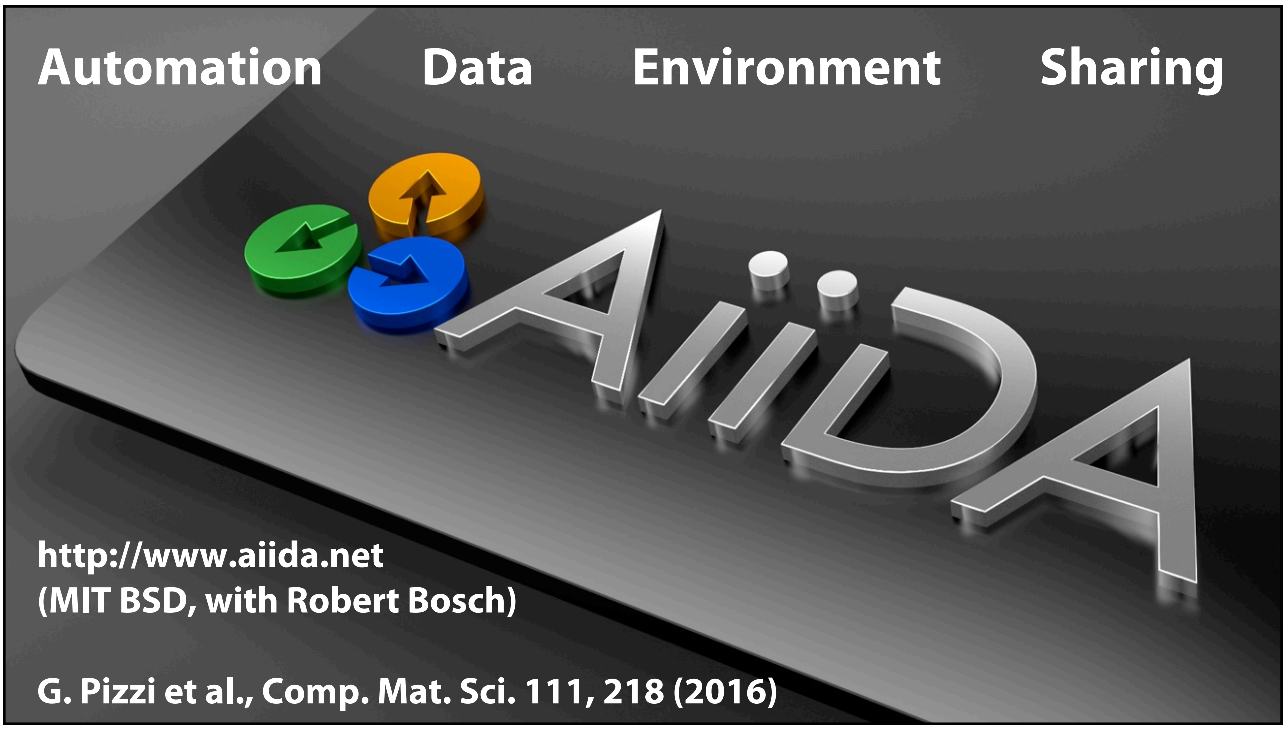
ADES MODEL FOR COMPUTATIONAL SCIENCE

ADES

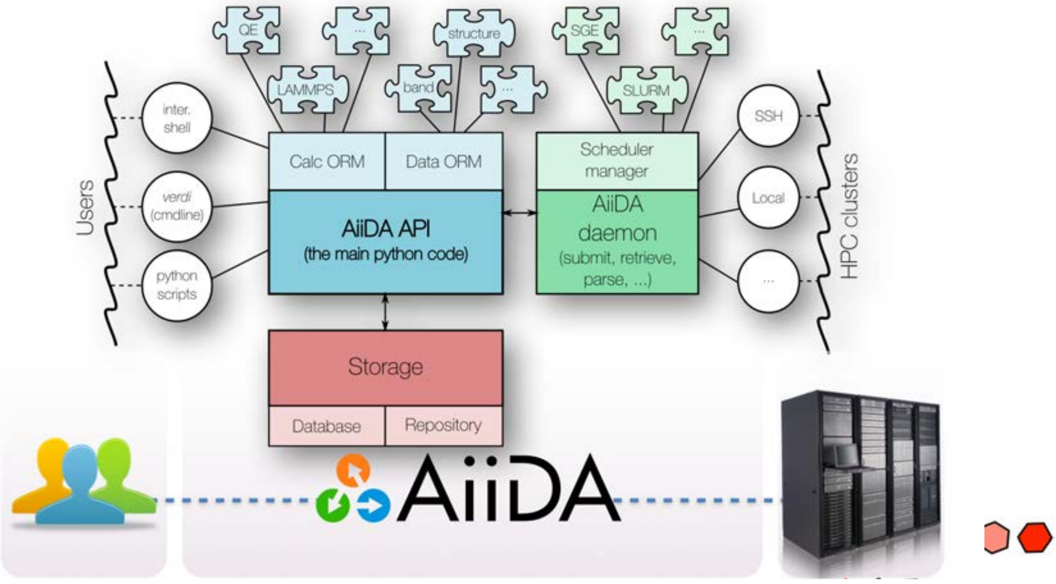
Automation	Data	Environment	Sharing
Remote management Coupling to data High-throughput	Storage Database Provenance	High-level workspace Scientific workflows Data analytics	Social ecosystem Repository pipelines Standardization

