

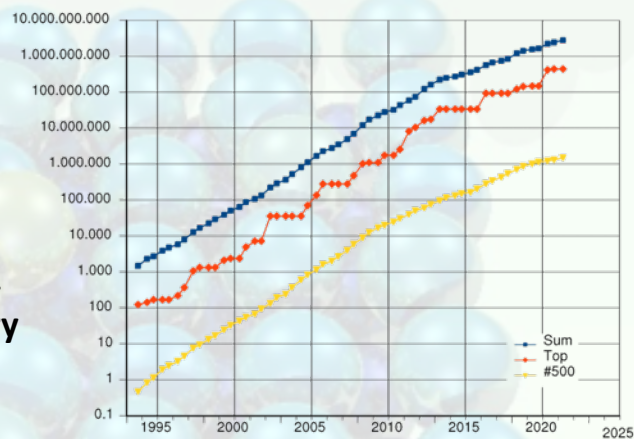
# DIGITAL INFRASTRUCTURES EMPOWERING MATERIALS DISCOVERY

Nicola Marzari, EPFL & PSI

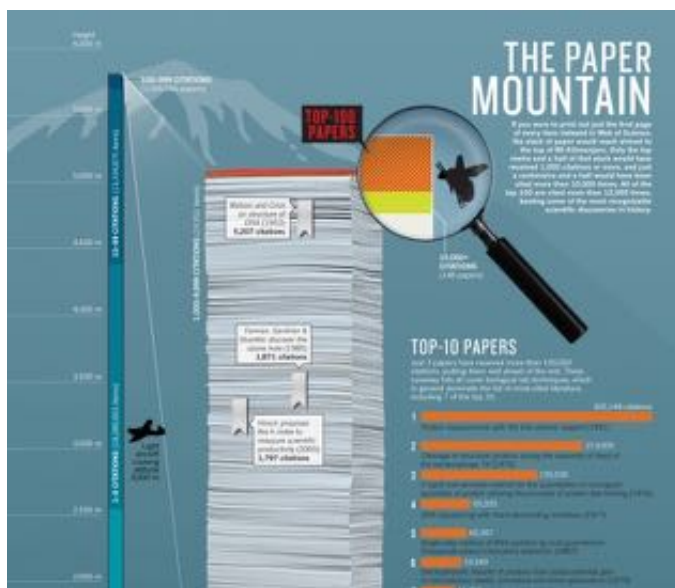
## THE RISE OF COMPUTATIONAL SCIENCE

A calculation that took **one year in 1993** takes **30 seconds in 2022** (1-million-fold increase).

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



## IMPACT OF COMPUTATIONAL QUANTUM MECHANICS



**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**



## MOST CITED PAPERS IN THE HISTORY OF APS

	Journal	# cites	Title	Author(s)
1	PRL (1996)	78085	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
2	PRB (1988)	67303	Development of the Colle-Salvetti Correlation-Energy ...	Lee, Yang, Parr
3	PRB (1996)	41683	Efficient Iterative Schemes for Ab Initio Total-Energy ...	Kresse and Furthmüller
4	PR (1965)	36841	Self-Consistent Equations Including Exchange and Correlation ...	Kohn and Sham
5	PRA (1988)	36659	Density-Functional Exchange-Energy Approximation ...	Becke
6	PRB (1976)	31865	Special Points for Brillouin-Zone Integrations	Monkhorst and Pack
7	PRB (1999)	30940	From Ultrasoft Pseudopotentials to the Projector Augmented ...	Kresse and Joubert
8	PRB (1994)	30801	Projector Augmented-Wave Method	Bloch
9	PR (1964)	30563	Inhomogeneous Electron Gas	Hohenberg and Kohn
10	PRB (1993)	19903	Ab initio Molecular Dynamics for Liquid Metals	Kresse and Hafner
11	PRB (1992)	17286	Accurate and Simple Analytic Representation of the Electron ...	Perdew and Wang
12	PRB (1990)	15618	Soft Self-Consistent Pseudopotentials in a Generalized ...	Vanderbilt
13	PRB (1992)	15142	Atoms, Molecules, Solids, and Surfaces - Applications of the ...	Perdew, Chevary, ...
14	PRB (1981)	14673	Self-Interaction Correction to Density-Functional Approx. ...	Perdew and Zunger
15	PRB (1986)	13907	Density-Functional Approx. for the Correlation-Energy ...	Perdew
16	RMP (2009)	13513	The Electronic Properties of Graphene	Castro Neto et al.
17	PR (1934)	12353	Note on an Approximation Treatment for Many-Electron Systems	Møller and Plesset
18	PRB (1972)	11840	Optical Constants on Noble Metals	Johnson and Christy
19	PRB (1991)	11580	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier and Martins
20	PRL (1980)	10784	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley and Alder

Marzari  
(11 Apr 2019)



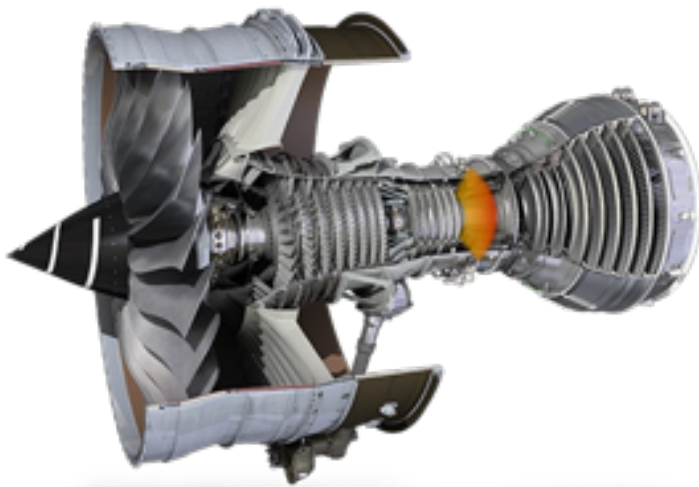
## THE RISE OF MATERIALS SCIENCE

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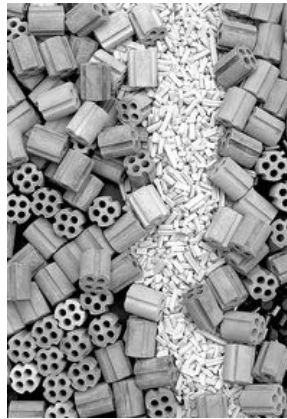
## IF WE FLY AGAIN...

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## THE MOST IMPORTANT MATERIAL EVER?

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## MATERIALS ARE KEY TO SOCIETAL WELL BEING

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We need novel materials for:

- **Energy harvesting, conversion, storage, efficiency**
- **Environmental protection and reparation**
- **High-tech and high-value industries**
- **Information and communication technologies**
- **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)



## COMPUTATIONAL MATERIALS DESIGN AND DISCOVERY

### 3 Technologies That Could Create Trillion-Dollar Markets Over the Next Decade

By Greg Satell | Updated April 21, 2019 9:00 a.m. ET



Yet today, we're in the midst of a **materials revolution**. Powerful simulation techniques, combined with increased computing power and machine learning, are enabling researchers to automate much of the discovery process, vastly accelerating the development of new materials

BARRON'S (April 2019)



## THE COLOUR OF MATERIALS: REFLECTIVITY IN THE OPTICAL LIMIT

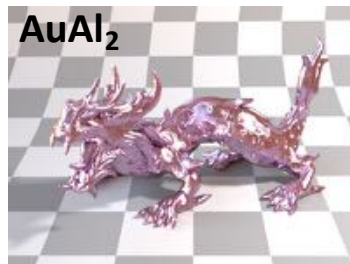
Os



Cs



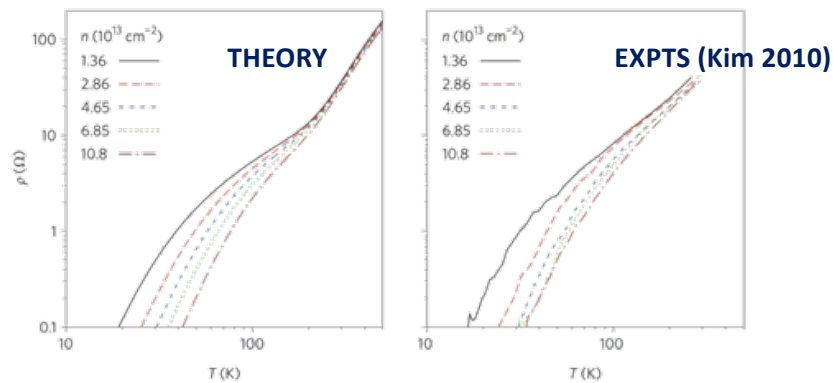
AuAl<sub>2</sub>



G. Prandini, G.M. Rignanese, and N. Marzari,  
*npj Computational Materials* 5, 129 (2019)



## PHONON-LIMITED RESISTIVITY IN DOPED GRAPHENE

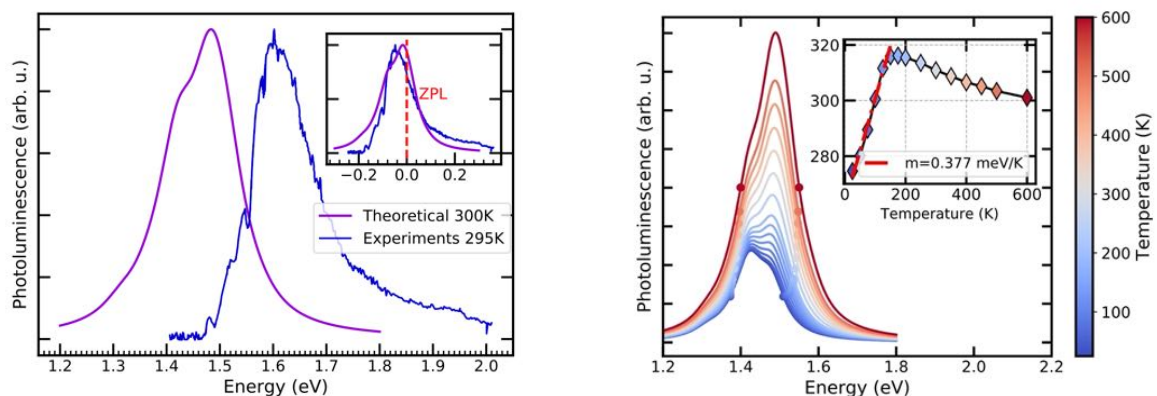


**Figure 1** | Electrical resistivity of graphene as a function of temperature and doping ( $\rho$ , electrical resistivity;  $T$ , temperature;  $n$ , carrier density). Left panel: first-principles results obtained using a combination of density-functional perturbation theory, many-body perturbation 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* 14, 1113 (2014)  
 T. Y. Kim, C.-H. Park, and N. Marzari, *Nano Letters* 16, 2439 (2016)



