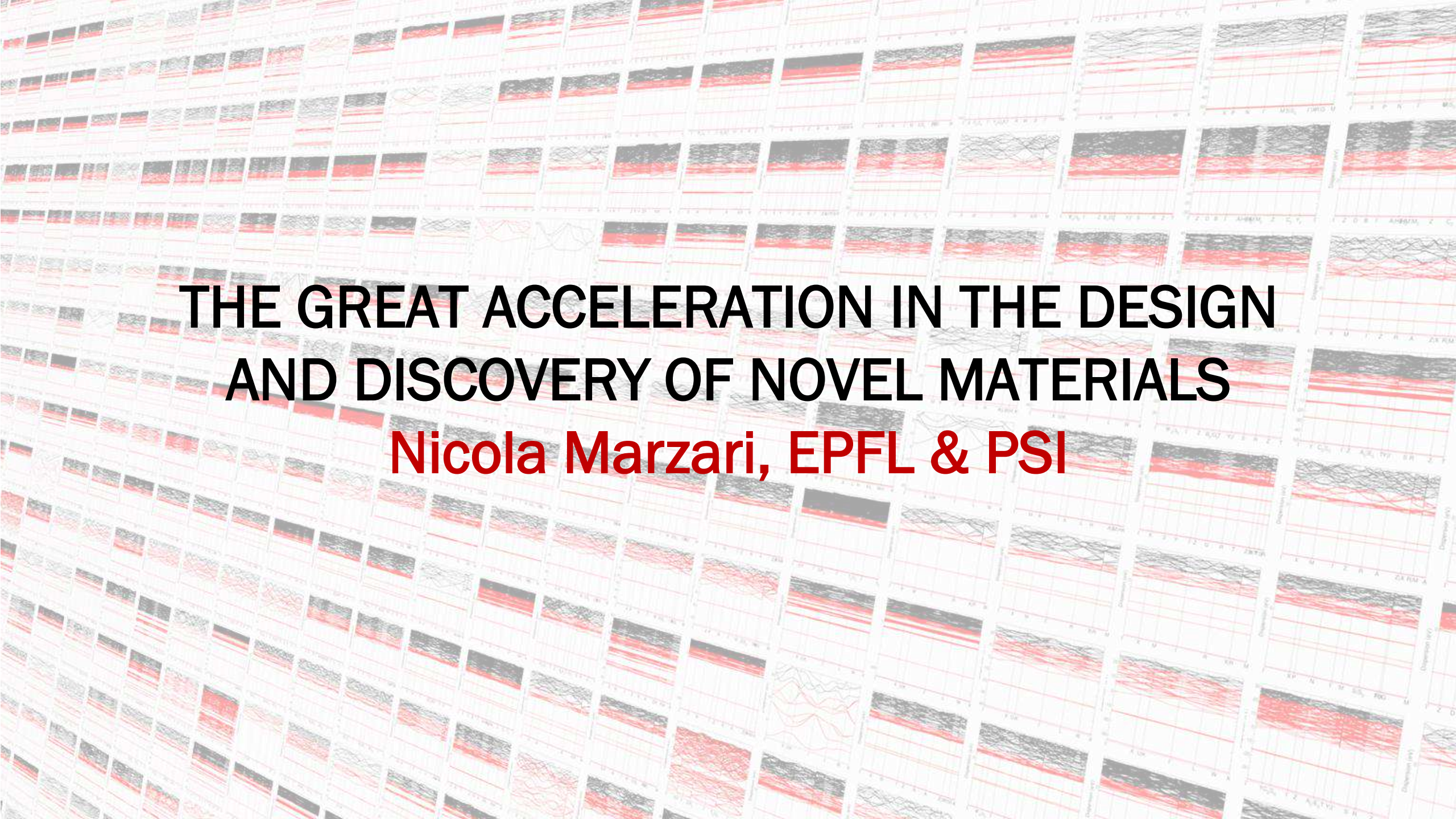


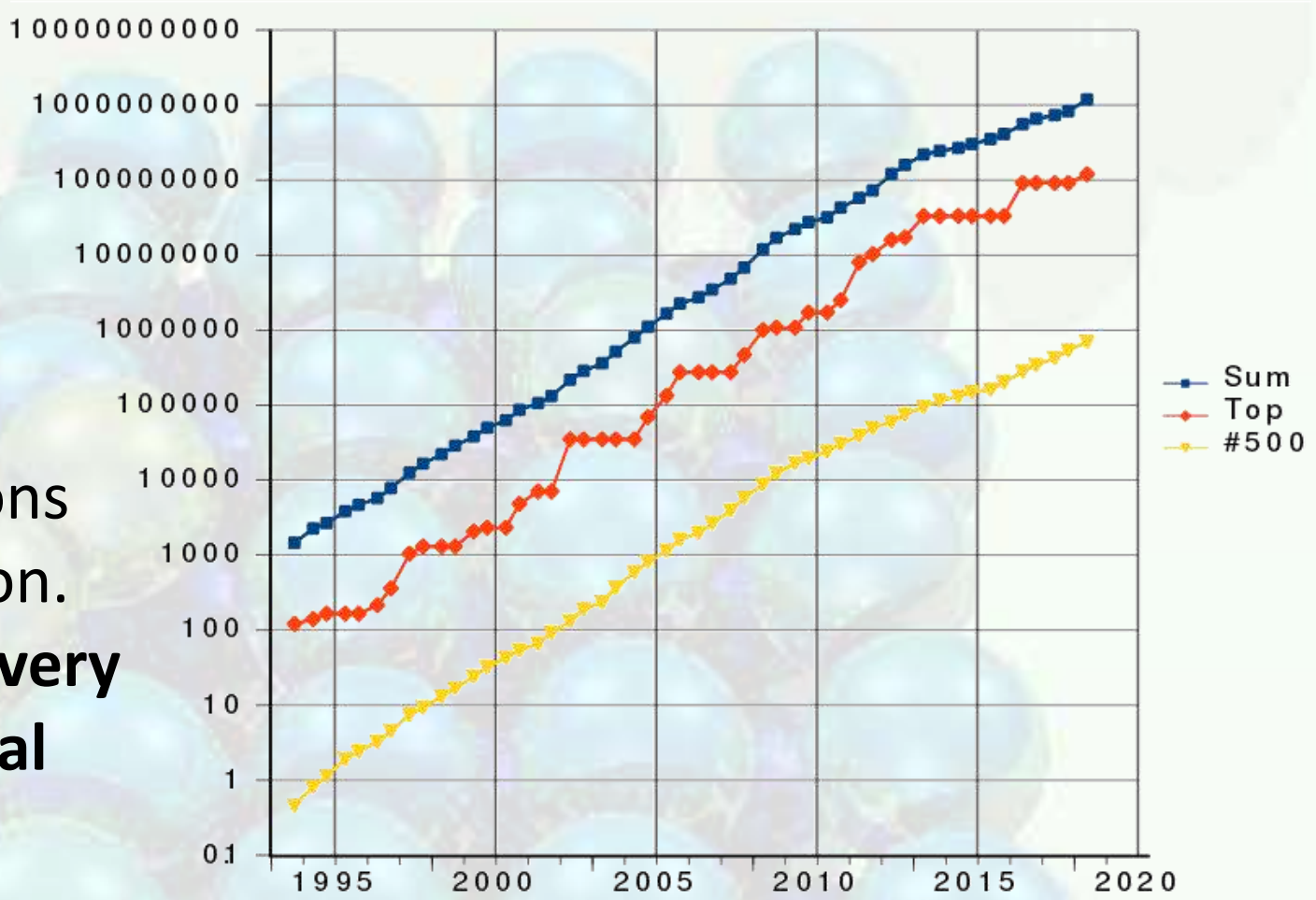
THE GREAT ACCELERATION IN THE DESIGN AND DISCOVERY OF NOVEL MATERIALS

Nicola Marzari, EPFL & PSI

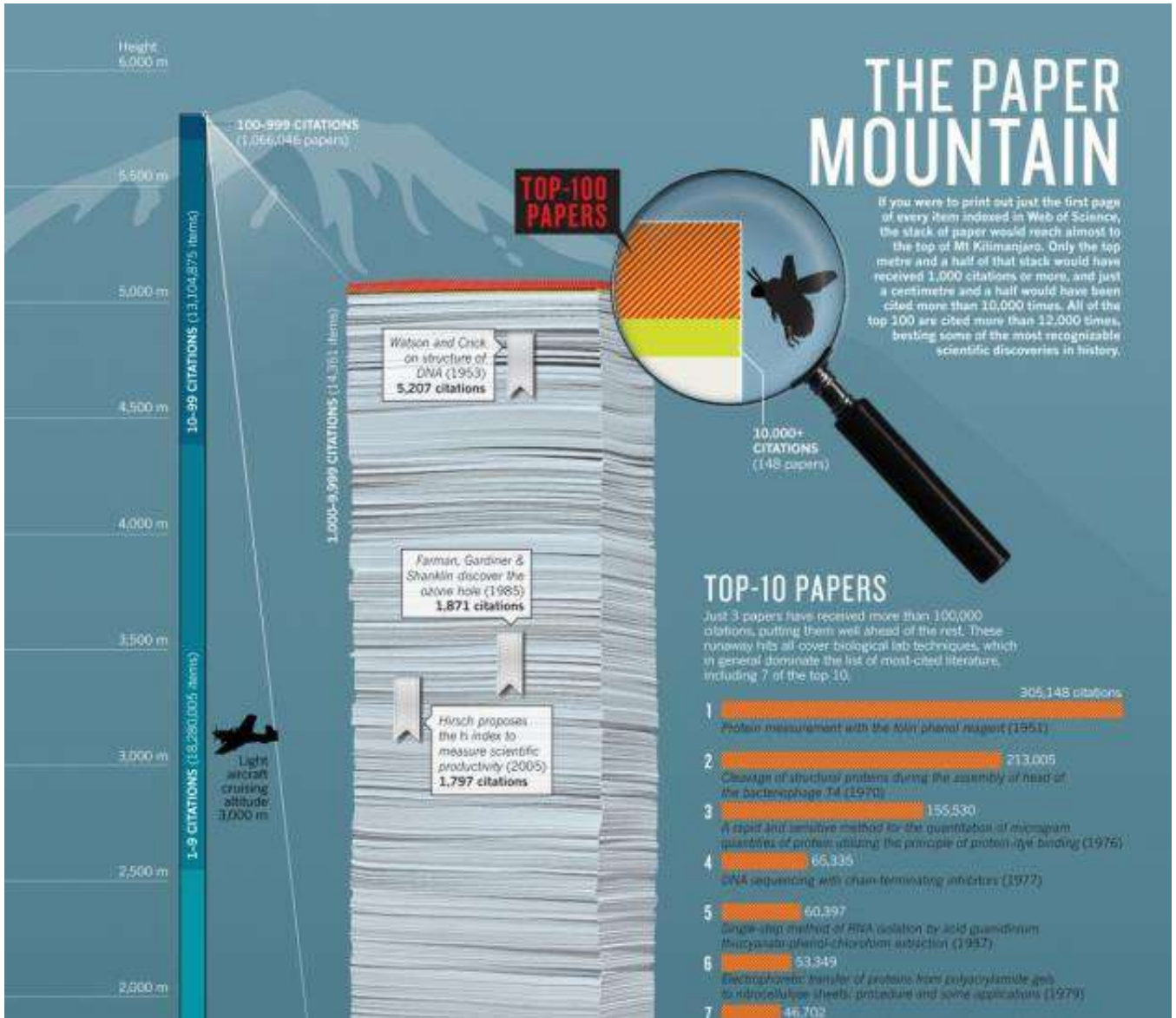
THE RISE OF COMPUTATIONAL SCIENCE

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



THE TOP 100 PAPERS:

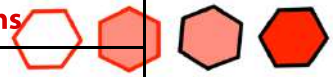
12 papers on density-functional theory in the top-100 most cited papers in the entire scientific-medical-engineering literature, ever.