Low-level pillars — *User-level pillars*

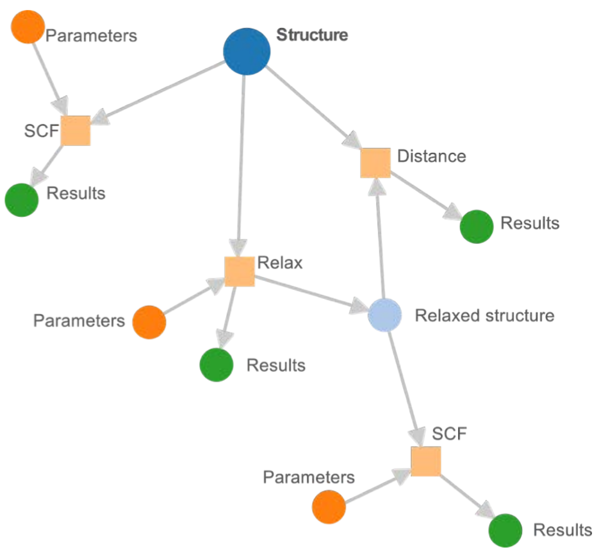
G. Pizzi et al., Comp. Mat. Sci. 111, 218 (2016)



MATERIALS' INFORMATICS PYTHON FRAMEWORK

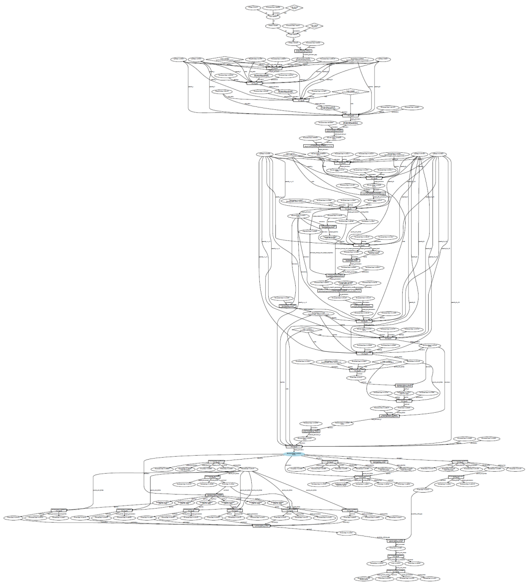


WORKFLOWS AS DIRECTED ACYCLIC GRAPHS

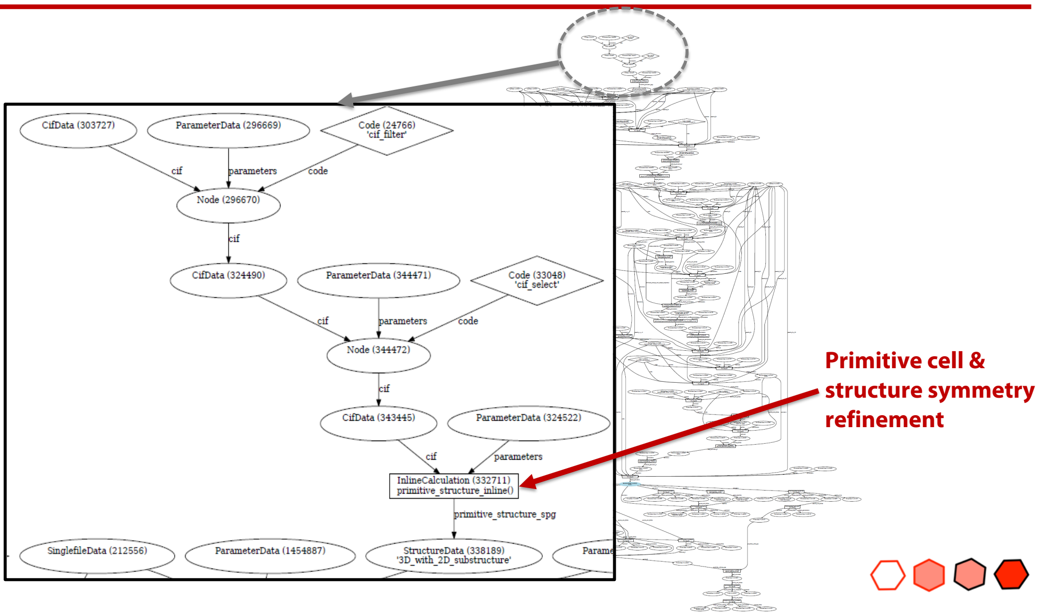


Nodes:
Calculations
Codes
Data

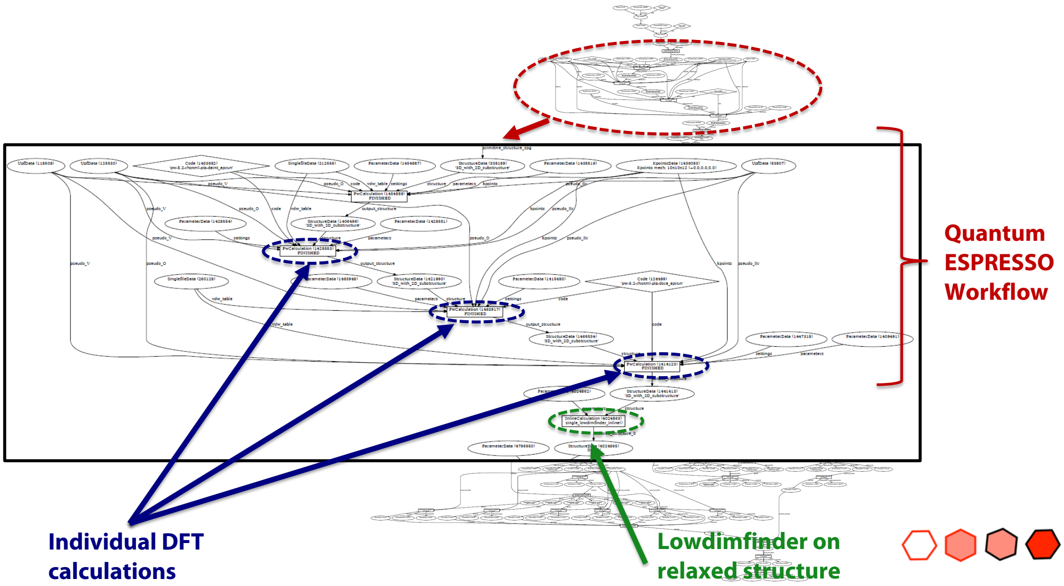
LET'S START FROM A MATERIAL ($VOBr_2$)