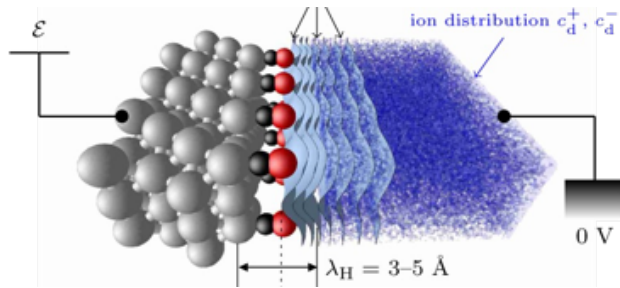
## READ-OUT OF A QUBIT: PHOTOLUMINESCENCE OF A DEFECT



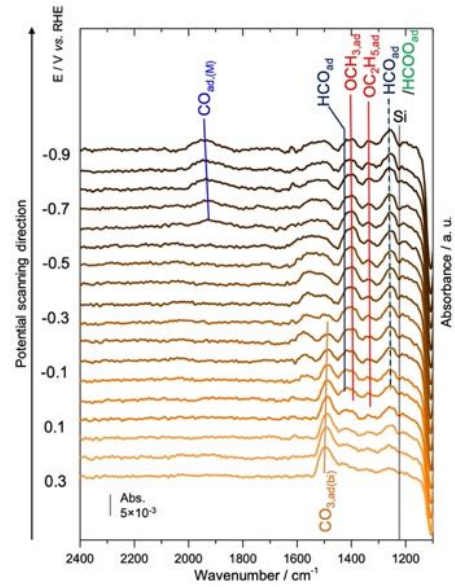
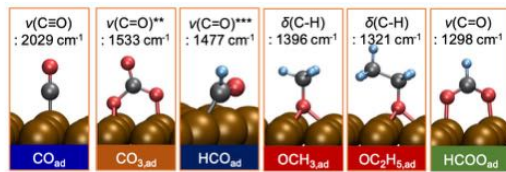
F. Libbi, P.M. de Melo, Z. Zanoli, M. Verstraete, and N. Marzari, *Phys. Rev. Lett.* 128, 167401 (2022)



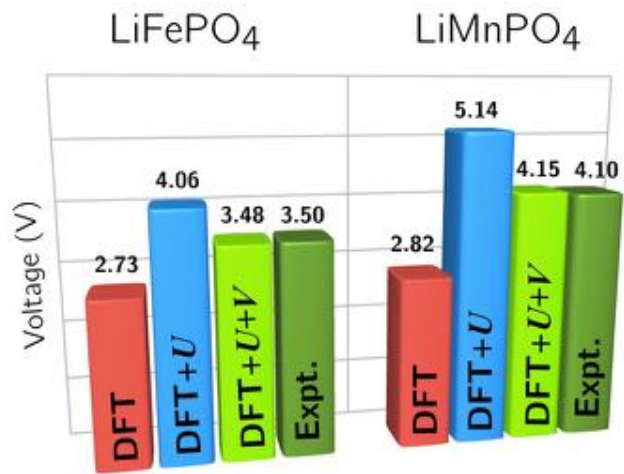
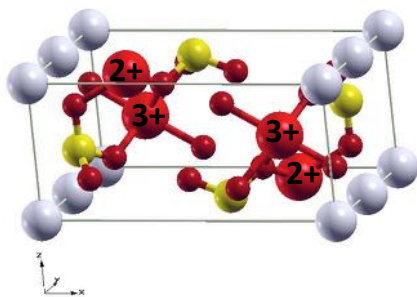
## OPERANDO SPECTROSCOPIES



O. Andreussi *et al.*, *J. Chem. Phys.* **136**, 064102 (2012)  
 F. Nattino *et al.*, *J. Chem. Phys.* **150**, 041722 (2019)



## LI-ION CATHODES



M. Cococcioni and N. Marzari, *Phys. Rev. Materials* **3**, 033801 (2019)  
 I. Timrov *et al.*, *arXiv* (2022)



## SOME NEW PHYSICS DRIVEN BY THERMOELECTRICS

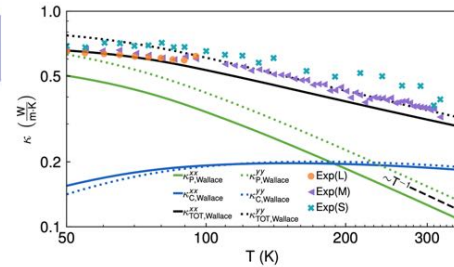
nature  
physics

ARTICLES

<https://doi.org/10.1038/s41567-019-0520-4>

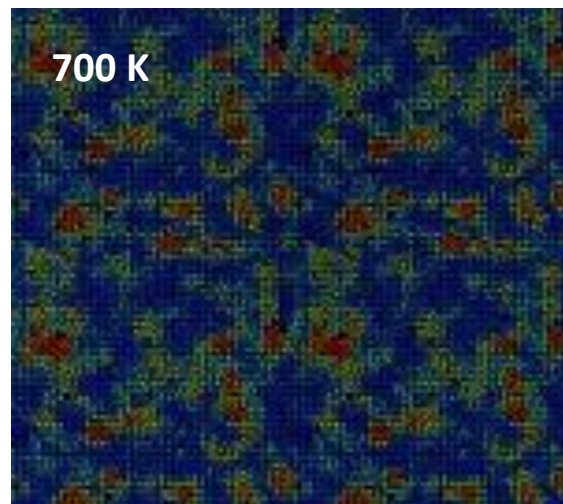
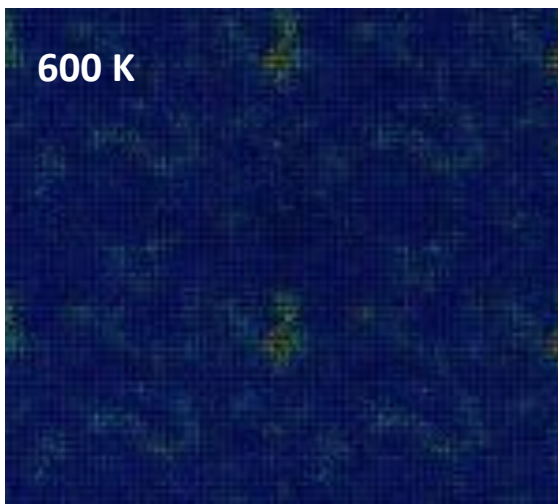
### Unified theory of thermal transport in crystals and glasses

Michele Simoncelli<sup>1</sup>, Nicola Marzari<sup>1</sup> and Francesco Mauri<sup>2\*</sup>



$$\kappa^{\alpha\beta} = \kappa_{\text{P}}^{\alpha\beta} + \frac{\hbar^2}{k_B T^2} \frac{1}{V N_c} \sum_{\mathbf{q}} \sum_{s \neq s'} \frac{\omega(\mathbf{q})_s + \omega(\mathbf{q})_{s'}}{2} V^\alpha(\mathbf{q})_{s,s'} V^\beta(\mathbf{q})_{s',s} \times \\ \times \frac{\omega(\mathbf{q})_s \bar{N}^T(\mathbf{q})_s [\bar{N}^T(\mathbf{q})_s + 1] + \omega(\mathbf{q})_{s'} \bar{N}^T(\mathbf{q})_{s'} [\bar{N}^T(\mathbf{q})_{s'} + 1]}{4[\omega(\mathbf{q})_{s'} - \omega(\mathbf{q})_s]^2 + [\Gamma(\mathbf{q})_s + \Gamma(\mathbf{q})_{s'}]^2}$$

## BEYOND EXPERIMENTAL RESOLUTION: 2D MELTING OF AL(100)



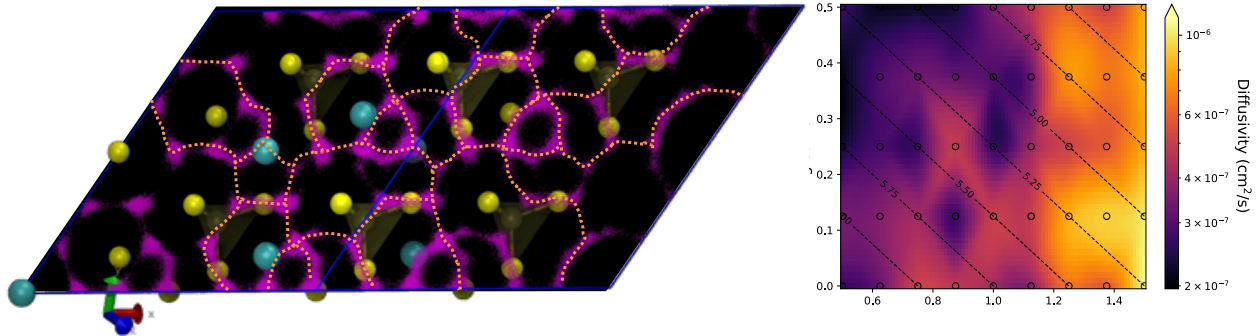
N. L. Nguyen, L. Kahle, F. Baletto, and N. Marzari (in preparation, 2022)





## ENGINEERING SOLID-STATE ELECTROLYTES

Cl-doped argyrodite ( $\text{Li}_6\text{PS}_5\text{Cl}$ )



S. Mui, L. Ercole, N. Marzari, 2 patents filed with  SOLVAY (2022)



## RELIABLY, REPRODUCIBLY, HIGH-THROUGHPUT

VOLUME 88, NUMBER 25

PHYSICAL REVIEW LETTERS

24 JUNE 2002

### Combined Electronic Structure and Evolutionary Search Approach to Materials Design

G. H. Jóhannesson, T. Bligaard, A. V. Ruban, H. L. Skriver, K. W. Jacobsen, and J. K. Nørskov

*Center for Atomic-Scale Materials Physics, Department of Physics, Technical University of Denmark, DK-2800, Lyngby, Denmark*

(Received 20 February 2002; published 10 June 2002)

We show that density functional theory calculations have reached an accuracy and speed making it possible to use them in conjunction with an evolutionary algorithm to search for materials with specific properties. The approach is illustrated by finding the most stable four component alloys out of the 192 016 possible fcc and bcc alloys that can be constructed out of 32 different metals. A number of well known and new "super alloys" are identified in this way.