NATURE, OCT 2014

MOST CITED PAPERS IN THE HISTORY OF APS

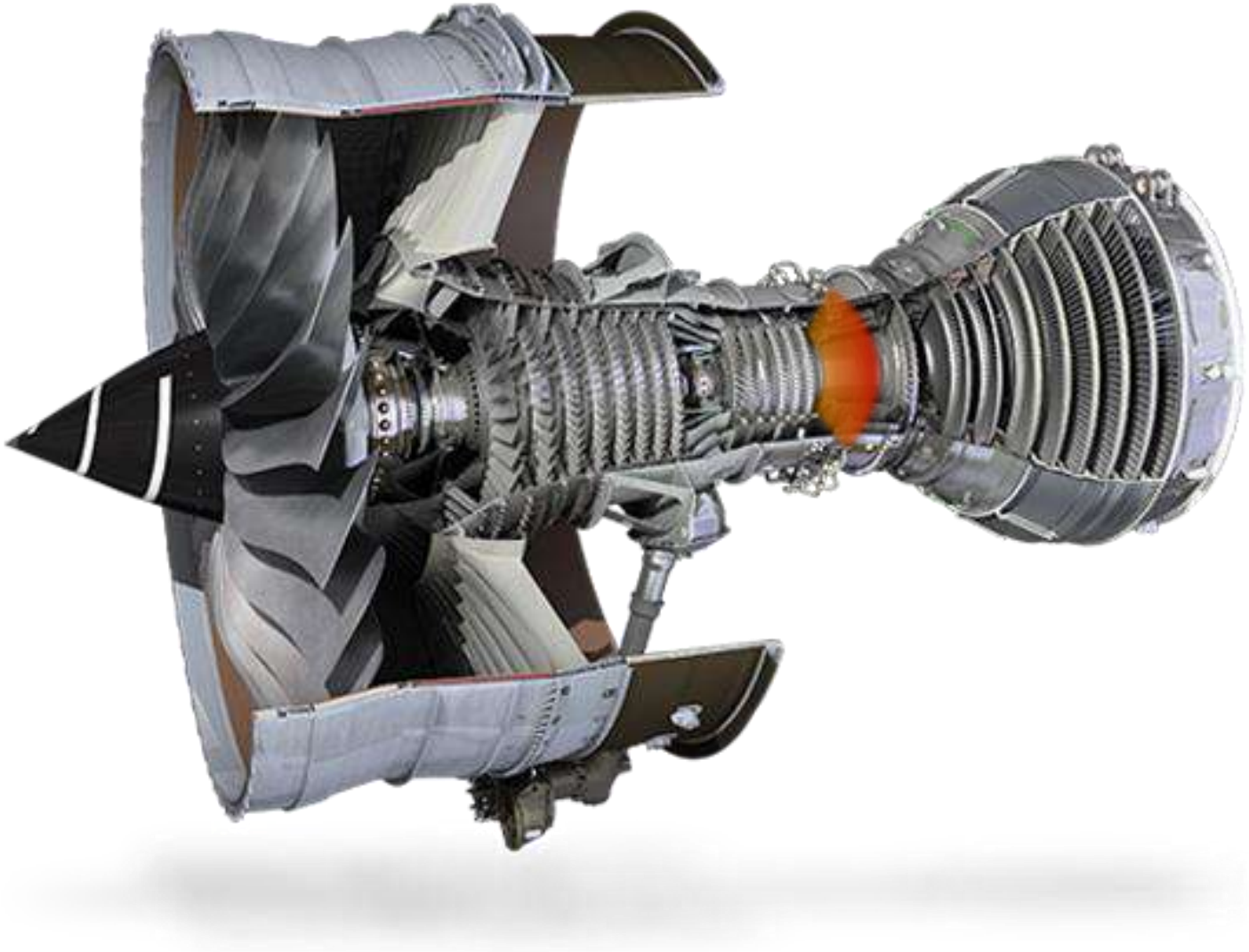
	Journal	# cites	Title	Author(s)
1	PRL (1996)	78085	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
2	PRB (1988)	67303	Development of the Colle-Salvetti Correlation-Energy …	Lee, Yang, Parr
3	PRB (1996)	41683	Efficient Iterative Schemes for Ab Initio Total-Energy …	Kresse and Furthmuller
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)

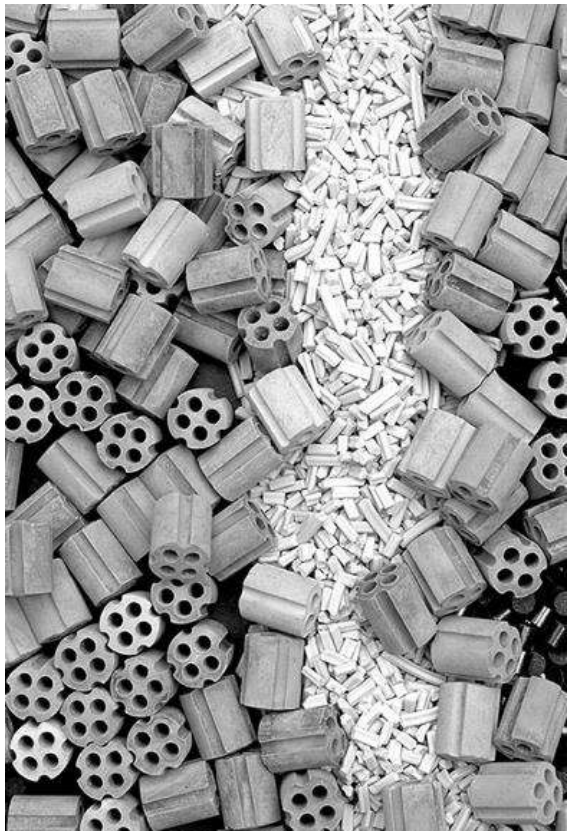


THE RISE OF MATERIALS SCIENCE

IF WE FLY AGAIN…



THE MOST IMPORTANT MATERIAL EVER?



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)

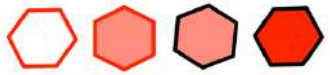
COMPUTATIONAL MATERIALS DESIGN AND DISCOVERY

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)



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

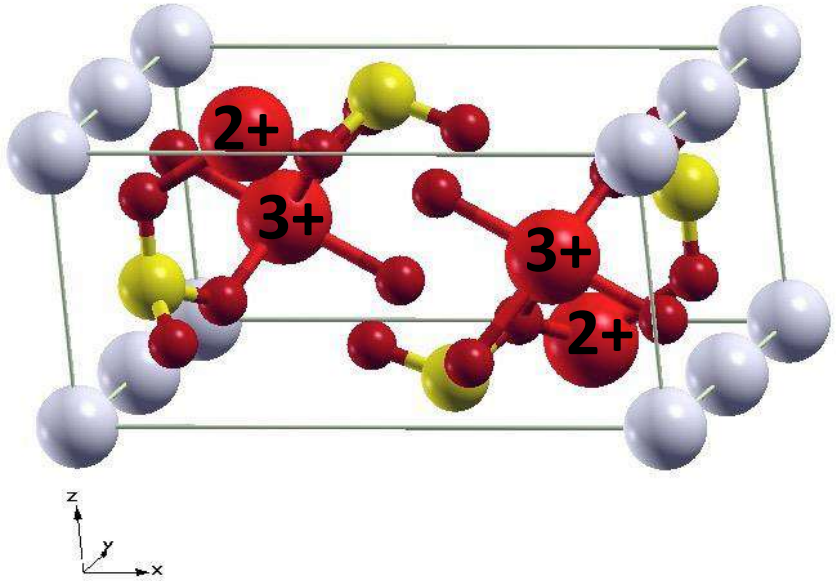
1) PREDICTIVE ACCURACY

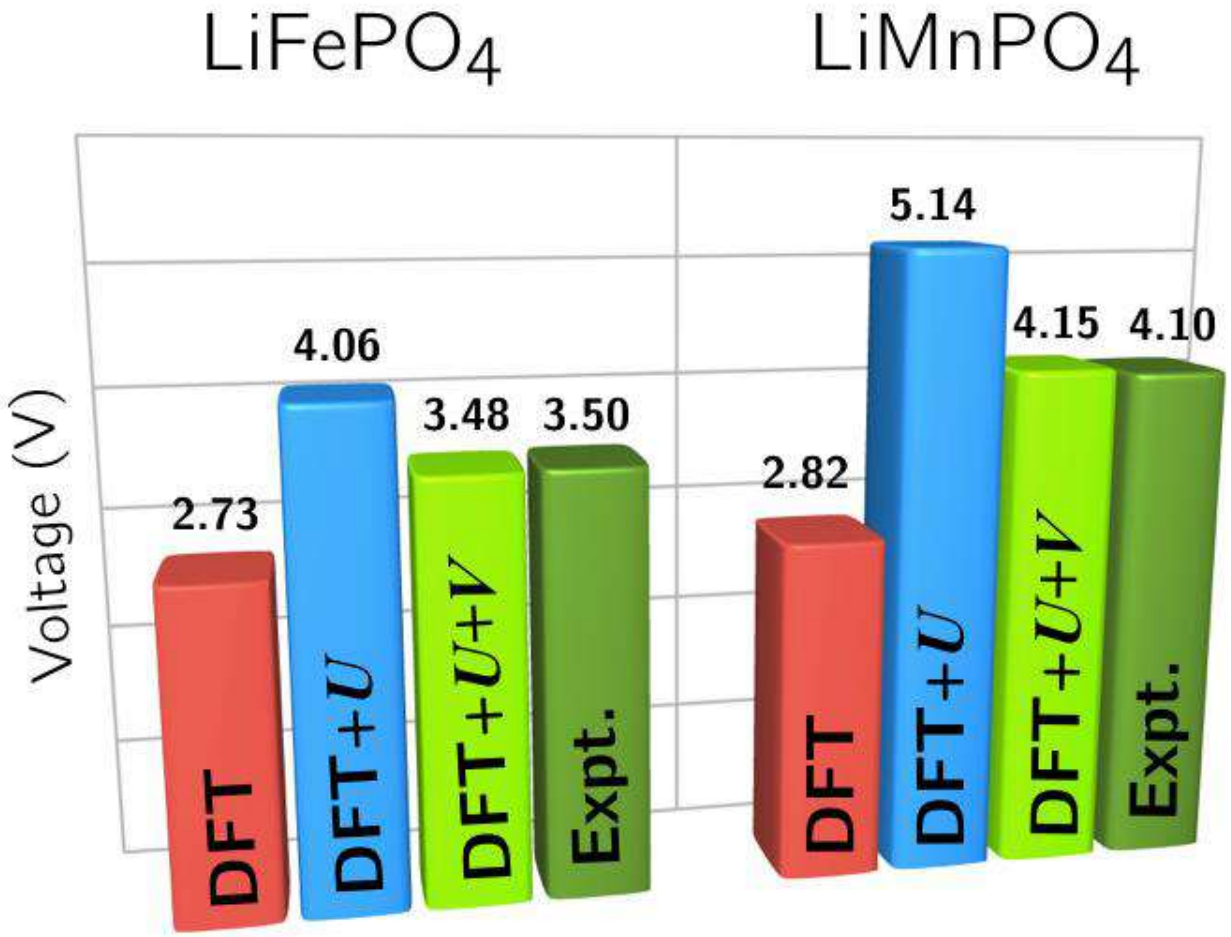
2) REALISTIC COMPLEXITY

3) MATERIALS' INFORMATICS

HUBBARD FUNCTIONALS (DFT+U+V)

