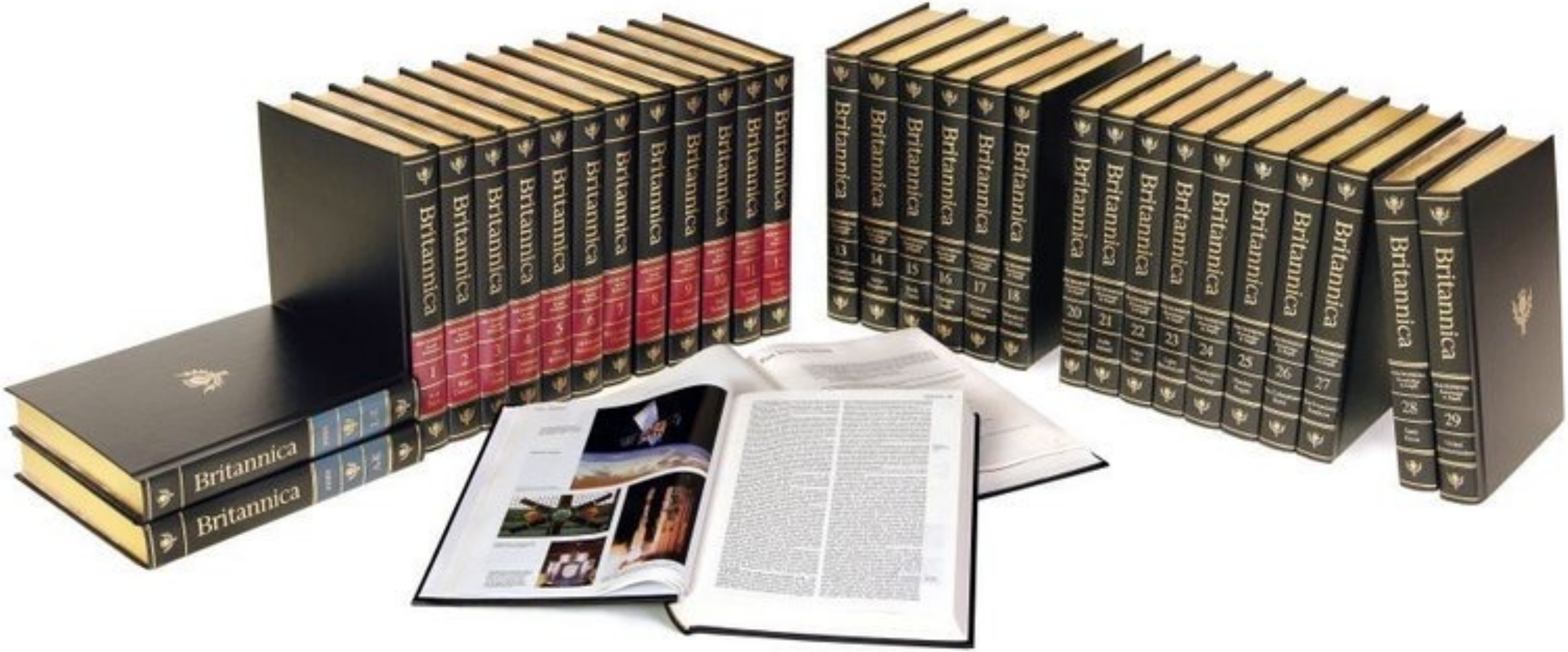
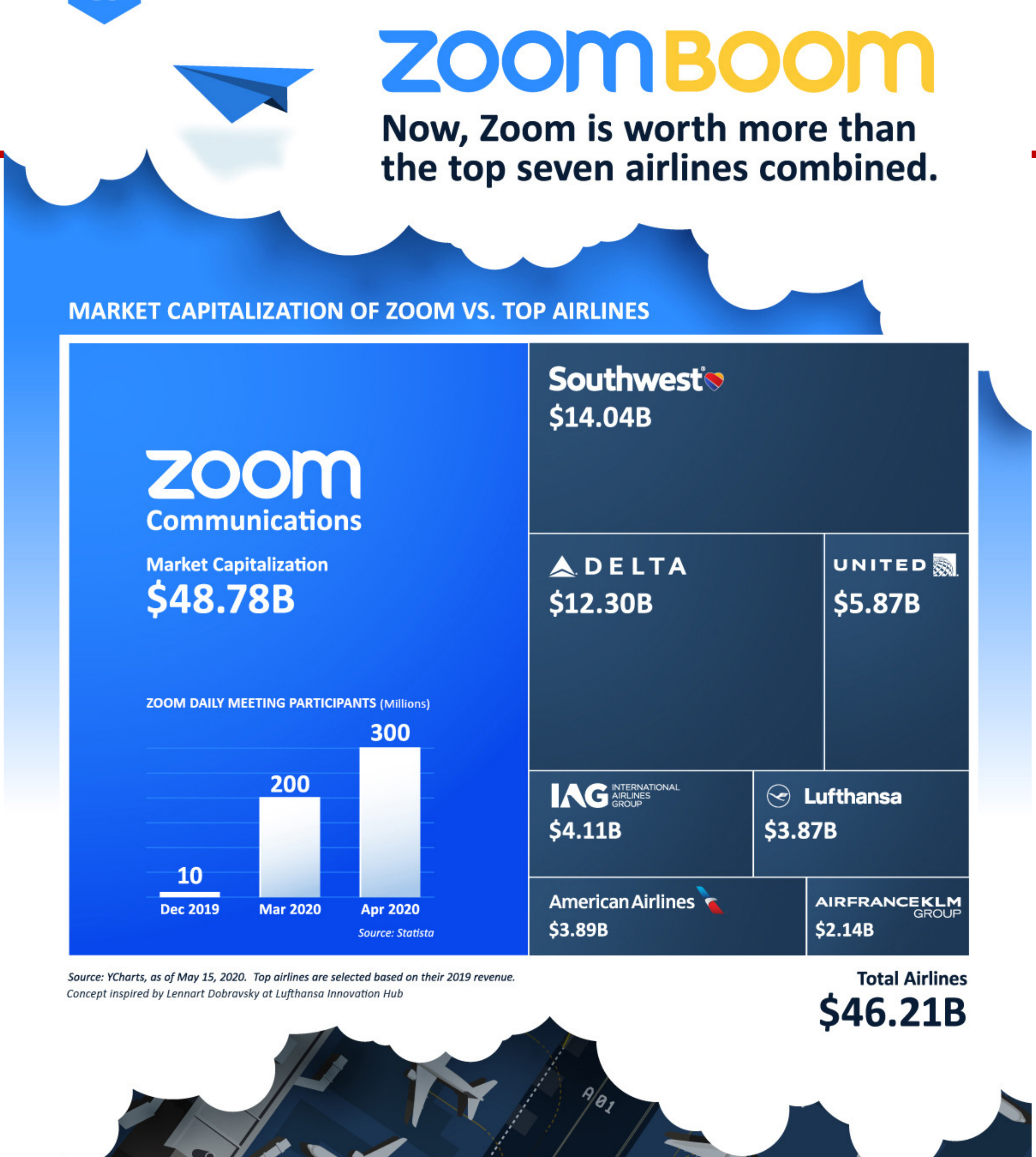
THE DIGITAL INFRASTRUCTURES FOR 21st CENTURY SCIENCE

NICOLA MARZARI, EPFL

@ NASA/JPL-Caltech


Britannica


Kodachrome 64
24 EXP FILM
Kodachrome 25
36
Kodachrome 200
24 EXP FILM
KM 135-36
KR 135-36
PERFORATED ONE EDGE
PERFORATION UNE RANGÉE
EINSEITIG PERFORIERT
FILM FOR COLOR SLIDES
Kodachrome
FILM FOR COLOR SLIDES
36 EXP 64
Kodachrome
POUR DIAPOSITIVES COULEUR
36 POSES 64
PKR-64
36



ZOOM BOOM

Now, Zoom is worth more than the top seven airlines combined.

MARKET CAPITALIZATION OF ZOOM VS. TOP AIRLINES

Source: YCharts, as of May 15, 2020. Top airlines are selected based on their 2019 revenue.
Concept inspired by Lennart Dobravsky at Lufthansa Innovation Hub

Total Airlines
$46.21B

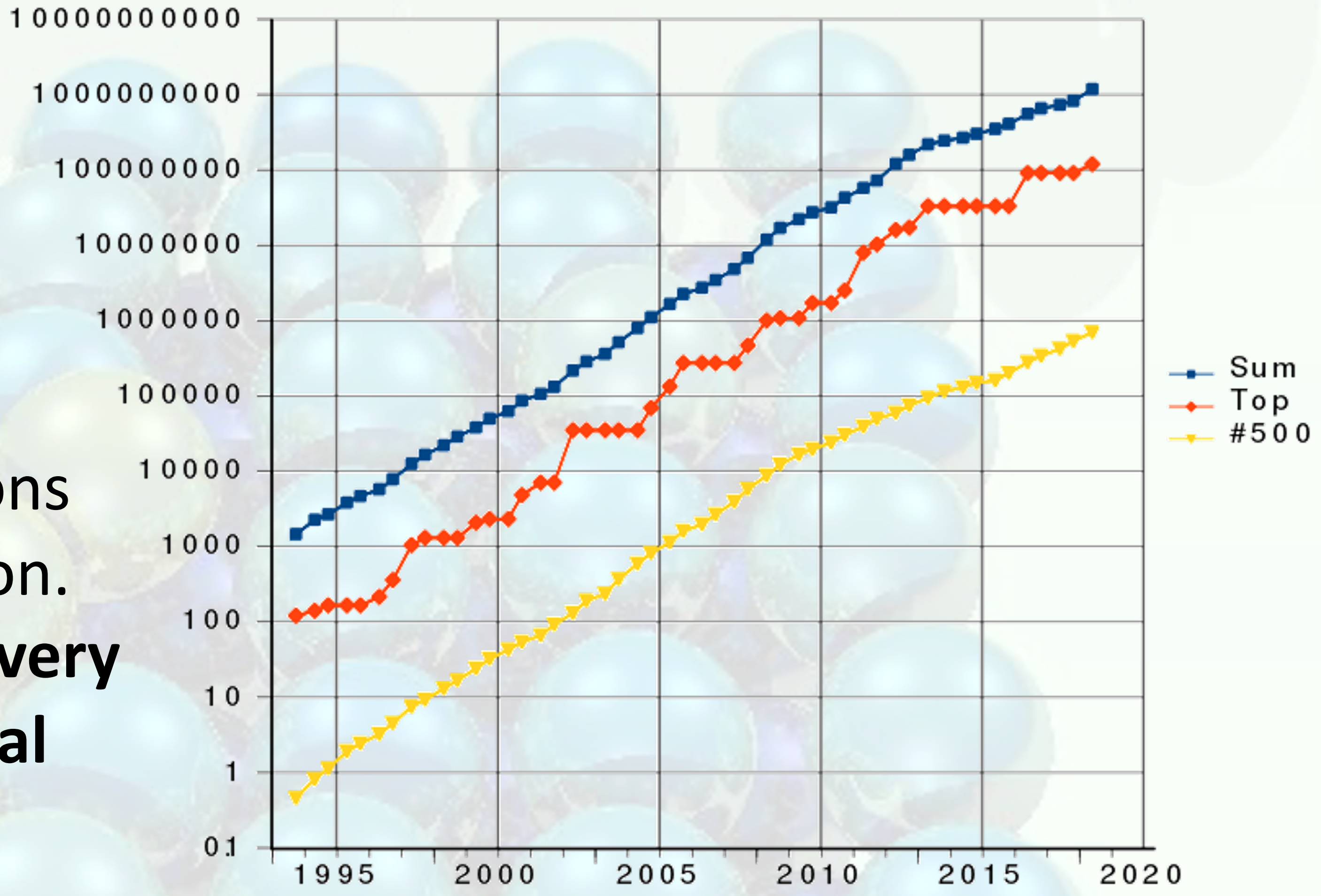
FORTUNE COOKIE #1

UNDERESTIMATING DIGITAL IS NOT GOOD FOR YOU

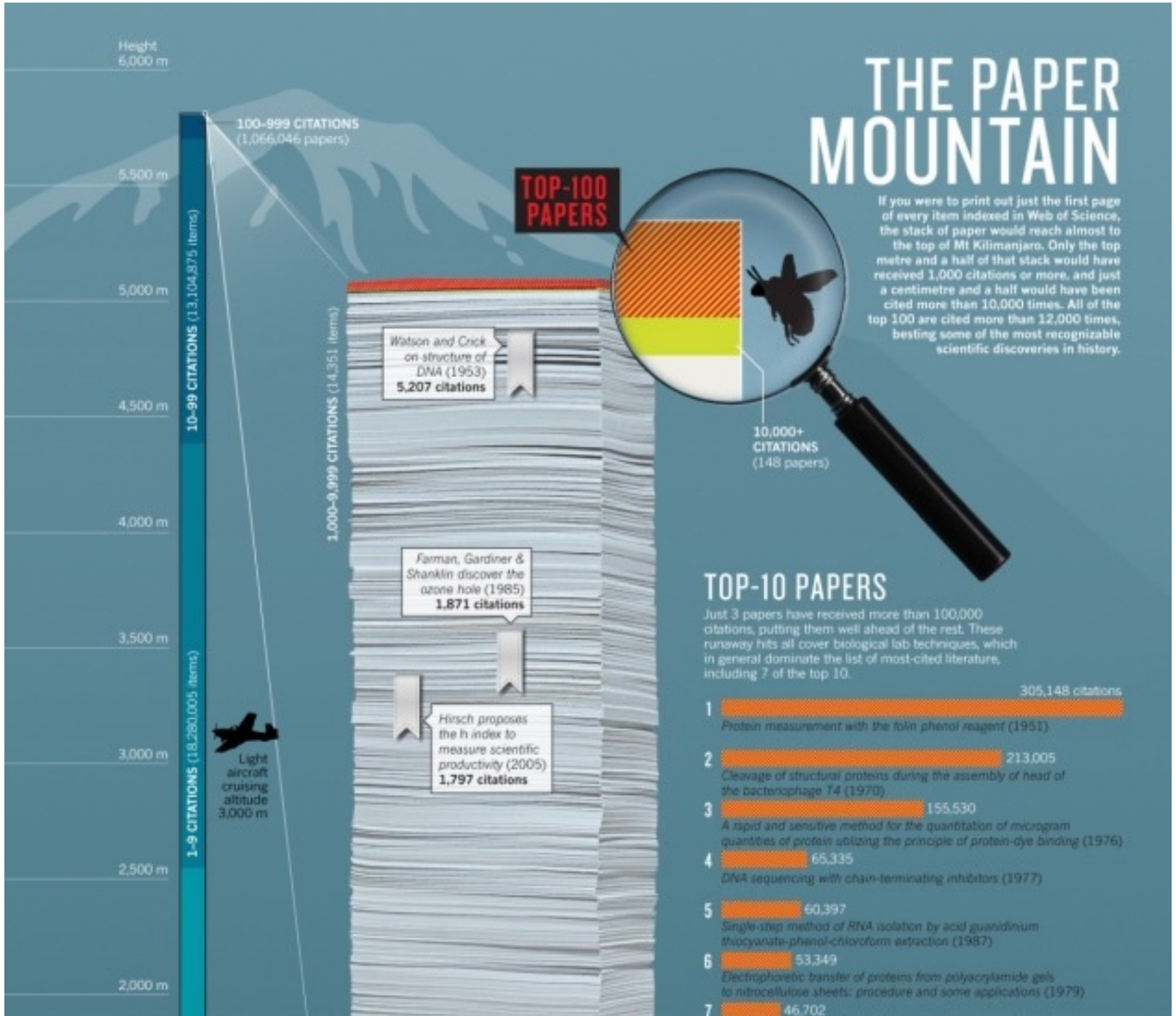
100% GROWTH EVERY 14-16 MONTHS

A calculation that took **one year in 1992** takes **one second in 2021** (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.**



IMPACT OF COMPUTATIONAL QUANTUM MECHANICS



If you were to print out just the first page of every item indexed in Web of Science, the stack of paper would reach almost to the top of Mt Kilimanjaro. Only the top metre and a half of that stack would have received 1,000 citations or more, and just a centimetre and a half would have been cited more than 10,000 times. All of the top 100 are cited more than 12,000 times, besting some of the most recognizable scientific discoveries in history.

Just 3 papers have received more than 100,000 citations, putting them well ahead of the rest. These runaway hits all cover biological lab techniques, which in general dominate the list of most-cited literature, including 7 of the top 10.

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 Furthmuller
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	Blochl
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	Moller 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)

FORTUNE COOKIE #2

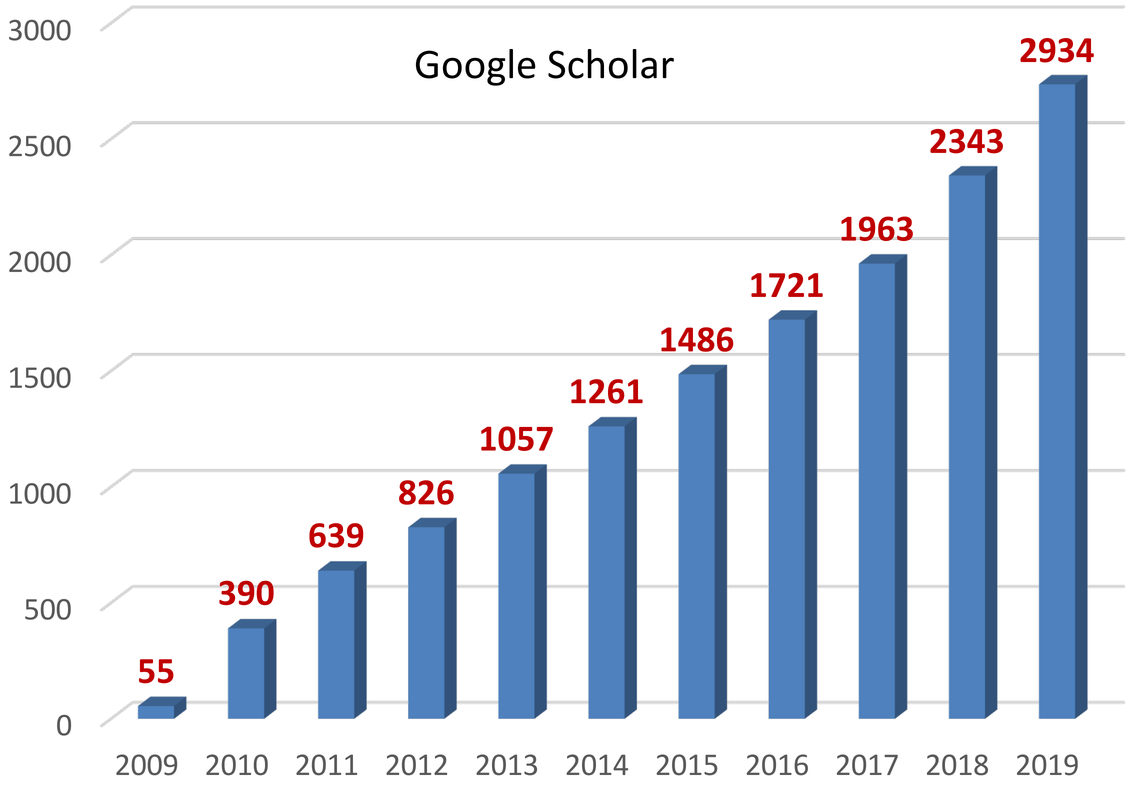
COMPUTATIONAL SCIENCE IS HERE, WITH MAJOR IMPACT

SOME EU INFRASTRUCTURES IN THE PHYSICAL SCIENCES

- ESA **5.72 € billion/year** (2019)
- ITER **22 to 65 $ billion** (2007-35)
- CERN **1.3 CHF billion/year** (2019)

QUANTUM ESPRESSO vs CERN

www.quantum-espresso.org




CERN Scientific Information Service

Library - Archive - Open Access

List of CERN publications in 2019

1762 CERN publications were selected for inclusion in the list corresponding to the CERN 2019 annual report. Of these 944 were articles in journals, 714 were contributions published in conference proceedings, 62 were reports, books, book chapters or conference proceedings.

CERN (2019): 944 articles, 714 proceedings

QE (2019, Web of Science): ~2300 articles

FORTUNE COOKIE #3

MAYBE WE SHOULD DO MORE

THE RISE OF MATERIALS SCIENCE

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)

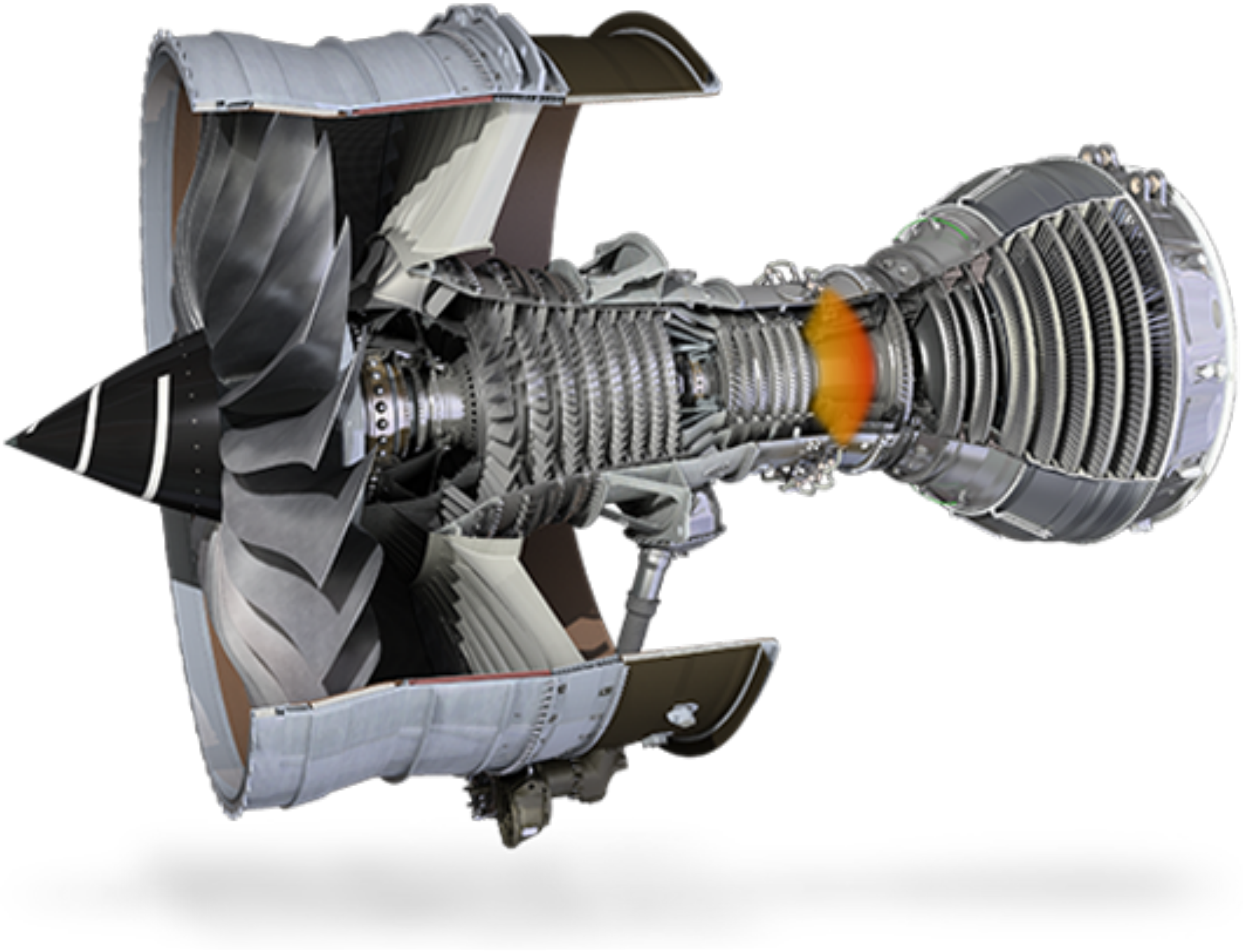
MATERIALS ARE KEY TO SOCIETAL WELL BEING

We need novel materials for:

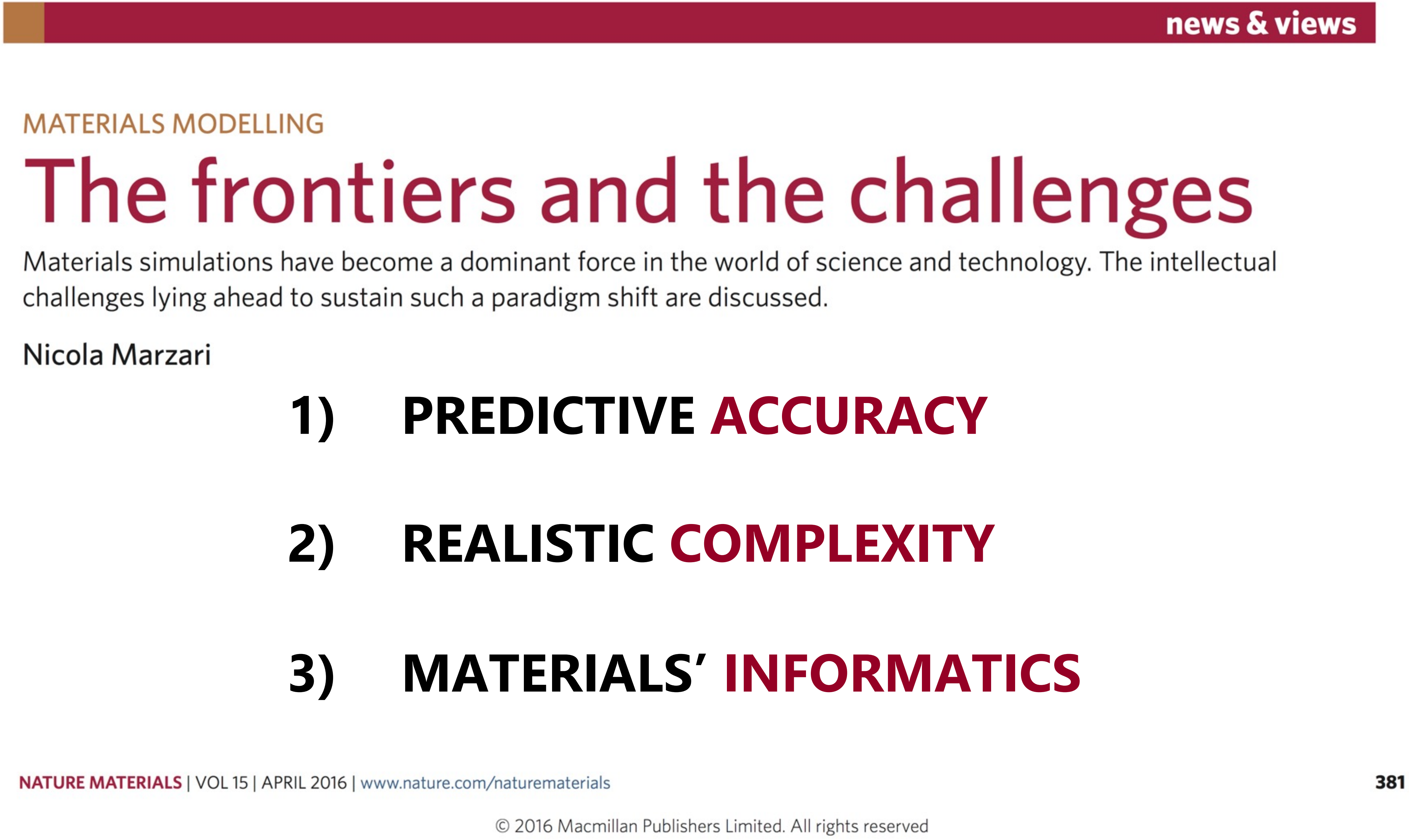
- **Energy harvesting, conversion, storage, efficiency**
- **Environmental protection and reparation**
- **High-tech and high-value industries**
- **Information and communication technologies**
- **Health care and biomedical engineering**
- **Pharmaceuticals** (crystallization, stability, polytypes)
- **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)

A FEW EASY PIECES

IF WE FLY AGAIN…



THE MOST IMPORTANT MATERIAL EVER?