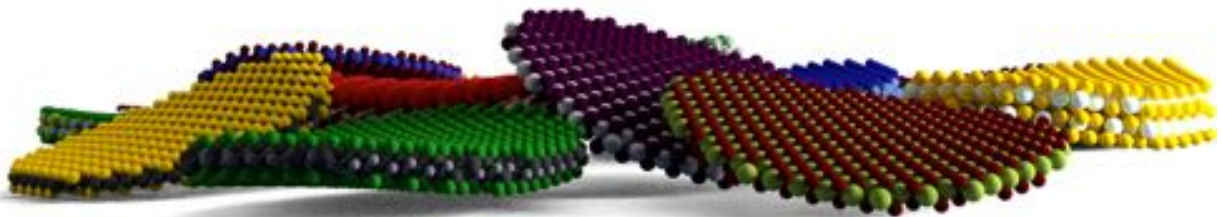
DOI: 10.1103/PhysRevLett.88.255506

PACS numbers: 81.05.Bx, 61.66.Dk, 71.15.Mb

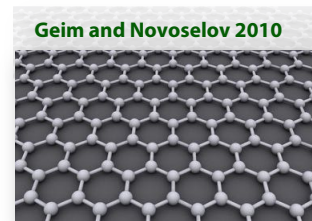
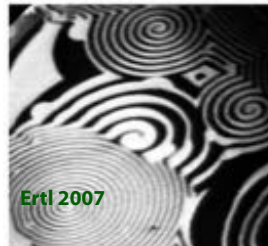
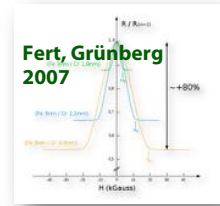
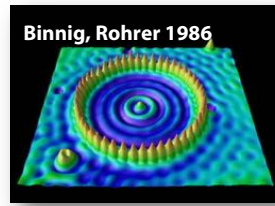
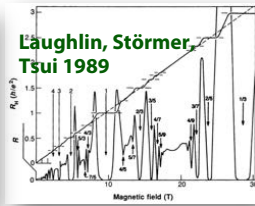




## EXAMPLE: COMPUTATIONAL EXFOLIATION OF ALL KNOWN INORGANIC MATERIALS



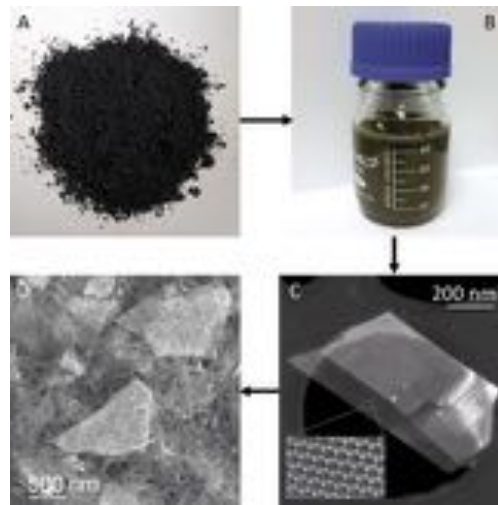
## PHYSICS AND CHEMISTRY IN LOW DIMENSIONS



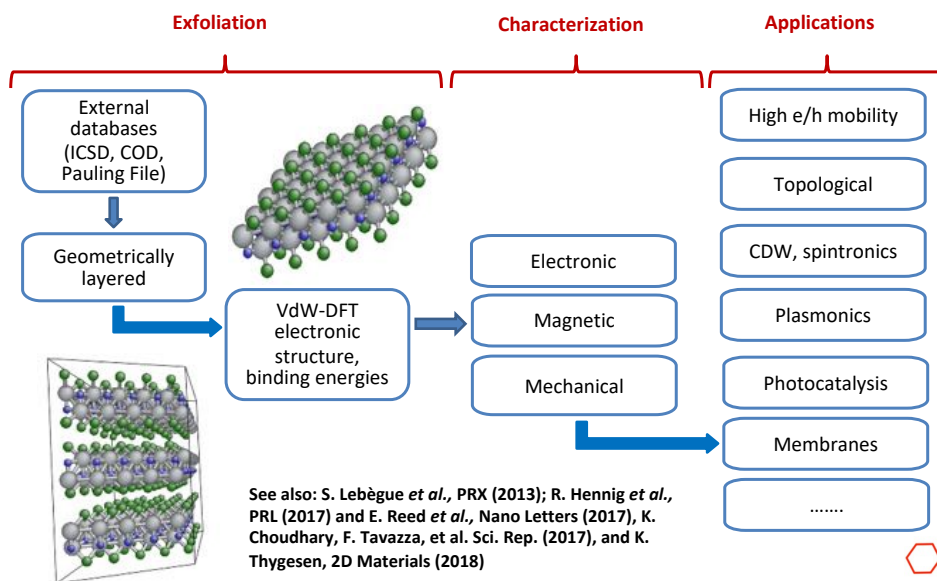
## HOW DO WE PRODUCE 2D MATERIALS?



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

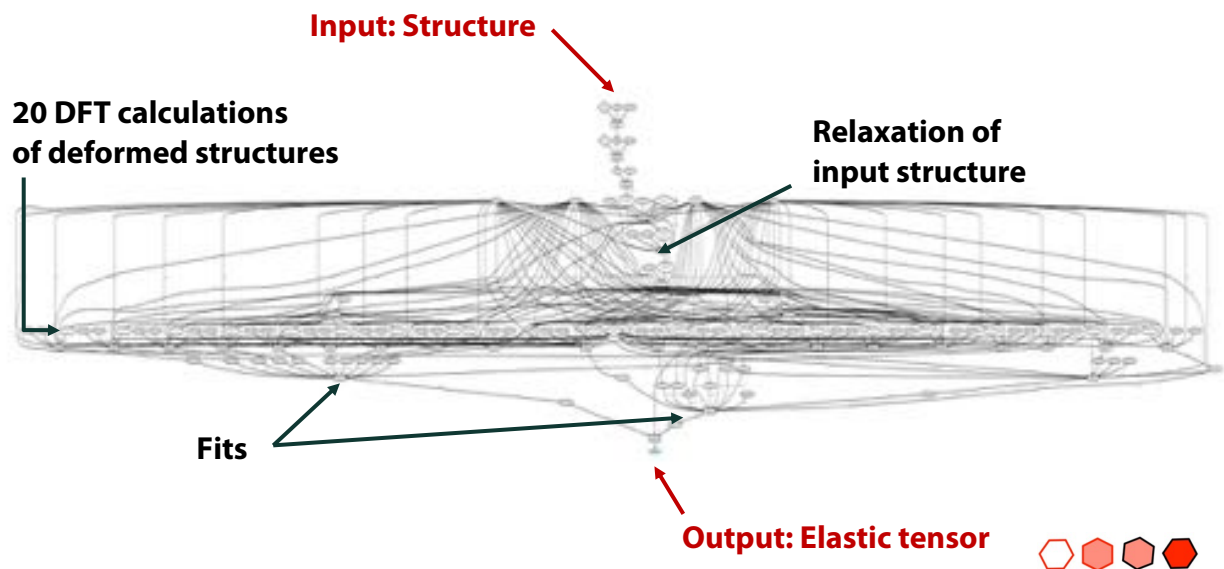


## HIGH-THROUGHPUT COMPUTATIONAL EXFOLIATION



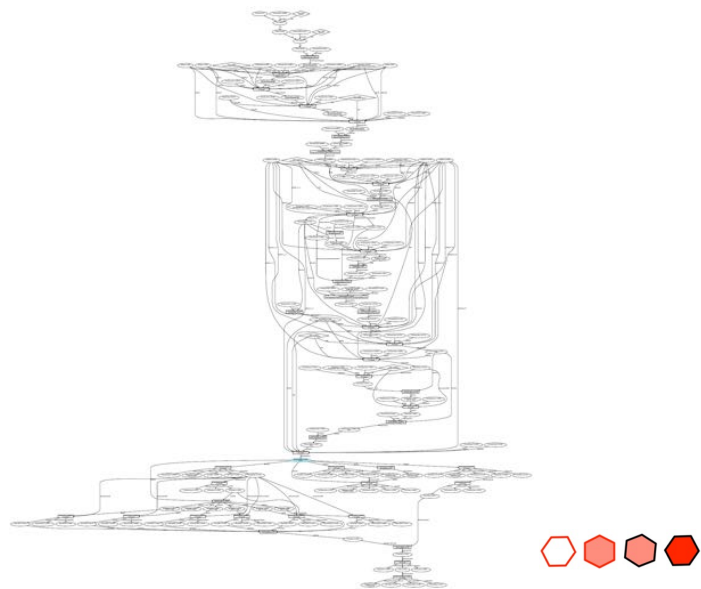
## AUTOMATIC WORKFLOWS: FROM STRUCTURE TO PROPERTY

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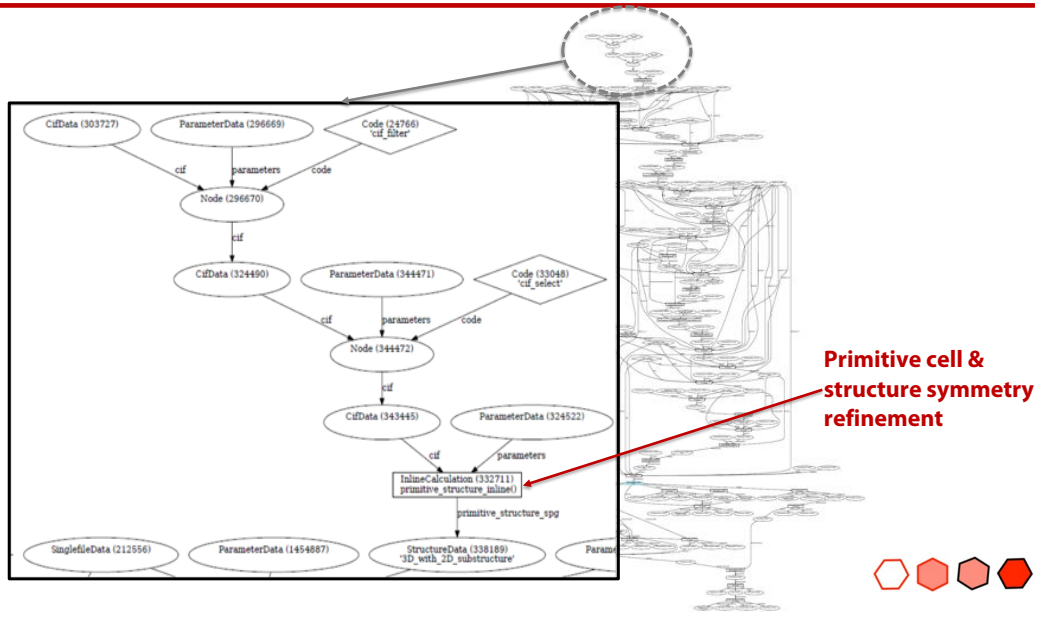