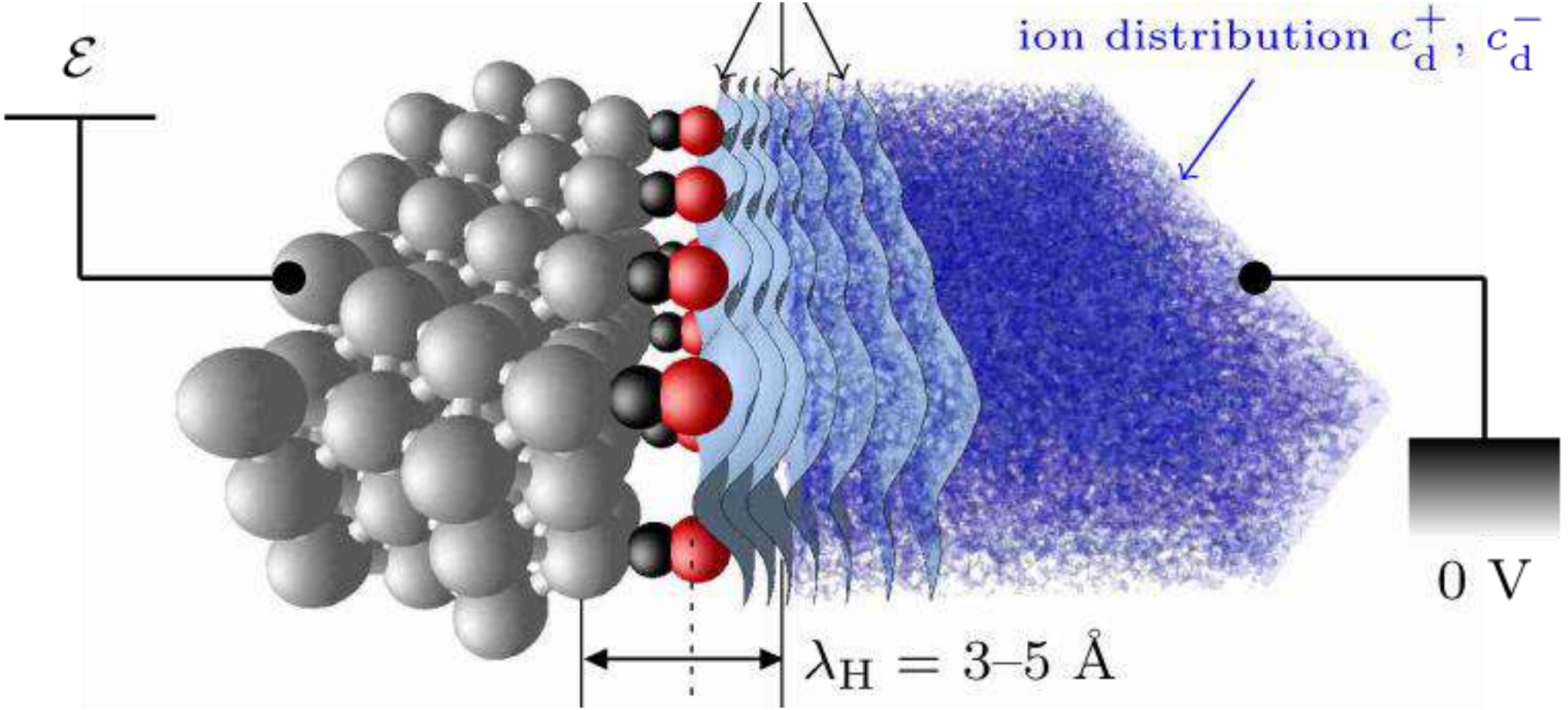
$Li_{0.5}FePO_4$





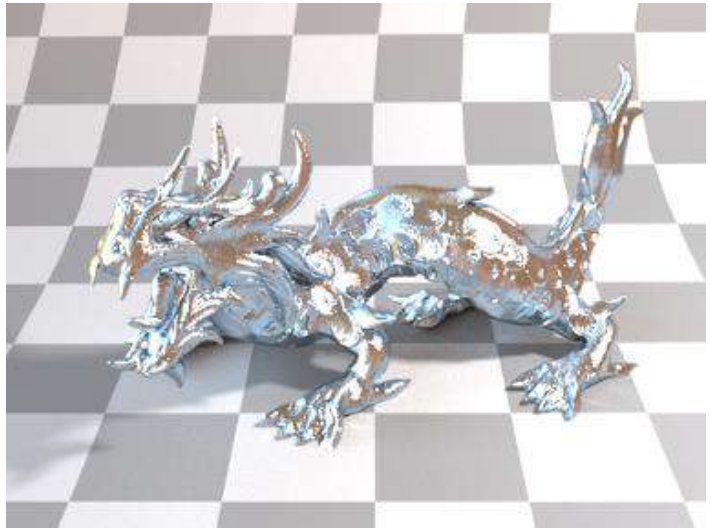
M. Cococcioni and N. Marzari, Phys. Rev. Materials 3, 033801 (2019).

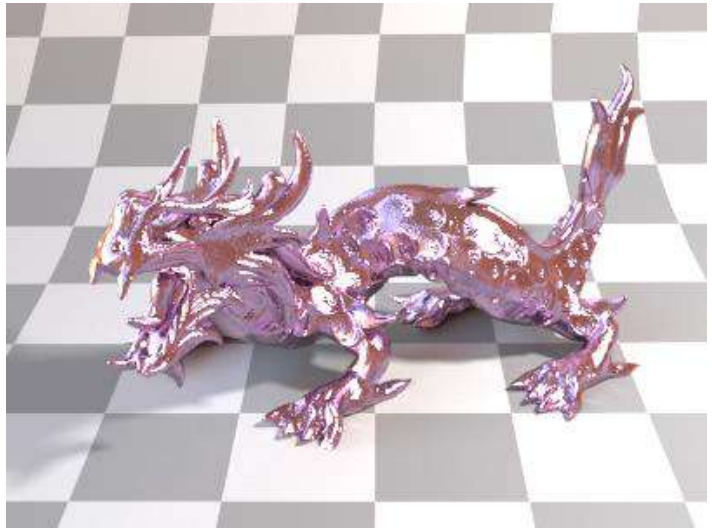
COMPLEXITY: MULTI-SCALE MODELING FOR ELECTROCHEMISTRY



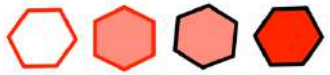
O. Andreussi *et al.*, J. Chem. Phys. 136, 064102 (2012)
F. Nattino *et al.*, J. Chem. Phys. 150, 041722 (2019)

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

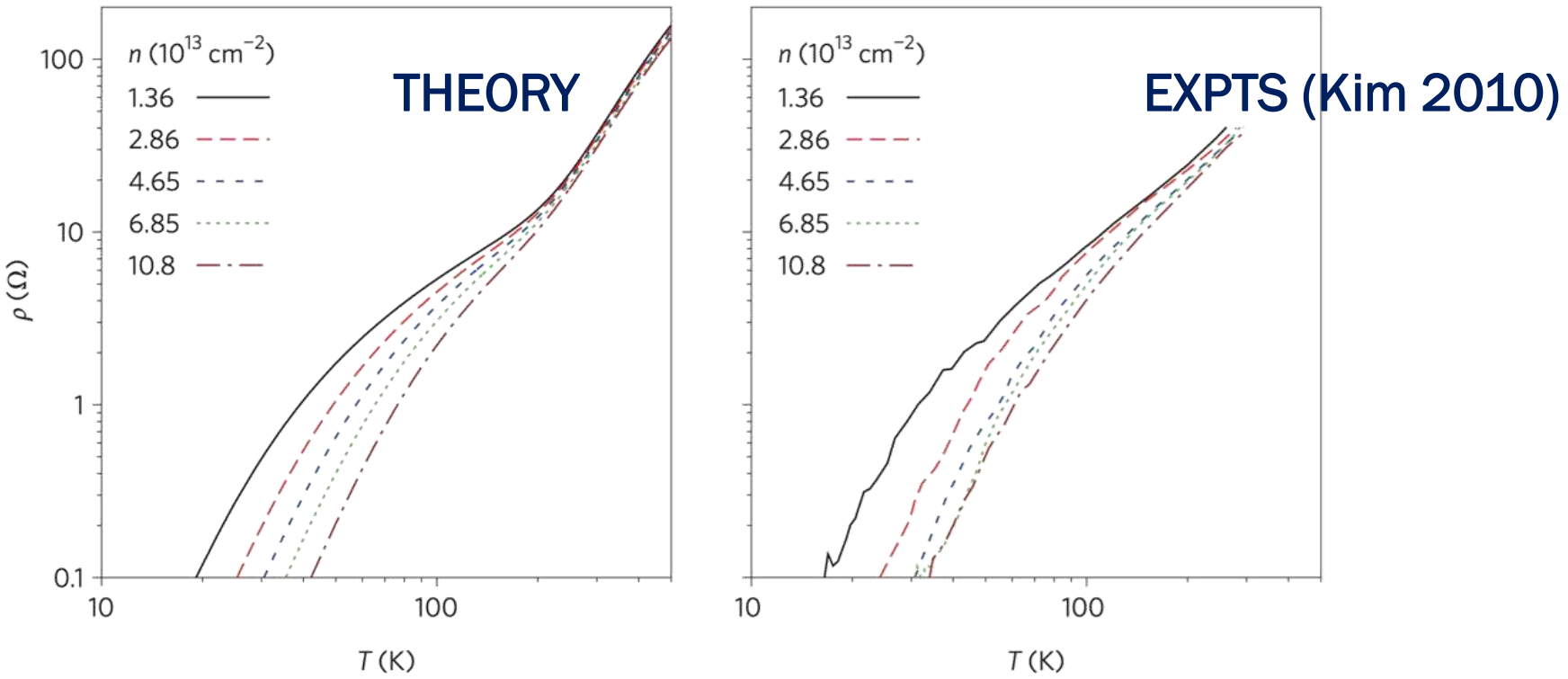


Figure 1 | Electrical resistivity of graphene as a function of temperature and doping (ρ, electrical resistivity; T, temperature; n, carrier density). Left panel: first-principles results obtained using a combination of density-functional perturbation theory, many-body perturbation theory and Wannier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

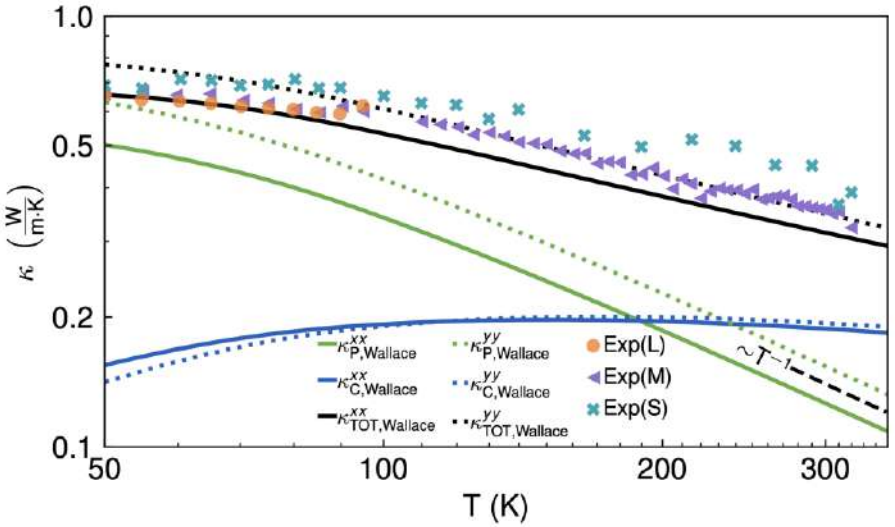
nature physics

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

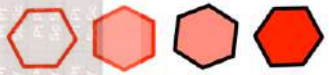
VOLUME 88, NUMBER 25 PHYSICAL REVIEW LETTERS 24 JUNE 2002

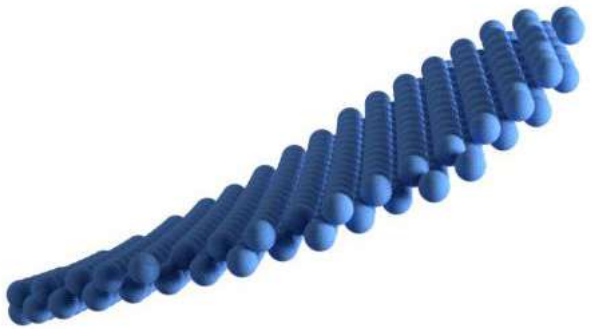
Combined Electronic Structure and Evolutionary Search Approach to Materials Design

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)

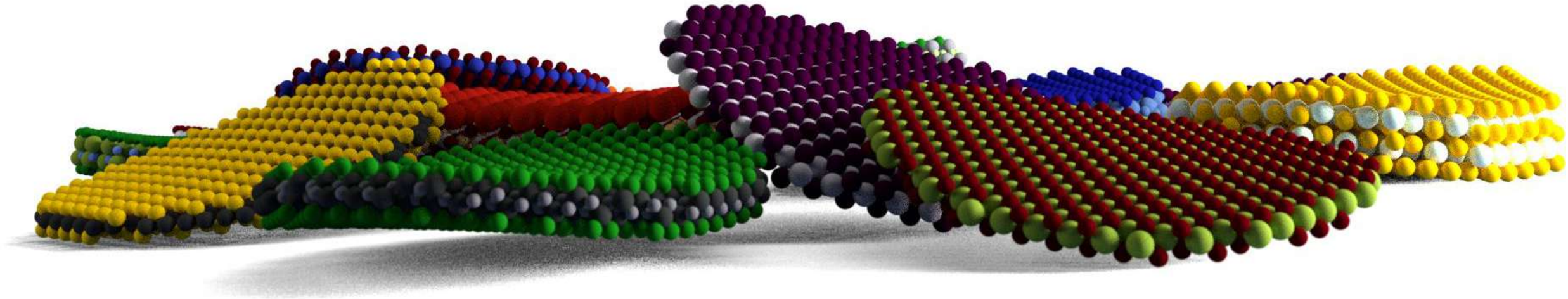
We show that density functional theory calculations have reached an accuracy and speed making it possible to use them in conjunction with an evolutionary algorithm to search for materials with specific properties. The approach is illustrated by finding the most stable four component alloys out of the 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