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**

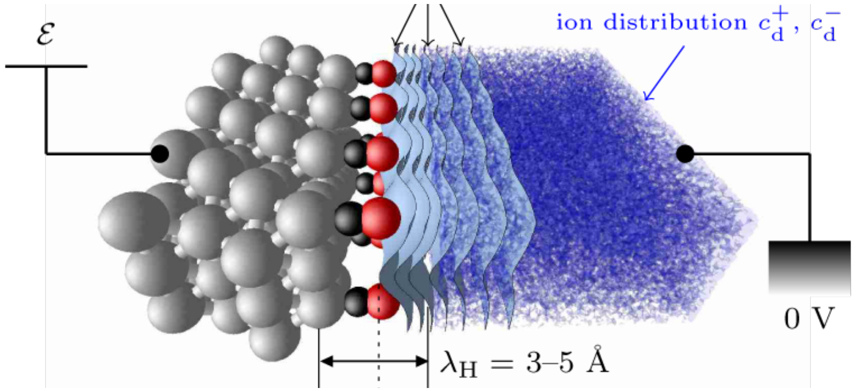
2) **REALISTIC COMPLEXITY**

3) **MATERIALS' INFORMATICS**

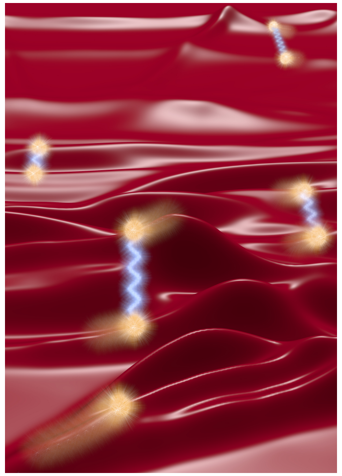
NATURE MATERIALS | VOL 15 | APRIL 2016 | www.nature.com/naturematerials 381

ADDRESSING THE REALISTIC COMPLEXITY OF MATERIALS

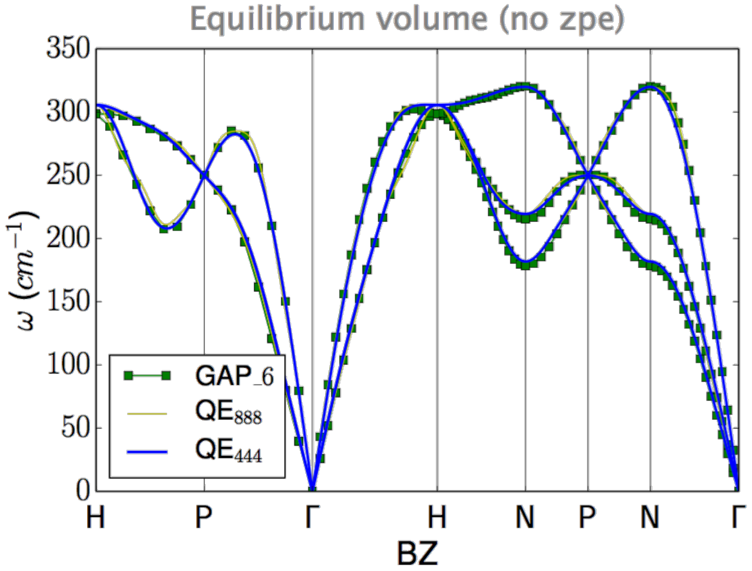
- COMPLEX SYSTEMS



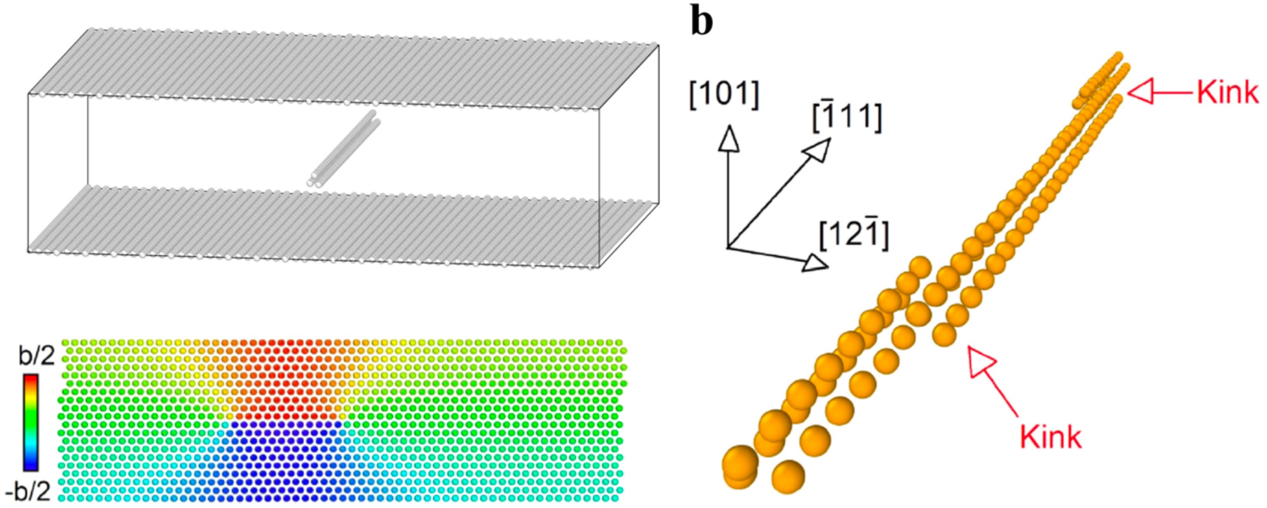
- COMPLEX PROCESSES



MACHINE-LEARNING QUANTUM MECHANICS



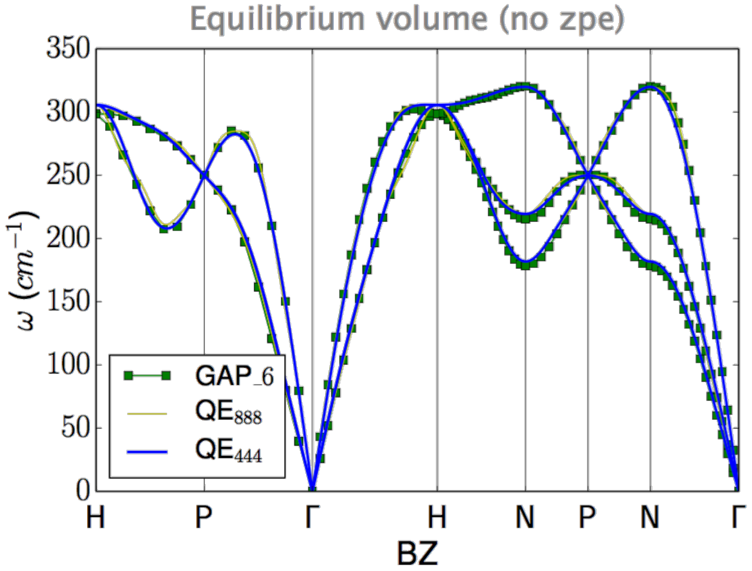
Dislocation glide by kink-pair nucleation and propagation



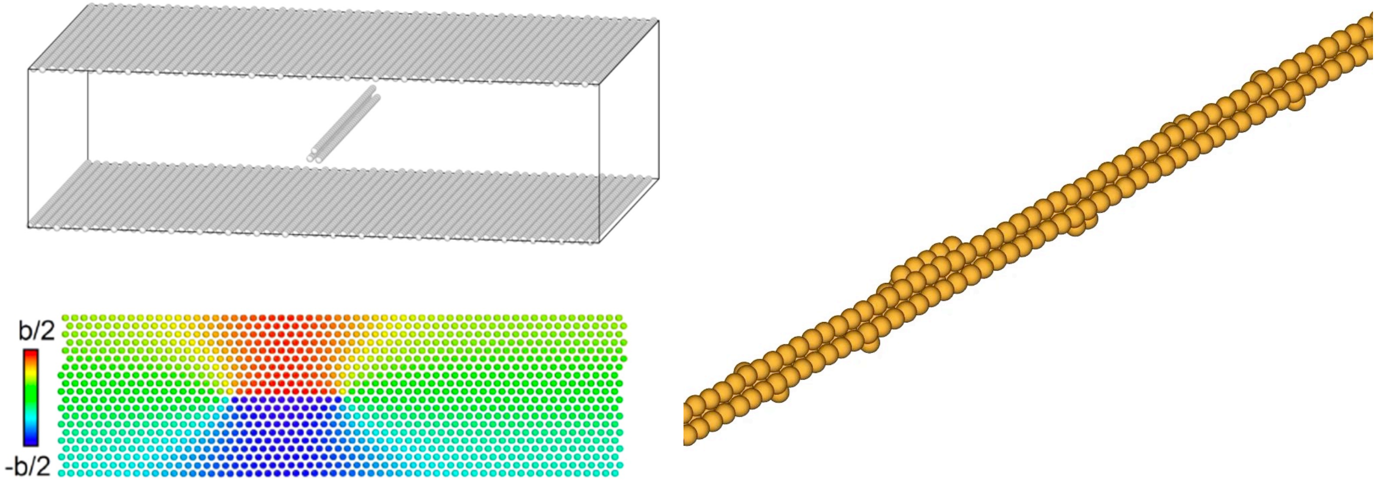
D. Dragoni, T. Duff, G. Csányi, and N. Marzari,
Phys. Rev. Materials 2, 013808 (2018)

F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W. A. Curtin,
npj Comput Mater 4, 69 (2018)

MACHINE-LEARNING QUANTUM MECHANICS



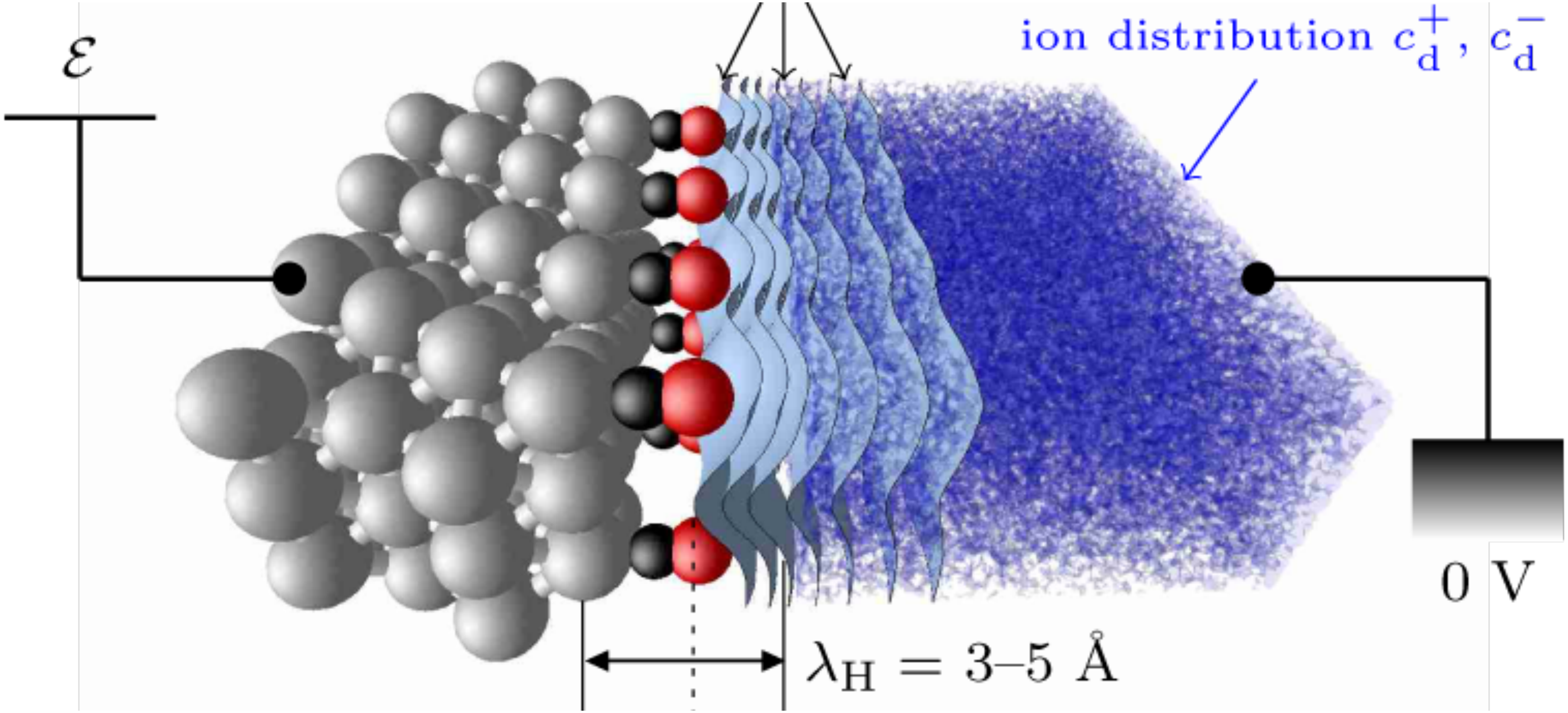
Dislocation glide by kink-pair nucleation and propagation



D. Dragoni, T. Duff, G. Csányi, and N. Marzari,
Phys. Rev. Materials 2, 013808 (2018)

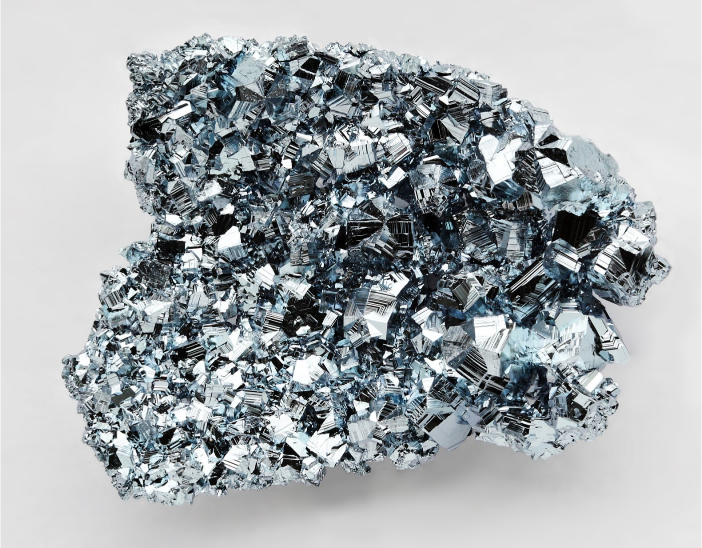
F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W. A. Curtin,
npj Comput Mater 4, 69 (2018)

COMPLEXITY: MULTI-SCALE MODELING FOR ELECTROCHEMISTRY



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

COMPLEXITY: PREDICTING THE COLOUR OF A MATERIAL



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

COMPLEXITY: MULTI-PHYSICS MODELING OF TRANSPORT

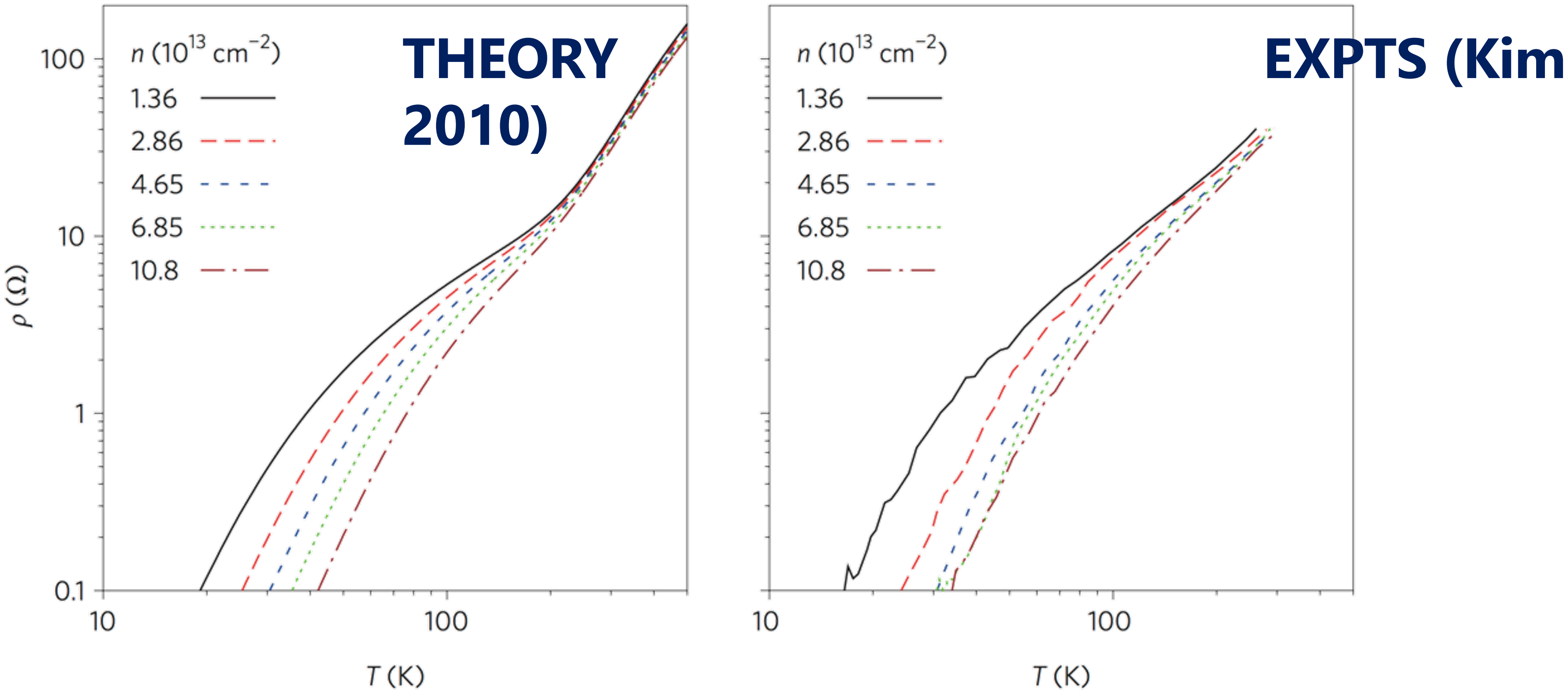
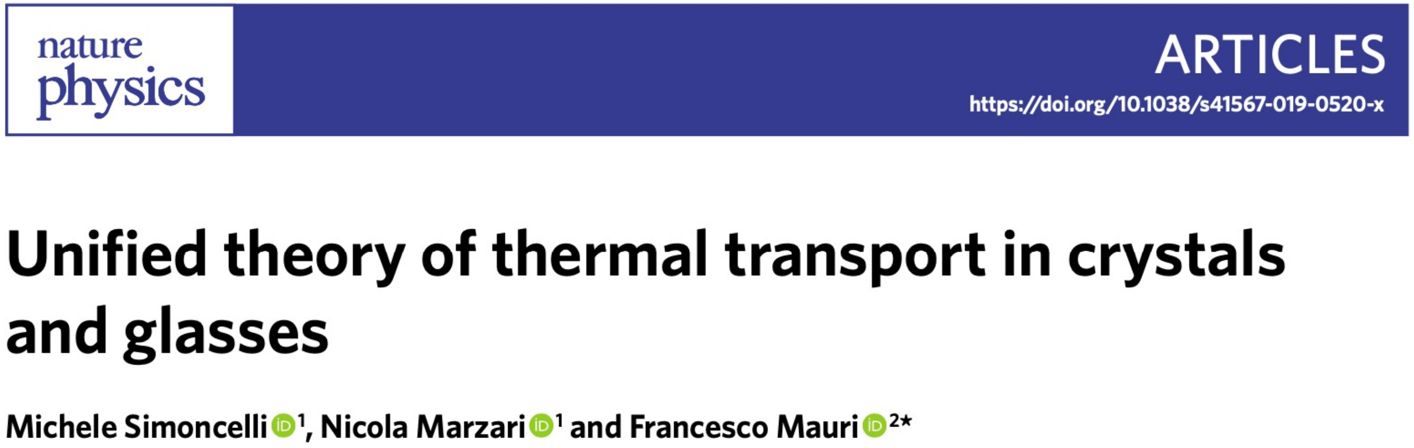


Figure 1 | Electrical resistivity of graphene as a function of temperature and doping (ρ, electrical resistivity; T, temperature; n, carrier density). Left panel: first-principles results obtained using a combination of density-functional perturbation theory, many-body perturbation theory and Wannier 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)

THERMOELECTRICS AND THERMAL BARRIER COATINGS

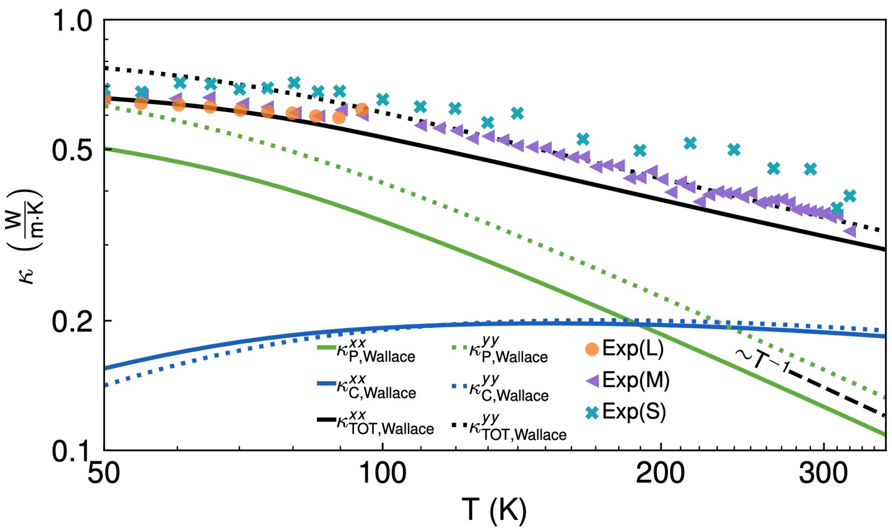

nature physics

ARTICLES

https://doi.org/10.1038/s41567-019-0520-x

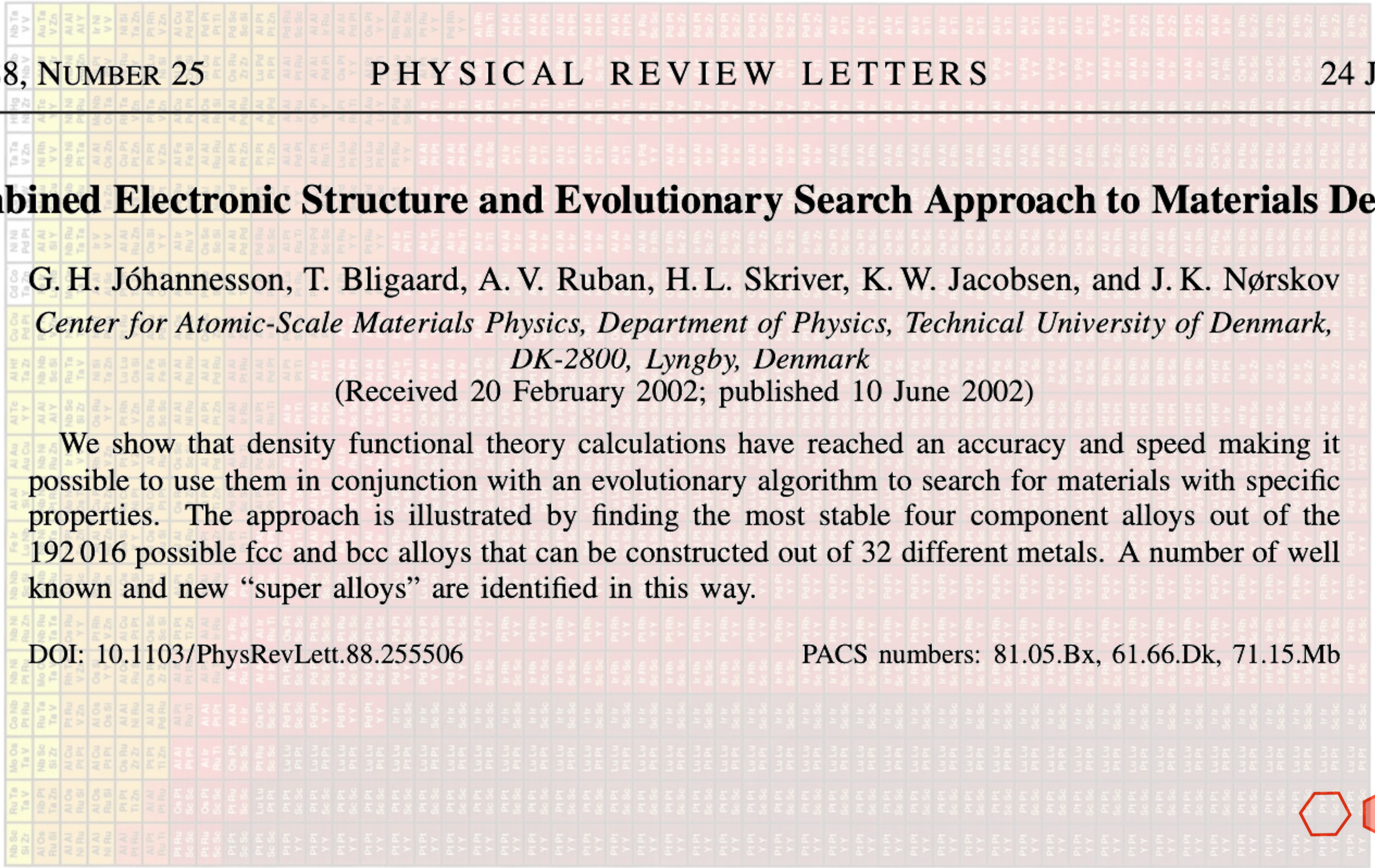
Unified theory of thermal transport in crystals and glasses

Michele Simoncelli [1], **Nicola Marzari** [1] **and Francesco Mauri** [2*]



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

RELIABLY, REPRODUCIBLY, HIGH-THROUGHPUT



VOLUME 88, NUMBER 25 PHYSICAL REVIEW LETTERS 24 JUNE 2002

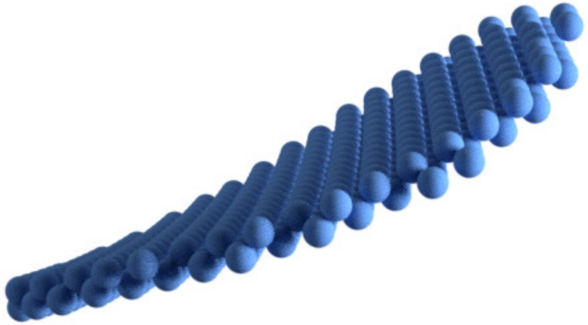
Combined Electronic Structure and Evolutionary Search Approach to Materials Design

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

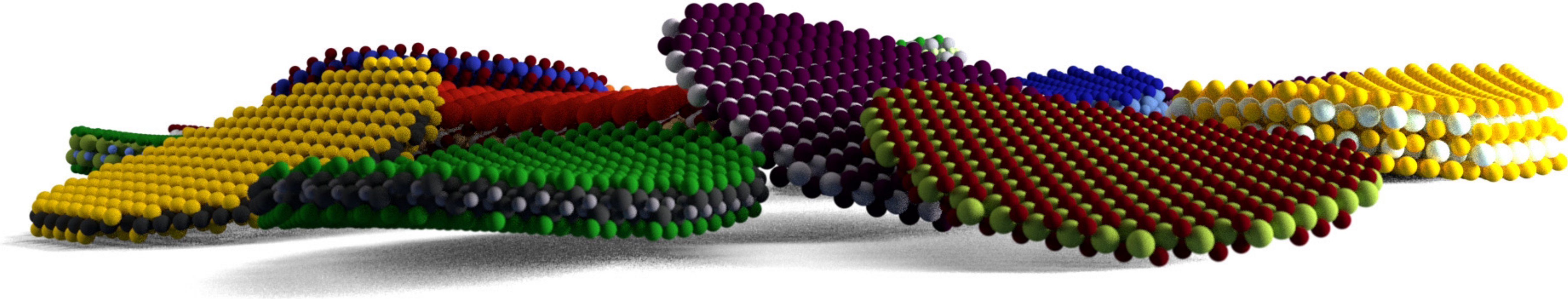
(Received 20 February 2002; published 10 June 2002)

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.