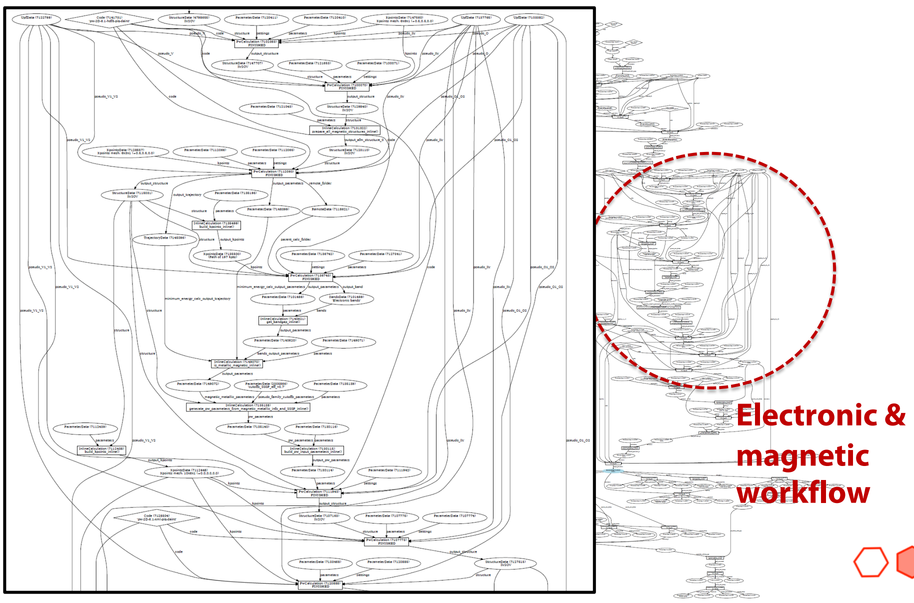
FROM ICSD TO A WORKING STRUCTURE



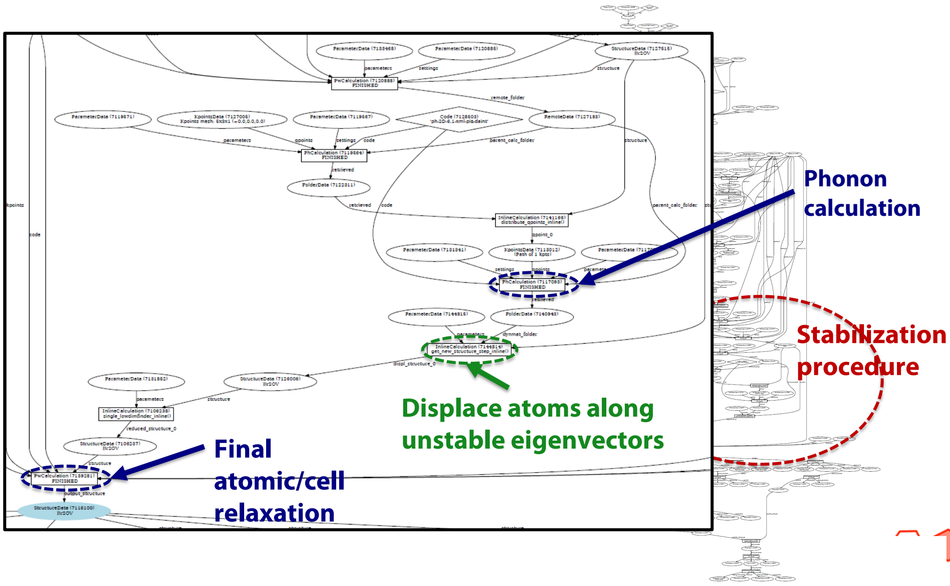
3D RELAXATION



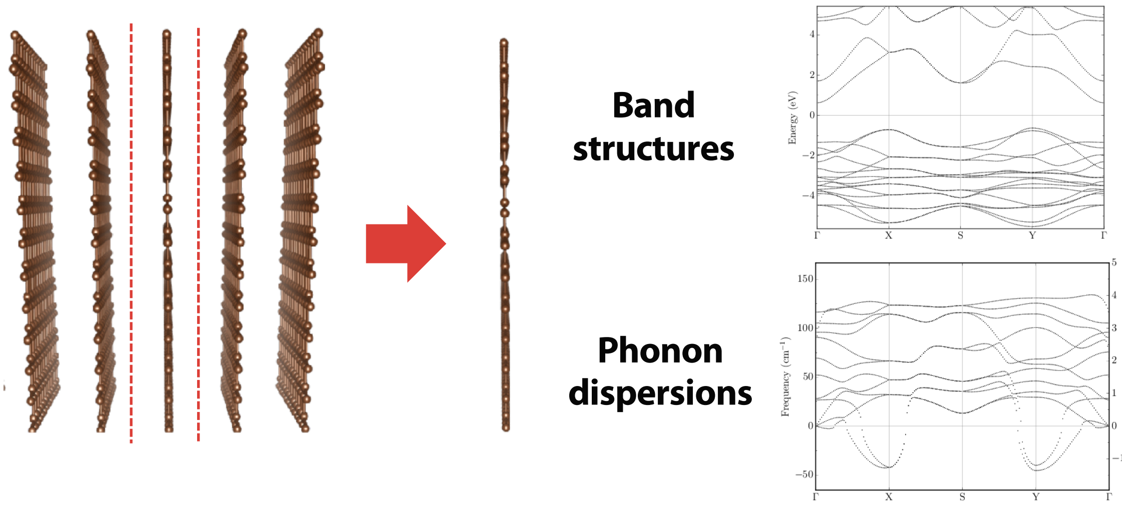
MAGNETIC SCREENING OF THE 2D MONOLAYER



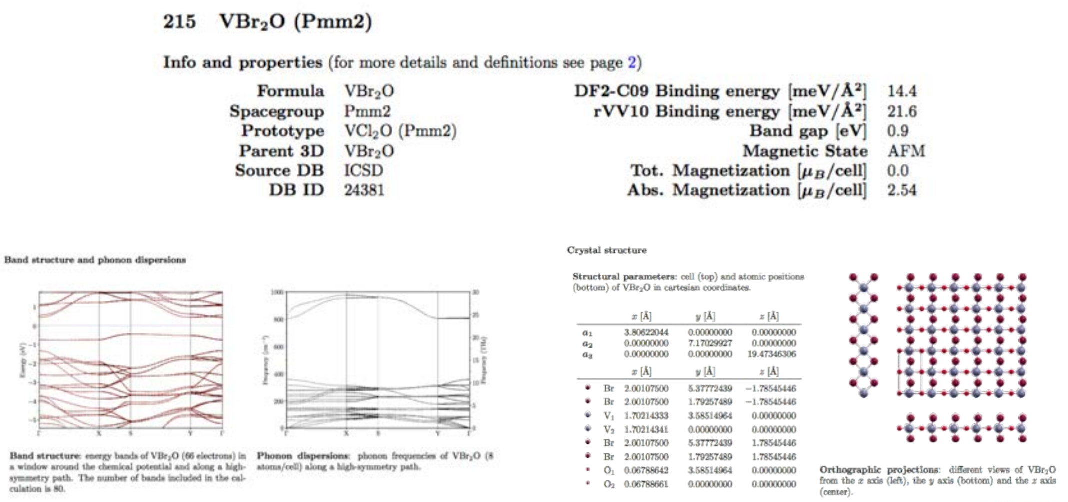
REMOVING MECHANICAL INSTABILITIES



STABILITY ANALYSIS: MAGNETIC AND MECHANICAL



FINALLY…


215 VBr_2O (Pmm2)

Info and properties (for more details and definitions see page 2)

Formula	VBr_2O	**DF2-C09 Binding energy** [meV/Å²]	14.4
Spacegroup	Pmm2	**rVV10 Binding energy** [meV/Å²]	21.6
Prototype	VCl_2O (Pmm2)	**Band gap** [eV]	0.9
Parent 3D	VBr_2O	**Magnetic State**	AFM
Source DB	ICSD	**Tot. Magnetization** [μ_B/cell]	0.0
DB ID	24381	**Abs. Magnetization** [μ_B/cell]	2.54

Band structure and phonon dispersions

Band structure: energy bands of VBr_2O (66 electrons) in a window around the chemical potential and along a high-symmetry path. The number of bands included in the calculation is 80.

Phonon dispersions: phonon frequencies of VBr_2O (8 atoms/cell) along a high-symmetry path.