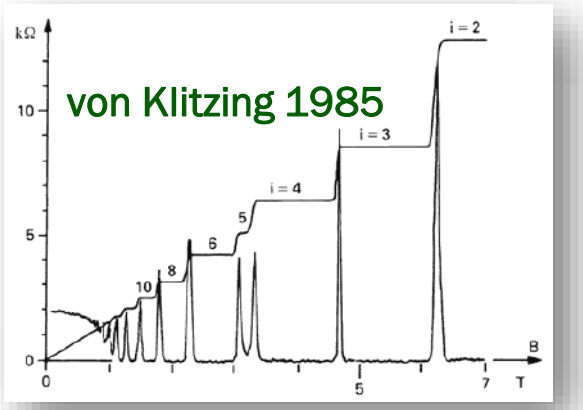


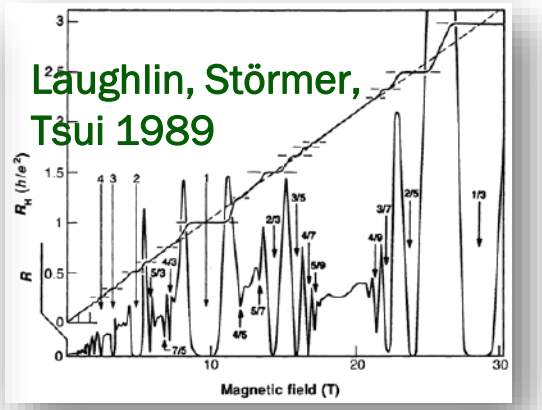


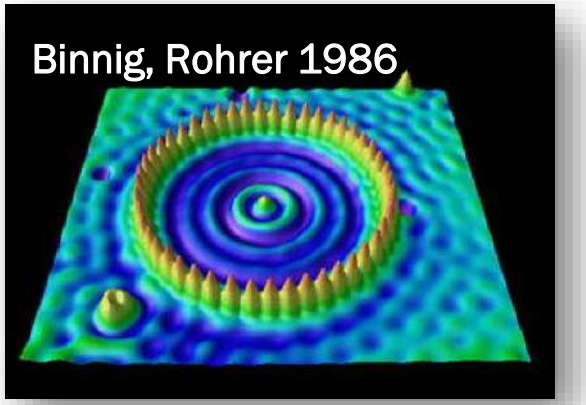
EXAMPLE: COMPUTATIONAL EXFOLIATION OF ALL KNOWN INORGANIC MATERIALS

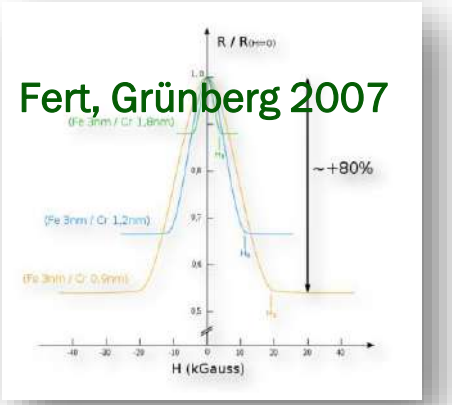


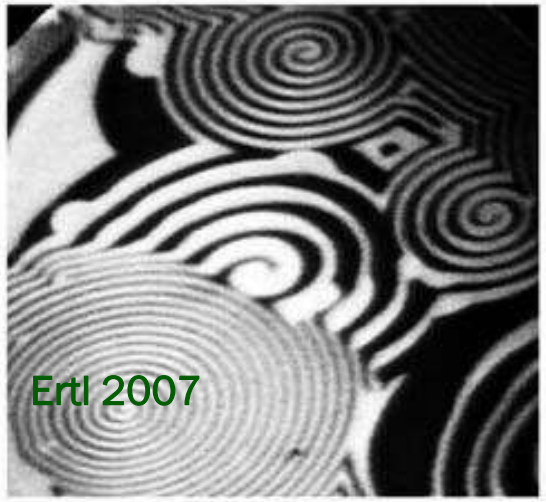
PHYSICS AND CHEMISTRY IN LOW DIMENSIONS

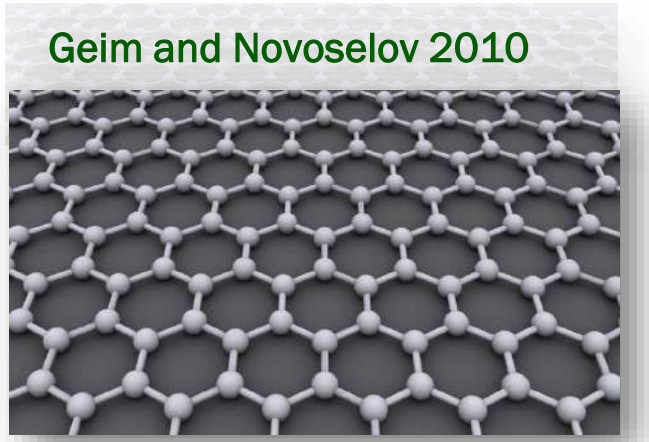




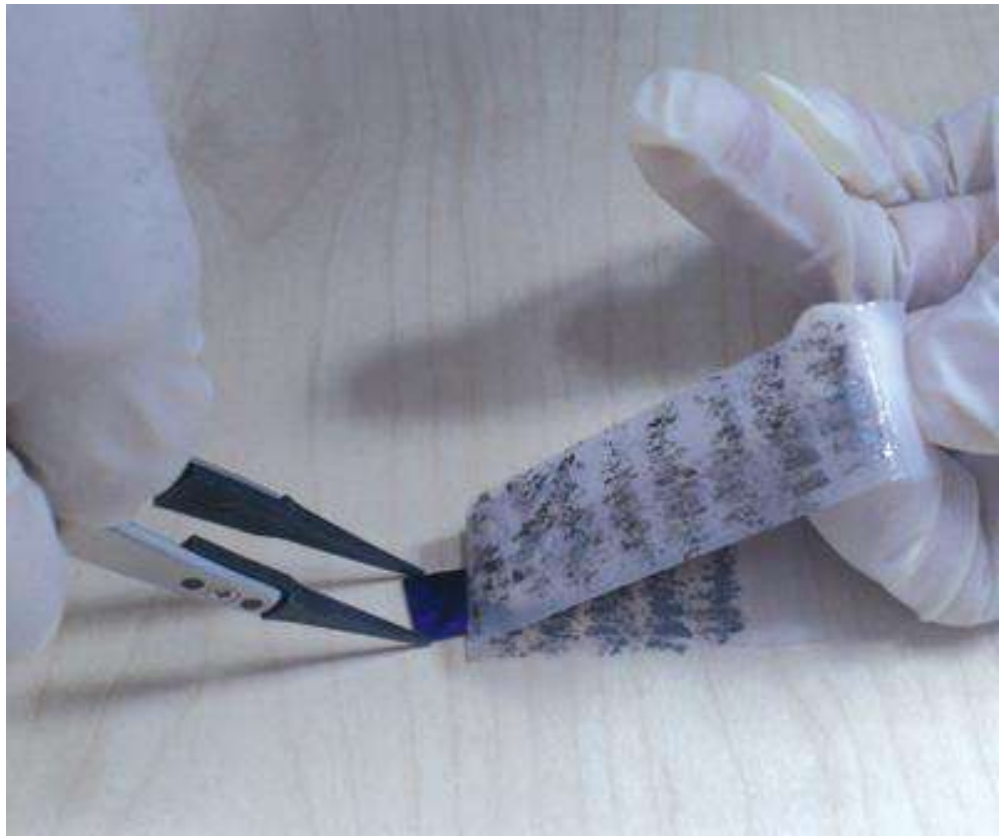


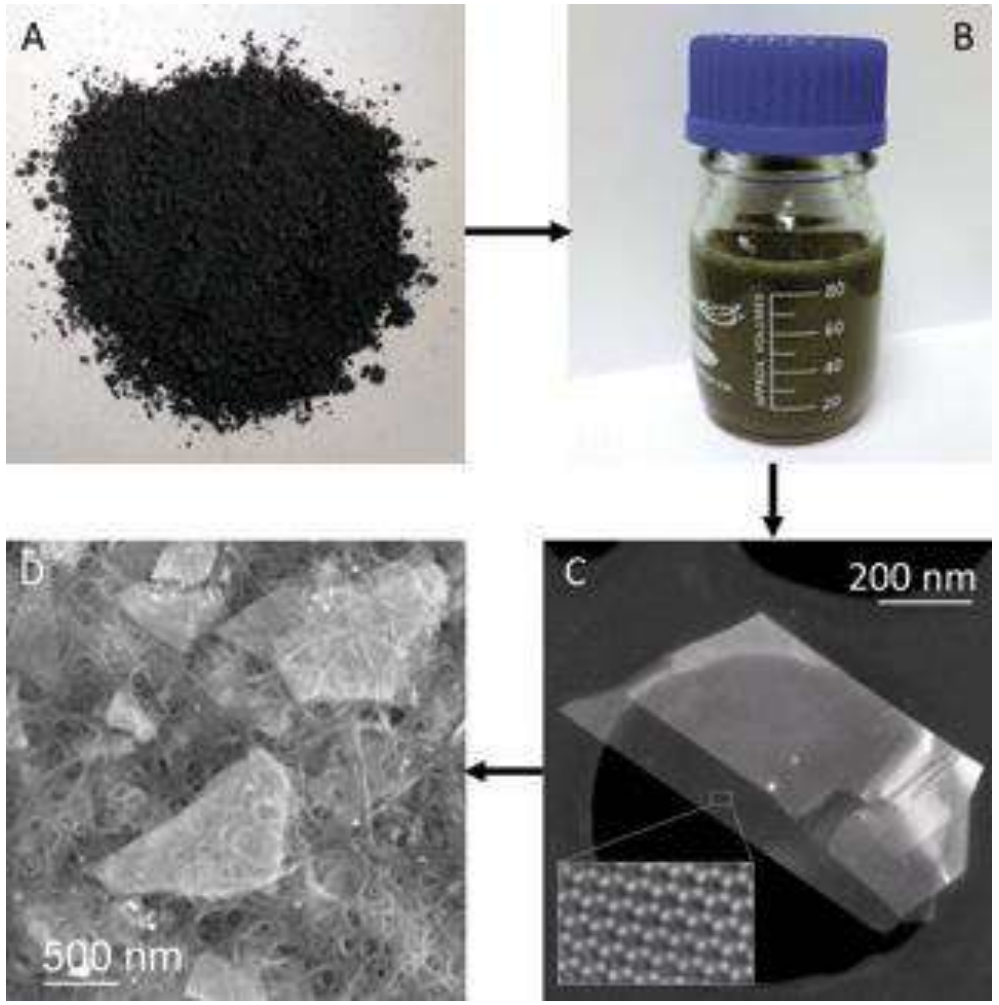






HOW DO WE PRODUCE 2D MATERIALS?





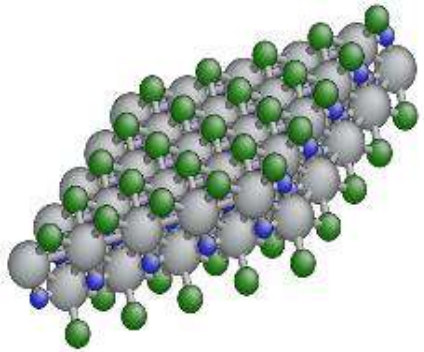
Mechanical (e.g. Geim/Novoselov, fig. from Nature/NUS) **or liquid exfoliation** (e.g. Nicolosi/Coleman, fig. from Science), **electrochemical intercalation**. Also, bottom-up: **CVD and wet chemical synthesis.**

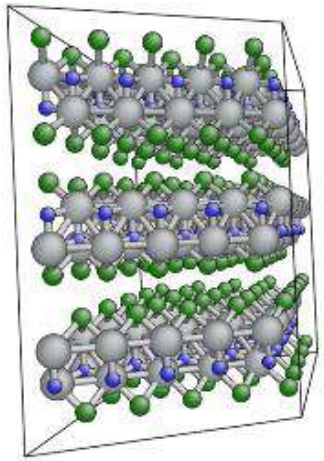
HIGH-THROUGHPUT COMPUTATIONAL EXFOLIATION

Exfoliation | **Characterization** | **Applications**

External databases (ICSD, COD, Pauling File)