## LET'S START FROM A MATERIAL ( $\text{VOBr}_2$ )

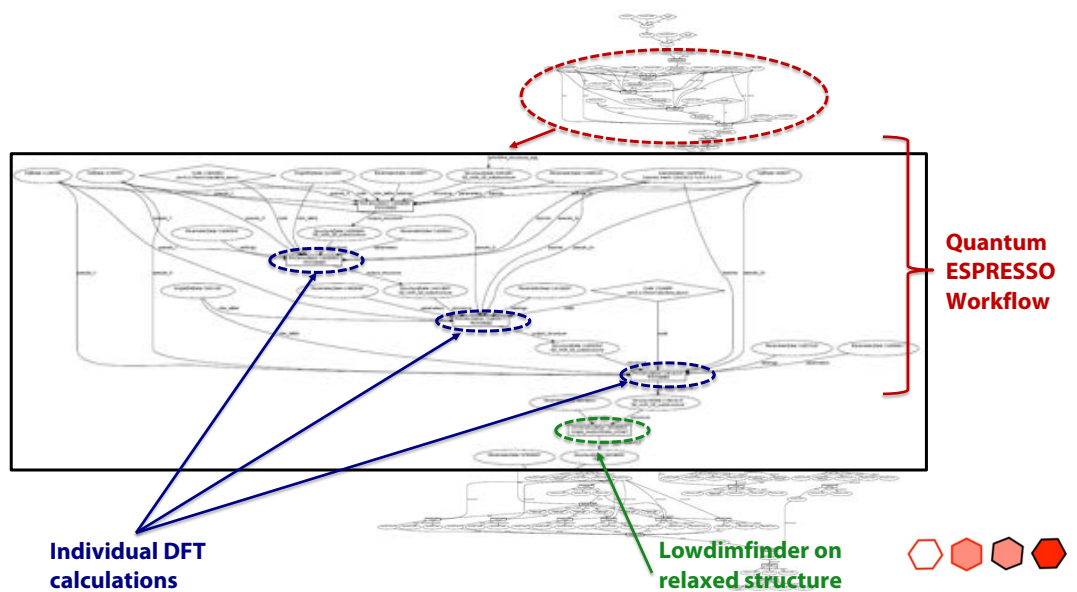
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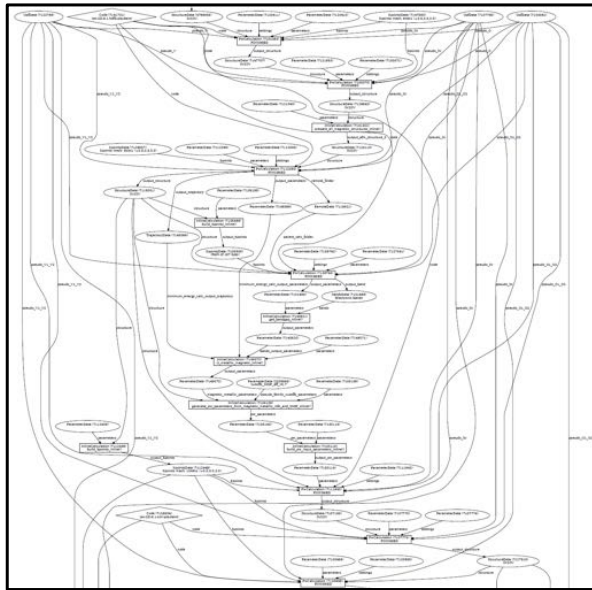
## FROM DATABASE ENTRY TO A WORKING STRUCTURE



## 3D RELAXATION



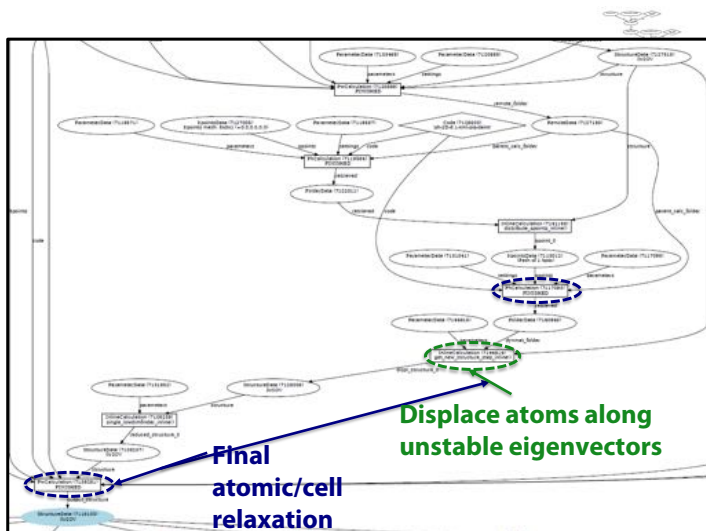
## MAGNETIC SCREENING OF THE 2D MONOLAYER



**Electronic & magnetic workflow**



## REMOVING MECHANICAL INSTABILITIES



**Phonon calculation**

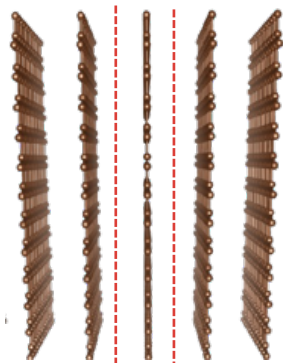
**Stabilization procedure**

**Displace atoms along unstable eigenvectors**

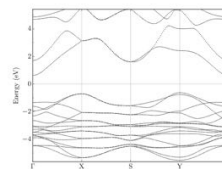
**Final atomic/cell relaxation**



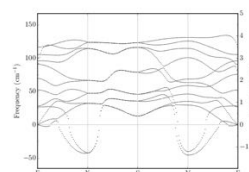
# ALL AUTOMATED...



**Band structures**



**Phonon dispersions**



# FINALLY...

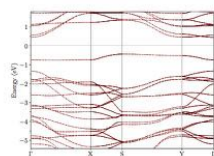
## 215 VBr<sub>2</sub>O (Pmm2)

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

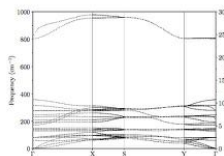
Formula VBr<sub>2</sub>O  
 Spacegroup Pmm2  
 Prototype VCl<sub>2</sub>O (Pmm2)  
 Parent 3D VBr<sub>2</sub>O  
 Source DB ICSD  
 DB ID 24381

DF2-C09 Binding energy [meV/Å<sup>2</sup>] 14.4  
 rVV10 Binding energy [meV/Å<sup>2</sup>] 21.6  
 Band gap [eV] 0.9  
 Magnetic State AFM  
 Tot. Magnetization [ $\mu_B$ /cell] 0.0  
 Abs. Magnetization [ $\mu_B$ /cell] 2.54

### Band structure and phonon dispersions



Band structure: energy bands of VBr<sub>2</sub>O (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.

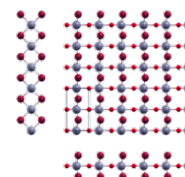


Phonon dispersions: phonon frequencies of VBr<sub>2</sub>O (8 atoms/cell) along a high-symmetry path.

### Crystal structure

Structural parameters: cell (top) and atomic positions (bottom) of VBr<sub>2</sub>O in cartesian coordinates.

	$x$ [Å]	$y$ [Å]	$z$ [Å]
$a_1$	3.86622044	0.00000000	0.00000000
$a_2$	0.00000000	7.17629927	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 <sub>1</sub>	1.70214333	3.58514964	0.00000000
* V <sub>2</sub>	1.70214341	0.00000000	0.00000000
• Br	2.00107500	5.37772439	1.78545446
• Br	2.00107500	1.79257489	1.78545446
• O <sub>1</sub>	0.06788642	3.58514964	0.00000000
• O <sub>2</sub>	0.06788661	0.00000000	0.00000000



Orthographic projections: different views of VBr<sub>2</sub>O from the  $x$  axis (left), the  $y$  axis (bottom) and the  $z$  axis (center).



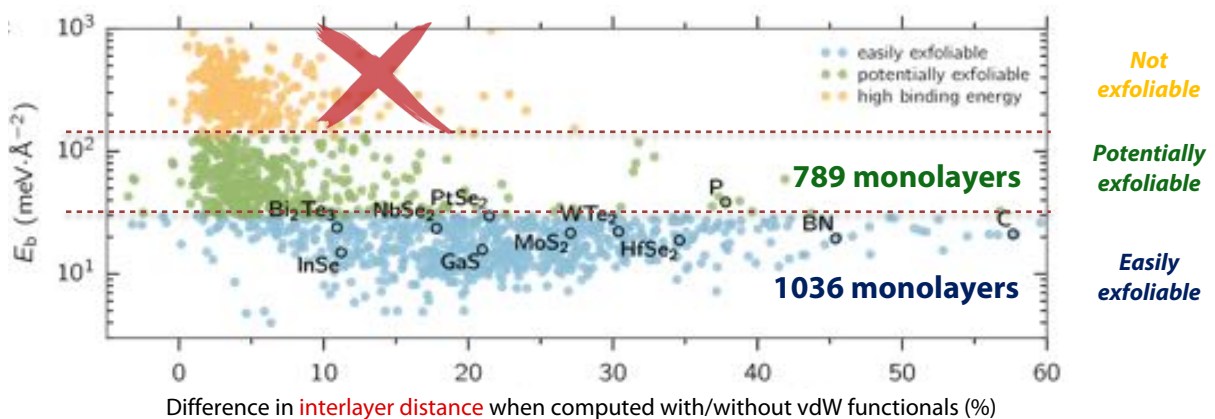
## HOW MANY CANDIDATES? GEOMETRIC SCREENING

	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

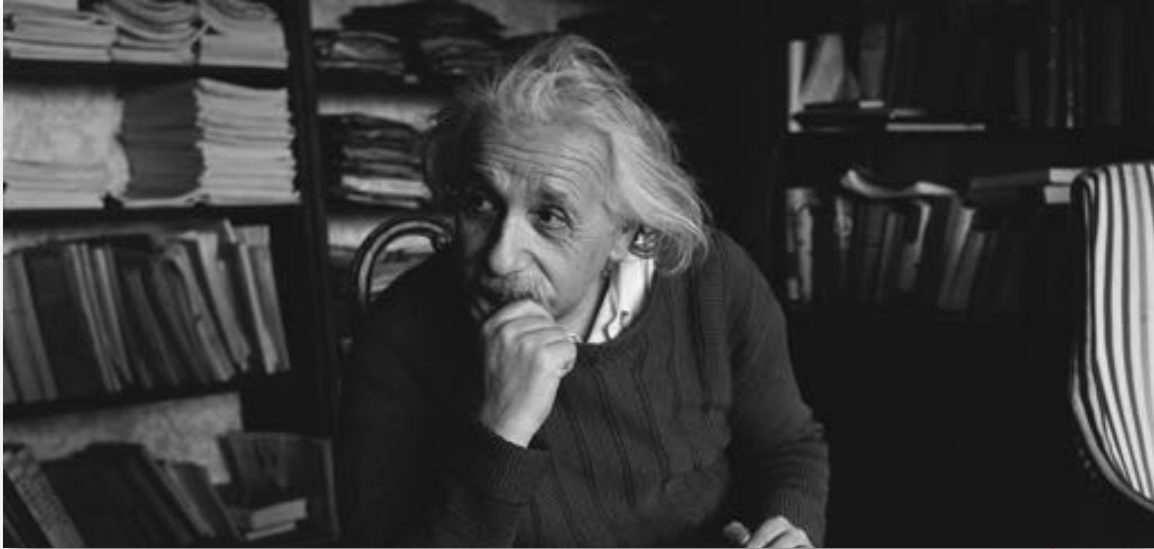


- $E_b < 30 \text{ meV}/\text{Å}^2$  (DF2-C09) or  $E_b < 35 \text{ meV}/\text{Å}^2$  (rVV10) → 2D, easily exfoliable
- In-between → 2D, potentially exfoliable
- $E_b > 130 \text{ meV}/\text{Å}^2$  → not 2D (discarded)