Crystal structure

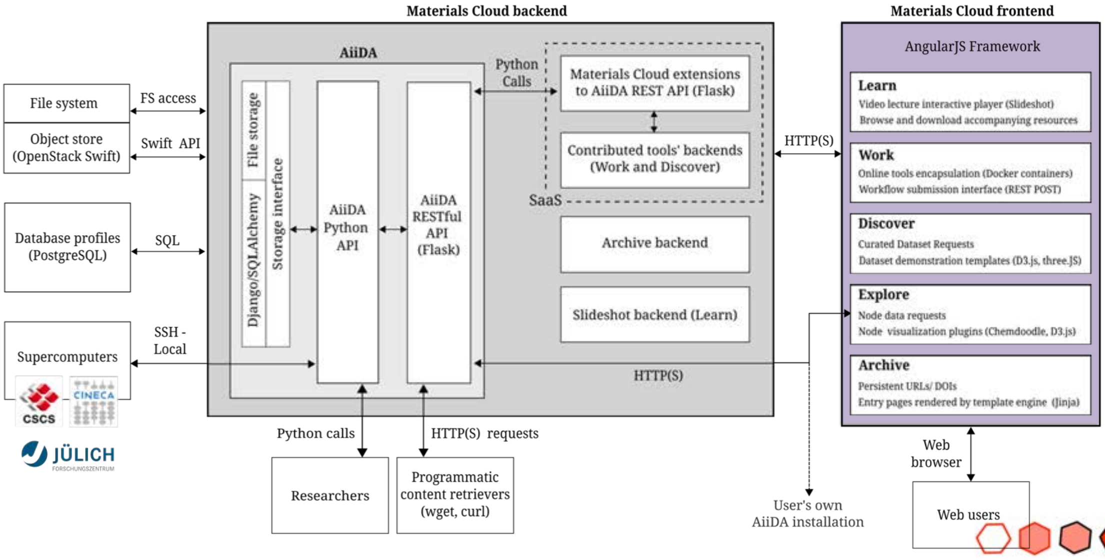
Structural parameters: cell (top) and atomic positions (bottom) of VBr_2O in cartesian coordinates.

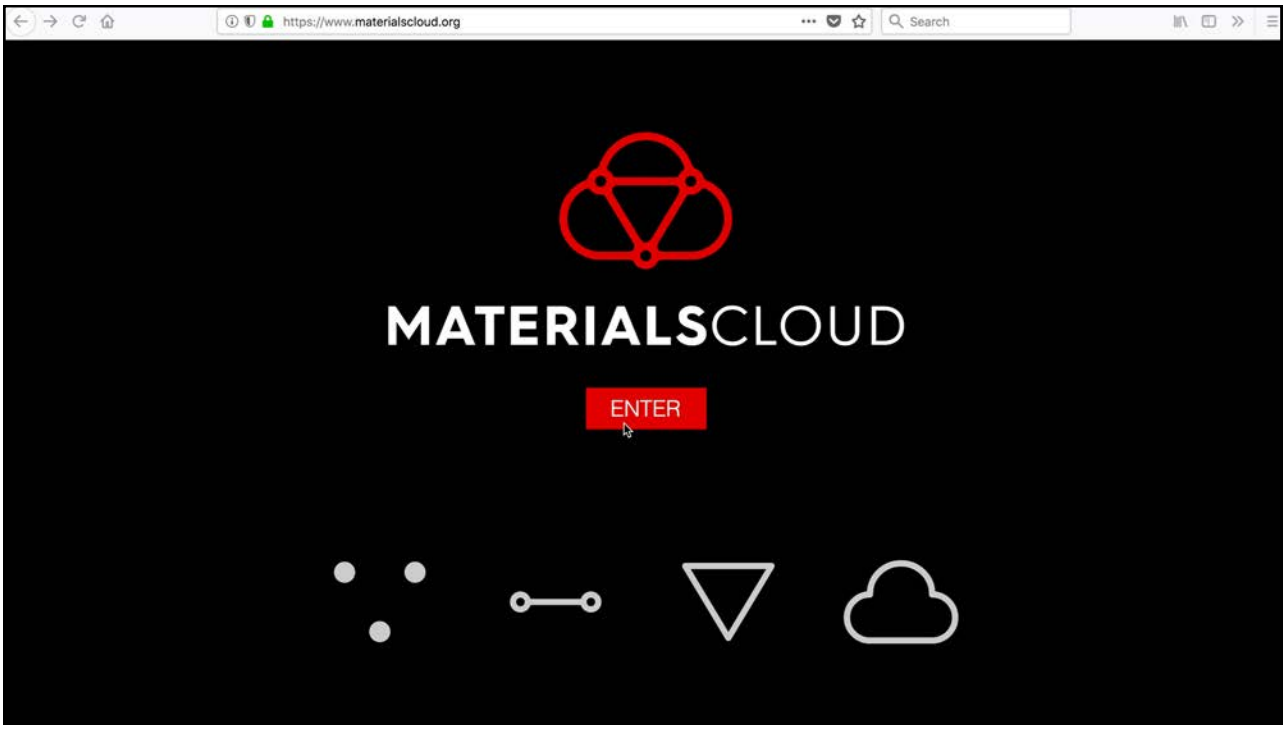
	x [Å]	y [Å]	z [Å]
a_1	3.80622044	0.00000000	0.00000000
a_2	0.00000000	7.17029927	0.00000000
a_3	0.00000000	0.00000000	19.47346306

	x [Å]	y [Å]	z [Å]
Br	2.00107500	5.37772439	−1.78545446
Br	2.00107500	1.79257489	−1.78545446
V_1	1.70214333	3.58514964	0.00000000
V_2	1.70214341	0.00000000	0.00000000
Br	2.00107500	5.37772439	1.78545446
Br	2.00107500	1.79257489	1.78545446
O_1	0.06788642	3.58514964	0.00000000
O_2	0.06788661	0.00000000	0.00000000