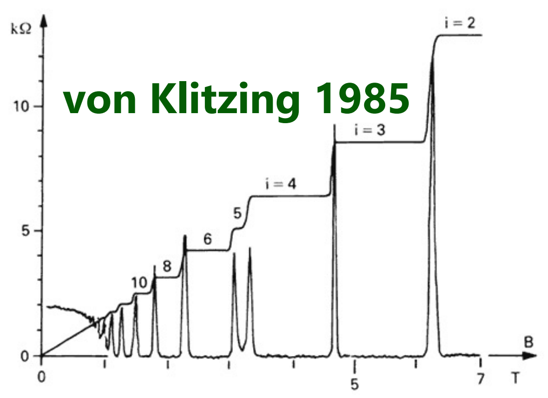
DOI: 10.1103/PhysRevLett.88.255506 PACS numbers: 81.05.Bx, 61.66.Dk, 71.15.Mb

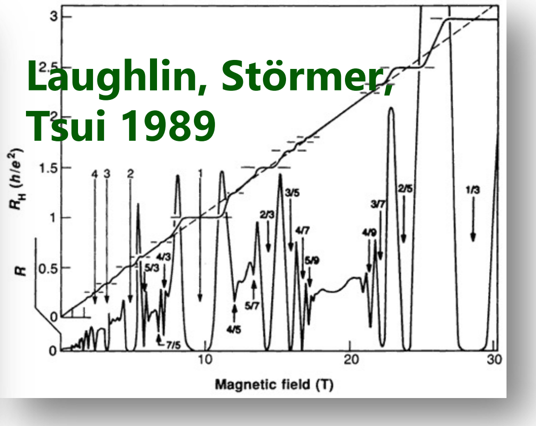


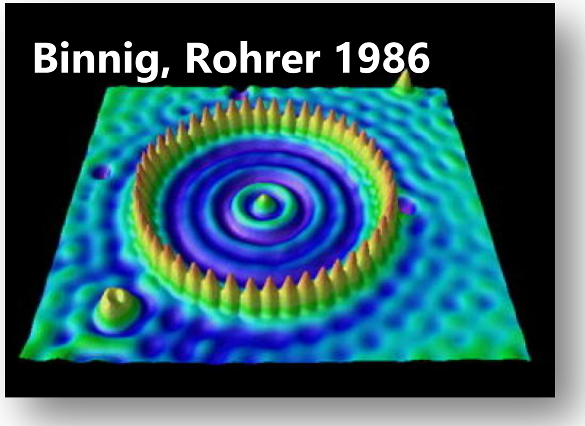
EXAMPLE: COMPUTATIONAL EXFOLIATION OF ALL KNOWN INORGANIC MATERIALS

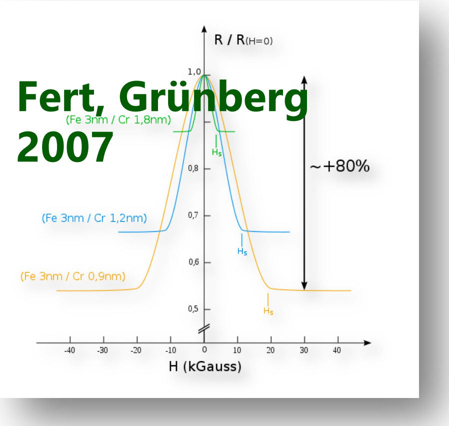


PHYSICS AND CHEMISTRY IN LOW DIMENSIONS


von Klitzing 1985

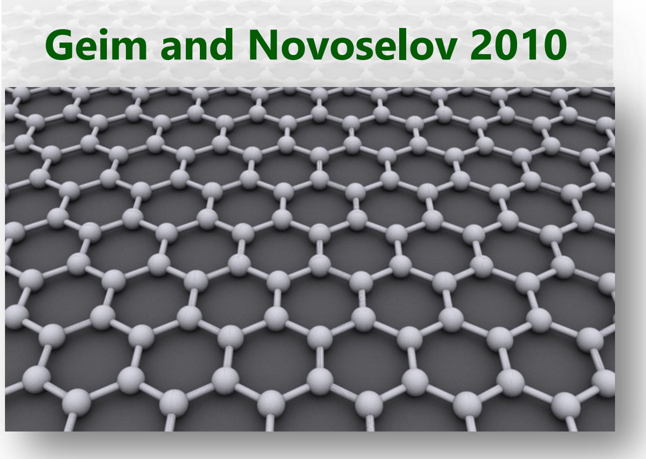

Laughlin, Störmer, Tsui 1989


Binnig, Rohrer 1986

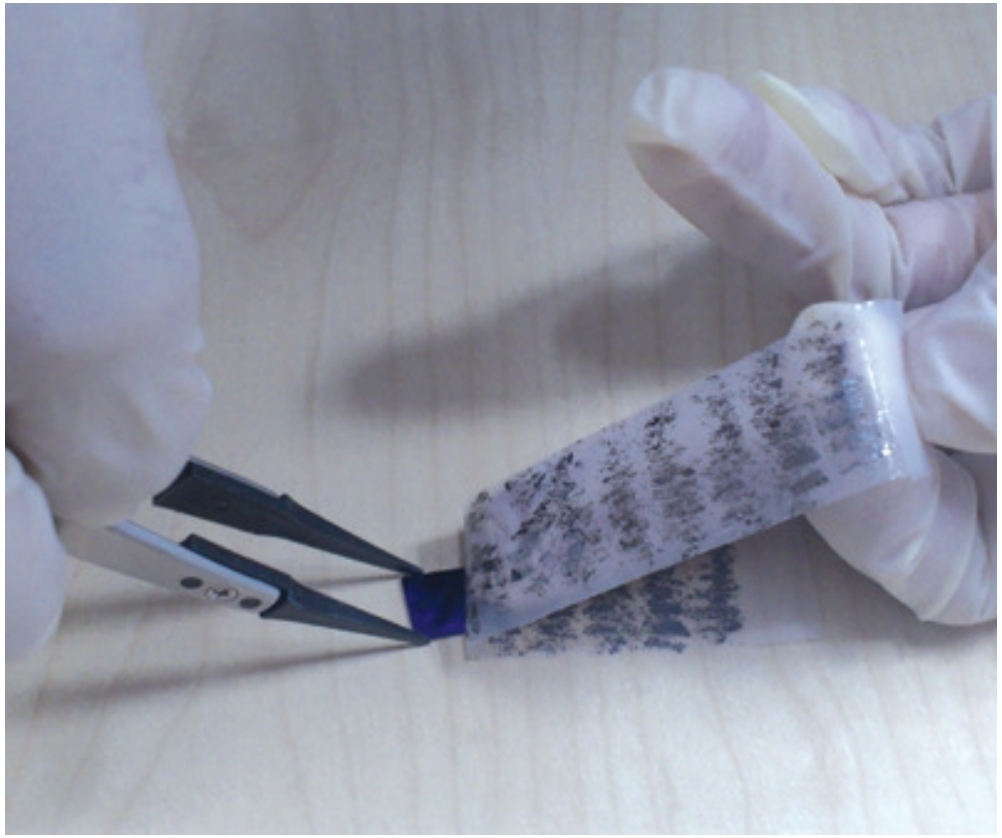

Fert, Grünberg 2007

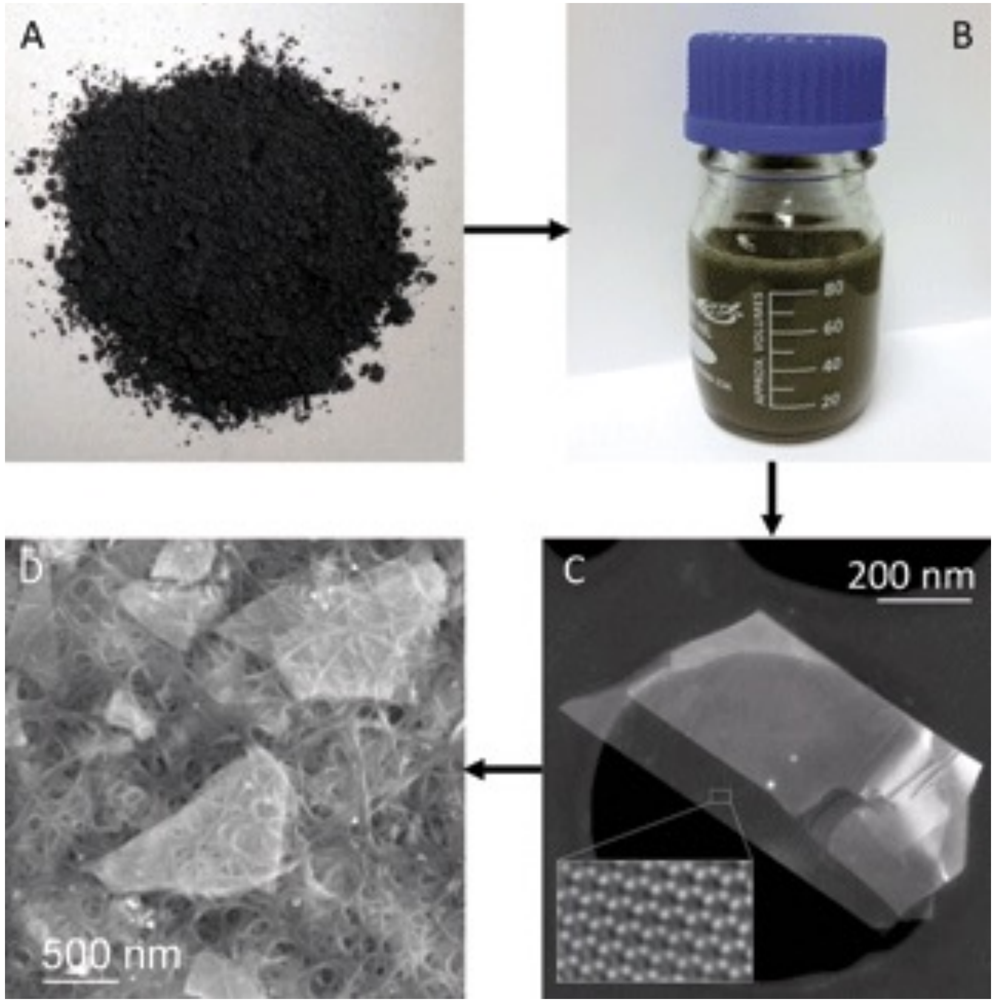

Bednorz and Müller 1987


Ertl 2007


Geim and Novoselov 2010

HOW DO WE PRODUCE 2D MATERIALS?





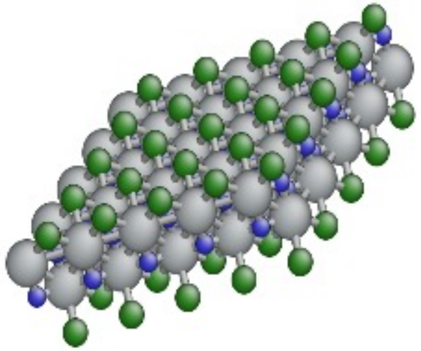
Mechanical (e.g. Geim/Novoselov, fig. from Nature/NUS) **or liquid exfoliation** (e.g. Nicolosi/Coleman, fig. from Science), **electrochemical intercalation**. Also, bottom-up: **CVD and wet chemical synthesis.**

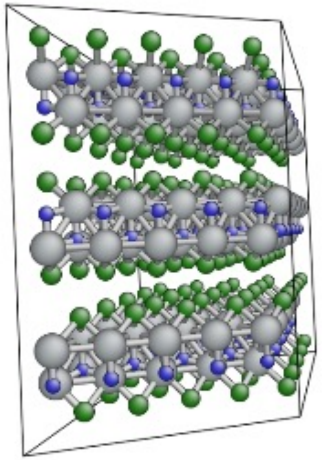
HIGH-THROUGHPUT COMPUTATIONAL EXFOLIATION

Exfoliation

External databases (ICSD, COD)

Geometrically layered





VdW-DFT electronic structure, binding energies

Characterization

Electronic

Magnetic

Mechanical

Applications

High e/h mobility

Topological

CDW, spintronics

Plasmonics

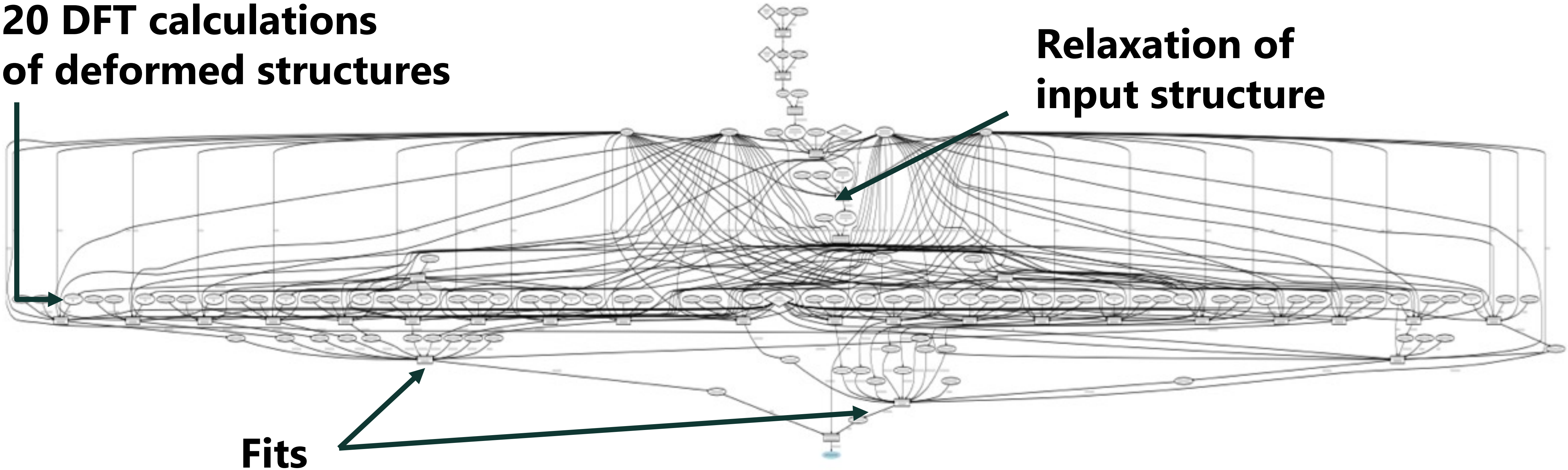
Photocatalysis

Membranes

…….

See also: S. Lebègue *et al.,* PRX (2013); R. Hennig *et al.,* PRL (2017) and E. Reed *et al.,* Nano Letters (2017), K. Choudhary, F. Tavazza, et al. Sci. Rep. (2017), and K. Thygesen, 2D Materials (2018)

AUTOMATIC WORKFLOWS: FROM STRUCTURE TO PROPERTY



Input: Structure

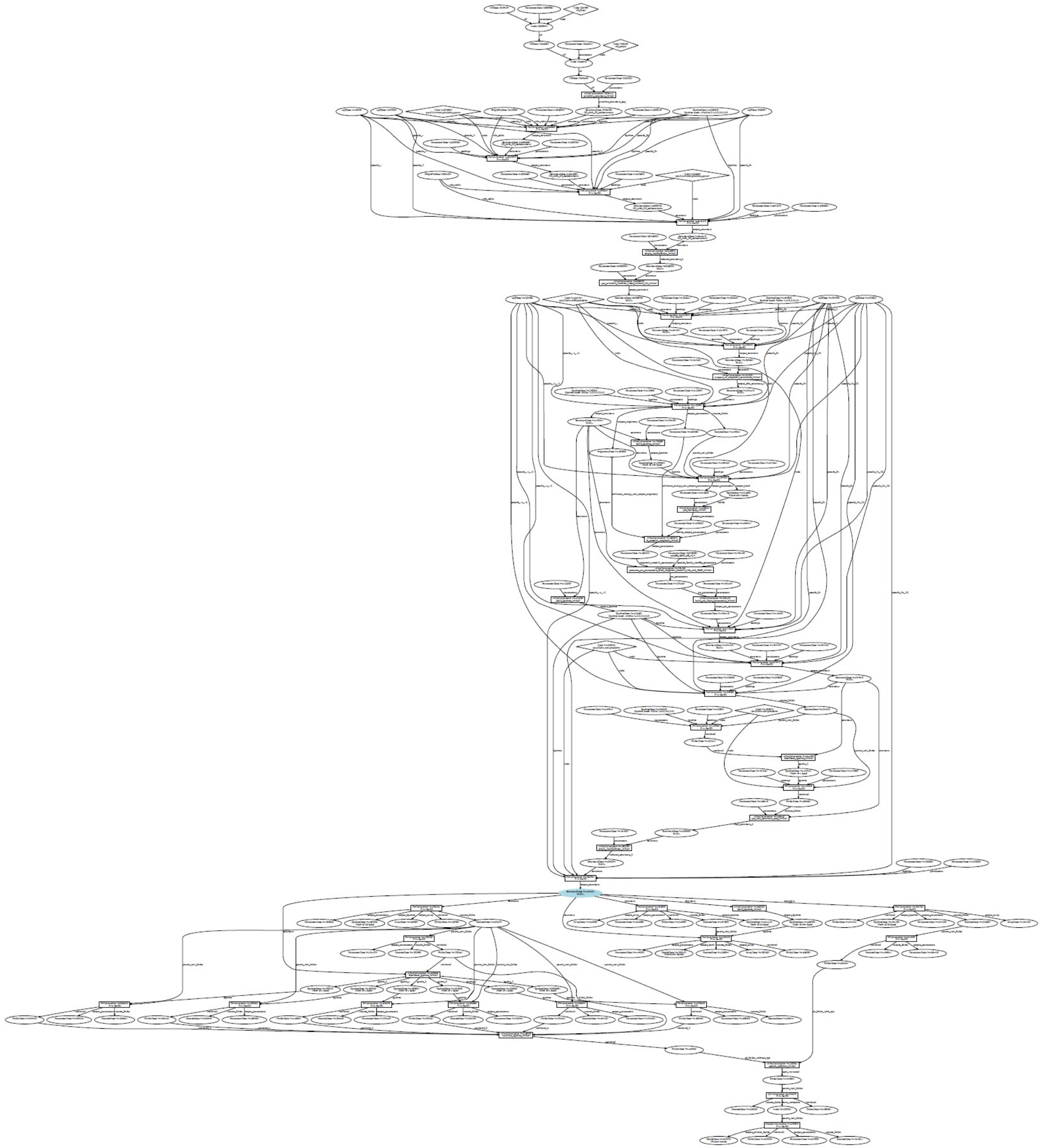
20 DFT calculations of deformed structures