Geometrically layered





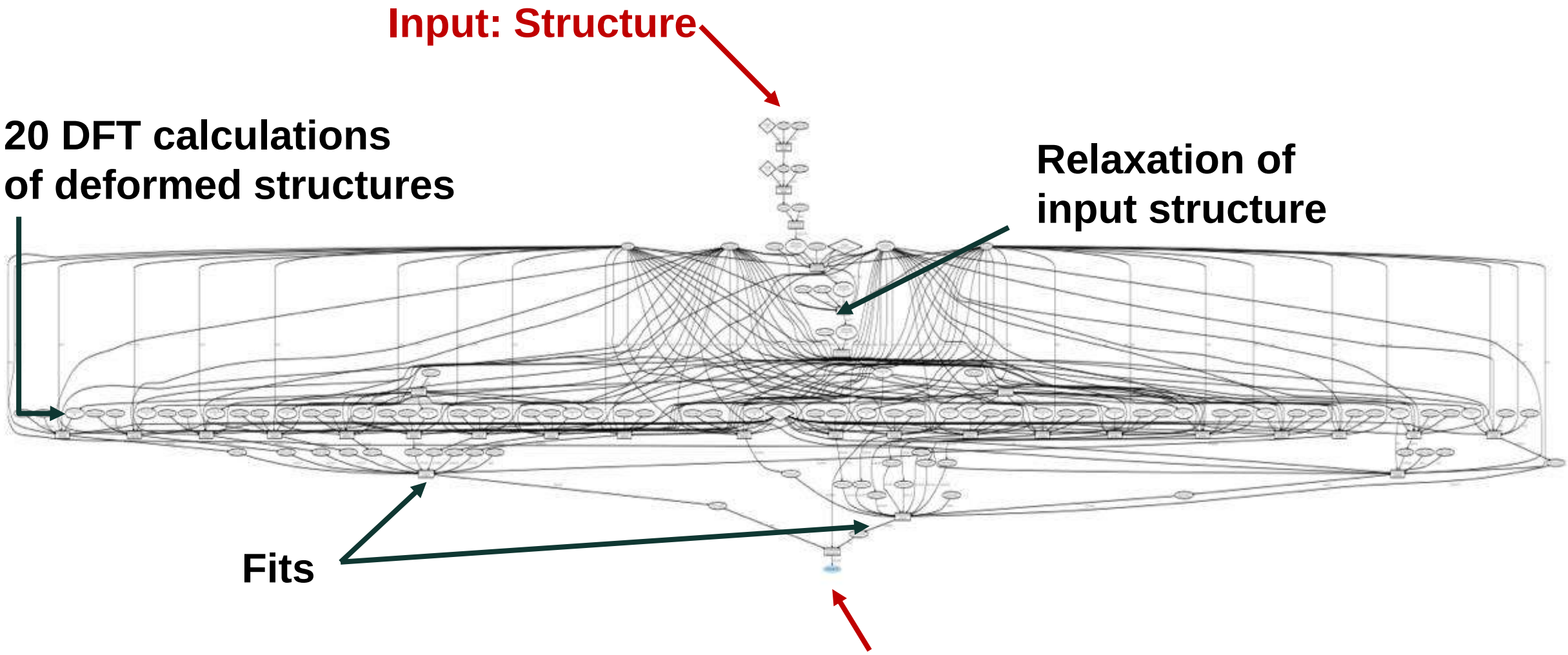
VdW-DFT electronic structure, binding energies

- Electronic
- Magnetic
- Mechanical

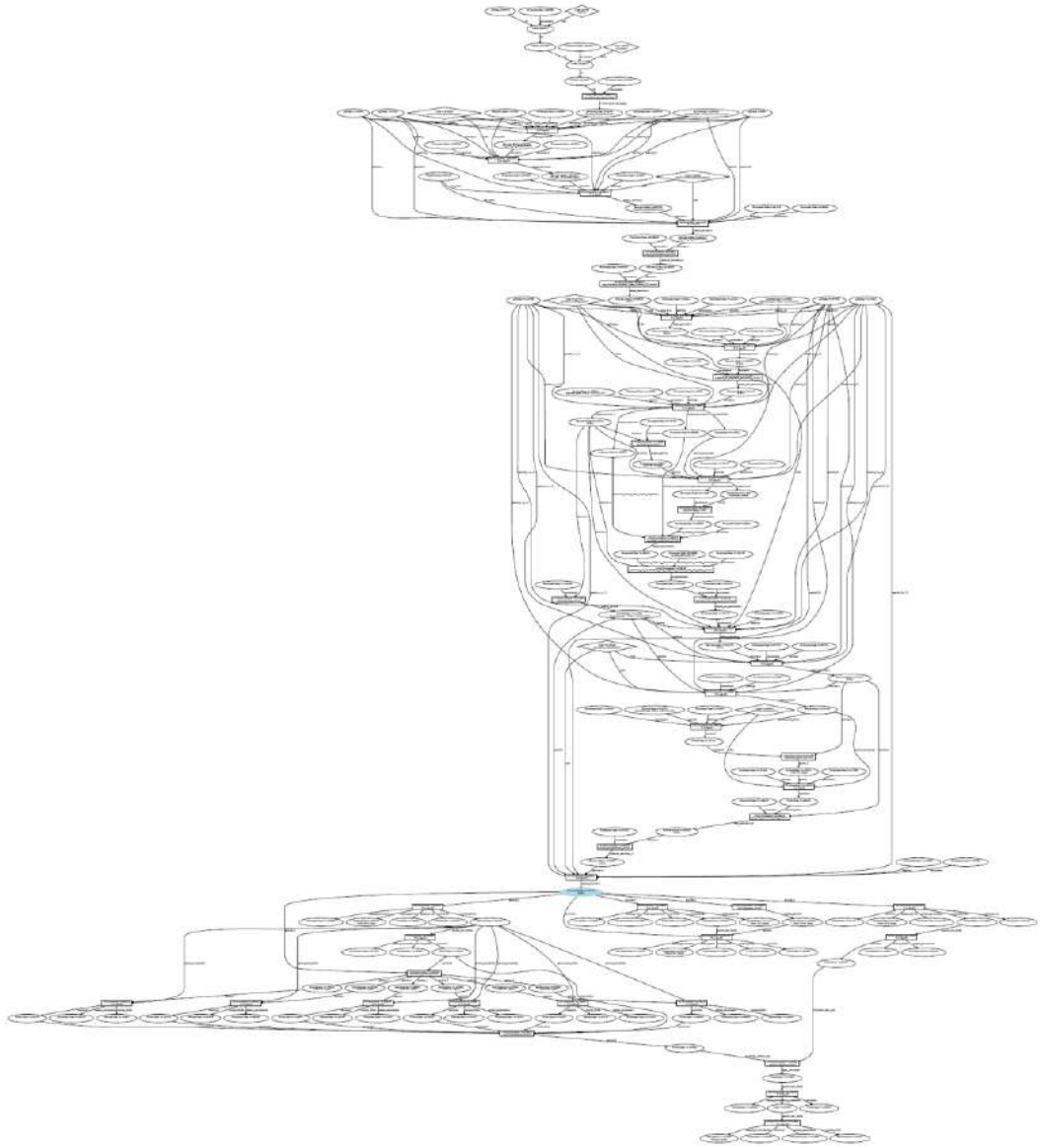
- High e/h mobility
- Topological
- CDW, spintronics
- Plasmonics
- Photocatalysis
- Membranes
- .....

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)

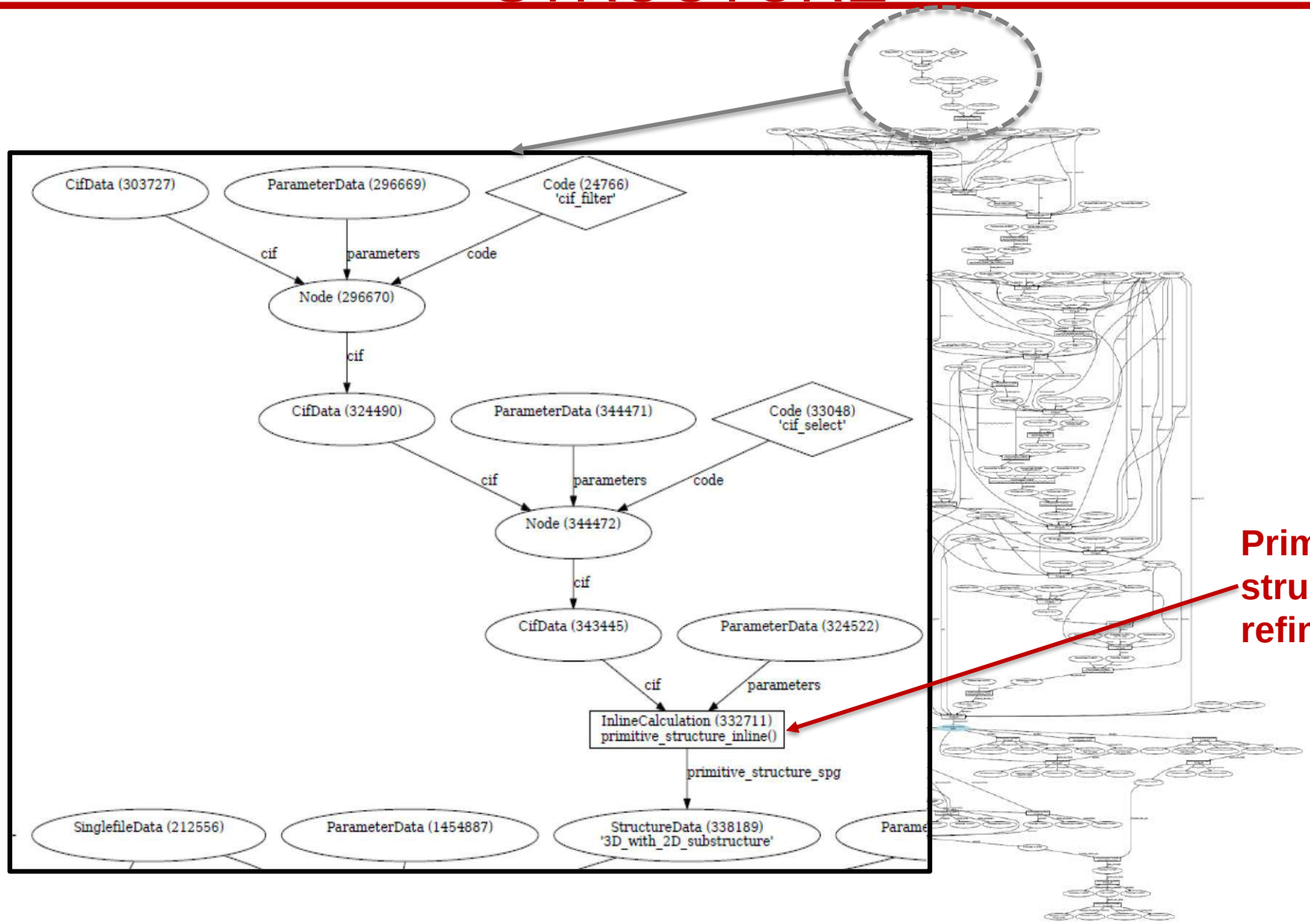
AUTOMATIC WORKFLOWS: FROM STRUCTURE TO PROPERTY