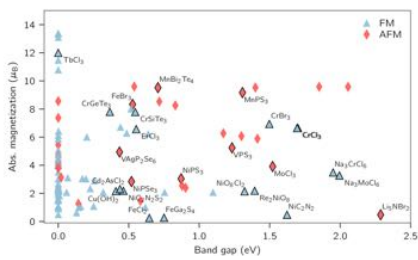




## WHAT TO DO NEXT?

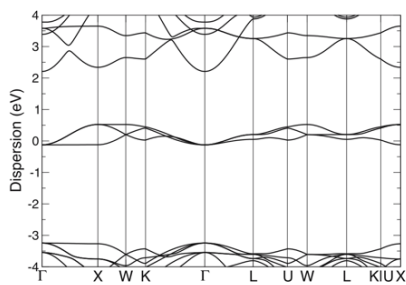


## FROM ELECTRONICS...

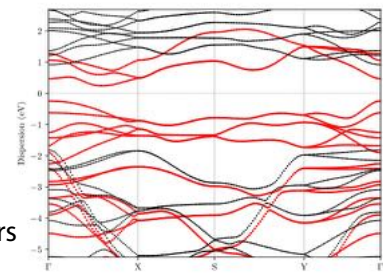


Magnetic metals  
and insulators

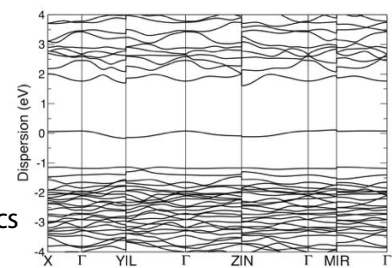
Half-semiconductors



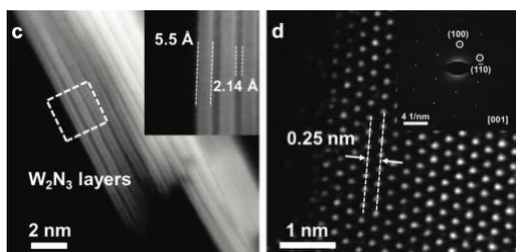
Transparent  
conductors



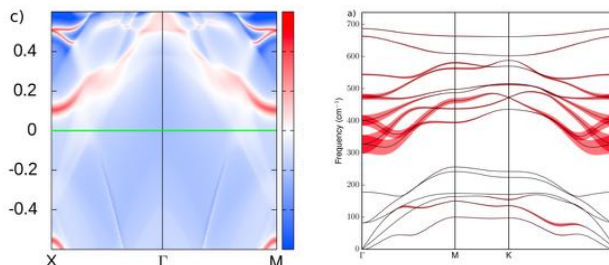
Plasmonics



## ...TO THE LARGEST SUPERCONDUCTING $T_c$ IN 2D...

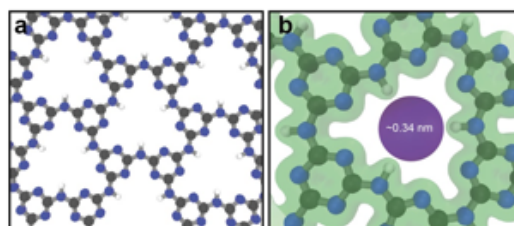
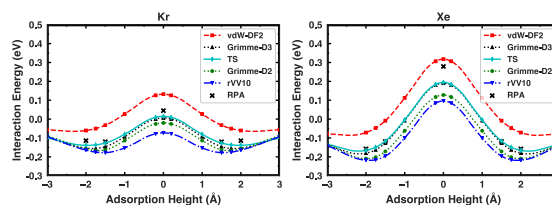
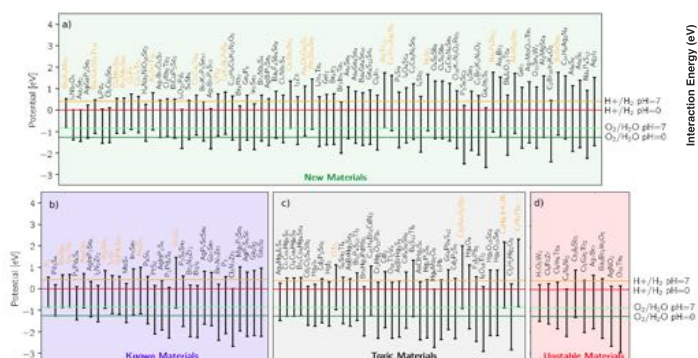


H. Jun *et al.*, *Advanced Materials* 31, 1902709 (2019)



D. Campi, S. Kumari, and N. Marzari, *Nano Letters* 21, 3435 (2021)

## ...TO MATERIALS: PHOTOCATALYSIS, MEMBRANES



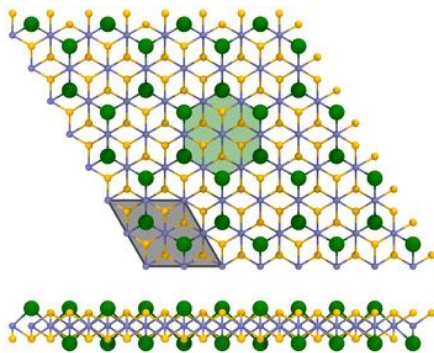
Science Advances (2019), and under review (2022)



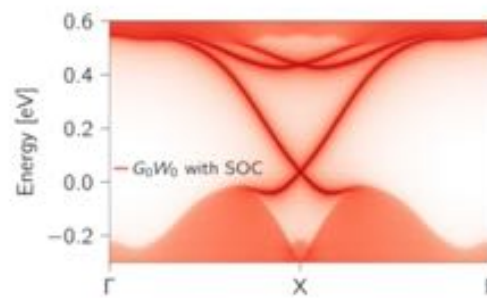
## THE DISCOVERY OF JACUTINGAITE



## THE DISCOVERY OF JACUTINGAITE



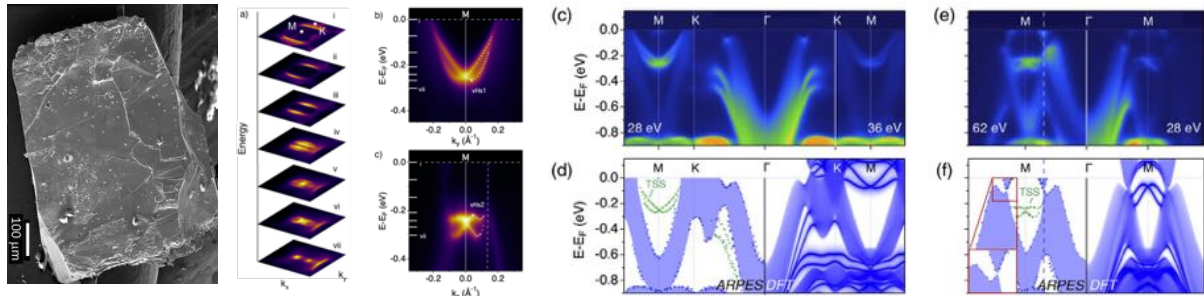
Classified as potentially exfoliable  
(binding energy of  $60 \text{ meV } \text{Å}^{-2}$ )



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



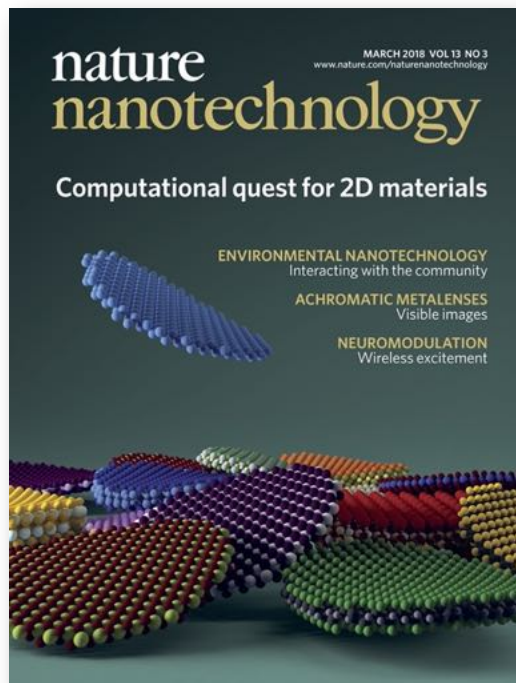
## ROOM-TEMPERATURE KANE-MELE QSHI



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

I. Cucchi, *et al.*, *Phys. Rev. Lett.* **124**, 106402 (2020)

A. Marrazzo, N. Marzari, and M. Gibertini, *Phys. Rev. Res.* **2**, 012063(R) (2020)



## THERE IS PLENTY OF ROOM AT THE TOP

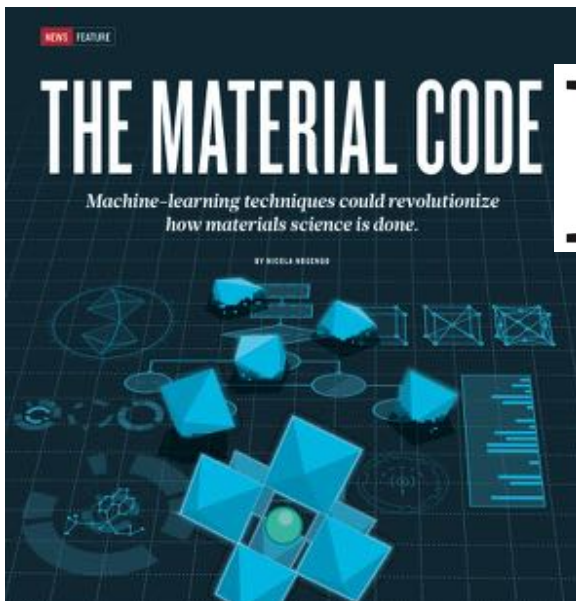
- High electron/hole mobility devices
- Topological insulators, quantum computing
- Ferromagnetic/spintronics in 2D
- Charge-density waves and superconductors
- Plasmonics, transparent conductors

### 3D layered parents:

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

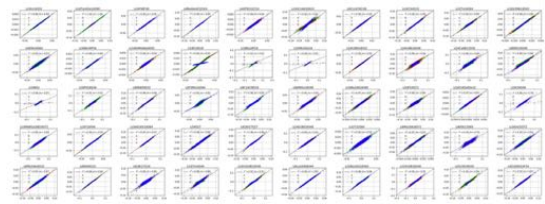
N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi and N. Marzari, *Nature Nanotechnology* **13**, 246 (2018)