Relaxation of input structure

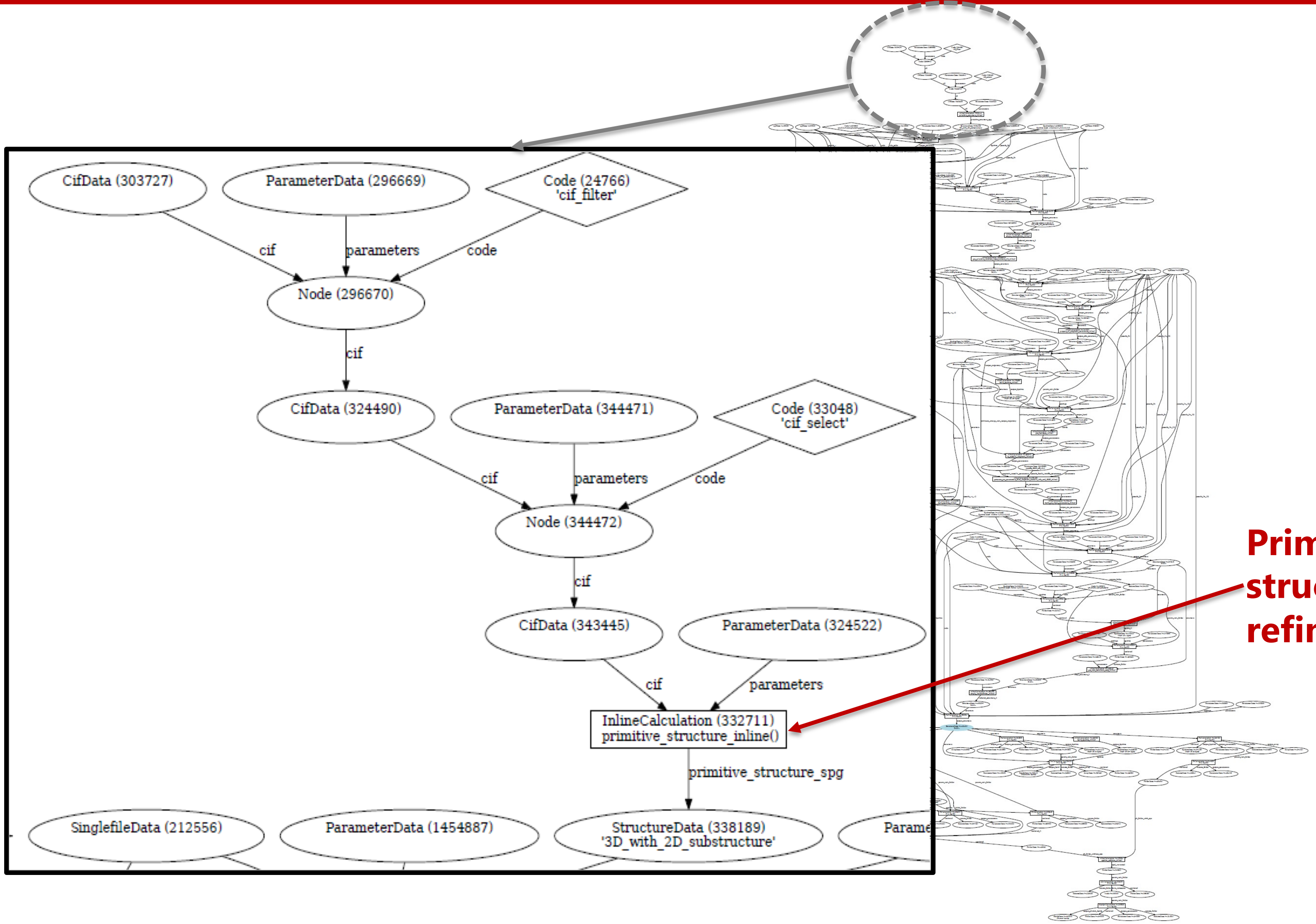
Fits

Output: Elastic tensor

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

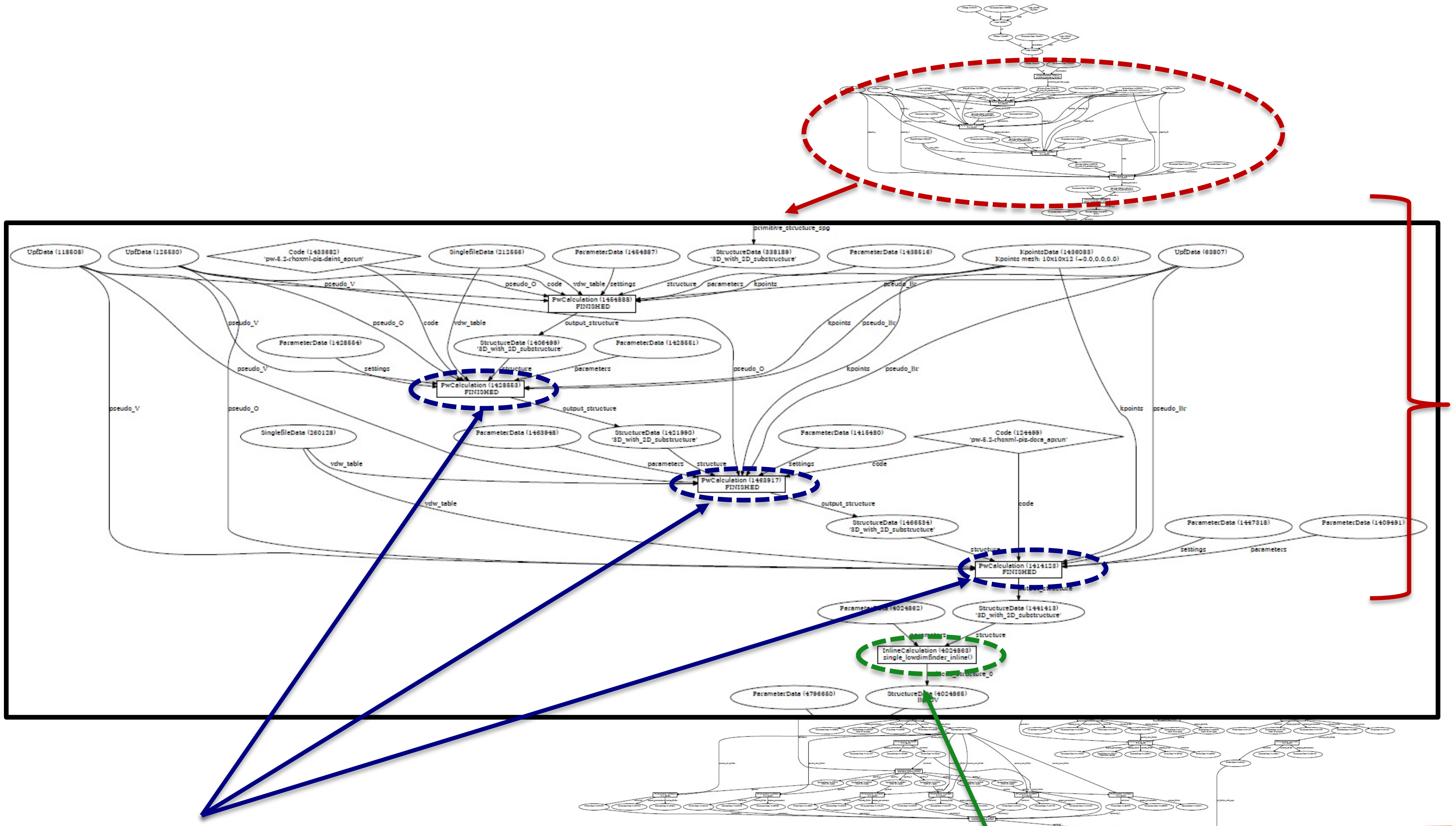


FROM DATABASE ENTRY TO A WORKING STRUCTURE



Primitive cell & structure symmetry refinement

3D RELAXATION

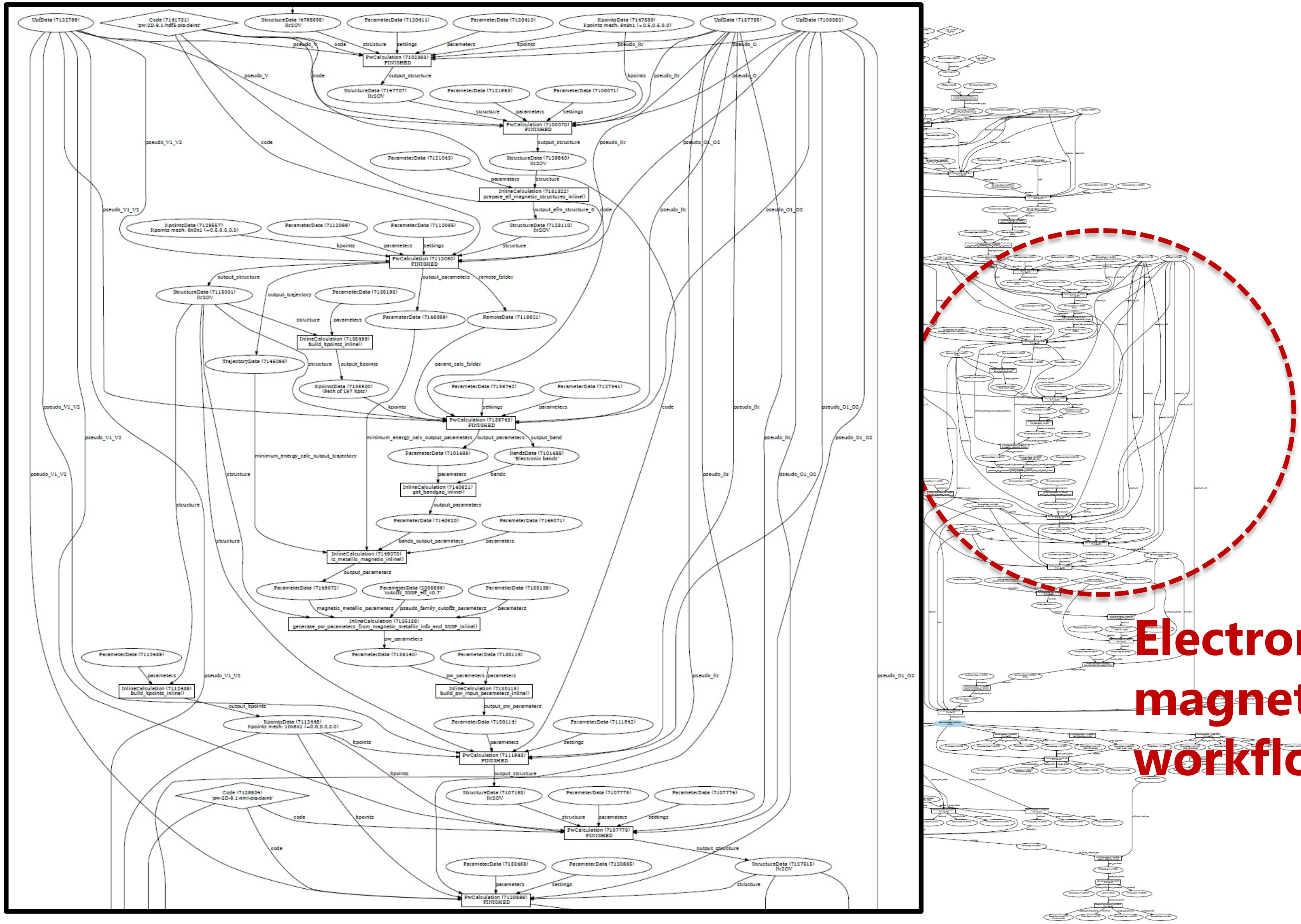


Quantum ESPRESSO Workflow

Individual DFT calculations

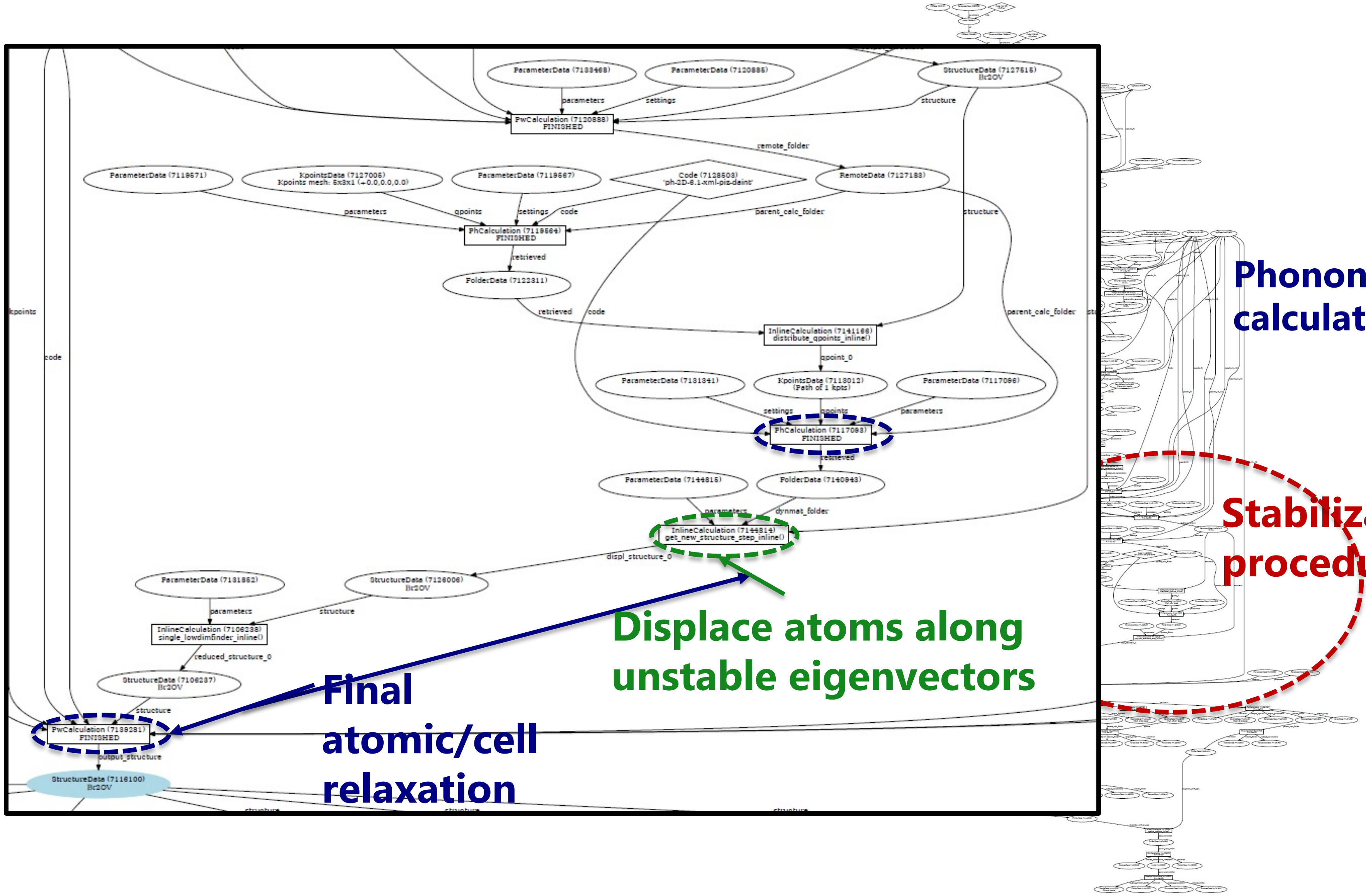
Lowdimfinder on relaxed structure

MAGNETIC SCREENING OF THE 2D MONOLAYER



Electronic & magnetic workflow

REMOVING MECHANICAL INSTABILITIES



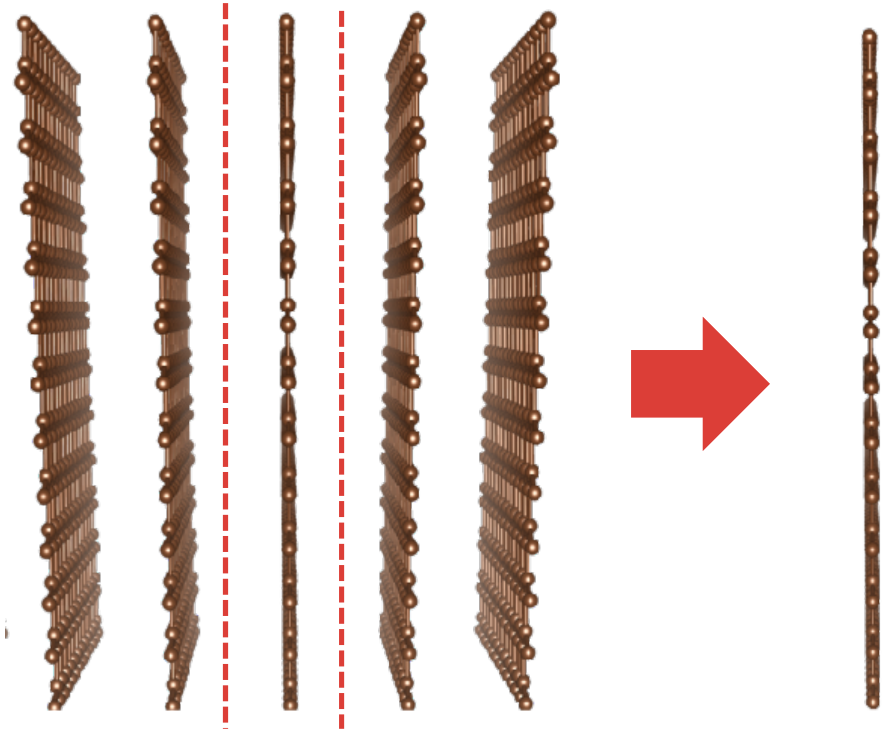
Phonon calculation

Stabilization procedure

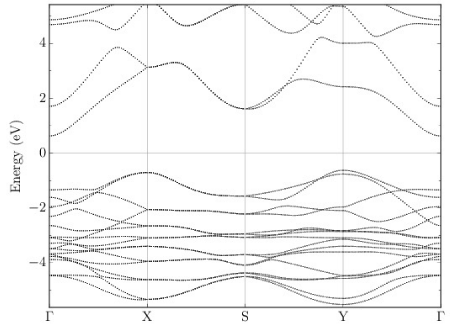
Displace atoms along unstable eigenvectors

Final atomic/cell relaxation

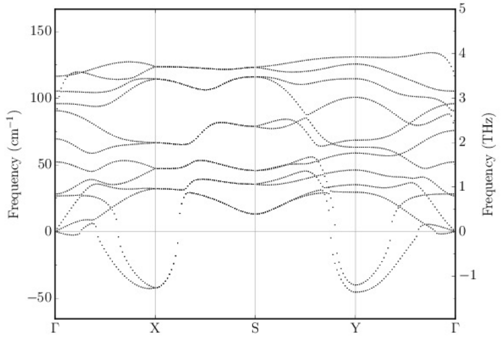
ALL AUTOMATED…



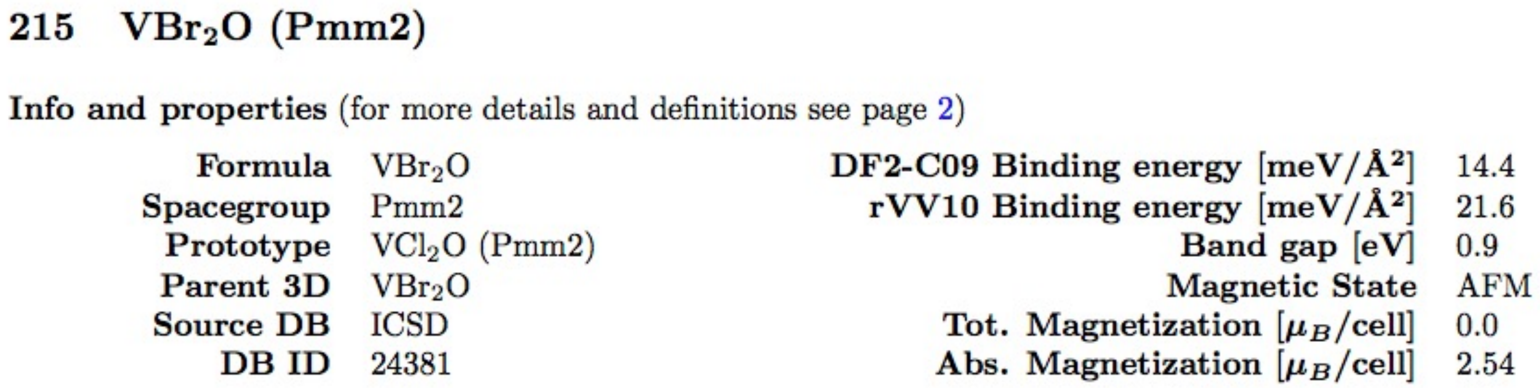
Band structures



Phonon dispersions



FINALLY…

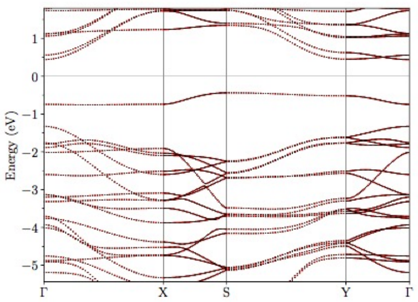


215 VBr_2O (Pmm2)

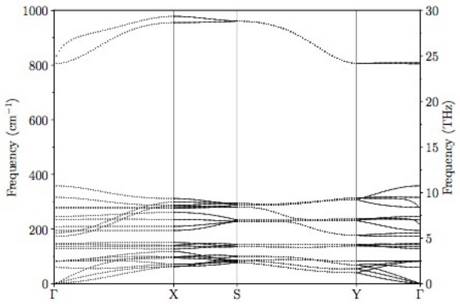
Info and properties (for more details and definitions see page 2)

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

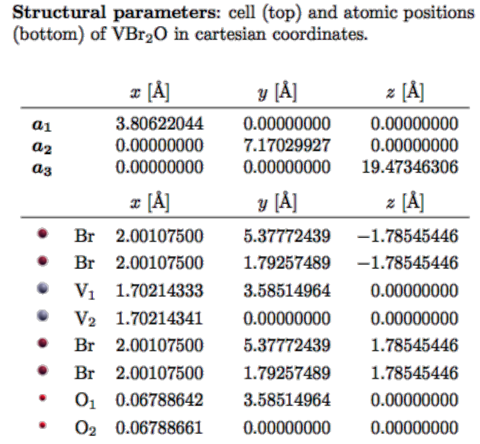


Band structure: energy bands of VBr_2O (66 electrons) in a window around the chemical potential and along a high-symmetry path. The number of bands included in the calculation is 80.



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

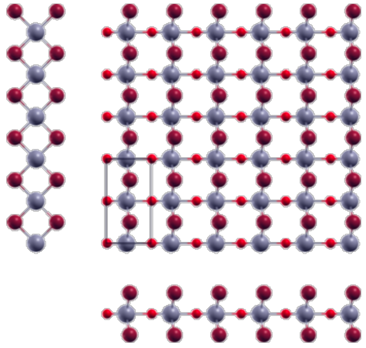
Crystal structure



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

	x [Å]	y [Å]	z [Å]
$\boldsymbol{a}_1$	3.80622044	0.00000000	0.00000000
$\boldsymbol{a}_2$	0.00000000	7.17029927	0.00000000
$\boldsymbol{a}_3$	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



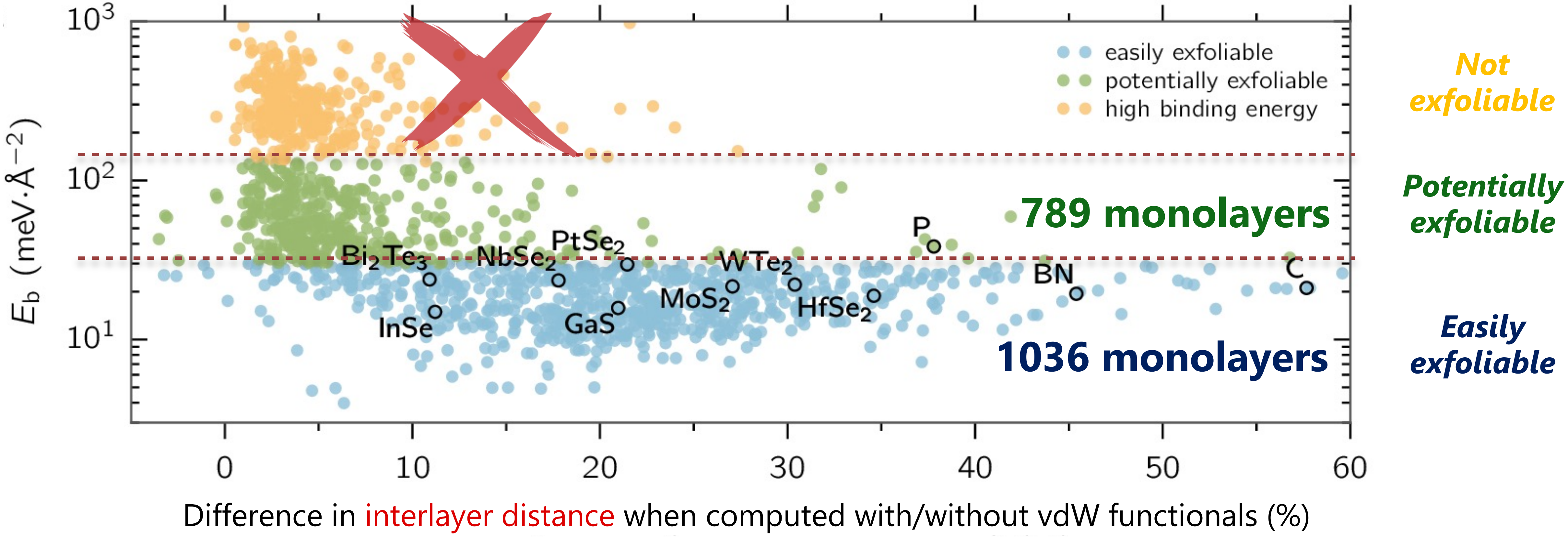
Orthographic projections: different views of VBr_2O from the x axis (left), the y axis (bottom) and the z axis (center).

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**

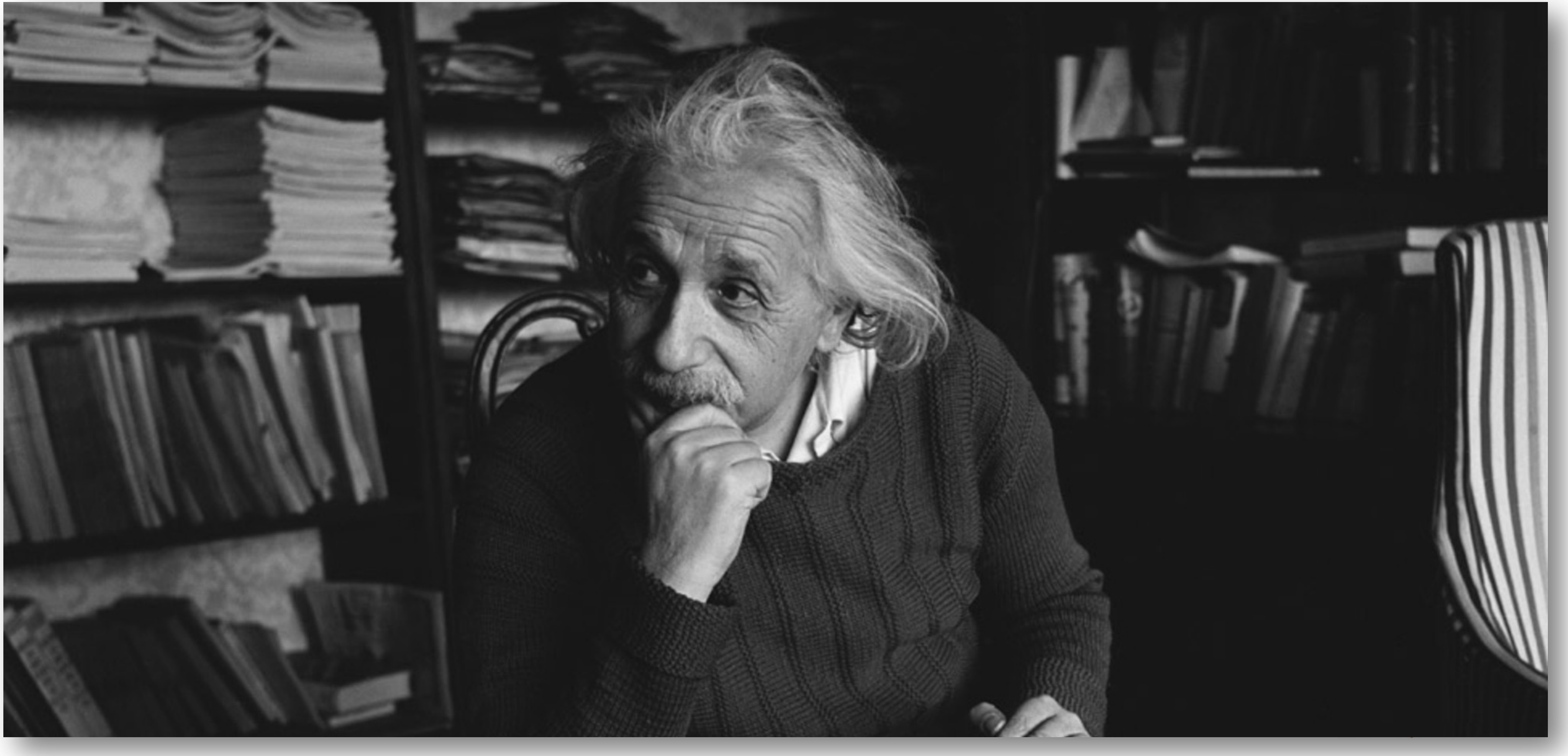
[*] **At this level unicity is not tested**

HOW MANY CANDIDATES? QUANTUM SCREENING

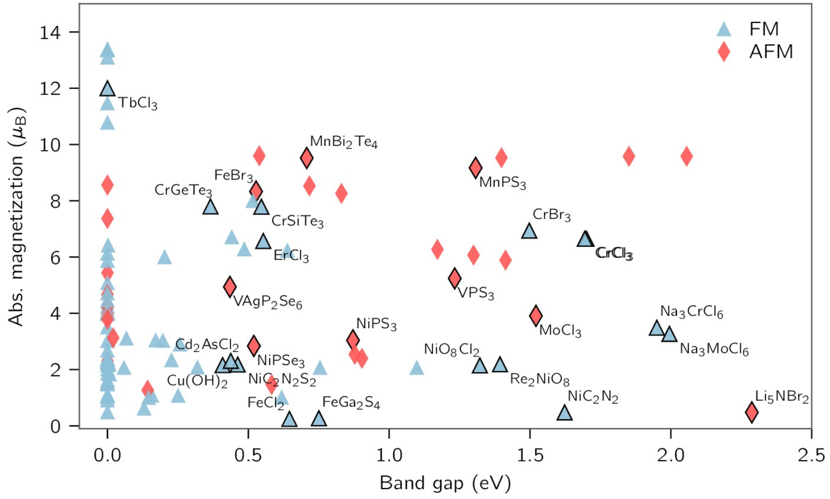


- ***E_b < 30 meV/Å² (DF2-C09) or E_b < 35 meV/Å² (rVV10) → 2D, easily exfoliable***
- ***In-between → 2D, potentially exfoliable***
- ***E_b > 130 meV/Å² → not 2D (discarded)***

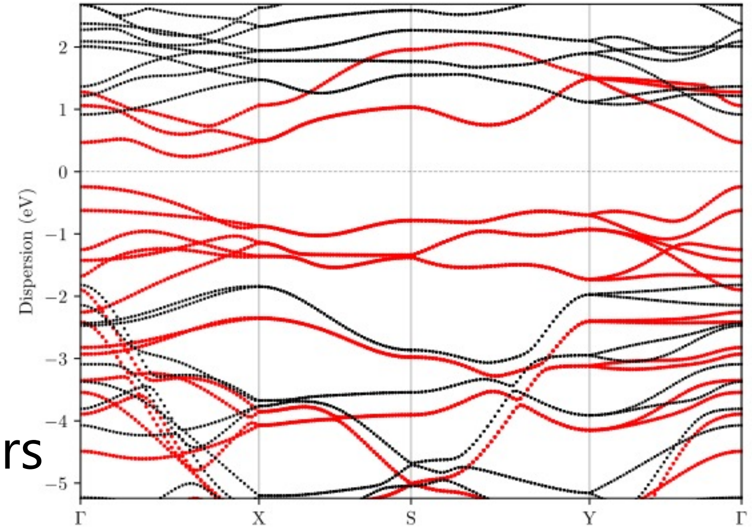
WHAT TO DO NEXT?