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

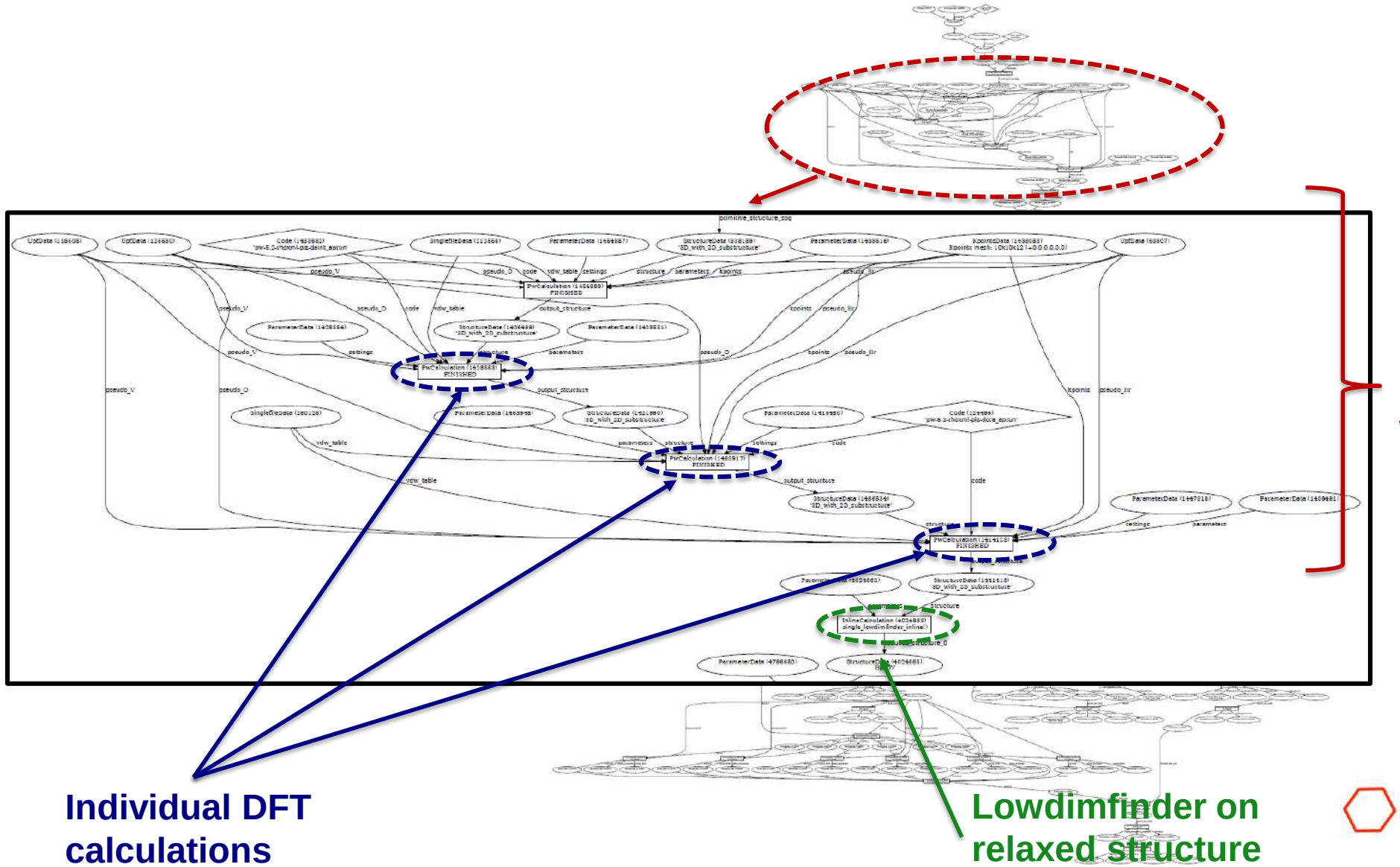


FROM DATABASE ENTRY TO A WORKING STRUCTURE

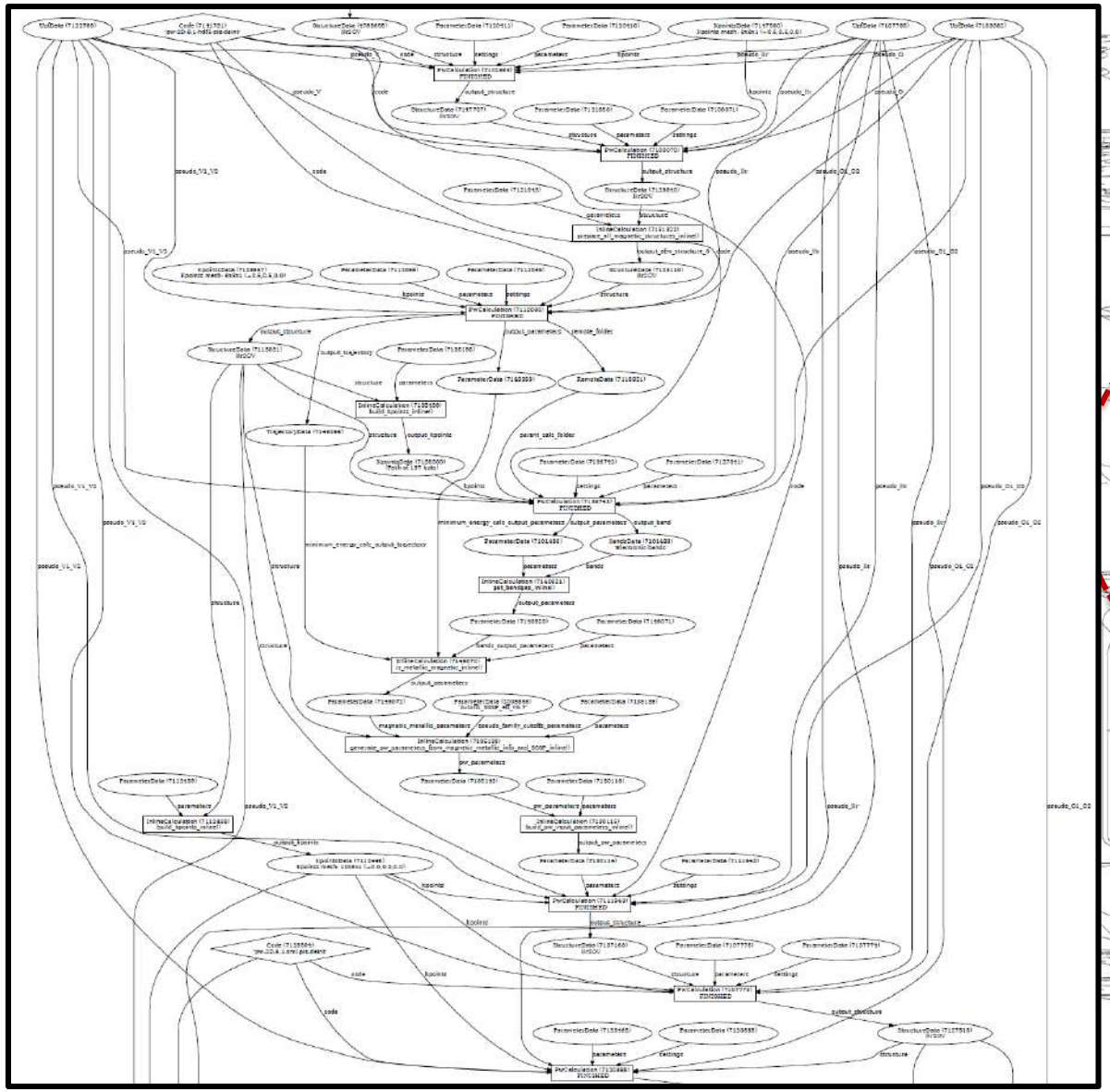


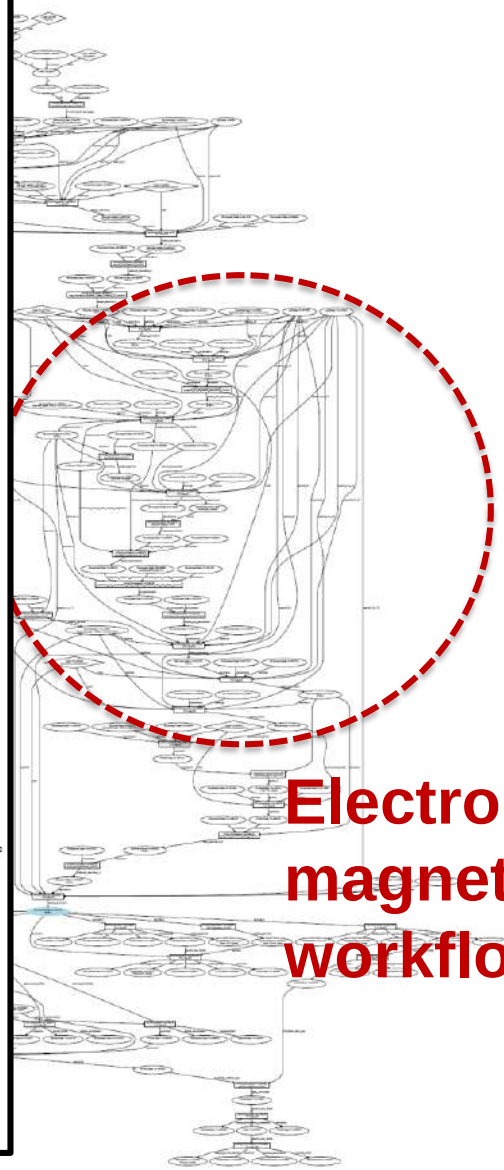
Primitive cell & structure symmetry refinement

3D RELAXATION



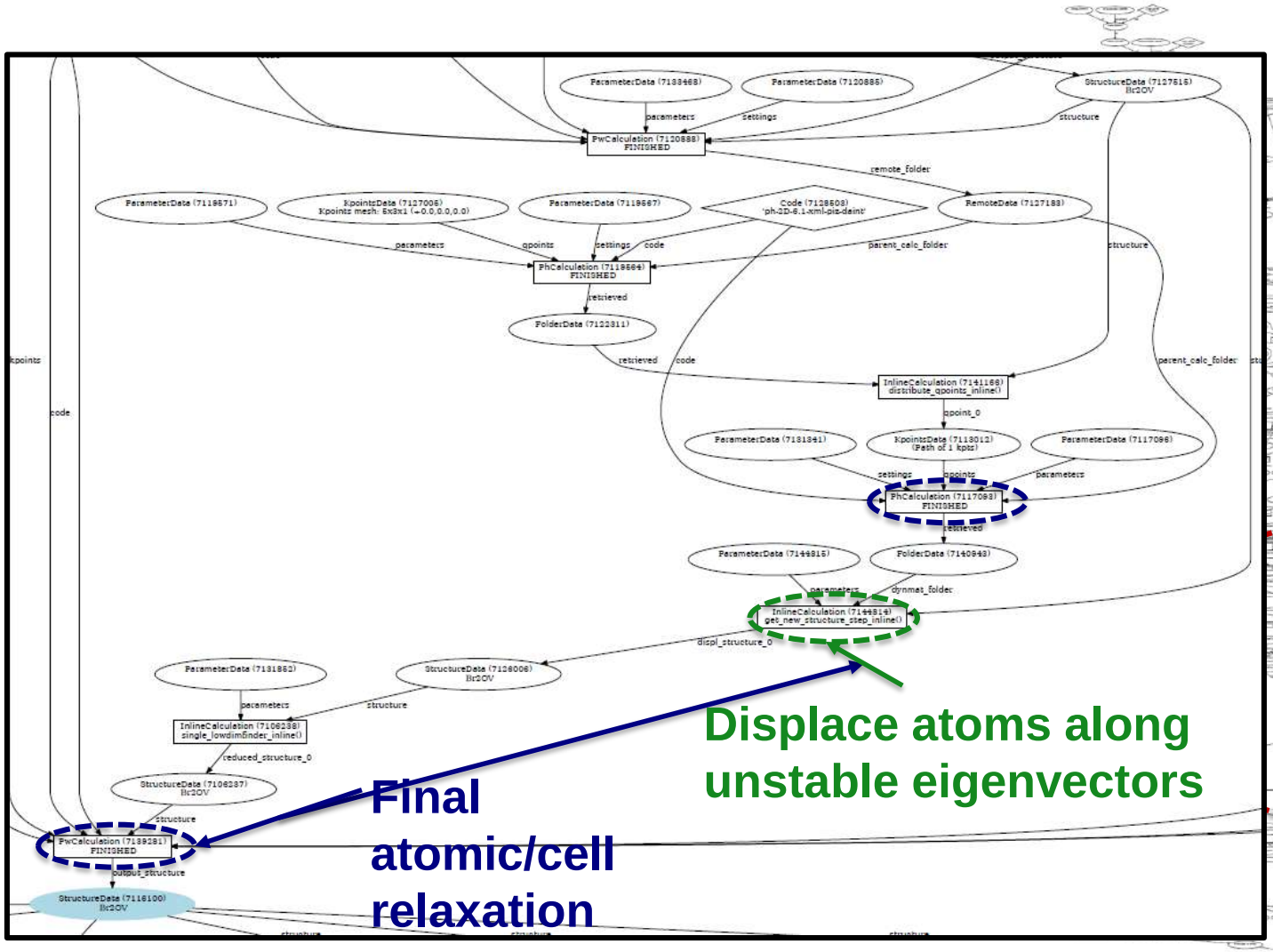
MAGNETIC SCREENING OF THE 2D MONOLAYER



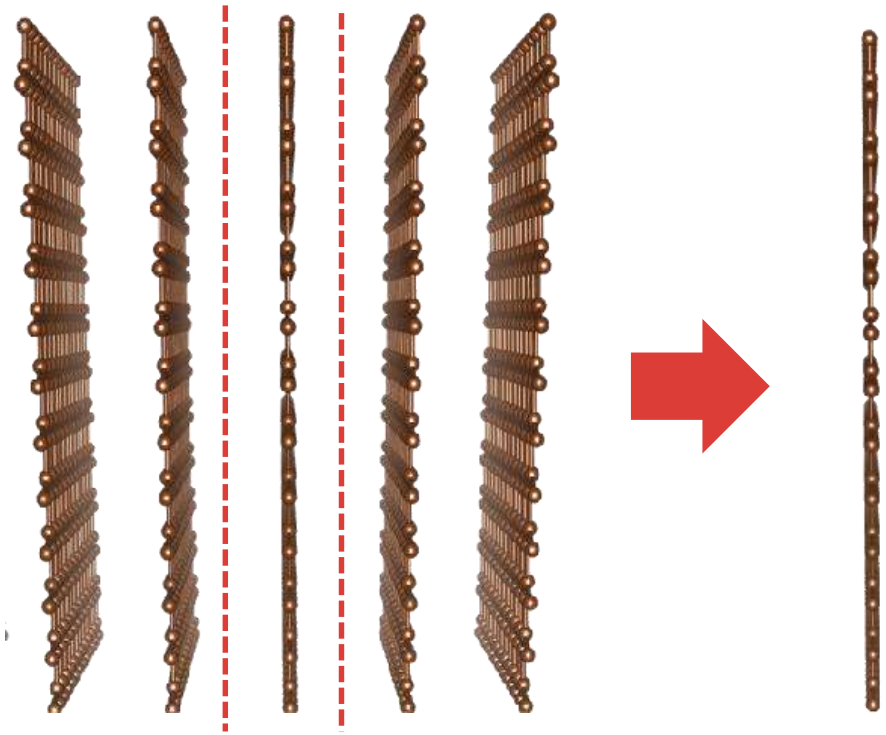


Electronic & magnetic workflow

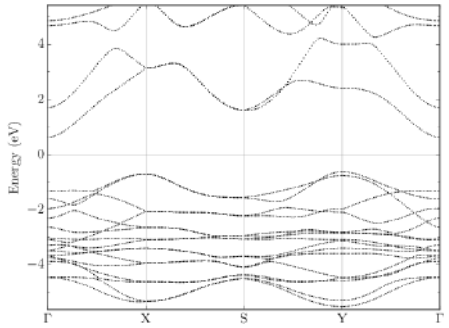
REMOVING MECHANICAL INSTABILITIES



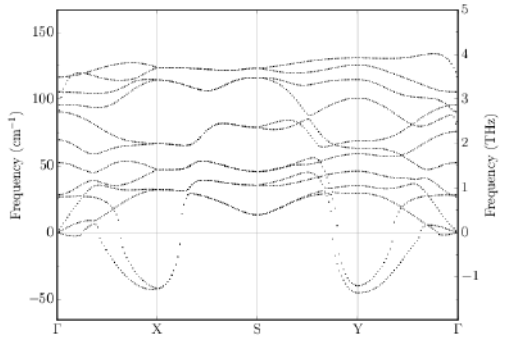
ALL AUTOMATED…



Band structures



Phonon dispersions



FINALLY…

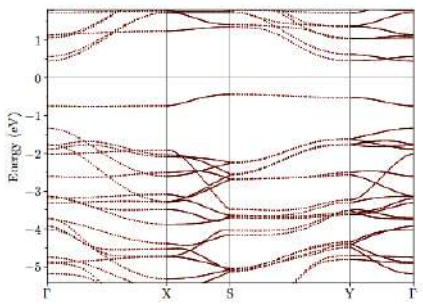
215 VBr_2O (Pmm2)