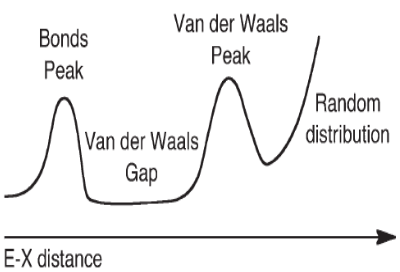
Orthographic projections: different views of VBr_2O from the x axis (left), the y axis (bottom) and the z axis (center).

SERVICES AND DISSEMINATION: http://www.materialscloud.org



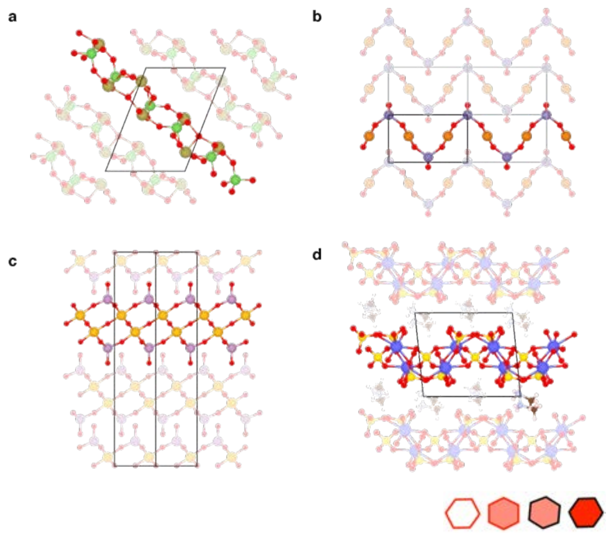


GEOMETRIC IDENTIFICATION OF LAYERED MATERIALS



S. Alvarez, Dalton Transactions (2013)

$$d_{i,j} < r_i^{vdw} + r_j^{vdw} - \Delta$$

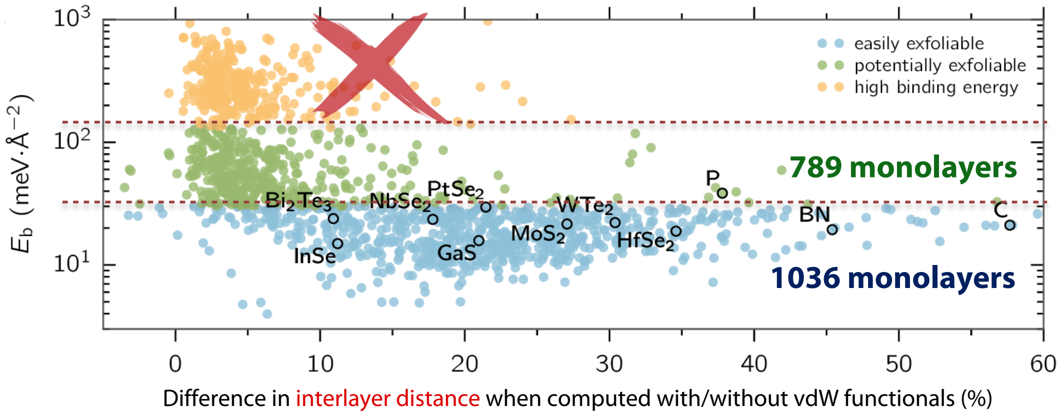


HOW MANY CANDIDATES? GEOMETRIC SCREENING

	Unique to COD	Unique to ICSD	Common to both	Total
Entries analyzed	307616	172370		479986*
CIF inputs	99212	87070		186282*
Unique 3D structures	60354	34548	13521	108423
Layered 3D structures	1180	3257	1182	5619