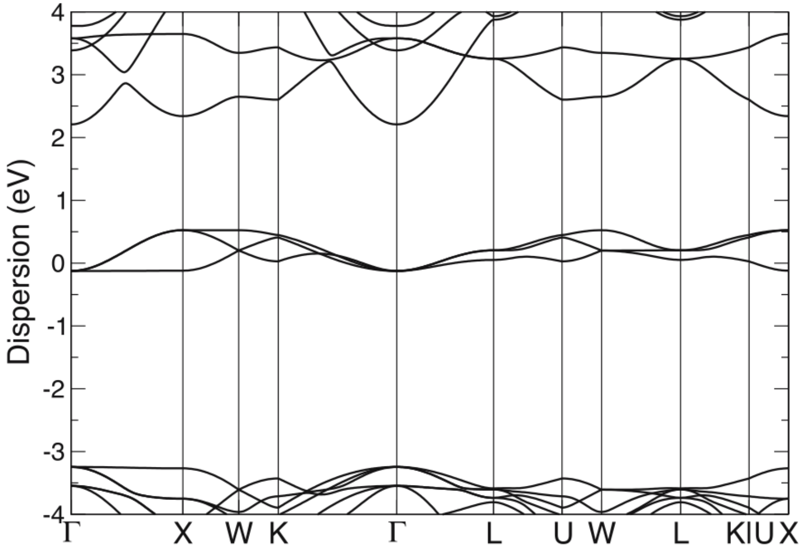
FROM ELECTRONICS...



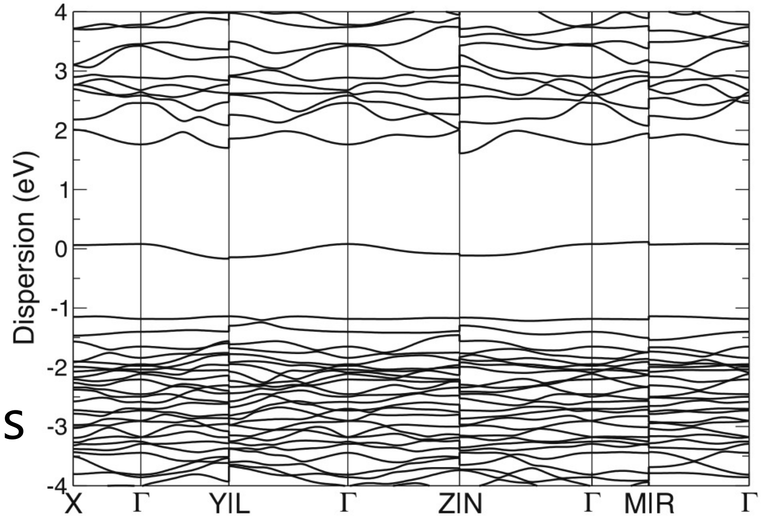
Magnetic metals
and insulators



Half-semiconductors

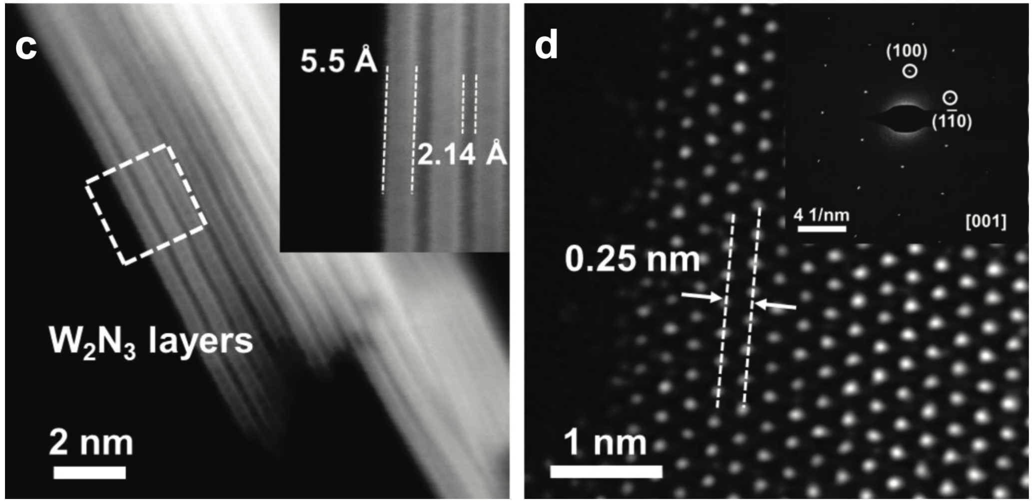


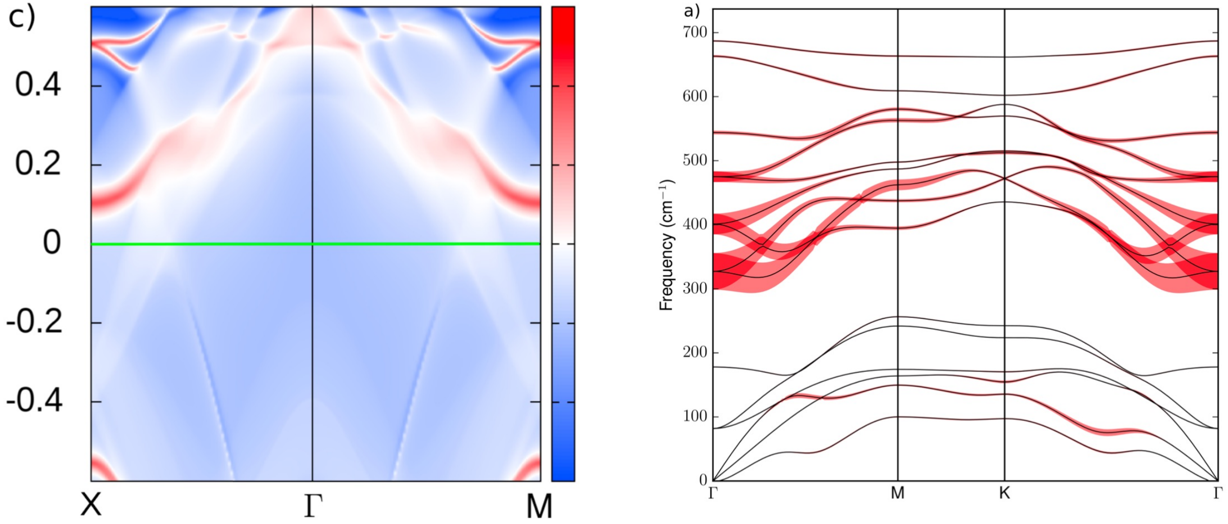
Transparent
conductors



Plasmonics

…TO THE LARGEST SUPERCONDUCTING Tc IN 2D…

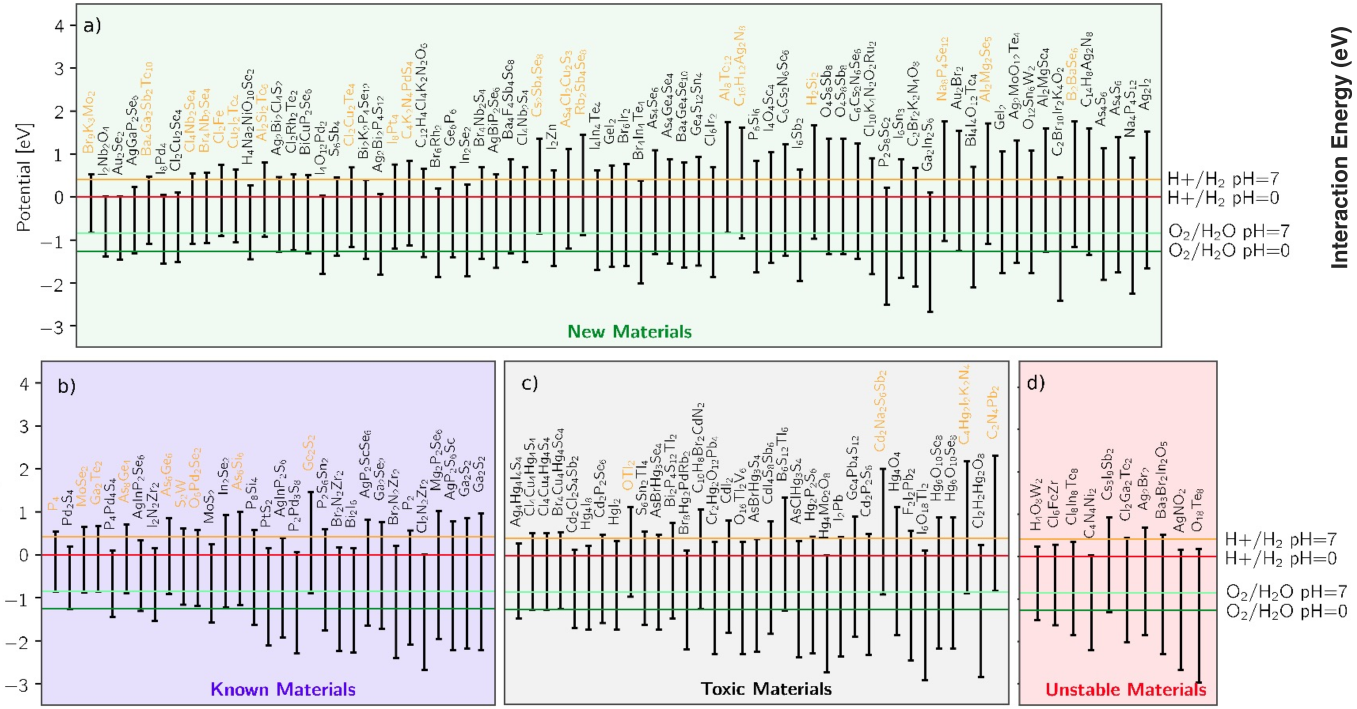


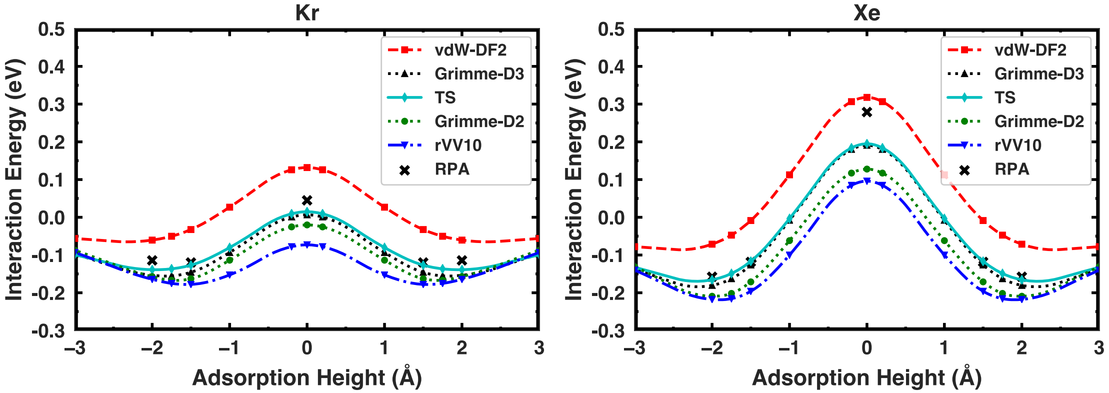


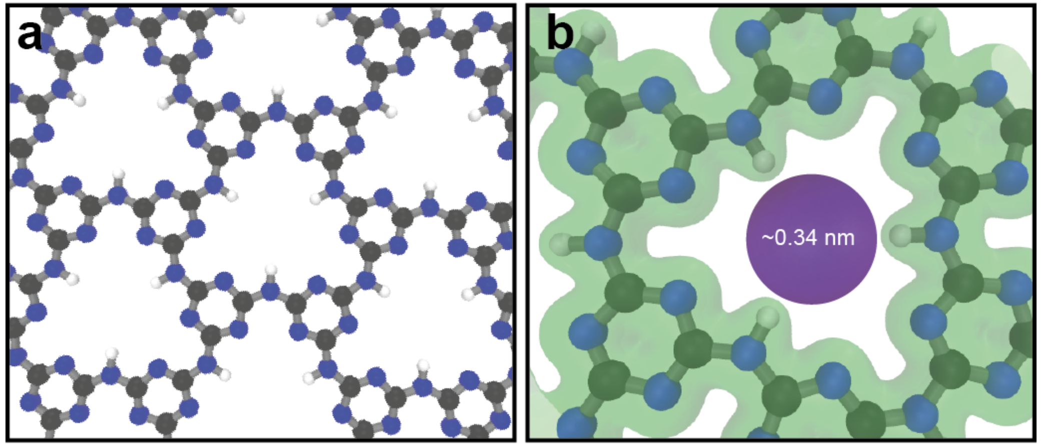
H. Jun *et al.*, Advanced Materials 31, 1902709 (2019)

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

…TO MATERIALS: PHOTOCATALYSIS, MEMBRANES

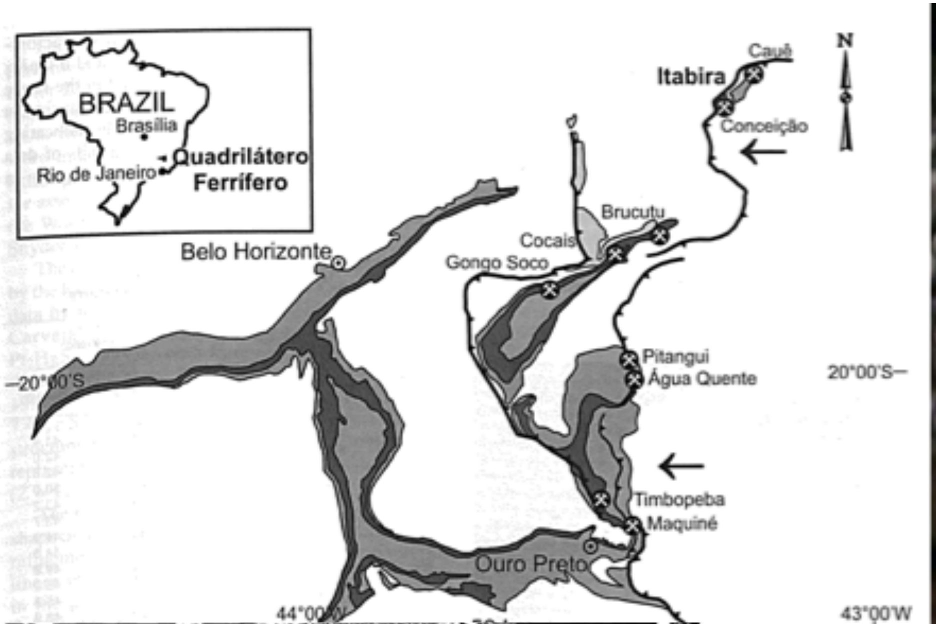


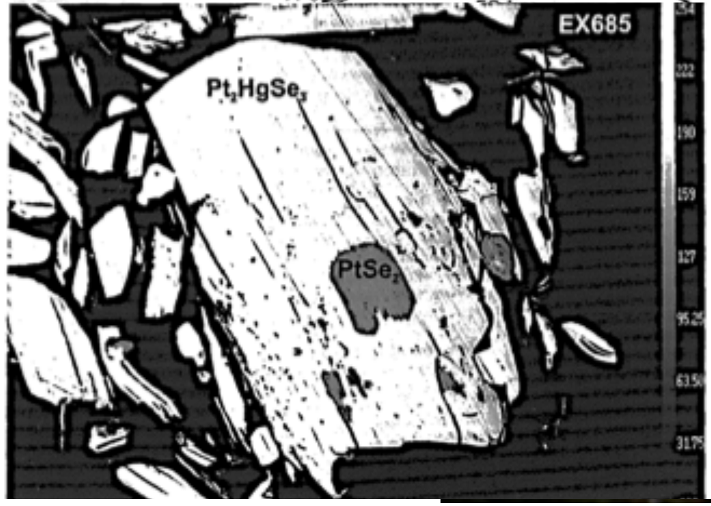




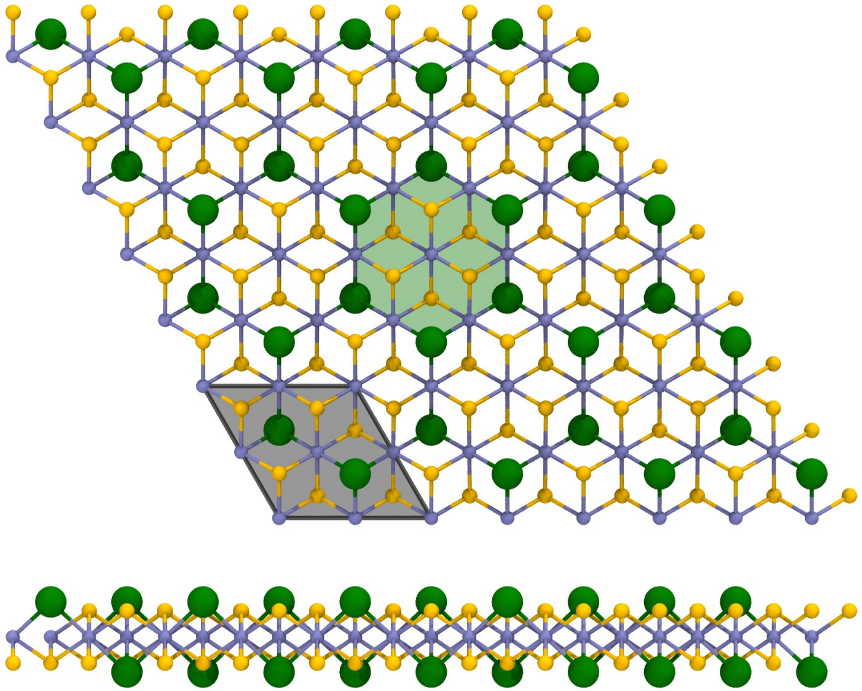
Science Advances (2019), and under review (2021)

THE DISCOVERY OF JACUTINGAITE

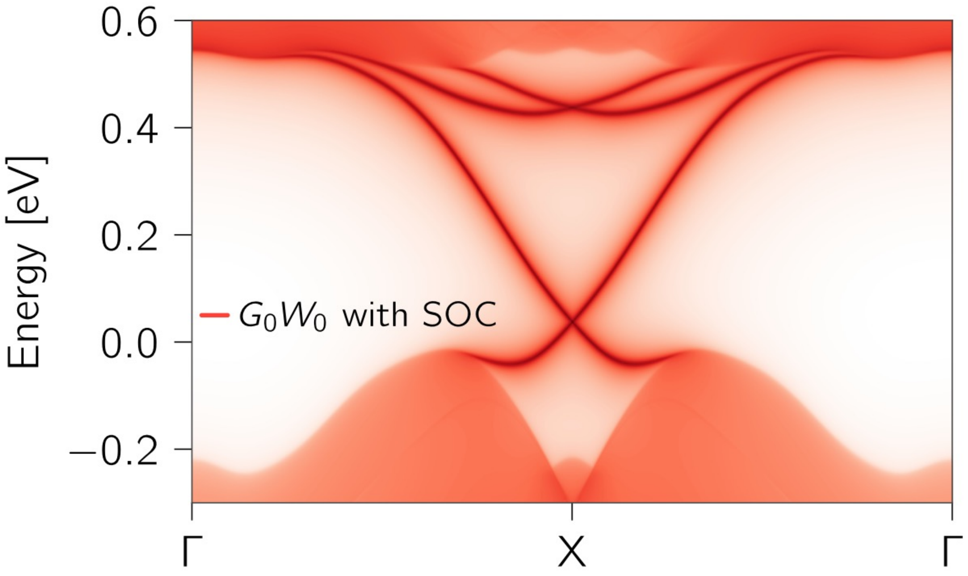




THE DISCOVERY OF JACUTINGAITE

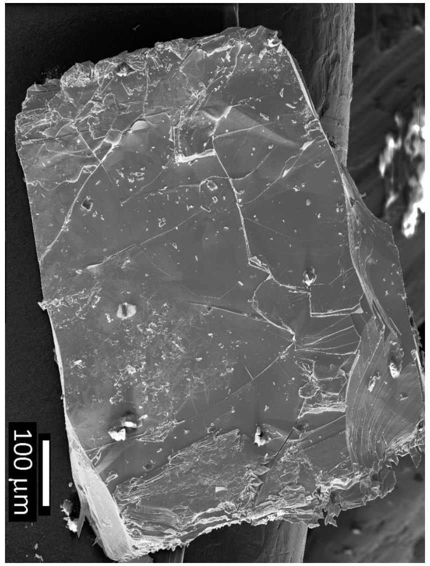


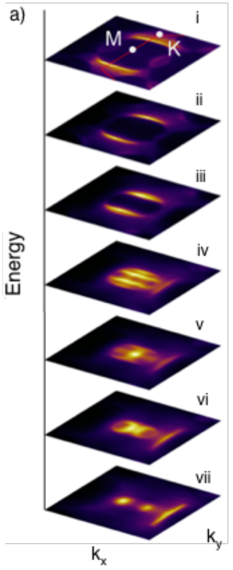
Classified as potentially exfoliable
(binding energy of 60 meV Å^{-2})

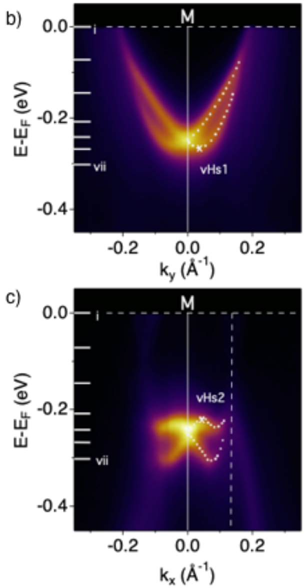


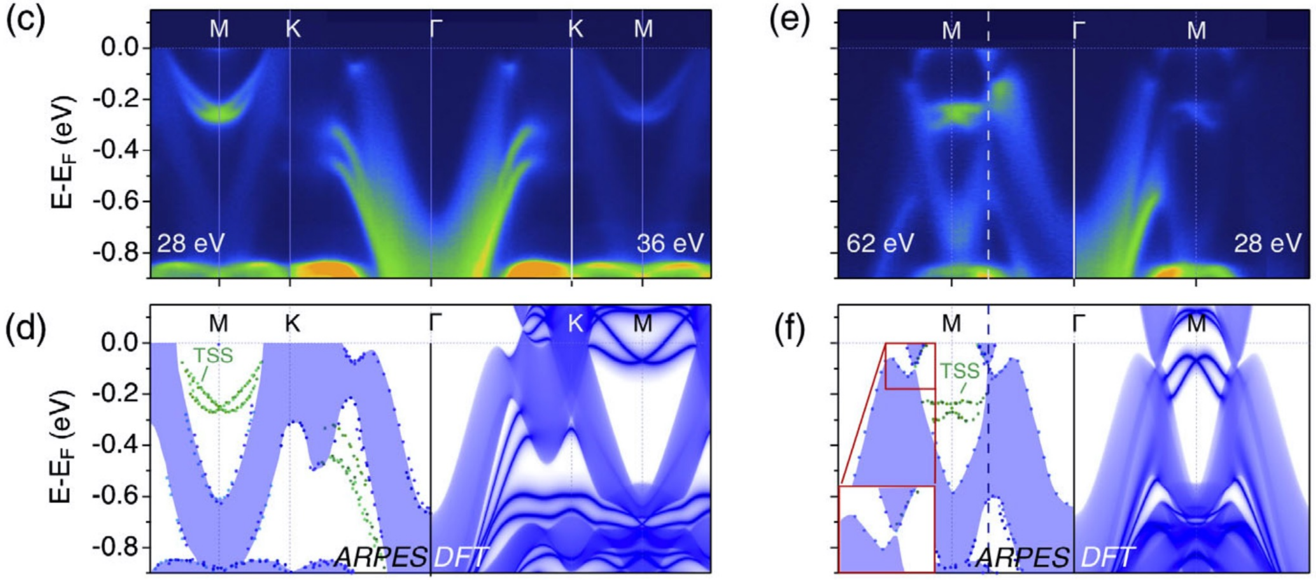
A. Marrazzo *et al.*, Phys. Rev. Lett. 120, 117701 (2018)