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

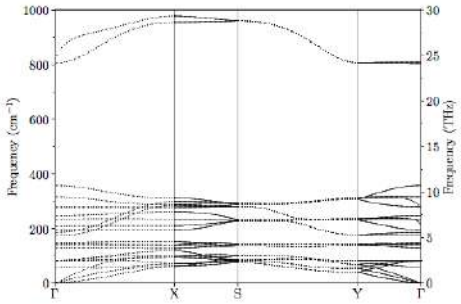
Formula	VBr_2O
Spacegroup	Pmm2
Prototype	VCl_2O (Pmm2)
Parent 3D	VBr_2O
Source DB	ICSD
DB ID	24381

DF2-C09 Binding energy [meV/Å²]	14.4
rVV10 Binding energy [meV/Å²]	21.6
Band gap [eV]	0.9
Magnetic State	AFM
Tot. Magnetization [μ_B/cell]	0.0
Abs. Magnetization [μ_B/cell]	2.54

Band structure and phonon dispersions



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



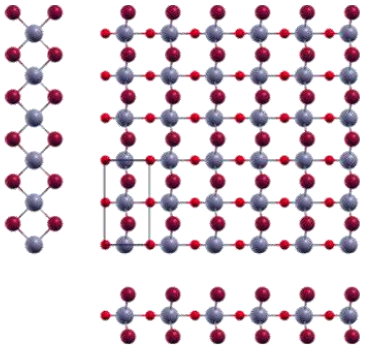
Phonon dispersions: phonon frequencies of VBr_2O (8 atoms/cell) along a high-symmetry path.

Crystal structure

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

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

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

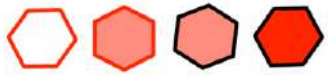


Orthographic projections: different views of VBr_2O from the x axis (left), the y axis (bottom) and the z axis (center).

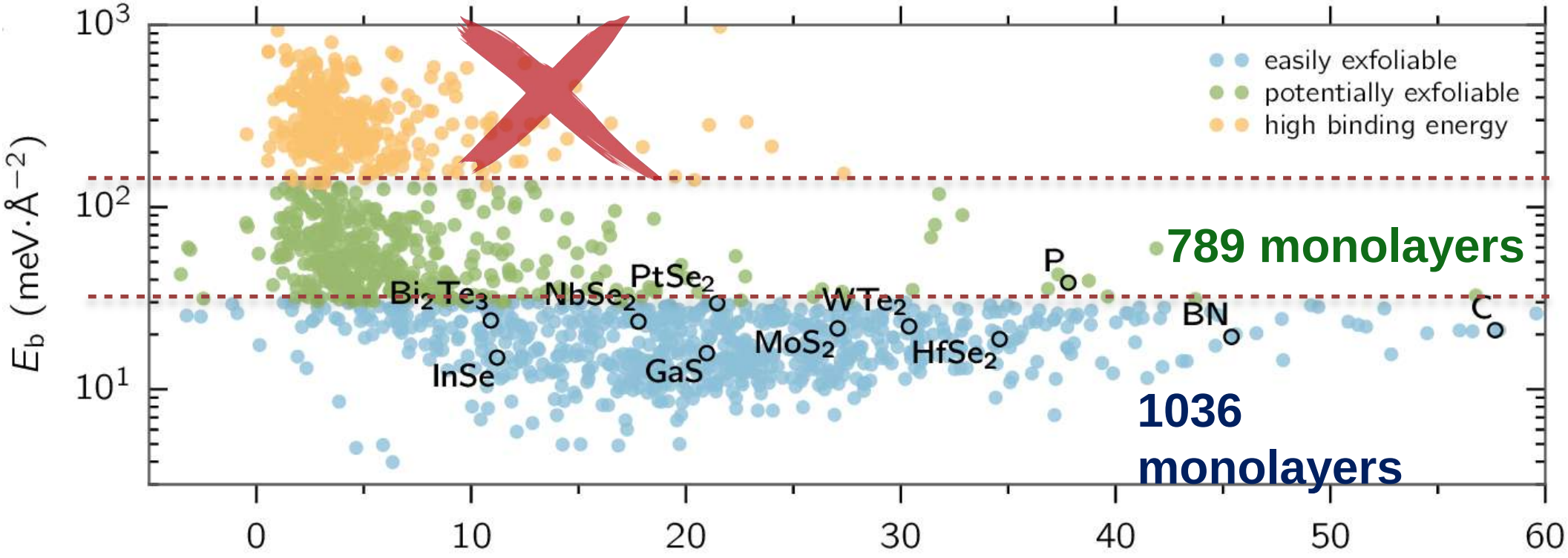
HOW MANY CANDIDATES? GEOMETRIC SCREENING

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

*At this level unicity is not tested



HOW MANY CANDIDATES? QUANTUM SCREENING



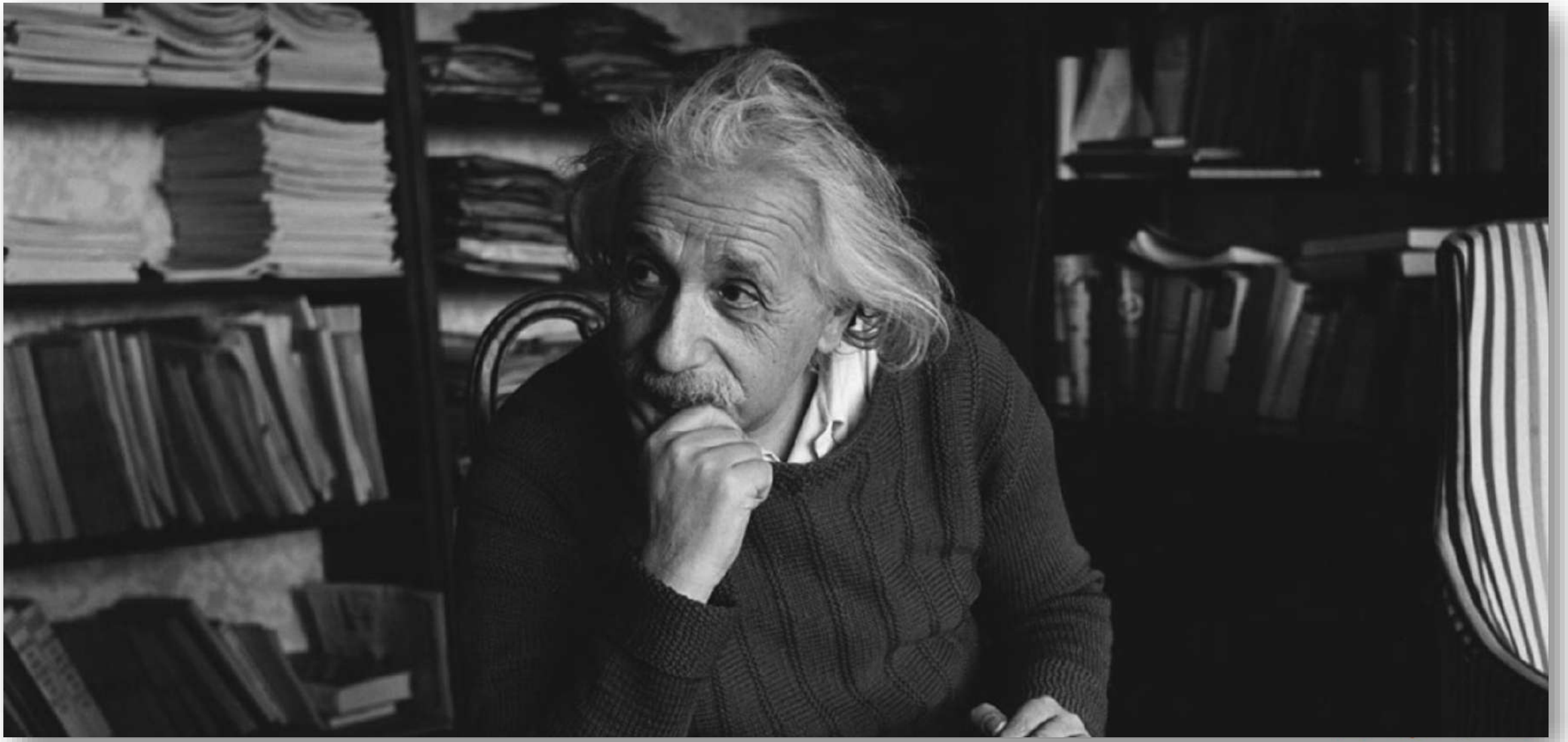
Not exfoliable

Potentially exfoliable

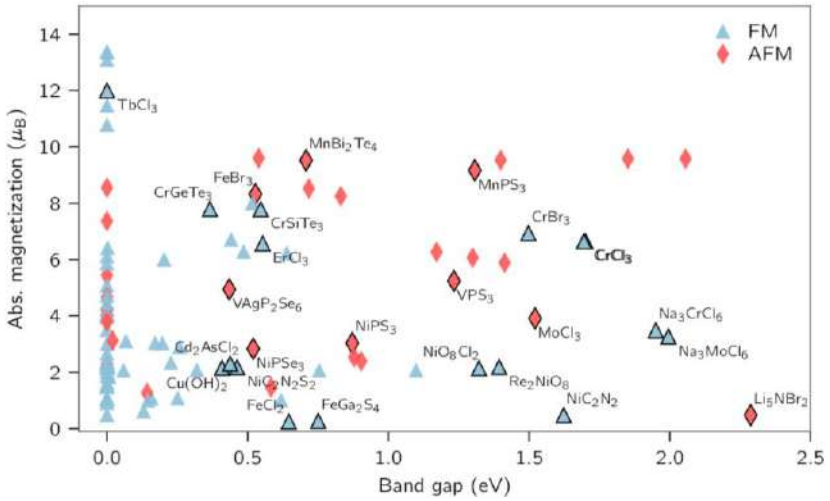
Easily exfoliable

- ***E_b < 30 meV/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)***

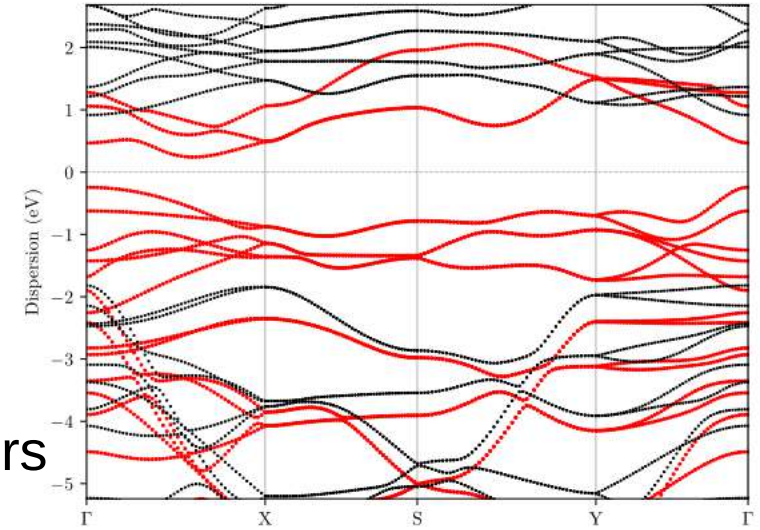
WHAT TO DO NEXT?