*At this level unicity is not tested

HOW MANY CANDIDATES? QUANTUM SCREENING



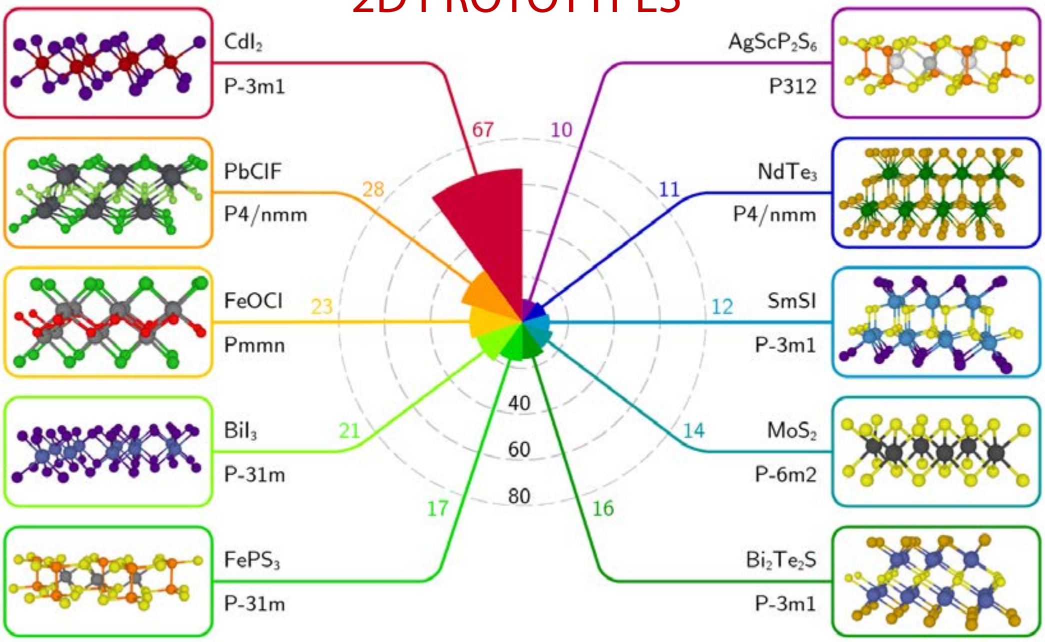
Not exfoliable

Potentially exfoliable

Easily exfoliable

- ***$E_b < 30$ meV/Å^2 (DF2-C09) or $E_b < 35$ meV/Å^2 (rVV10) → 2D, easily exfoliable***
- ***In-between → 2D, potentially exfoliable***
- ***$E_b > 130$ meV/Å^2 → not 2D (discarded)***

2D PROTOTYPES



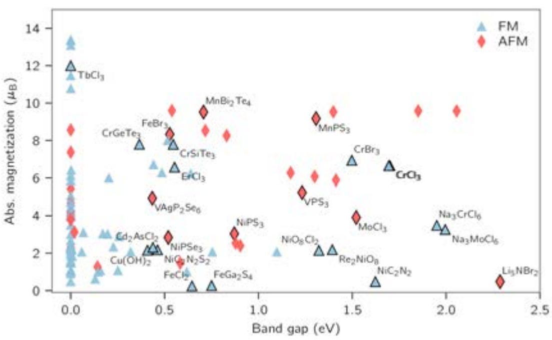
BROAD MATERIALS PORTFOLIO FOR ELECTRONICS

Luisier, Marzari,… IEEE Transactions on Electron Devices (2018)

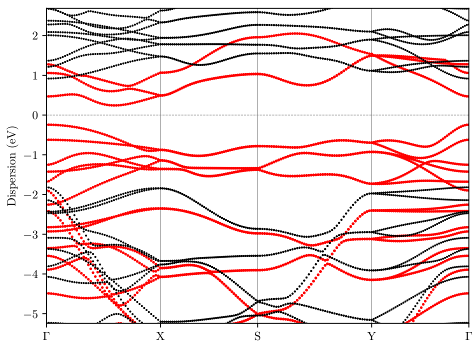
PHOTOCATALYTIC WATER SPLITTING

SOME FERMIOLOGY

Magnetic metals and insulators

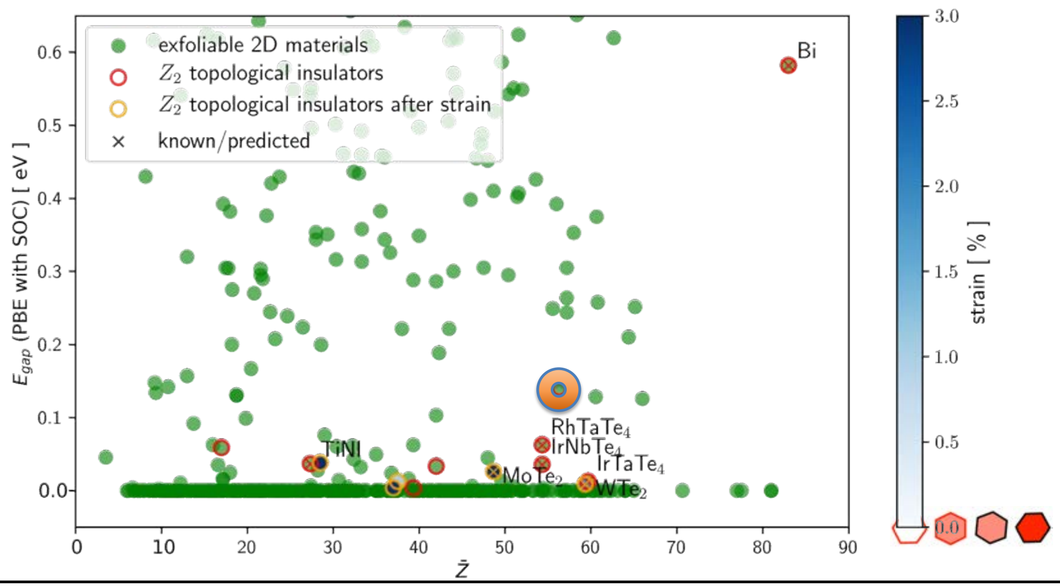


Half-semiconductors



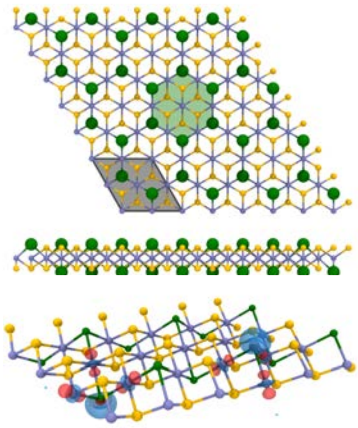
In collaboration with K. Thygesen (DTU)