## MACHINE LEARNING AS THE GREAT ACCELERATOR

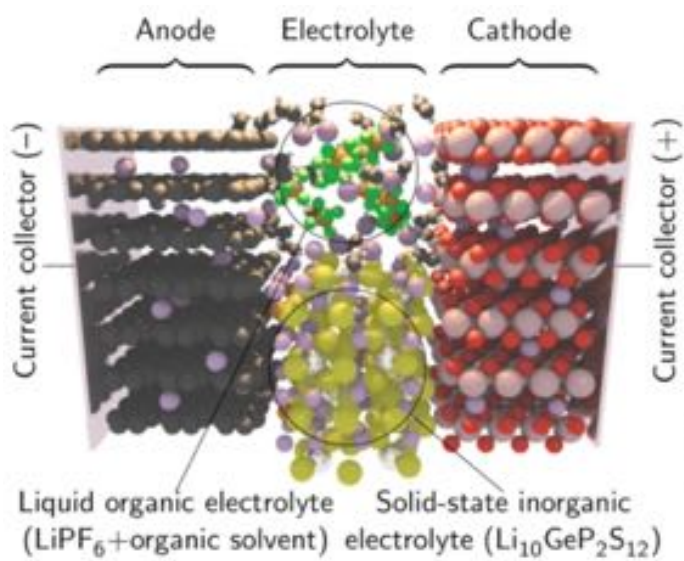


Nature, May 2016

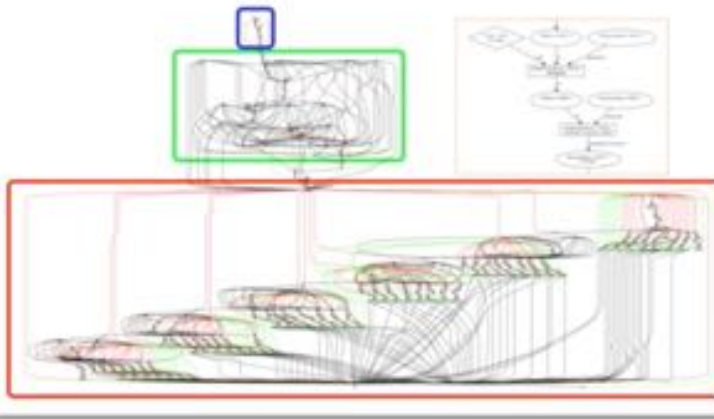
**I**t's a strong contender for the geekiest video ever made: a close-up of a smartphone with line upon line of numbers and symbols scrolling down the screen. But when visitors stop by Nicola Marzari's office, which overlooks Lake Geneva, he can hardly wait to show it off. "It's from 2010," he says, "and this is my cellphone calculating the electronic structure of silicon in real time!"



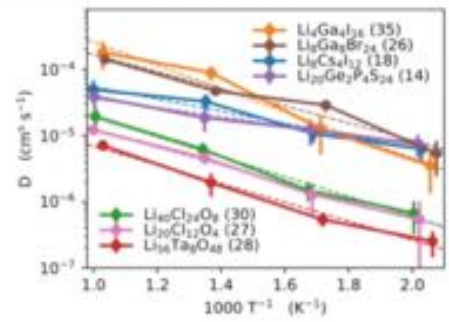
## ALL SOLID-STATE BATTERIES



## AUTOMATED SCREENING



### Fast-ionic conductors



Arrhenius behavior of tracer diffusion (from MSD) for best Li-ion conductors

L. Kahle, A. Marcolongo, and N. Marzari, Energy & Environmental Science 13, 928 (2020)



SCIENCE IN THE CLOUD:  
TOWARDS A DIGITAL INFRASTRUCTURE

## OPEN SCIENCE TECHNOLOGY STACK

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 **work environment** for non specialist where to run simulations



4. A **dissemination platform** for raw and curated data, simulation services, educational tools



Automation

Data

Environment

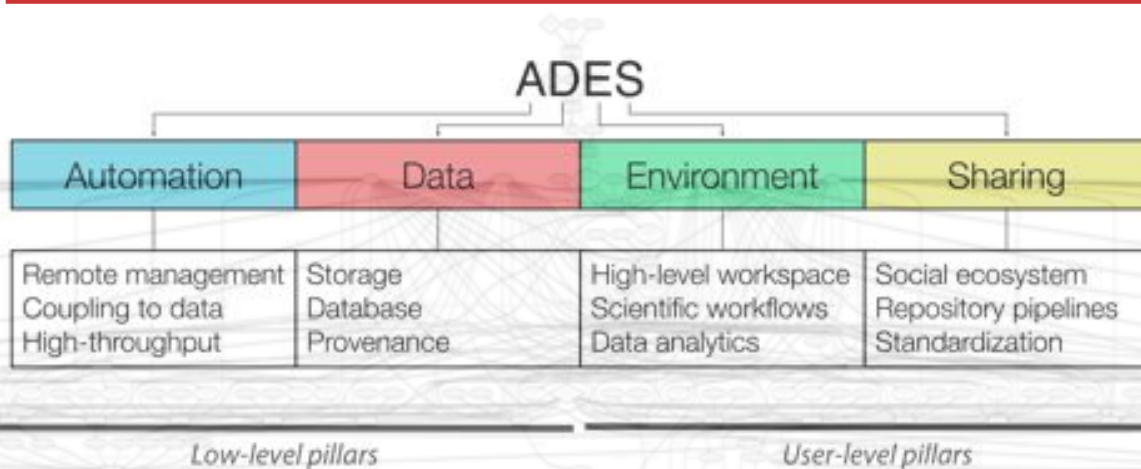
Sharing



<http://www.aiida.net>

S.P. Huber *et al.*, Nature Scientific Data (2020)  
G. Pizzi *et al.*, Comp. Mat. Sci. 111, 218 (2016)

## ADES MODEL FOR COMPUTATIONAL SCIENCE



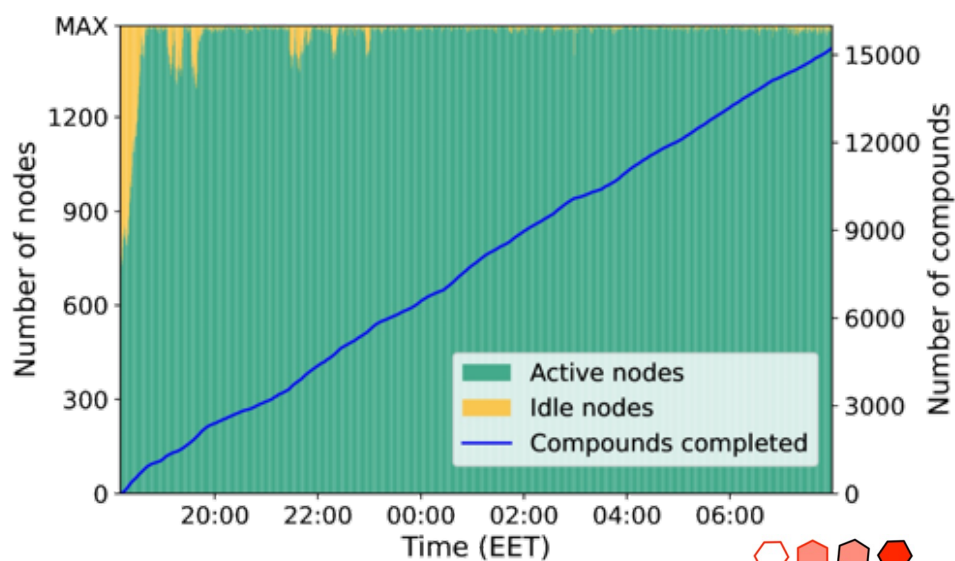
S.P. Huber *et al.*, *Nature Scientific Data* (2020)

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

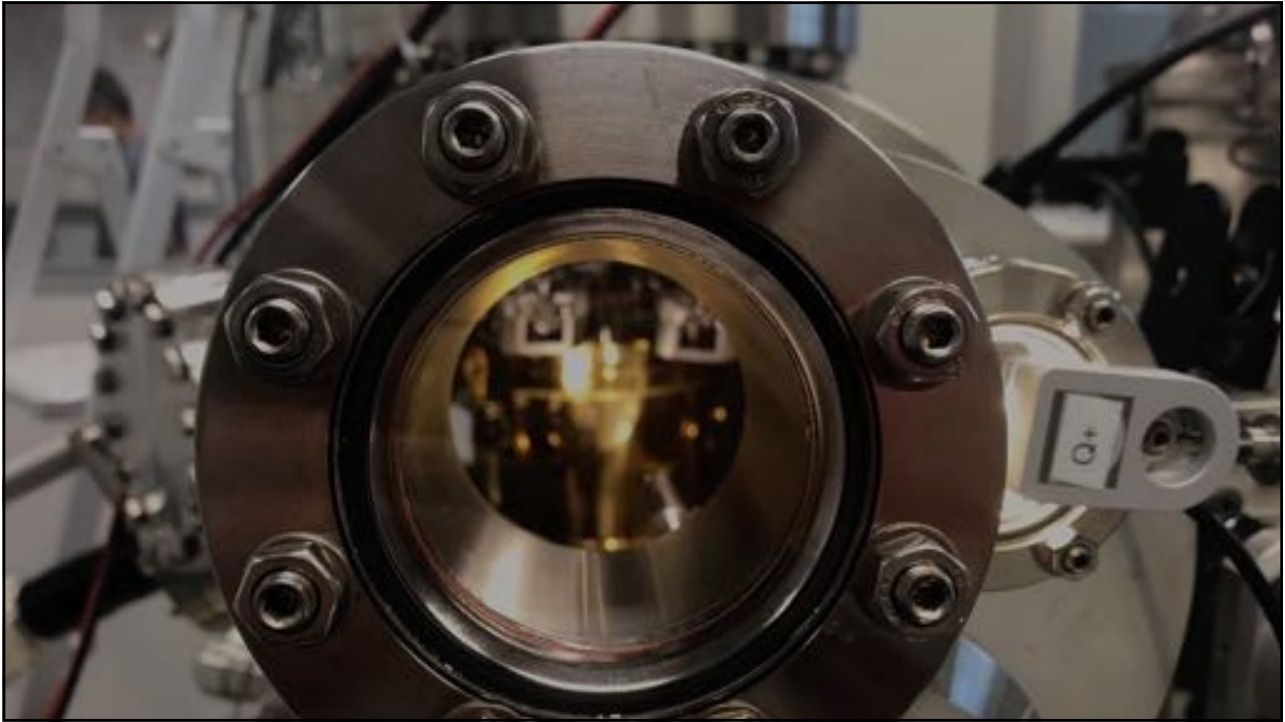


## LUMI-C HERO RUN

**12 hours and  
196,608 cores:**  
ran **55704 QE  
calculations**  
handled **7887  
errors on the fly**  
fully optimized  
geometries of  
**15324 different  
compounds**








## READY TO GO IN THE QUANTUM MOBILE

## READY TO GO IN THE QUANTUM MOBILE

---



20.11.2a

Search the docs ...

**Quantum Mobile**

Releases

**USERS**

- Launching Quantum Mobile
- Using Quantum Mobile
- VirtualBox FAQ
- Troubleshooting

**DEVELOPERS**

- Customize Quantum Mobile
- Build a Desktop VM
- Build a Cloud VM
- Build a Docker container
- Create a new ansible role

**MAINTAINERS**

- Developing Quantum Mobile
- Preparing releases

Theme by the Executable Book Project

←

### Quantum Mobile

#### What is Quantum Mobile

Quantum-Mobile is a Virtual Machine for computational materials science.