ROOM-TEMPERATURE KANE-MELE QSHI

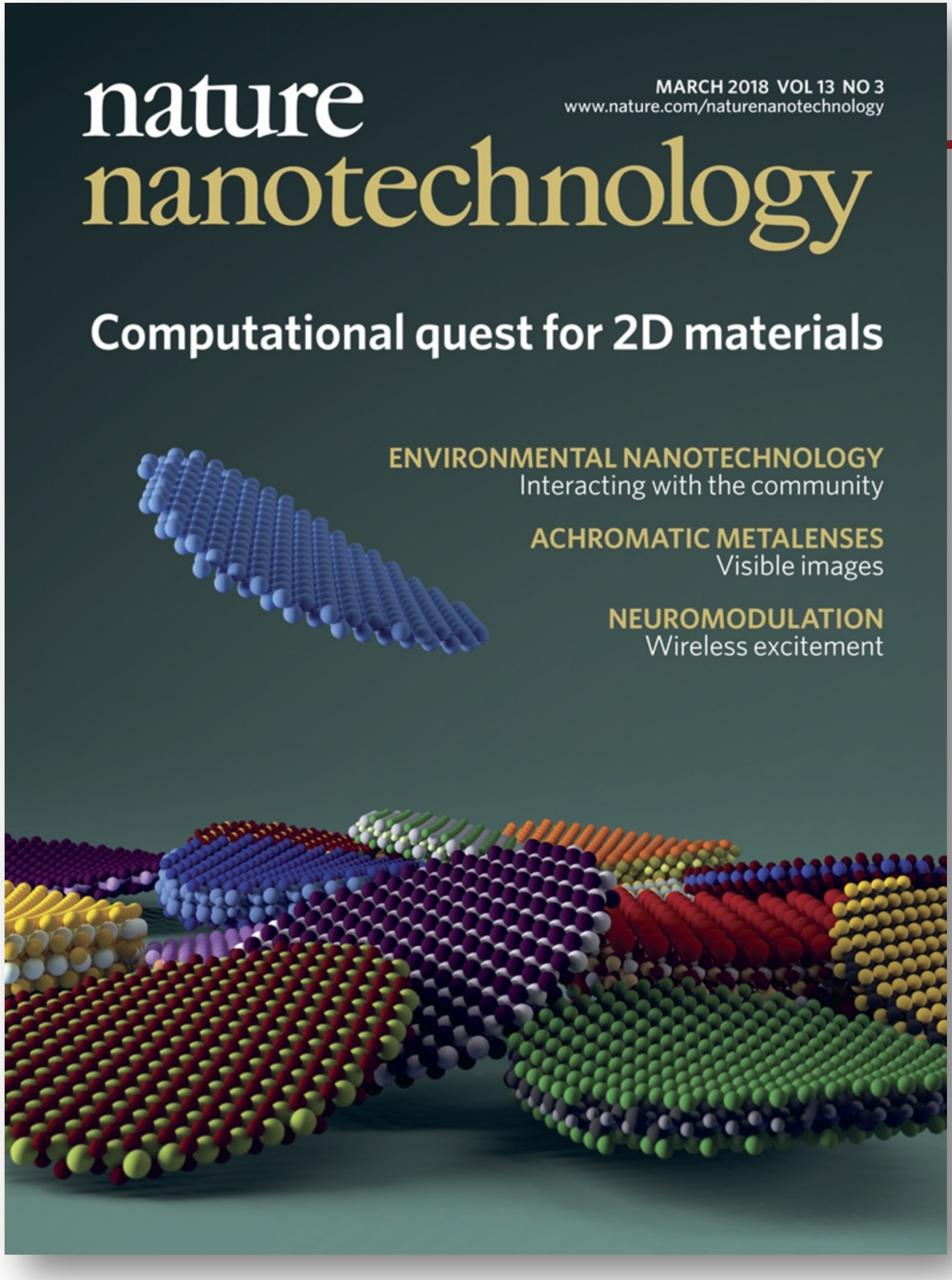








A. Marrazzo *et al.*, Phys. Rev. Lett. 120, 117701 (2018)
I. Cucchi, *et al.*, Phys. Rev. Lett. 124, 106402 (2020)
A. Marrazzo, N. Marzari, and M. Gibertini, Phys. Rev. Res. 2, 012063(R) (2020)



nature nanotechnology

MARCH 2018 VOL 13 NO 3
www.nature.com/naturenanotechnology

Computational quest for 2D materials

ENVIRONMENTAL NANOTECHNOLOGY
Interacting with the community

ACHROMATIC METALENSES
Visible images

NEUROMODULATION
Wireless excitement

THERE IS PLENTY OF ROOM AT THE TOP

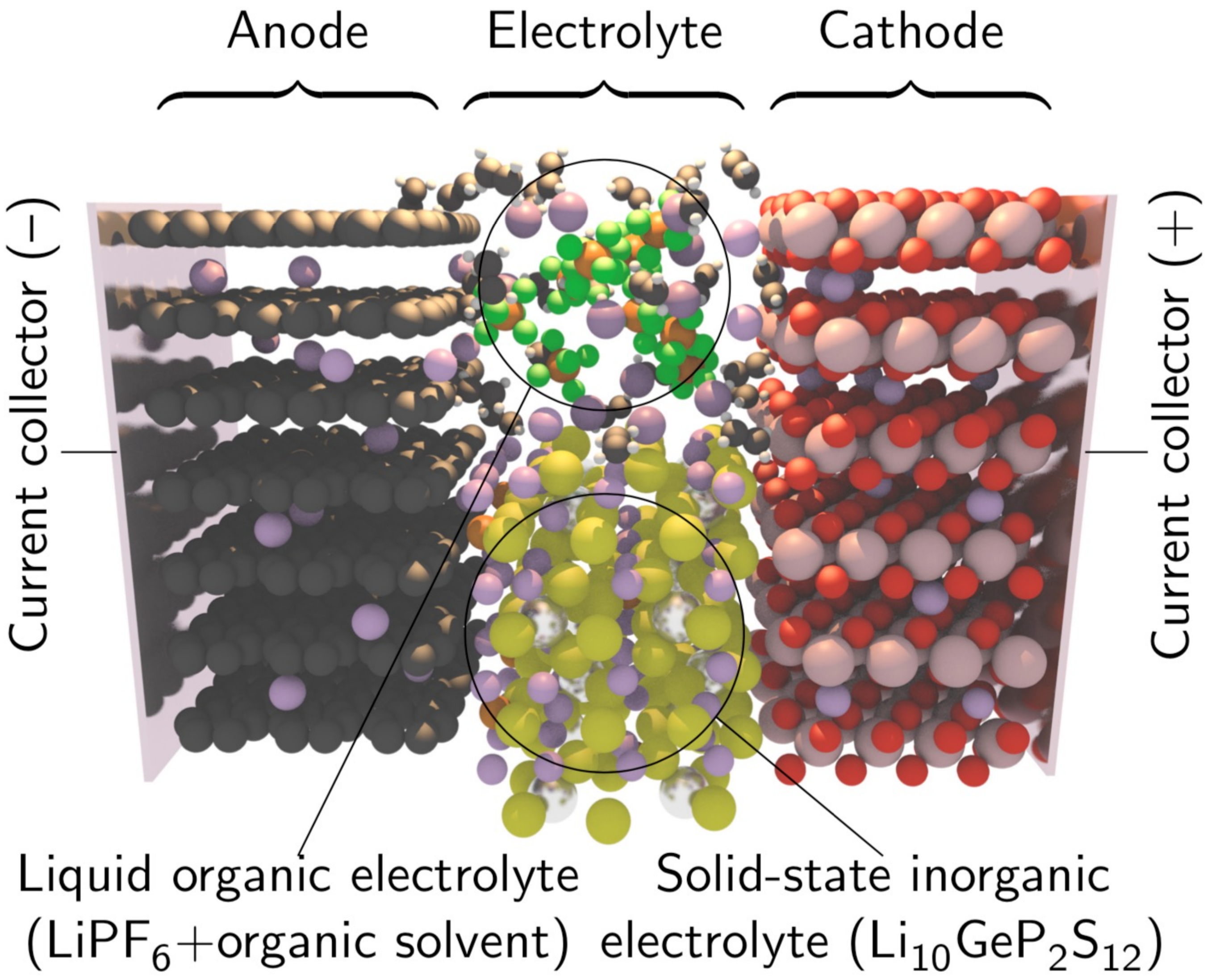
- High electron/hole mobility devices
- Topological insulators, quantum computing
- Ferromagnetic/spintronics in 2D
- Charge-density waves and superconductors
- Plasmonics, transparent conductors

3D layered parents:

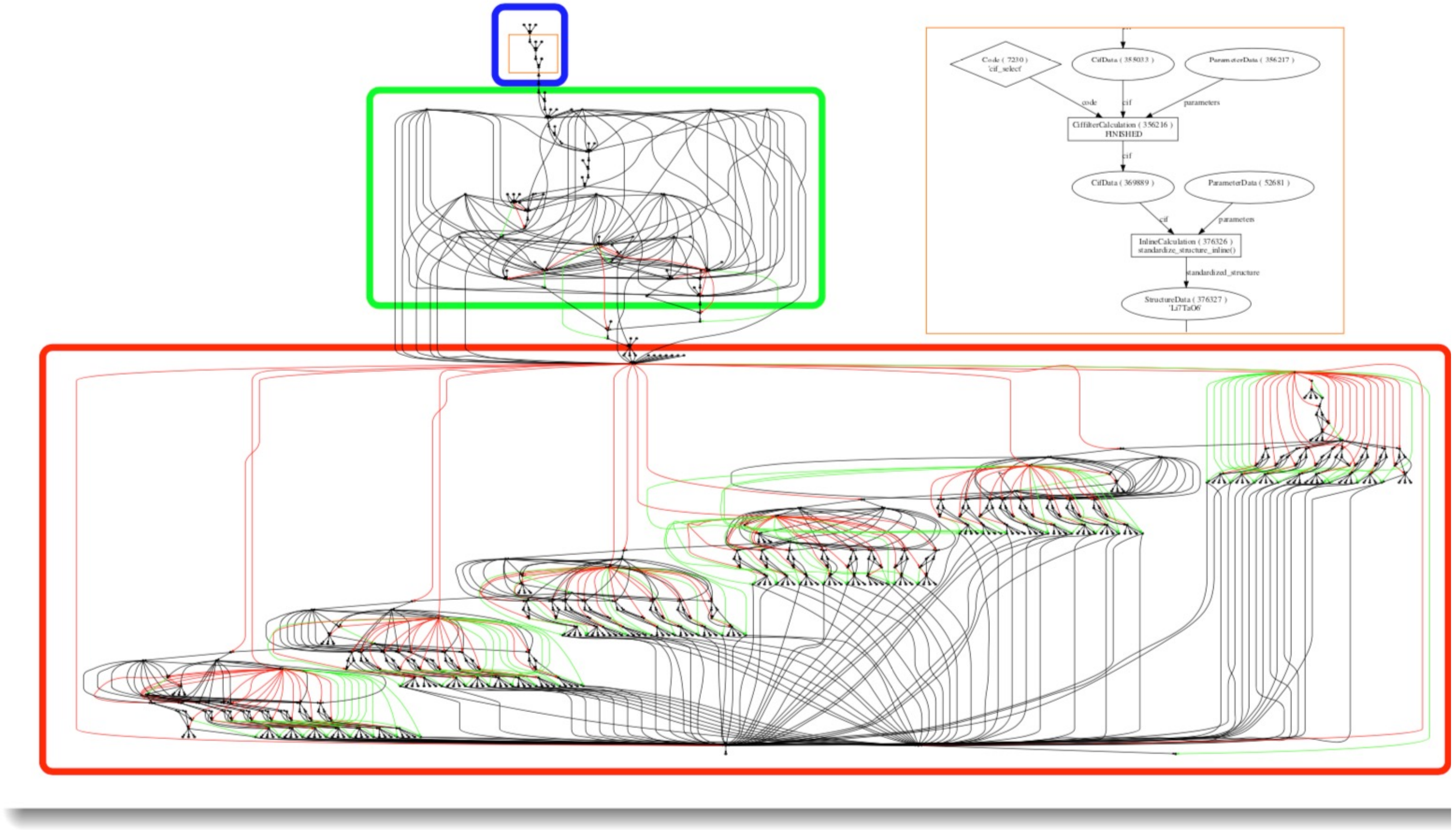
- Solid-state ionic conductors
- Hydrogen or oxygen evolution catalysts
- Membranes for filtration/separation
- Piezo, ferro, and thermoelectrics

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)

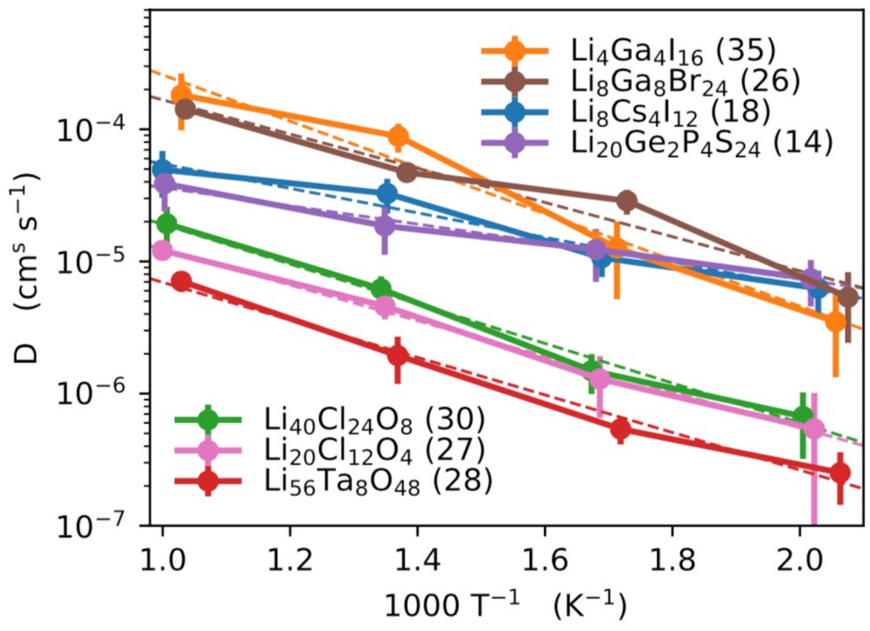
ALL SOLID-STATE BATTERIES



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**

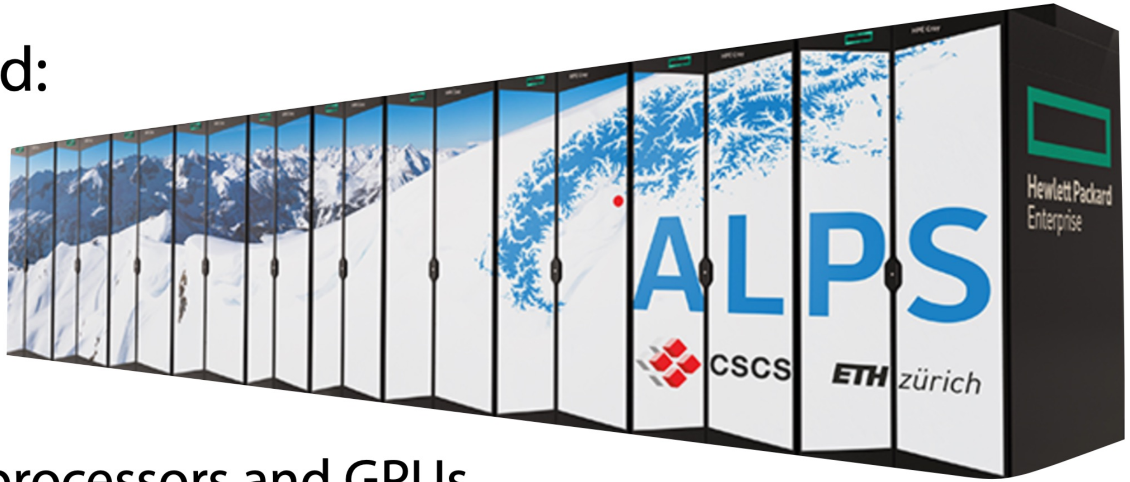
2. An **operating system** for high-throughput computational science, data provenance and reproducibility – http://aiida.net

3. A **work environment** for non specialist where to run simulations

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

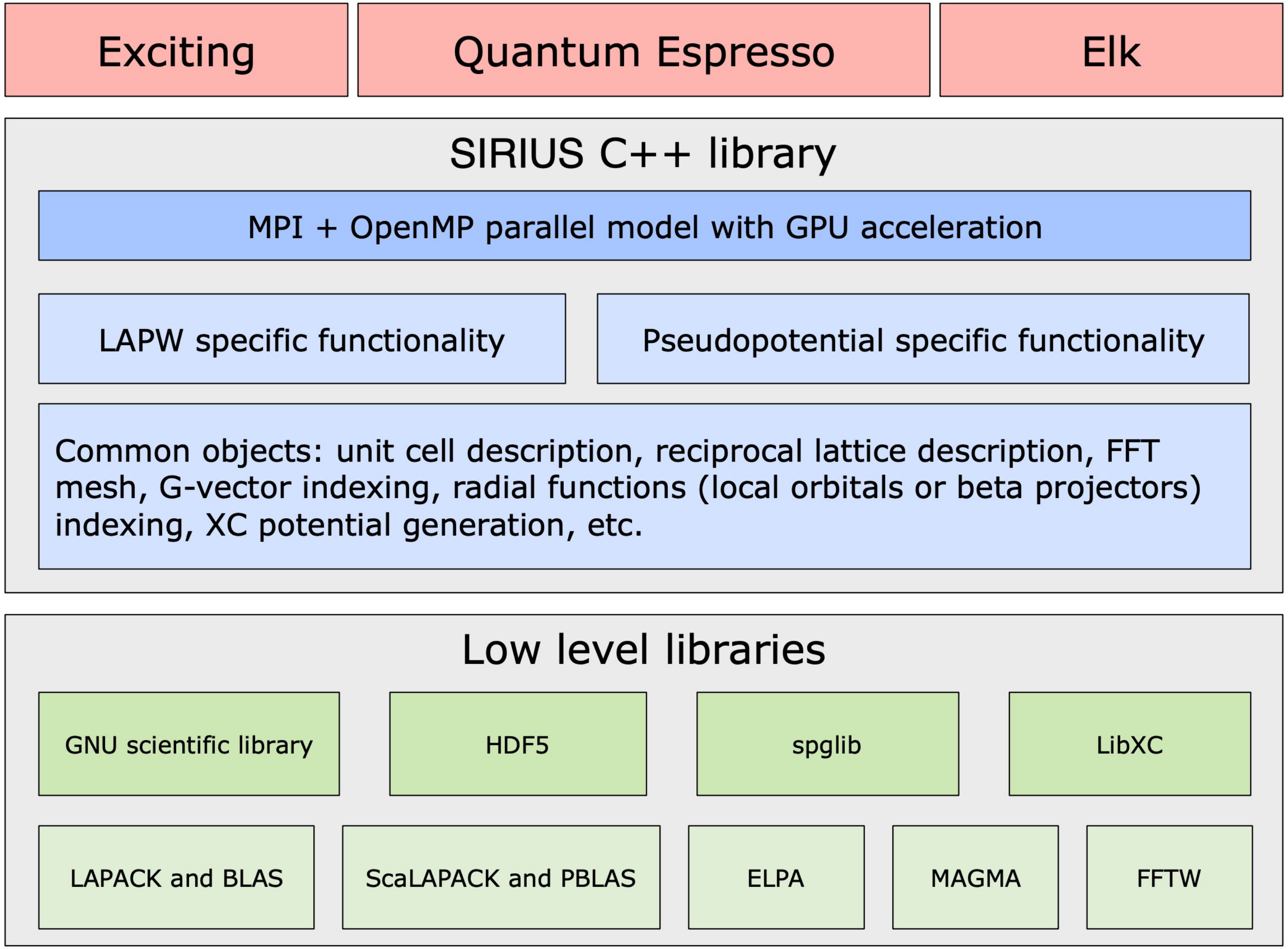
EXASCALE THROUGH HPC AND HTC

- **Pre-exascale systems** are being deployed:
  - Switzerland’s next flagship supercomputing infrastructure (Alps)
    CSCS, NVIDIA GPUs
  - EuroHPC LUMI consortium
    Finland, owned in part by Switzerland; AMD processors and GPUs



- Objective: **ensure the technology stack (AiiDA, SIRIUS, quantum engines) can run at scale**

THE SIRIUS MODEL: DOMAIN-SPECIFIC LIBRARY



Exciting

Quantum Espresso

Elk

SIRIUS C++ library

MPI + OpenMP parallel model with GPU acceleration

LAPW specific functionality

Pseudopotential specific functionality

Common objects: unit cell description, reciprocal lattice description, FFT mesh, G-vector indexing, radial functions (local orbitals or beta projectors) indexing, XC potential generation, etc.