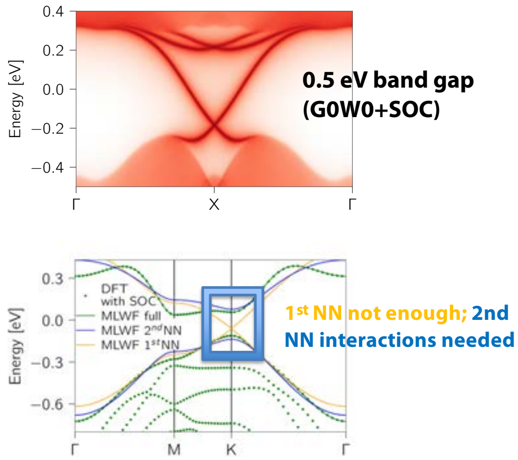
Z_2 TOPOLOGICAL INSULATORS



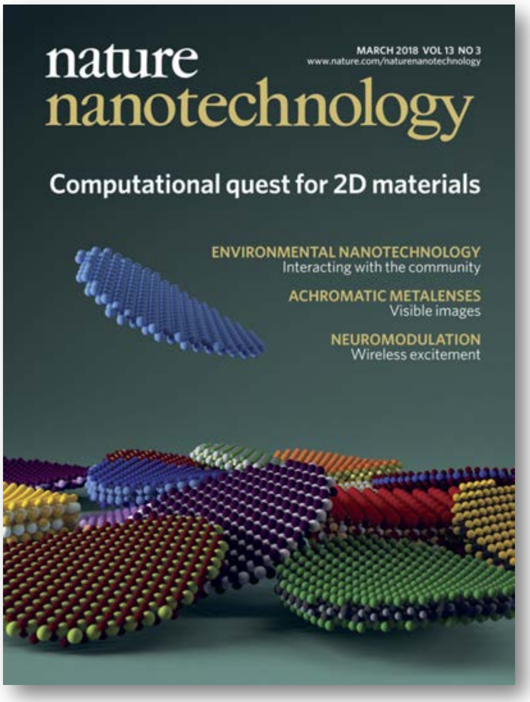
THE DISCOVERY OF JACUTINGAITE

MONOLAYER JACUTINGAITE AS A KANE-MELE QSHI





A. Marrazzo *et al.*, Phys. Rev. Lett. 120 117701 (2018)



THERE IS PLENTY OF ROOM AT THE TOP

- High electron/hole mobility devices
- Topological insulators, quantum computing
- Ferromagnetic/spintronics in 2D
- Charge-density waves and superconductors
- Plasmonics, transparent conductors

3D layered parents:

- Solid-state ionic conductors
- Hydrogen or oxygen evolution catalysts
- Membranes for filtration/separation
- Piezo, ferro, and thermoelectrics

N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi and N. Marzari, Nature Nanotechnology 13, 246 (2018)

2D ACKNOWLEDGMENTS

Nicolas Mounet
CERN

Marco Gibertini
U. of Geneva

Philippe Schwaller
IBM

Davide Campi

Andrius Merkys
Vilnius

Antimo Marrazzo

Thibault Sohier

Ivano E. Castelli
DTU

Andrea Cepellotti
UC Berkeley

Giovanni Pizzi

SUPPORT FROM

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

http://epfl.ch

École Polytechnique Fédérale de Lausanne

MARVEL

http://nccr-marvel.ch

Swiss National Centre for Computational Design and Discovery of Novel Materials

MAX DRIVING THE EXASCALE TRANSITION

http://max-centre.eu

H2020 Centre of Excellence MaX: Materials Design at the Exascale

nffa.eu

PRACE

EMMC

FNSNF Swiss National Science Foundation

PASC Platform for Advanced Scientific Computing

Swiss National Science Foundation
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
Max-Planck-EPFL Centre
PASC
PRACE
IBM
Constellium
Innosuisse
Solvay
Varinor

SCIENCE CONCLUSIONS

There is a push **to accelerate invention and discovery in science and technology**, and especially to transform and accelerate the design and discovery of novel materials.

Key enablers:

- **the predictive accuracy of quantum simulations**
- **HPC/HTC capacity scaling**
- **the synergy of modeling and simulation with the ideas and tools of computer science**

DATA CONCLUSIONS

- In computational science, **data are generated, not harvested** (the workflows that create properties and data from a structure are key).
- **Importance of data-on-demand (**high-throughput pushes the development of robust workflows that can calculate properties automatically).
- I think there are three kind of data:
  - **Social (harvested, mostly uncontrolled conditions)**
  - **Experimental (harvested, controlled conditions)**
  - **Computational (generated, controlled conditions)**

FURTHER THOUGHTS ON COMPUTATIONAL SCIENCE

- **Computational science is central to the entire scientific and technological effort in the 21st century** – no other enabler can compete in terms of speed and acceleration
- Very few have understood its structural needs, and long-term opportunity
- As a side note, it is **a powerfully democratic force**, since it can be shared freely