Quantum-Mobile provides a uniform environment for quantum mechanical materials simulations. Simulation codes are set up and ready to be used either directly or through the **AiiDA** python framework for automated workflows and provenance tracking.

**Open source throughout**  
Based on [Ubuntu Linux](#)

**Pre-built images**  
Available for Linux, MacOS or Windows computers, using VirtualBox. Or deploy on cloud services like OpenStack or Amazon Elastic Compute Cloud using [ansible](#).


**Simulation codes pre-installed**  
[Abinit](#), [BigDFT](#), [CP2K](#), [Fleur](#), [Quantum ESPRESSO](#), [Siesta](#), [Wannier90](#), [Yambo](#), together with [AiiDA](#), [JupyterLab](#), and the [AiiDAlab](#) Jupyter environment.


**Tools pre-installed**  
[atomic](#), [pymatgen](#), [jmol](#), [cif2cell](#), [ase](#), [pymatgen](#), [seekpath](#), [spglib](#), [ewfhwf](#), [visualization](#) ([grace](#), [gnuplot](#), [matplotlib](#), [bekeh](#), [jupyter](#)), simulation environment ([slurm](#), [OpenMPI](#), [FFTW/LAPACK](#), [gcc](#), [gfortran](#), [singularity](#)).

**Modular setup**  
with individually tested [ansible roles](#). Build your own flavour tailored to your use case.

Contents

- What is Quantum Mobile
- Quantum Mobile Flavours
- Testimonials
- Acknowledgments





# COMMON WORKFLOWS



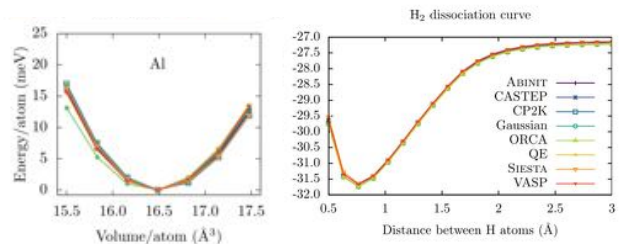
ARTICLE OPEN

Check for updates

## Common workflows for computing material properties using different quantum engines

Sebastian P. Huber<sup>1,2,3,4</sup>, Emanuele Bosoni<sup>5</sup>, Marnik Berx<sup>1</sup>, Jens Bröder<sup>2,4</sup>, Augustin Degomme<sup>6</sup>, Vladimir Dikan<sup>2</sup>, Kristjan Elmre<sup>7</sup>, Espen Flage-Larsen<sup>7,8</sup>, Alberto Garcia<sup>9</sup>, Luigi Genovese<sup>6</sup>, Dominik Gresch<sup>6</sup>, Conrad Johnston<sup>10</sup>, Guido Petretto<sup>11</sup>, Samuel Poncé<sup>12</sup>, Gian-Marco Rignanese<sup>11</sup>, Christopher J. Sewell<sup>1</sup>, Berend Smit<sup>12</sup>, Vasily Tseplyaev<sup>3,4</sup>, Martin Uhrin<sup>13</sup>, Daniel Wortmann<sup>14</sup>, Aliaksandr V. Yakutovich<sup>7,12</sup>, Austin Zadoks<sup>1</sup>, Pezhman Zarabadi-Poor<sup>13,14</sup>, Bonan Zhu<sup>14,15</sup>, Nicola Marzari<sup>1</sup> and Giovanni Pizzi<sup>16</sup>

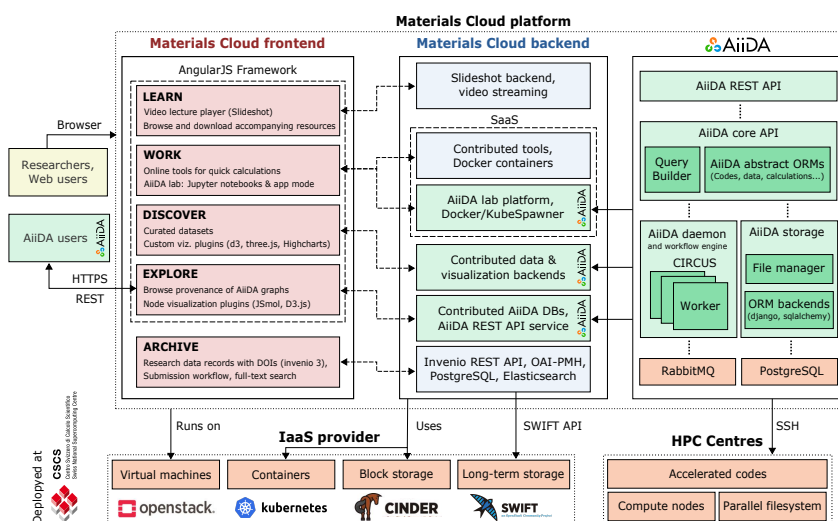
\$ aiiida-common-workflows launch eos siesta --structure=Al --protocol=precise



S. Huber et al., npj Computational Materials 7, 136 (2021)



# MATERIALS CLOUD



Indexed by

SCIENTIFIC DATA

re3data.org

FAIRsharing.org

GO FAIR

Google Dataset Search

B2FIND EUDAT

L. Talirz et al., Scientific Data 7, 299 (2020)



# MATERIALS CLOUD - DISCOVER

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: 10.26434/chemrxiv-2024-39911v1](https://doi.org/10.26434/chemrxiv-2024-39911v1)

Authors: Gianluca Prandini, Antonio 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: 10.26434/chemrxiv-2021-09081v2](https://doi.org/10.26434/chemrxiv-2021-09081v2)

Authors: Nicolas Mounet, Marco Gibertini, Philippe Schwofler, Davide Campi, Andrius Merkys, Antonio Marrazzo, Thibault Schrier, Ivano E. Castelli, Andrea Cepelloni, 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/s41565-021-0539-5 (2021).



2D topological insulators

Authors: Antonio Marrazzo, Marco Gibertini, Davide Campi, Nicolas Mounet & Nicola Marzari

Description: Results from screening exfoliable materials for 2D topological insulators (Quantum Spin Hall Insulators).

# MATERIALS CLOUD - ARCHIVE

## Latest records



Recommended by

SCIENTIFIC DATA

European Commission  
Open Research Europe

Swiss National Science Foundation

Indexed by

re3data.org  
re3data.org/10.26434/chemrxiv-2024-39911v1  
Materials Cloud Archive

FAIRsharing.org  
STANFORD, MIT, ETHZ, POLITECNICO

FAIR

Google  
Dataset Search

Collaborative  
EUDAT Data Infrastructure  
EUROPEAN COMMISSION

### Dynamic response of oxygen vacancies on the Deacon reaction over reduced single crystalline CeO<sub>2-x</sub>(111) surfaces

[DOI: 10.26434/chemrxiv-2024-39911v1](https://doi.org/10.26434/chemrxiv-2024-39911v1)

V. Koller, C. Sack, P. Lustenberger, M. V. Ganduglia-Pirovano, H. Over

The heterogeneously catalyzed HCl oxidation reaction (Deacon reaction) over ceria leads under typical reaction conditions to a reduction and surface chlorination of CeO<sub>2</sub>. The reduced single crystalline CeO<sub>2-x</sub>(111) model surface stabilizes various ordered surface structures, e.g.  $\sqrt{7} \times \sqrt{7}$ (R15.1°),  $\sqrt{3} \times \sqrt{3}$ , or  $\sqrt{4} \times \sqrt{4}$ , depending on the concentration of oxygen vacancies (VO). Saturating these phases with HCl at room temperature, followed by annealing to the process temperature of 700 K, leads in all cases to a uniformly covering  $\sqrt{3} \times \sqrt{3}$ (R30°) overlayer structure with identical Cl coverage and identical adsorption geometry. Low energy electron diffraction (LEED) fingerprinting, density functional theory (DFT) calculations and X-ray photoelectron spectroscopy (XPS) evidence that Cl adsorbs into the O-vacancy at the surface (Clvac) with a high adsorption energy (>2 eV). From thermal desorption spectroscopy (TDS) and XPS of Cl 2p the adsorption energy of Clvac and the water formation is ...

Latest version: v1

Publication date: May 24, 2022

### Efficient, interpretable graph neural network representation for angle-dependent properties and its application to optical spectroscopy

[DOI: 10.26434/chemrxiv-2024-39911v1](https://doi.org/10.26434/chemrxiv-2024-39911v1)

Tim Hsu, Tuan Anh Phan, Nathan Kalburt, Stephen Weitzner, James Chapman, Penghao Xiao, S. Roger Qu, Xiao Chen, Brandon Wood

Graph neural networks are attractive for learning properties of atomic structures thanks to their intuitive graph encoding of atoms and bonds. However, conventional encoding does not include angular information, which is critical for describing atomic arrangements in disordered systems. In this work, we extend the recently proposed ALIGNN encoding, which incorporates bond angles, to also include dihedral angles (ALIGNN-d). This simple extension leads to a memory-efficient graph representation that captures the complete geometry of atomic structures. ALIGNN-d is applied to predict the infrared optical response of dynamically disordered CuII aqua complexes, leveraging the intrinsic interpretability to elucidate the relative contributions of individual structural components. Bond and dihedral angles are found to be critical contributors to the fine structure of the absorption response, with distortions representing transitions between more common geometries exhibiting the strongest ...

Latest version: v1

Publication date: May 23, 2022

---

## LET'S BROADEN THE HORIZON




### THE BEZOS MANDATE: EXTERNALIZABLE SERVICE INTERFACES

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- 1) All teams will henceforth **expose their data and functionality through service interfaces.**
- 2) Teams must communicate with each other through these interfaces.
- 3) There will be no other form of interprocess communication allowed.
- 4) All service interfaces, without exception, must be designed **from the ground up to be externalizable.**



# IN ACTION: OPTIMADE UNIVERSAL REST API



**OPTIMADE**  
Open Databases Integration  
for Materials Design

About Documentation Specification Contributors Wiki GitHub Forum

### About us


Designing new materials suitable for specific applications is a long, complex, and costly process. Researchers think of new ideas based on intuition and experience. Their synthesis and evaluation require a tremendous amount of trial and error. In the last few years, there has been a major game change in materials design. Thanks to the exponential growth of computer power and the development of robust first-principles electronic structure codes, it has become possible to perform large sets of calculations automatically. This is the burgeoning area of high-throughput ab initio computation. Such calculations have been used to create large databases containing the calculated properties of existing and hypothetical materials, many of which have appeared online:

- the AFLOW distributed materials property repository
- the Harvard Clean Energy Project Database
- the Materials Cloud
- the Materials Project
- the NoMAD (Nowe Materials Discovery) Repository
- the Open Quantum Materials Database
- the Computational Materials Repository
- the Data Catalyst Genome
- the Materials Platform for Data Science
- the Joint Automated Repository for Various Integrated Simulations
- ...