Low level libraries

GNU scientific library

HDF5

spglib

LibXC

LAPACK and BLAS

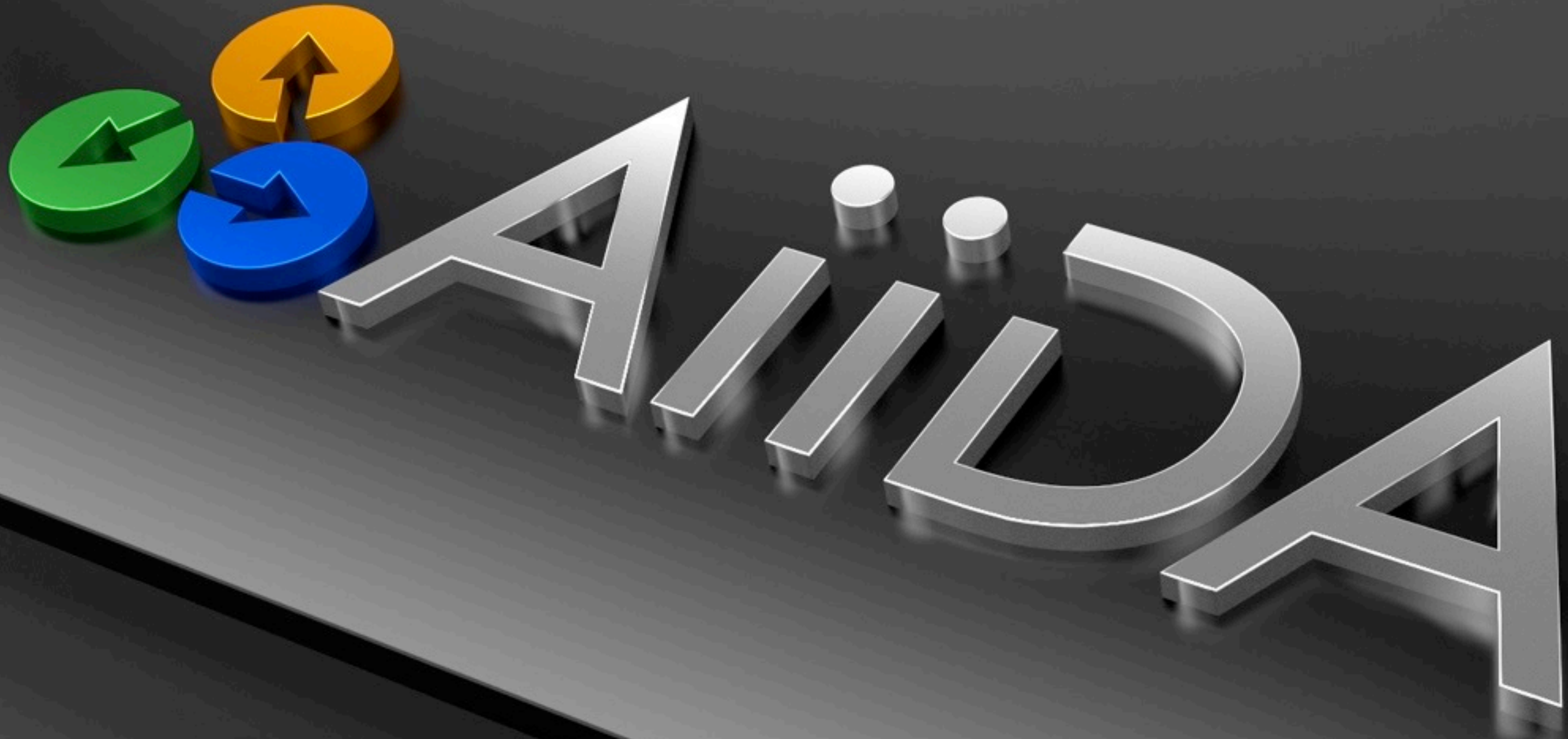
ScaLAPACK and PBLAS

ELPA

MAGMA

FFTW

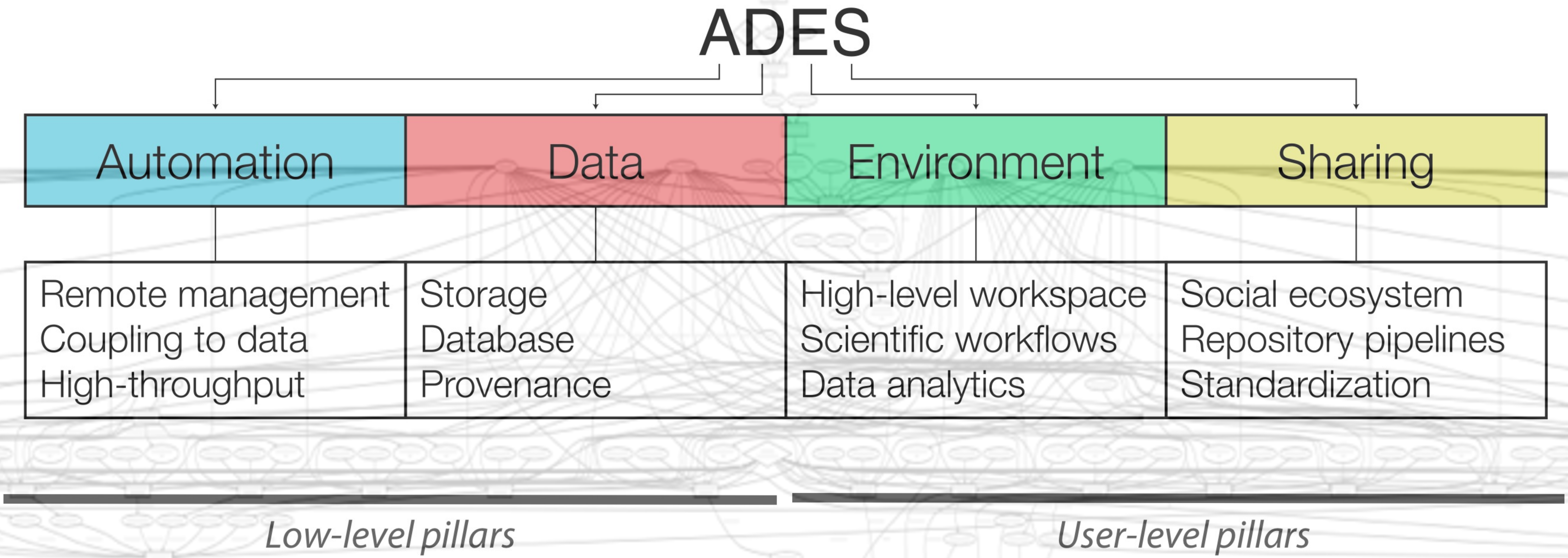
Automation Data Environment Sharing



http://www.aiida.net

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

ADES MODEL FOR COMPUTATIONAL SCIENCE



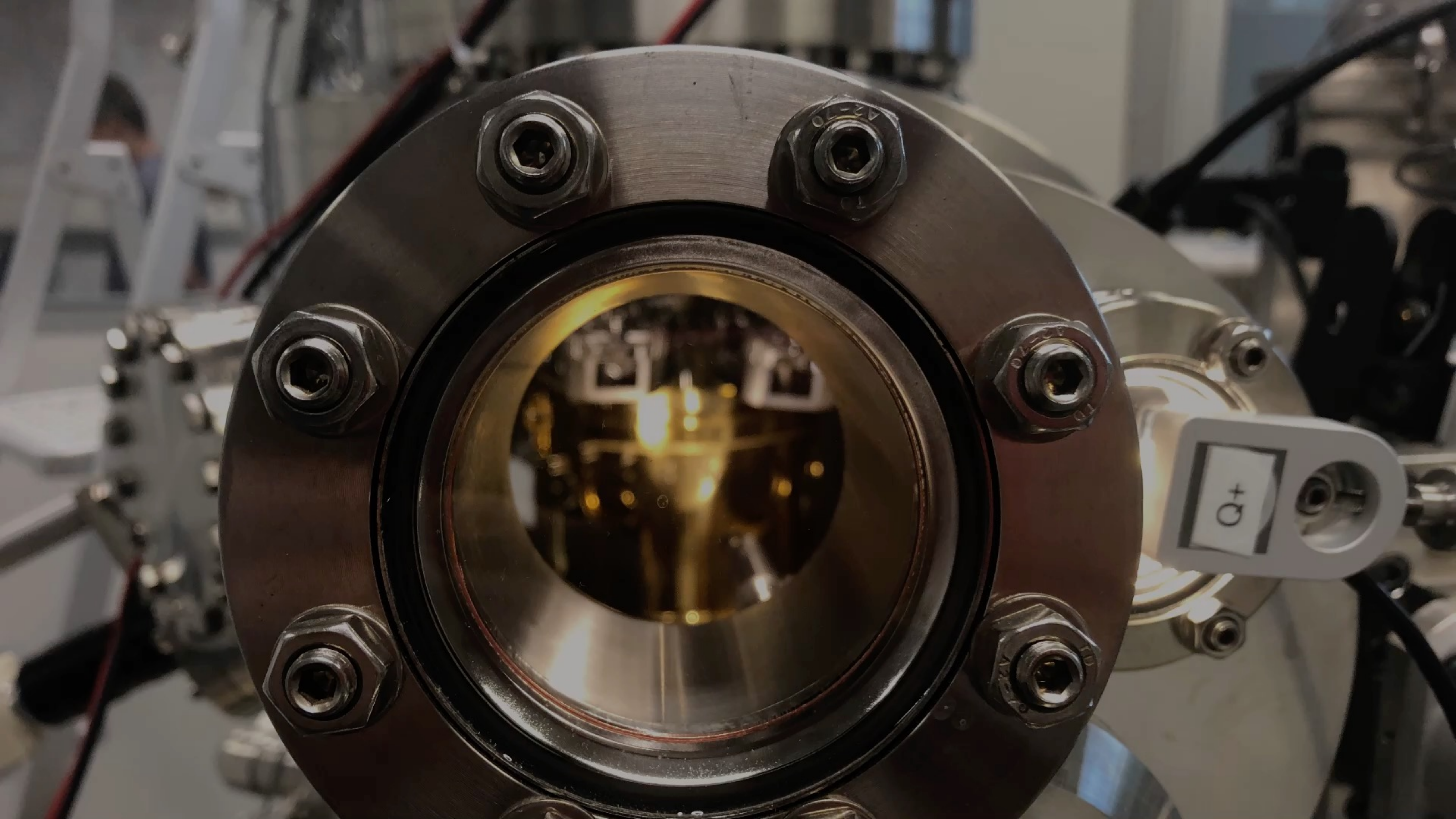
ADES

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

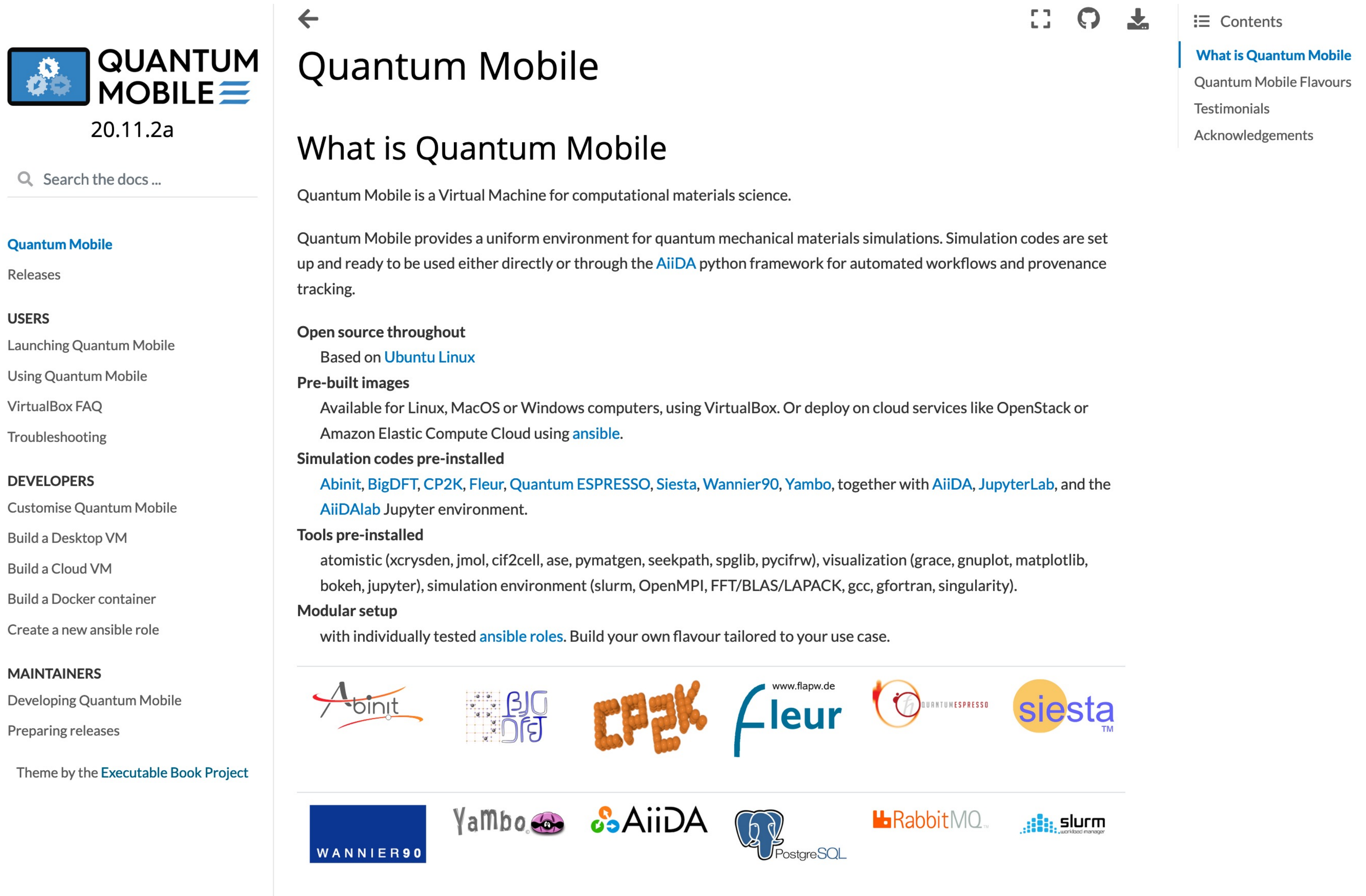
Low-level pillars

User-level pillars

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


Q+
A2-70

READY TO GO IN THE QUANTUM MOBILE



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

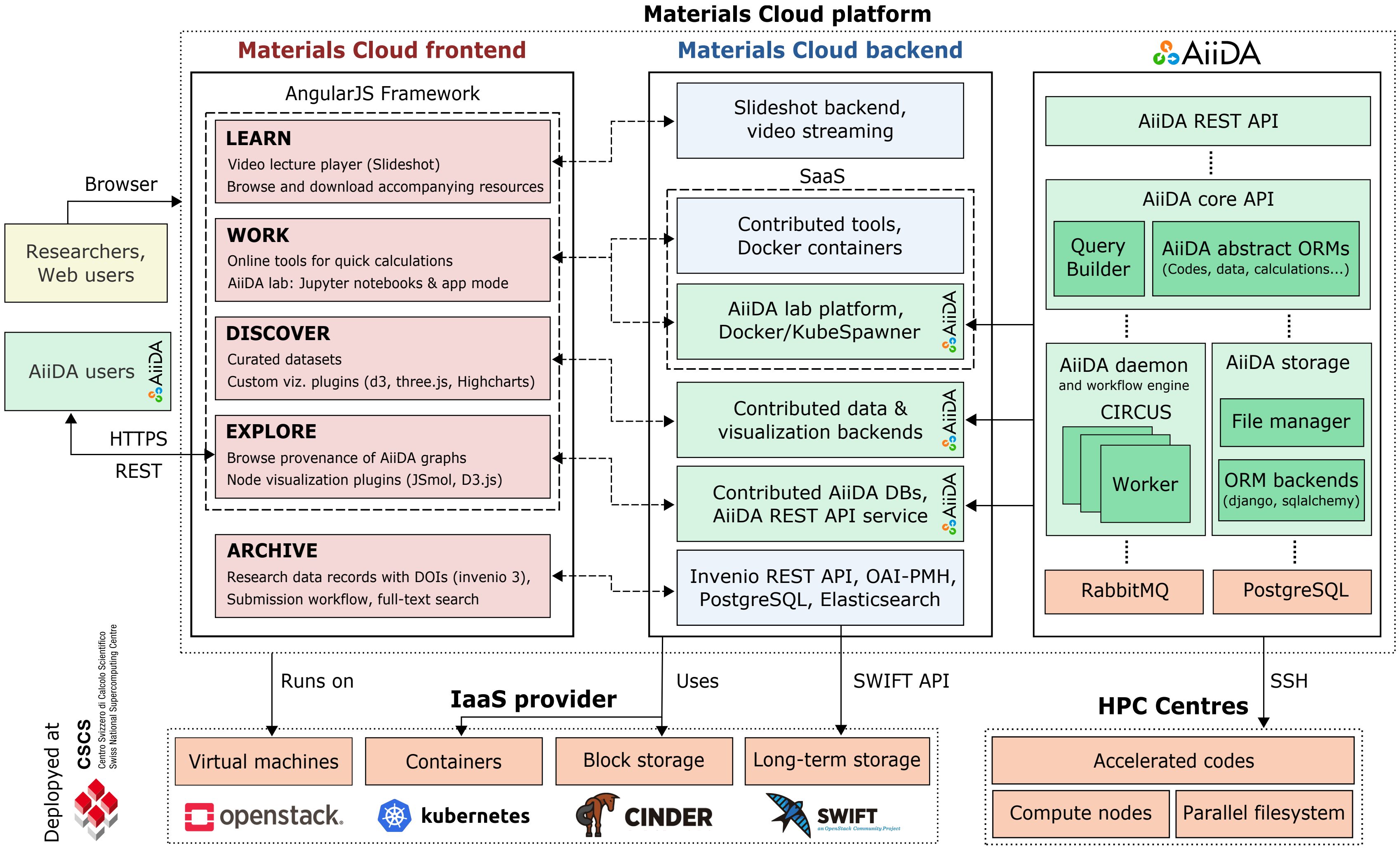
Pre-built images
Available for Linux, MacOS or Windows computers, using VirtualBox. Or deploy on cloud services like OpenStack or Amazon Elastic Compute Cloud using ansible.

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
atomistic (xcrysden, jmol, cif2cell, ase, pymatgen, seekpath, spglib, pycifrw), visualization (grace, gnuplot, matplotlib, bokeh, jupyter), simulation environment (slurm, OpenMPI, FFT/BLAS/LAPACK, gcc, gfortran, singularity).

Modular setup
with individually tested ansible roles. Build your own flavour tailored to your use case.

MATERIALS CLOUD



Materials Cloud platform

Browser

Researchers, Web users

AiiDA users

HTTPS
REST

Materials Cloud frontend

AngularJS Framework

LEARN
Video lecture player (Slideshot)
Browse and download accompanying resources

WORK
Online tools for quick calculations
AiiDA lab: Jupyter notebooks & app mode

DISCOVER
Curated datasets
Custom viz. plugins (d3, three.js, Highcharts)

EXPLORE
Browse provenance of AiiDA graphs
Node visualization plugins (JSmol, D3.js)

ARCHIVE
Research data records with DOIs (invenio 3),
Submission workflow, full-text search

Materials Cloud backend

Slideshot backend,
video streaming

SaaS

Contributed tools,
Docker containers

AiiDA lab platform,
Docker/KubeSpawner

Contributed data &
visualization backends

Contributed AiiDA DBs,
AiiDA REST API service

Invenio REST API, OAI-PMH,
PostgreSQL, Elasticsearch

AiiDA

AiiDA REST API

AiiDA core API

Query
Builder

AiiDA abstract ORMs
(Codes, data, calculations…)

AiiDA daemon
and workflow engine
CIRCUS
Worker

AiiDA storage
File manager
ORM backends
(django, sqlalchemy)

RabbitMQ

PostgreSQL

Runs on

Uses

SWIFT API

SSH

IaaS provider

Virtual machines | Containers | Block storage | Long-term storage

openstack. kubernetes CINDER SWIFT

HPC Centres

Accelerated codes

Compute nodes | Parallel filesystem

Deplopyed at
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

Indexed by

SCIENTIFIC DATA

re3data.org
REGISTRY OF RESEARCH DATA REPOSITORIES
http://doi.org/10.17616/R3ZJ5W
Materials Cloud Archive

FAIRsharing.org
standards, databases, policies

GO FAIR

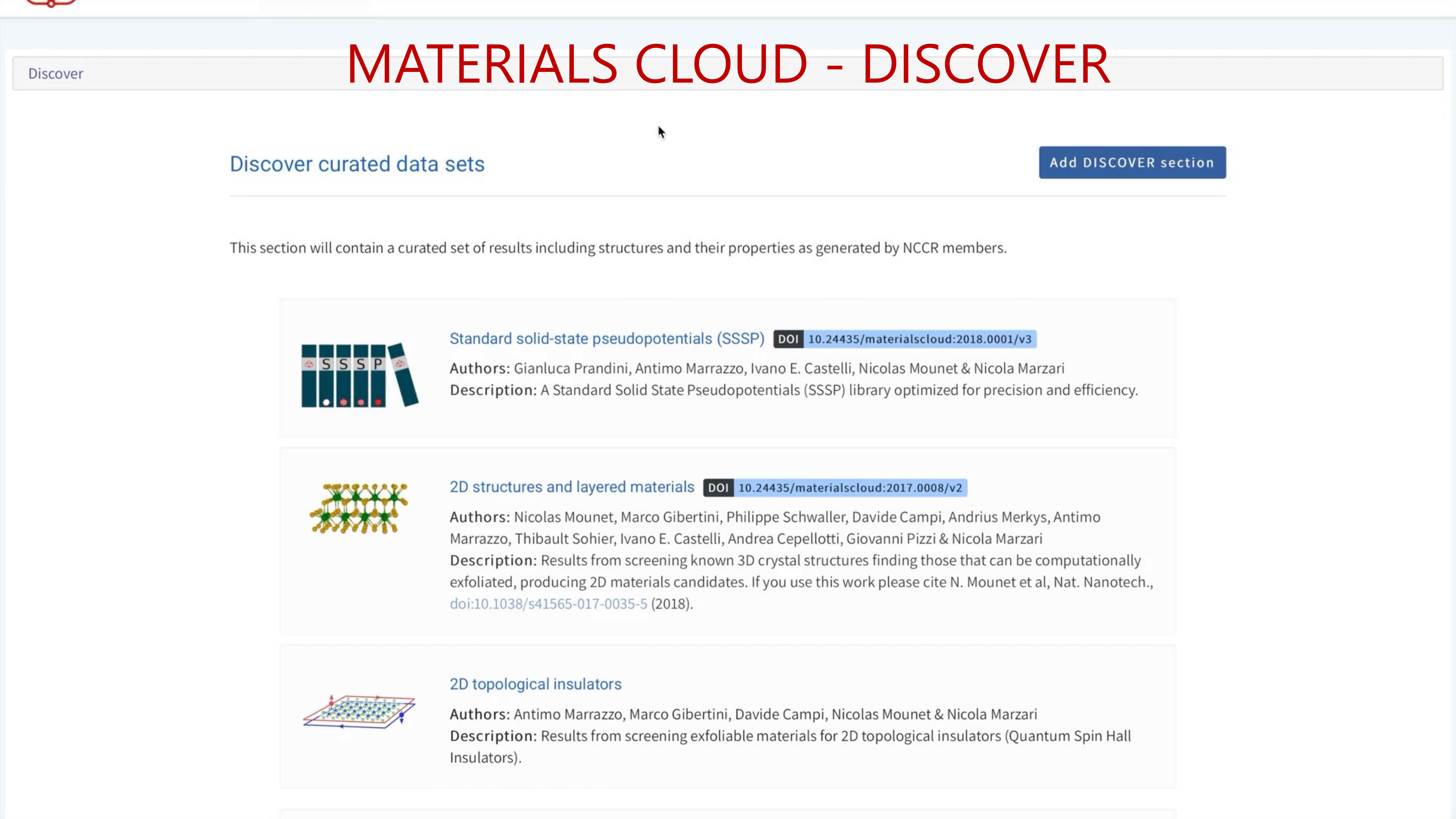
Google
Dataset Search

B2FIND

EUDAT

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

MATERIALS CLOUD - DISCOVER



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) 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.

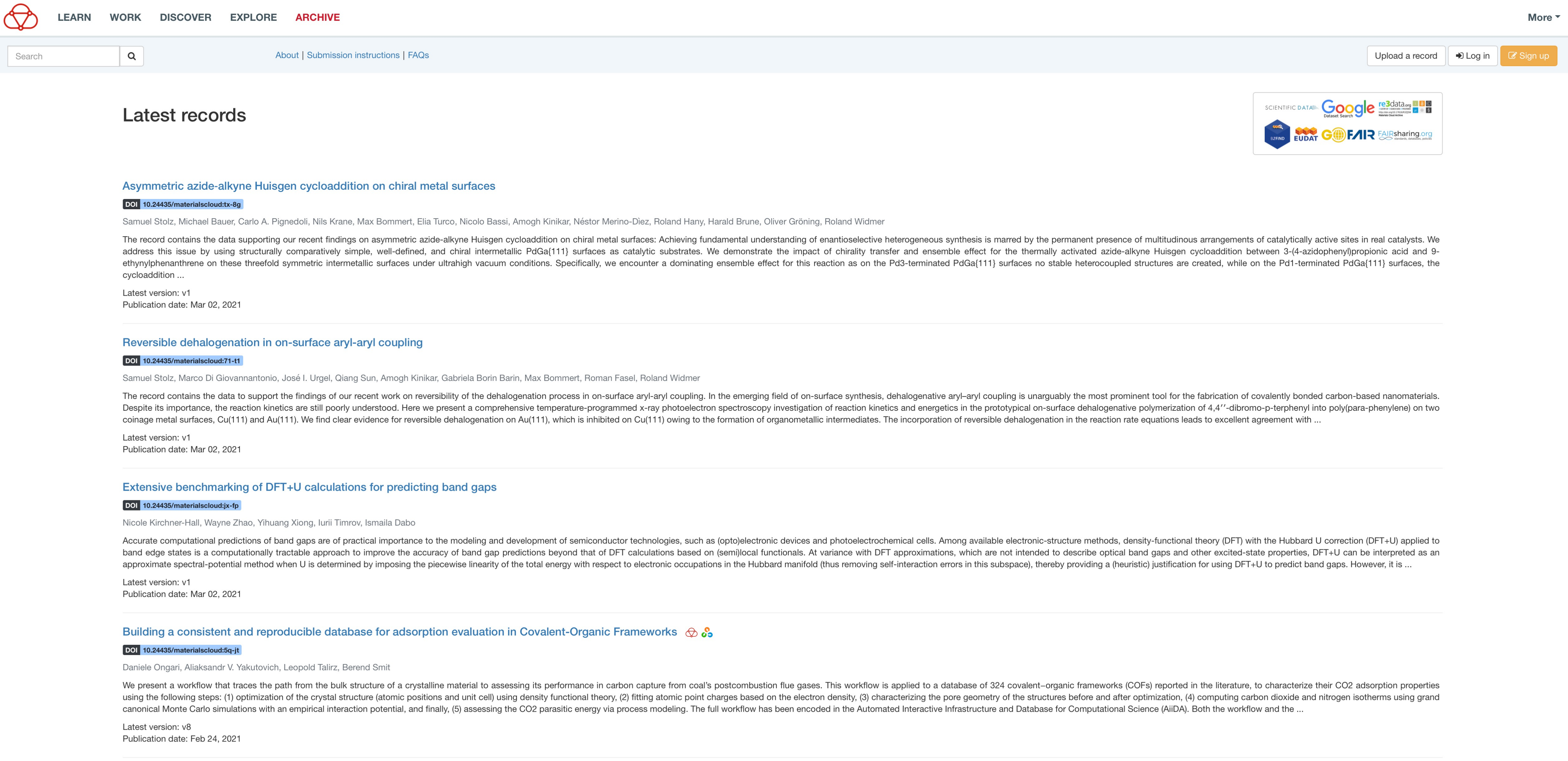
2D structures and layered materials DOI 10.24435/materialscloud:2017.0008/v2

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).

MATERIALS CLOUD - ARCHIVE



Latest records

Asymmetric azide-alkyne Huisgen cycloaddition on chiral metal surfaces

DOI 10.24435/materialscloud:tx-8g

Samuel Stolz, Michael Bauer, Carlo A. Pignedoli, Nils Krane, Max Bommert, Elia Turco, Nicolo Bassi, Amogh Kinikar, Néstor Merino-Díez, Roland Hany, Harald Brune, Oliver Gröning, Roland Widmer

The record contains the data supporting our recent findings on asymmetric azide-alkyne Huisgen cycloaddition on chiral metal surfaces: Achieving fundamental understanding of enantioselective heterogeneous synthesis is marred by the permanent presence of multitudinous arrangements of catalytically active sites in real catalysts. We address this issue by using structurally comparatively simple, well-defined, and chiral intermetallic PdGa{111} surfaces as catalytic substrates. We demonstrate the impact of chirality transfer and ensemble effect for the thermally activated azide-alkyne Huisgen cycloaddition between 3-(4-azidophenyl)propionic acid and 9-ethynylphenanthrene on these threefold symmetric intermetallic surfaces under ultrahigh vacuum conditions. Specifically, we encounter a dominating ensemble effect for this reaction as on the Pd3-terminated PdGa{111} surfaces no stable heterocoupled structures are created, while on the Pd1-terminated PdGa{111} surfaces, the cycloaddition ...

Latest version: v1
Publication date: Mar 02, 2021

Reversible dehalogenation in on-surface aryl-aryl coupling

DOI 10.24435/materialscloud:71-t1

Samuel Stolz, Marco Di Giovannantonio, José I. Urgel, Qiang Sun, Amogh Kinikar, Gabriela Borin Barin, Max Bommert, Roman Fasel, Roland Widmer

The record contains the data to support the findings of our recent work on reversibility of the dehalogenation process in on-surface aryl-aryl coupling. In the emerging field of on-surface synthesis, dehalogenative aryl–aryl coupling is unarguably the most prominent tool for the fabrication of covalently bonded carbon-based nanomaterials. Despite its importance, the reaction kinetics are still poorly understood. Here we present a comprehensive temperature-programmed x-ray photoelectron spectroscopy investigation of reaction kinetics and energetics in the prototypical on-surface dehalogenative polymerization of 4,4′′-dibromo-p-terphenyl into poly(para-phenylene) on two coinage metal surfaces, Cu(111) and Au(111). We find clear evidence for reversible dehalogenation on Au(111), which is inhibited on Cu(111) owing to the formation of organometallic intermediates. The incorporation of reversible dehalogenation in the reaction rate equations leads to excellent agreement with ...

Latest version: v1
Publication date: Mar 02, 2021

Extensive benchmarking of DFT+U calculations for predicting band gaps

DOI 10.24435/materialscloud:jx-fp

Nicole Kirchner-Hall, Wayne Zhao, Yihuang Xiong, Iurii Timrov, Ismaila Dabo

Accurate computational predictions of band gaps are of practical importance to the modeling and development of semiconductor technologies, such as (opto)electronic devices and photoelectrochemical cells. Among available electronic-structure methods, density-functional theory (DFT) with the Hubbard U correction (DFT+U) applied to band edge states is a computationally tractable approach to improve the accuracy of band gap predictions beyond that of DFT calculations based on (semi)local functionals. At variance with DFT approximations, which are not intended to describe optical band gaps and other excited-state properties, DFT+U can be interpreted as an approximate spectral-potential method when U is determined by imposing the piecewise linearity of the total energy with respect to electronic occupations in the Hubbard manifold (thus removing self-interaction errors in this subspace), thereby providing a (heuristic) justification for using DFT+U to predict band gaps. However, it is ...

Latest version: v1
Publication date: Mar 02, 2021

Building a consistent and reproducible database for adsorption evaluation in Covalent-Organic Frameworks

DOI 10.24435/materialscloud:5q-jt

Daniele Ongari, Aliaksandr V. Yakutovich, Leopold Talirz, Berend Smit

We present a workflow that traces the path from the bulk structure of a crystalline material to assessing its performance in carbon capture from coal's postcombustion flue gases. This workflow is applied to a database of 324 covalent–organic frameworks (COFs) reported in the literature, to characterize their CO2 adsorption properties using the following steps: (1) optimization of the crystal structure (atomic positions and unit cell) using density functional theory, (2) fitting atomic point charges based on the electron density, (3) characterizing the pore geometry of the structures before and after optimization, (4) computing carbon dioxide and nitrogen isotherms using grand canonical Monte Carlo simulations with an empirical interaction potential, and finally, (5) assessing the CO2 parasitic energy via process modeling. The full workflow has been encoded in the Automated Interactive Infrastructure and Database for Computational Science (AiiDA). Both the workflow and the ...