The Open Databases Integration for Materials Design (OPTIMADE) consortium aims to make materials databases interoperable by developing a common REST API.

LEARN WORK DISCOVER EXPLORE ARCHIVE

Work Tools OPTIMADE-Client



Currently valid OPTIMADE API version: v1.0.1  
Client version: 2021.2.23.1  
Source code: GitHub

Help improve the application: [Report a bug](#) [Suggest a feature/change](#)

This is a friendly client to search through databases and other implementations exposing an OPTIMADE REST API. To get more information about the OPTIMADE API, please see the [official web page](#). All providers are retrieved from the OPTIMADE consortium's list of providers.

Note: The structure property `asebuild` is currently not supported. Follow the [issue on GitHub](#) to learn more.

FAQ  
Log

### Query a provider's database

Select a provider: No provider chosen  
Showing 0 of 0 results

Apply filters: Basic | Fine

Basic

Chemistry

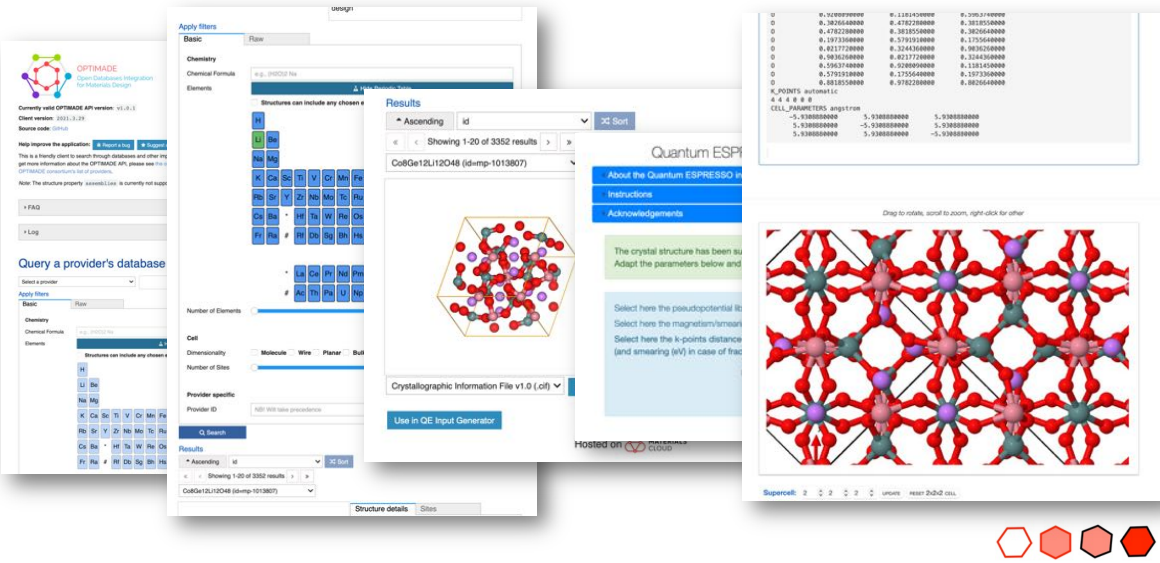
Chemical Formula

Elements

Structures can include any chosen elements (instead of all)

H	He
Li	Be
B	C
N	O
F	Ne

# IN ACTION: OPTIMADE UNIVERSAL REST API



Apply filters: Basic | Fine

Chemistry

Chemical Formula

Elements

Structures can include any chosen elements (instead of all)

Results

Showing 1-20 of 3352 results

Co8Ge12Lu12O48 (id=mp-1013807)

Crystallographic Information File v1.0 (.cif)

Use in QE Input Generator

Quantum ESPRESSO

About the Quantum ESPRESSO

Instructions

Acknowledgements

The crystal structure has been successfully adapted. Adapt the parameters below and select here the pseudopotential file. Select here the magnetism/ferromagnetism. Select here the k-points distance (and smearing (w)) in case of fractional k-points.

CELL\_PARAMETERS angstrom

```
5.9388880000 5.9388880000 5.9388880000
5.9388880000 -5.9388880000 5.9388880000
5.9388880000 5.9388880000 -5.9388880000
```

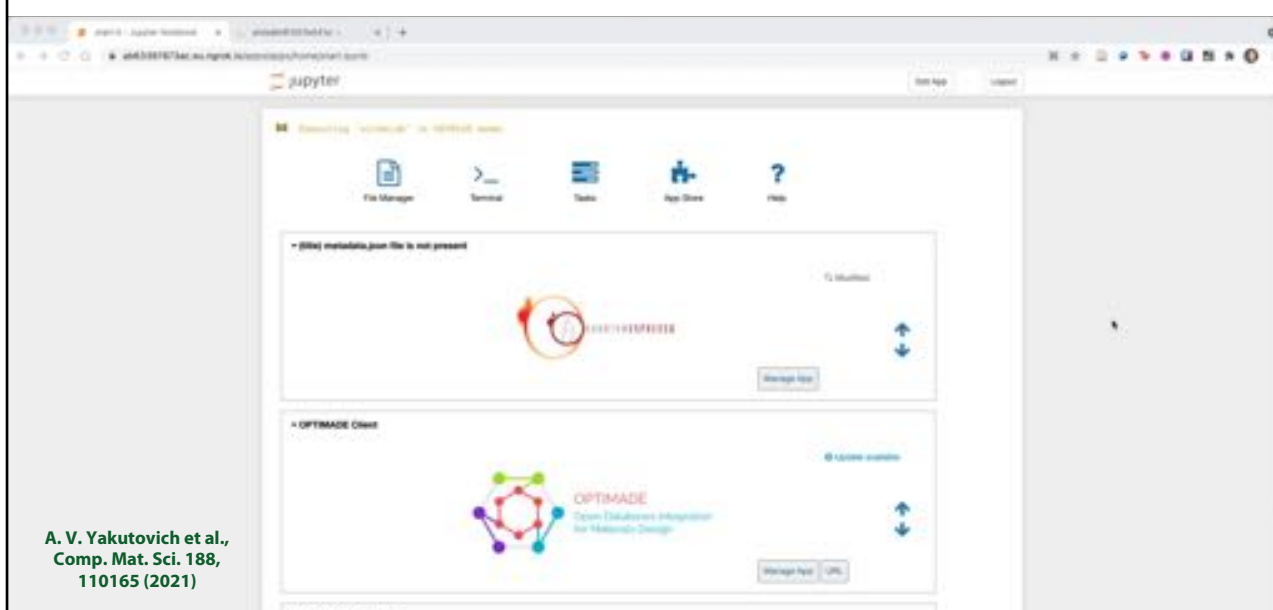
K\_POINTS automatic

```
4 4 4 0 0 0
```

Supercell: 2 2 2 units near 2x2x2 cell

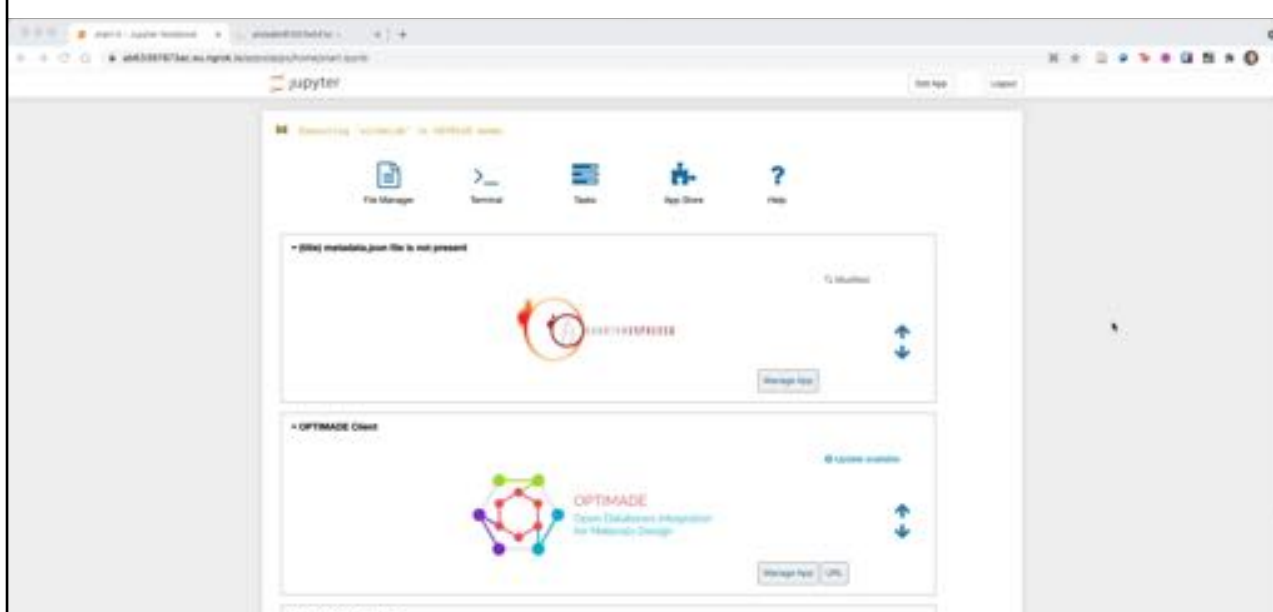
## QUANTUM-AS-A-SERVICE – AiiDALab deployment

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## QUANTUM-AS-A-SERVICE – AiiDALab deployment

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## SCIENCE CONCLUSIONS

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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

---

- I see three kind of data:
  - **Social (harvested, mostly uncontrolled conditions)**
  - **Experimental (harvested, controlled conditions)**
  - **Computational (generated, controlled conditions)**
- **Importance of data-on-demand** through reliable, robust workflows.
- **Value of data is in their reuse – curation is key, not the storage.**



## FURTHER THOUGHTS ON COMPUTATIONAL SCIENCE

---

- **Computational science is central to the entire scientific and technological effort in the 21<sup>st</sup> 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



## ACKNOWLEDGEMENTS

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# ACKNOWLEDGEMENTS



<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, 2018-22, ...)



<https://www.big-map.eu>  
**H2020 Battery Interface Genome – Materials Acceleration  
 Platform (Battery 2030+)**  
 (2020-23, ...)



<https://www.uni-bremen.de/mapex>  
**U Bremen Excellence Chair**  
 (2018-25, ...)

**Related projects:**  
 H2020 Nanoscience Foundries and Fine Analysis  
 H2020 European Materials Modelling Council



H2020 Marketplace  
 H2020 Intersect  
 H2020 DOME 4.0  
 H2020 OpenModel  
 H2020 NEP  
 H2020 EPFL Fellows  
 H2020 EPFL Innovators  
 H2020 Marie Curie  
 EPFL Open Science

PASC

PRACE

IBM

Constellium

Innosuisse

Solvay

Samsung



RICHEMONT

IBM

SWISS NATIONAL SCIENCE FOUNDATION

SAMSUNG

Richemont Varinor

nffa.eu



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