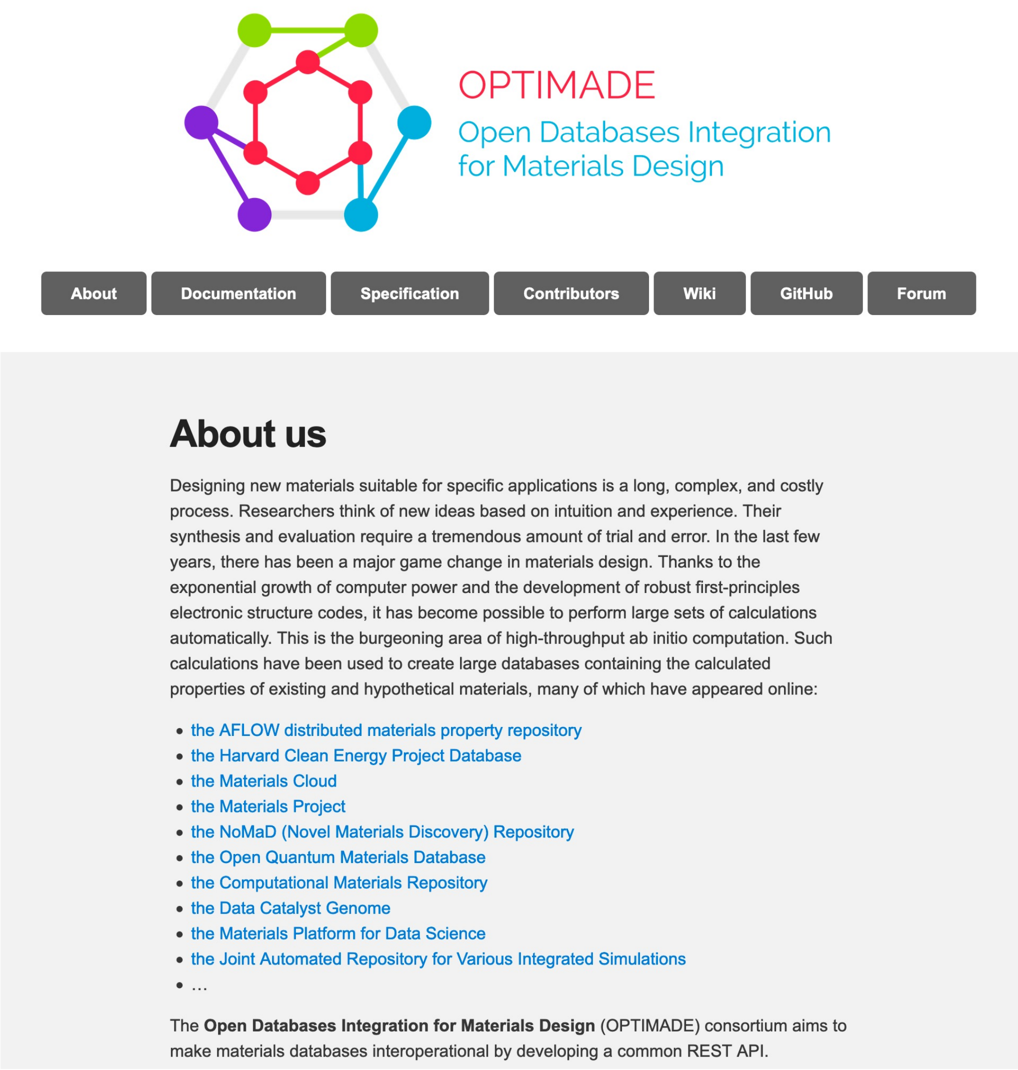
Latest version: v8
Publication date: Feb 24, 2021

LET’S BROADEN THE HORIZON

THE BEZOS MANDATE: EXTERNALIZABLE SERVICE INTERFACES

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

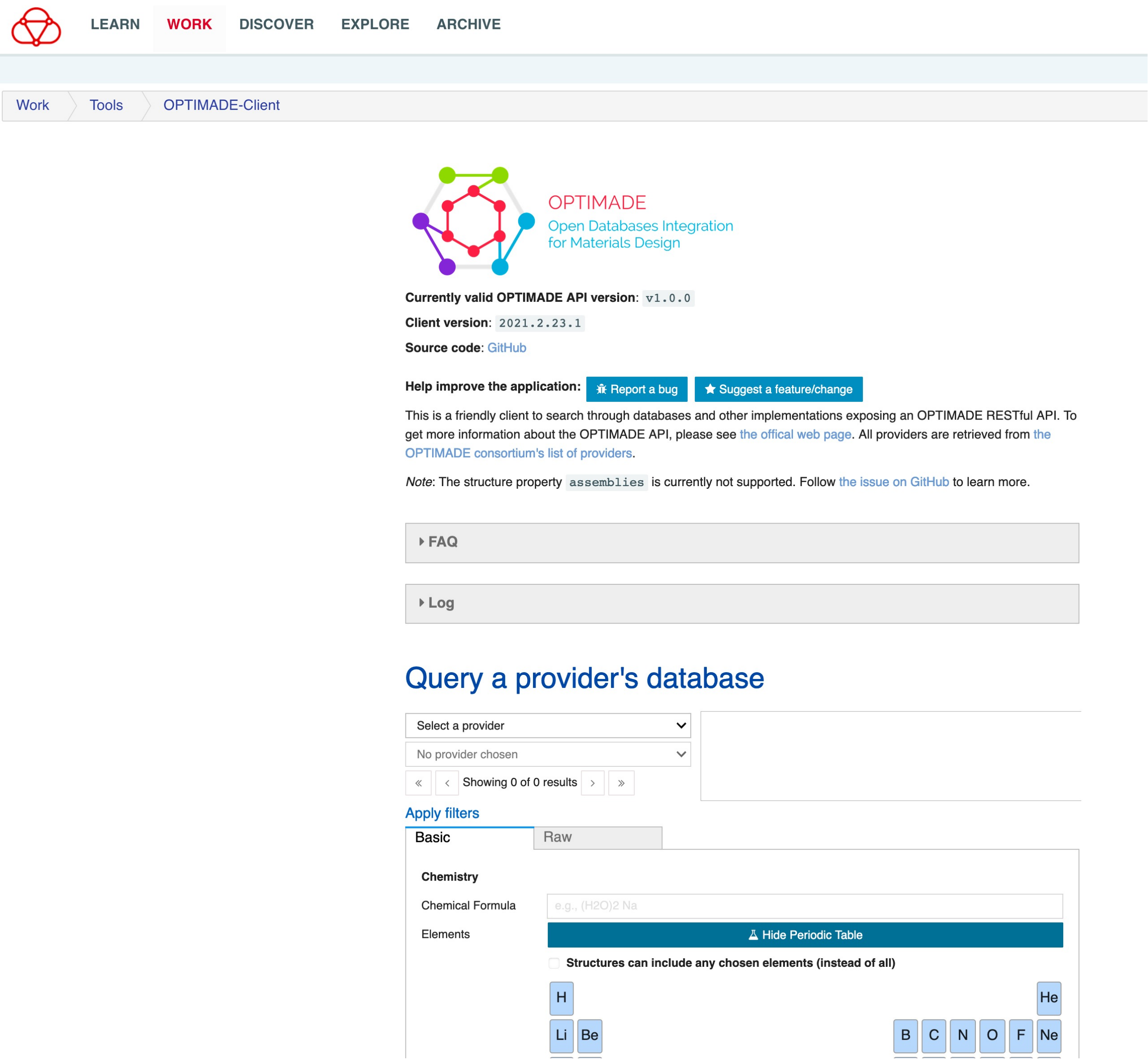


About us

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 (Novel 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 interoperational by developing a common REST API.



Currently valid OPTIMADE API version: `v1.0.0`

Client version: `2021.2.23.1`

Source code: GitHub

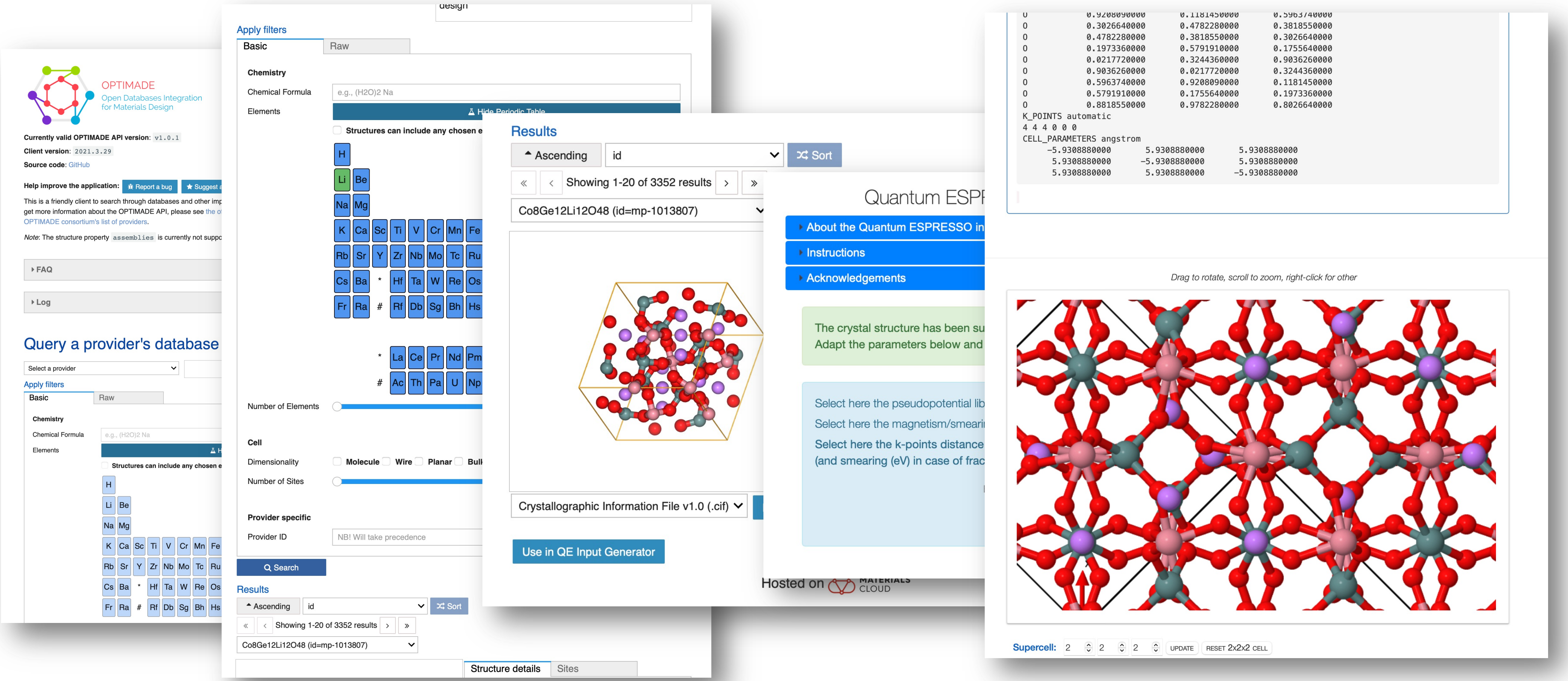
Help improve the application: Report a bug | Suggest a feature/change

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

Note: The structure property `assemblies` is currently not supported. Follow the issue on GitHub to learn more.

Query a provider's database

IN ACTION: OPTIMADE UNIVERSAL REST API



Currently valid OPTIMADE API version: `v1.0.1`

Client version: `2021.3.29`

Source code: GitHub

Help improve the application:

This is a friendly client to search through databases and other imp… get more information about the OPTIMADE API, please see the o… OPTIMADE consortium's list of providers.

Note: The structure property `assemblies` is currently not suppo…

Query a provider's database

Select a provider

Chemical Formula: e.g., (H2O)2 Na

☐ Structures can include any chosen e…

Dimensionality: ☐ Molecule ☐ Wire ☐ Planar ☐ Bul…

Provider ID: NB! Will take precedence

Ascending | id | Sort

Showing 1-20 of 3352 results

Co8Ge12Li12O48 (id=mp-1013807)

Crystallographic Information File v1.0 (.cif)

The crystal structure has been su…
Adapt the parameters below and…

Select here the pseudopotential lib…

Select here the magnetism/smeari…

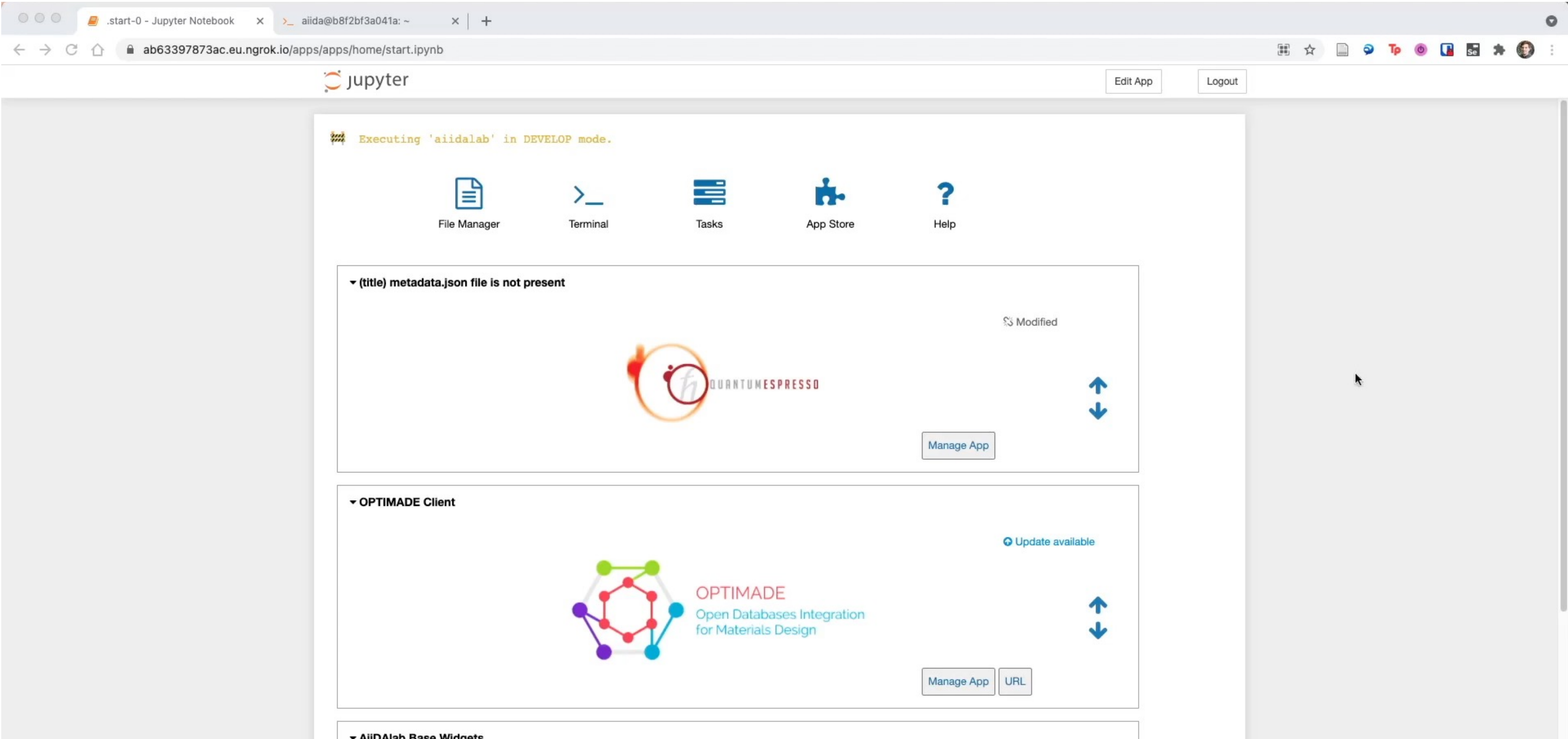
Select here the k-points distance (and smearing (eV) in case of frac…

```
O           0.9208090000       0.1181450000       0.5963740000
O           0.3026640000       0.4782280000       0.3818550000
O           0.4782280000       0.3818550000       0.3026640000
O           0.1973360000       0.5791910000       0.1755640000
O           0.0217720000       0.3244360000       0.9036260000
O           0.9036260000       0.0217720000       0.3244360000
O           0.5963740000       0.9208090000       0.1181450000
O           0.5791910000       0.1755640000       0.1973360000
O           0.8818550000       0.9782280000       0.8026640000
K_POINTS automatic
4 4 4 0 0 0
CELL_PARAMETERS angstrom
     -5.9308880000       5.9308880000       5.9308880000
      5.9308880000      -5.9308880000       5.9308880000
      5.9308880000       5.9308880000      -5.9308880000
```

Drag to rotate, scroll to zoom, right-click for other

Supercell: 2 2 2

QUANTUM-AS-A-SERVICE (AiiDAlab from Jul 2021)

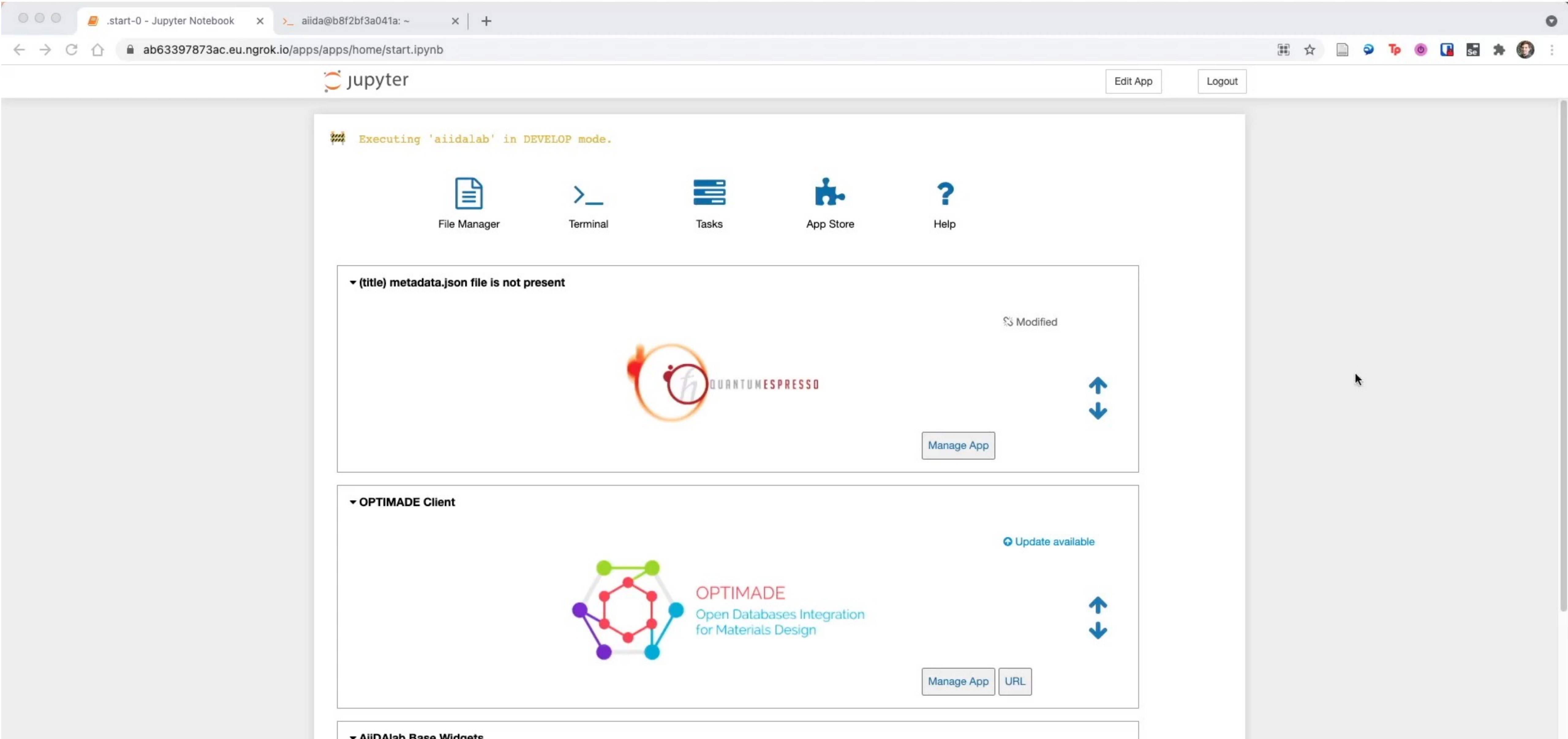


```
Executing 'aiidalab' in DEVELOP mode.
```

(title) metadata.json file is not present

OPTIMADE Client

QUANTUM-AS-A-SERVICE (AiiDAlab from Jul 2021)



ab63397873ac.eu.ngrok.io/apps/apps/home/start.ipynb

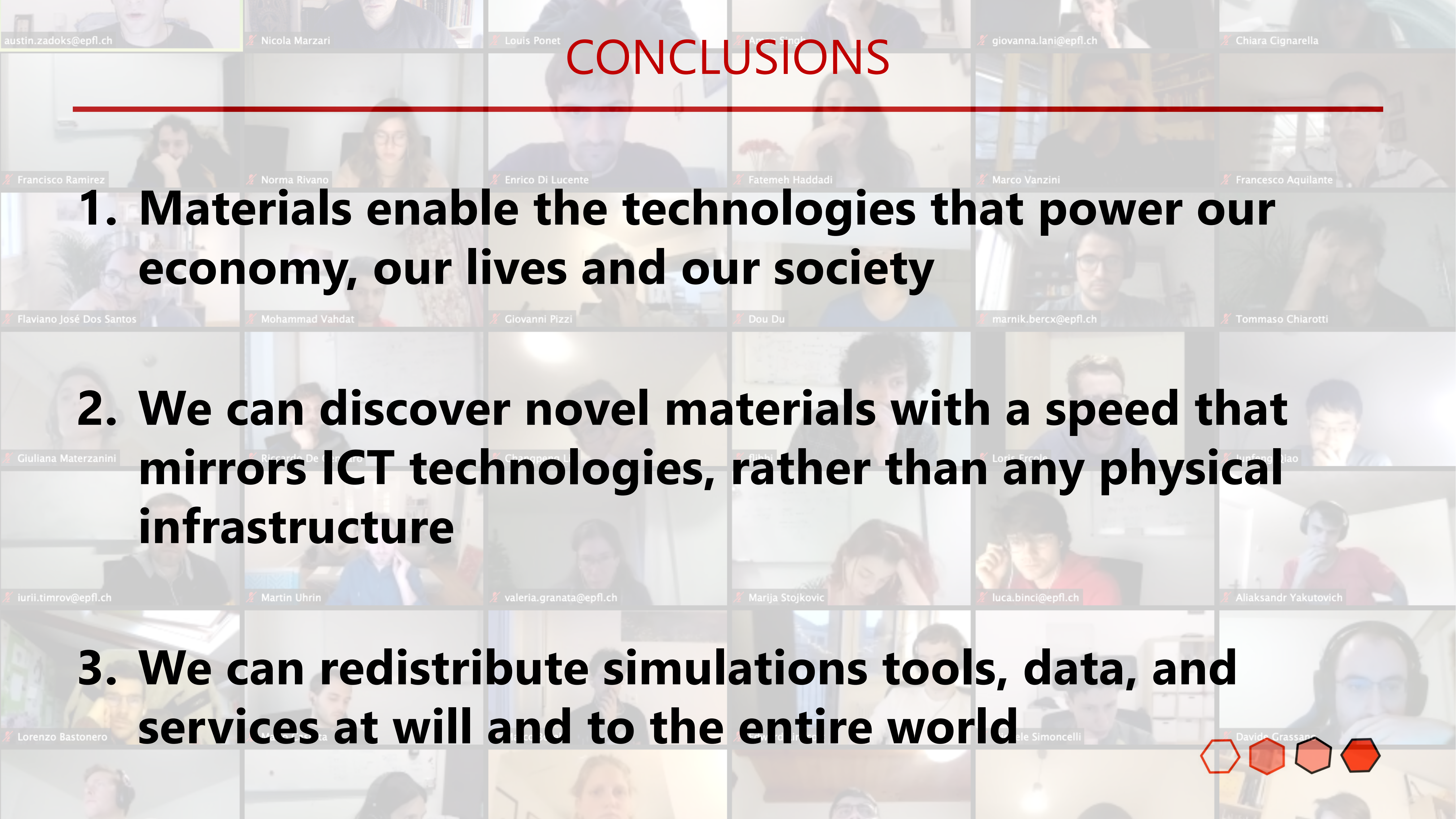
Executing 'aiidalab' in DEVELOP mode.

(title) metadata.json file is not present

OPTIMADE Client

AiiDAlab Base Widgets

CONCLUSIONS

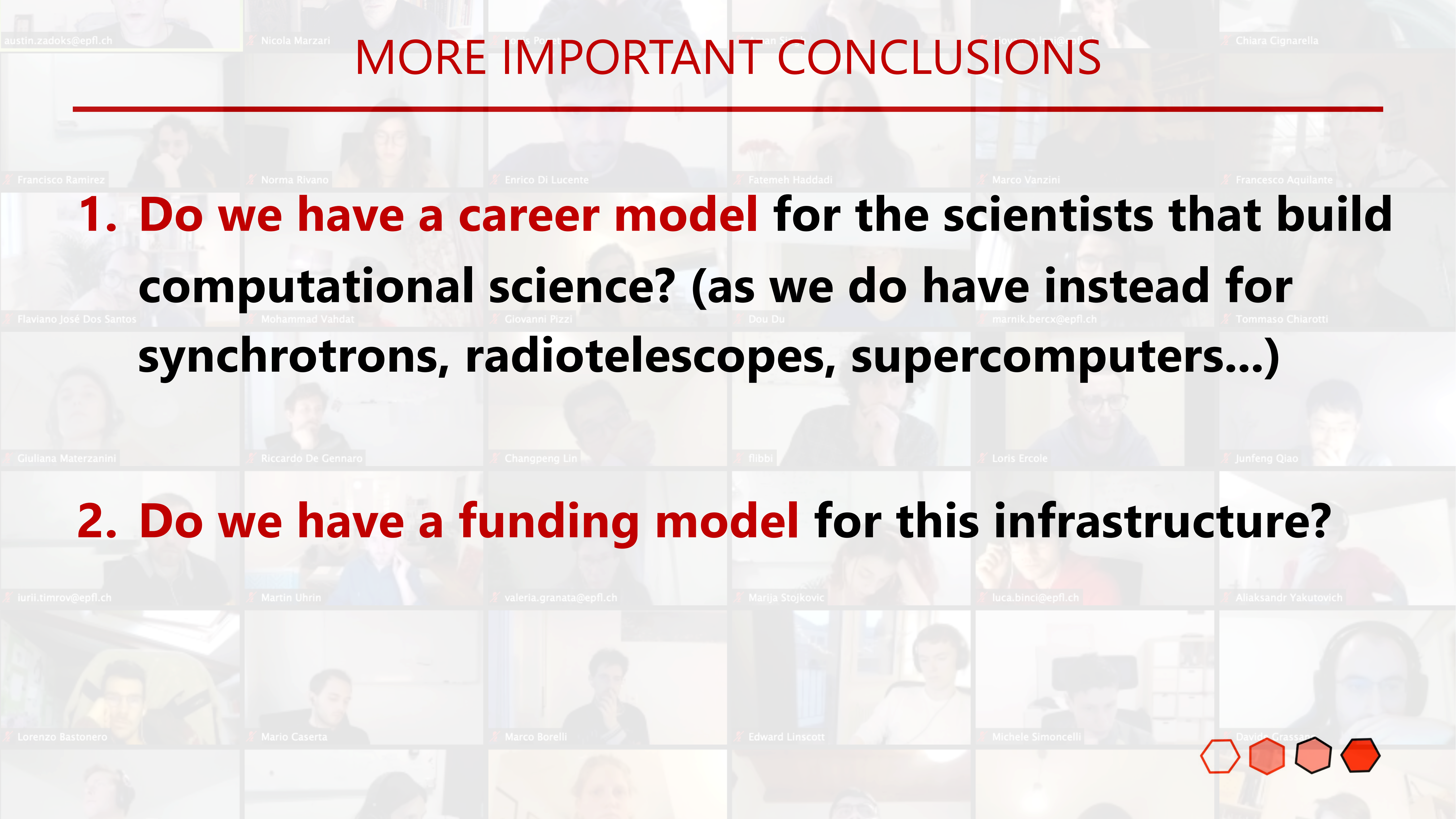


1. **Materials enable the technologies that power our economy, our lives and our society**

2. **We can discover novel materials with a speed that mirrors ICT technologies, rather than any physical infrastructure**

3. **We can redistribute simulations tools, data, and services at will and to the entire world**

MORE IMPORTANT CONCLUSIONS



1. **Do we have a career model for the scientists that build computational science? (as we do have instead for synchrotrons, radiotelescopes, supercomputers…)**

2. **Do we have a funding model for this infrastructure?**

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The Materials Cloud And AiiDA teams


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Joost VandeVondele (ETHZ,CSCS)


Thomas Schulthess (ETHZ,CSCS)

<u>http://www.aiida.net</u>
<u>http://www.materialscloud.org</u>

Contributors for the 40+ plugins: Quantum ESPRESSO, Wannier90, CP2K, FLEUR, YAMBO, SIESTA, VASP, CASTEP, CRYSTAL, …

Contributors to aiida-core and former AiiDA team members — Oscar Arbelaez, Michael Atambo, Valentin Bersier, Marco Borelli, Jocelyn Boullier, Jens Bröder, Ivano E. Castelli, Andrea Cepellotti, Keija Cui, Vladimir Dikan, Marco Dorigo, Y.-W. Fang, Fernando Gargiulo, Marco Gibertini, Davide Grassano, Dominik Gresch, Conrad Johnston, Rico Häuselmann, Daniel Hollas, Eric Hontz, Jianxing Huang, Christoph Koch, Espen Flage-Larsen, Ian Lee, Daniel Marchand, Antimo Marrazzo, Andrius Merkys, Simon Pintarelli, Nicolas Mounet, Tiziano Müller, Gianluca Prandini, Philip Rüßmann, Riccardo Sabatini, Ole Schütt, Phillippe Schwaller, Andreas Stamminger, Atsushi Togo, Daniele Tomerini, Nicola Varini, Martin Uhrin, Jason Yu, Austin Zadoks, Bonan Zhu, Mario Zic, Spyros Zoupanos

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NATIONAL CENTRE OF COMPETENCE IN RESEARCH

http://nccr-marvel.ch

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MAX DRIVING THE EXASCALE TRANSITION

http://max-centre.eu

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

BIG-MAP

https://www.big-map.eu

H2020 Battery Interface Genome – Materials Acceleration Platform (Battery 2030+) (2020-23)

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 Varinor

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