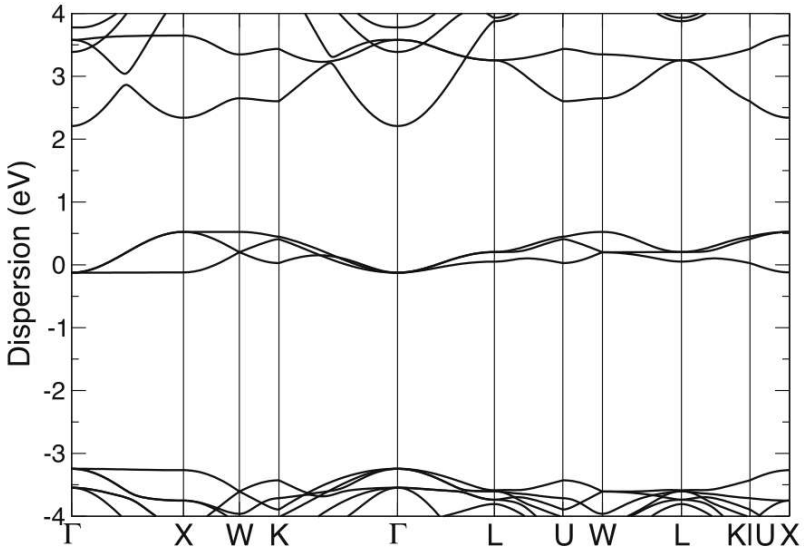
FROM ELECTRONICS…



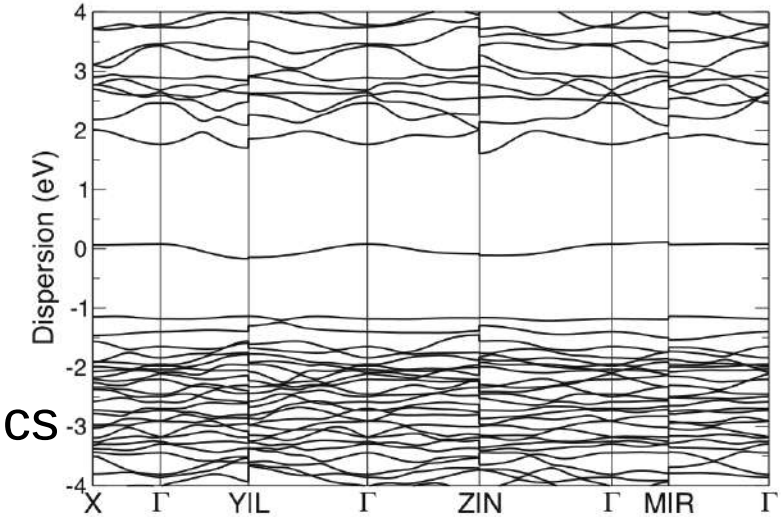
Magnetic metals and insulators



Half-semiconductors

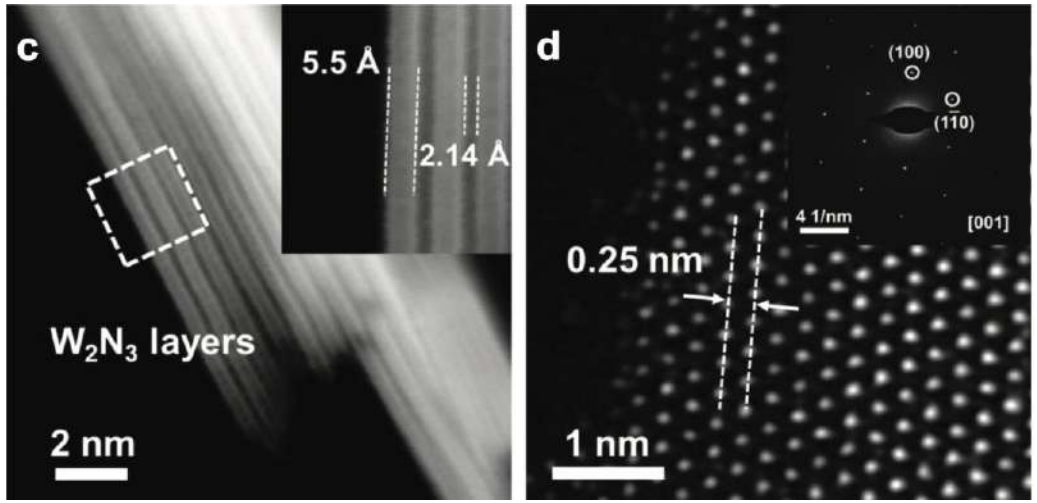


Transparent conductors

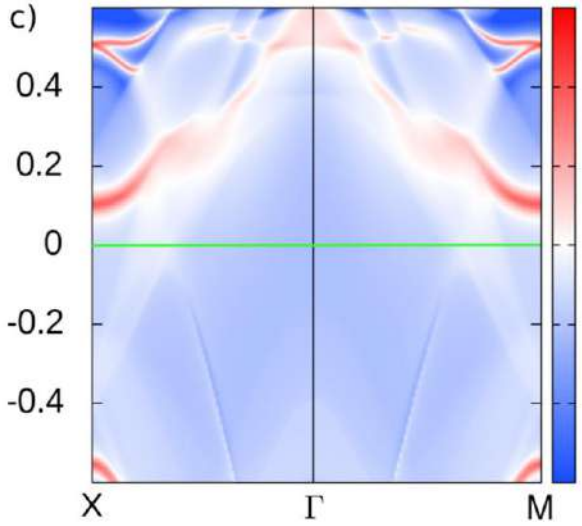


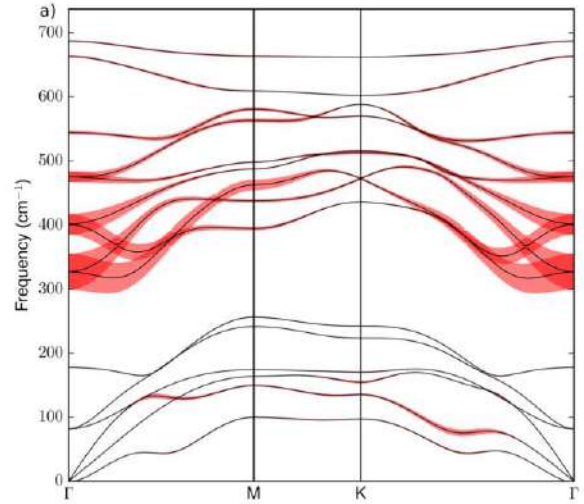
Plasmonics

…TO THE LARGEST SUPERCONDUCTING Tc IN 2D…



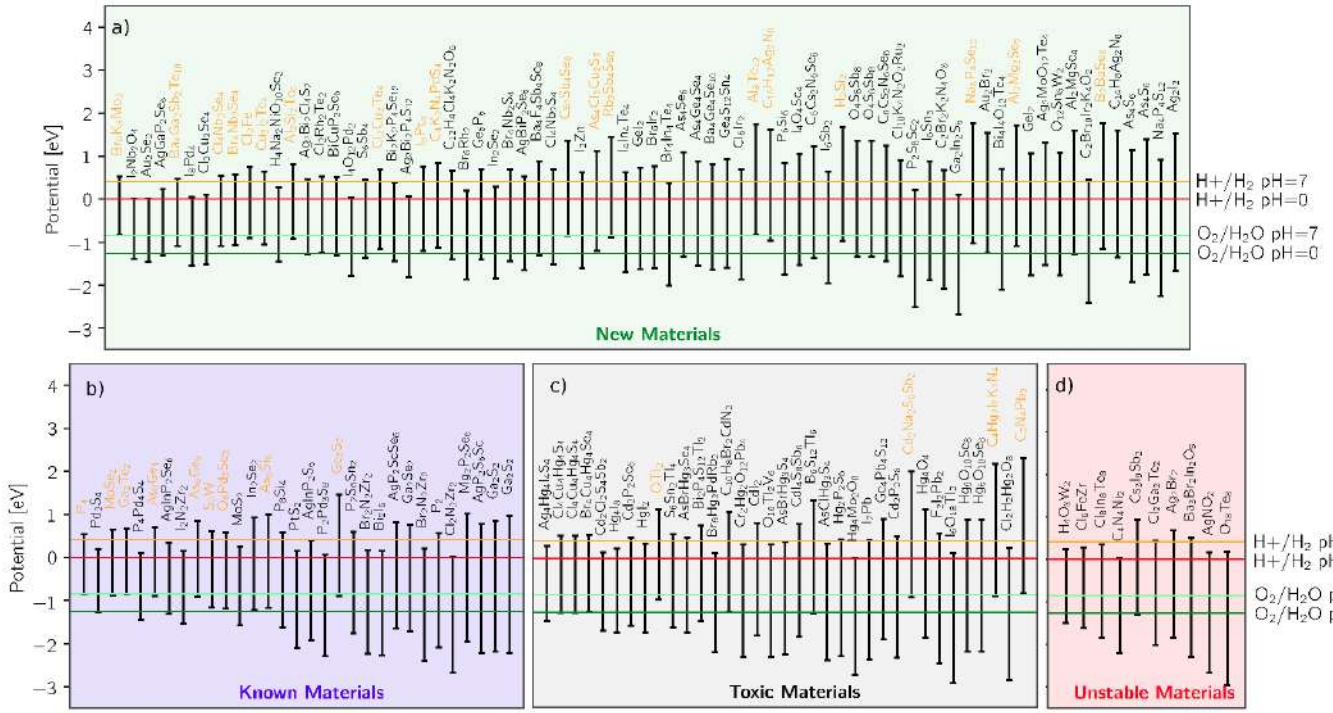
H. Jun *et al.,* Advanced Materials 31, 1902709 (2019)

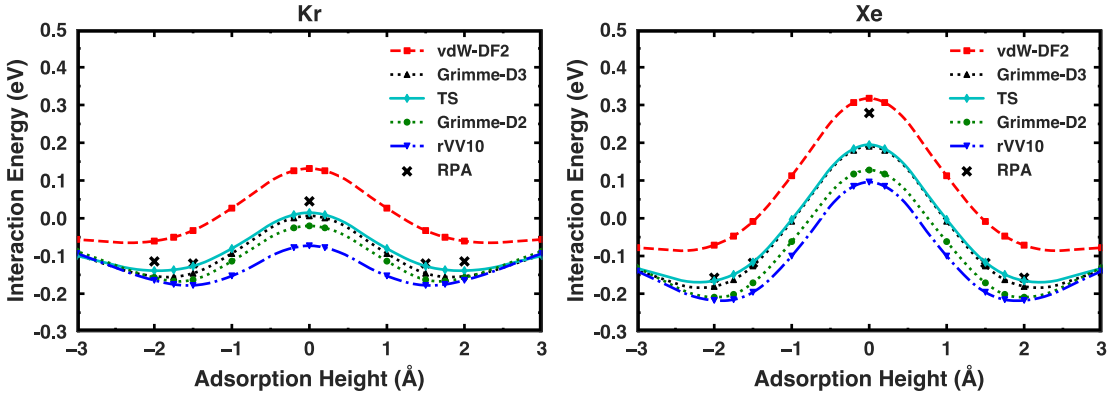


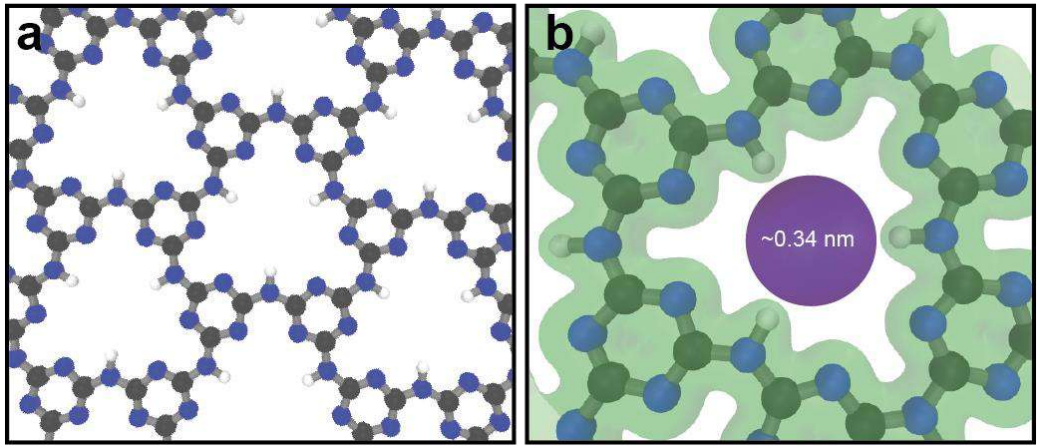


D. Campi, S. Kumari, and N. Marzari,
Nano Letters 21, 3435 (2021)

…TO MATERIALS: PHOTOCATALYSIS, MEMBRANES

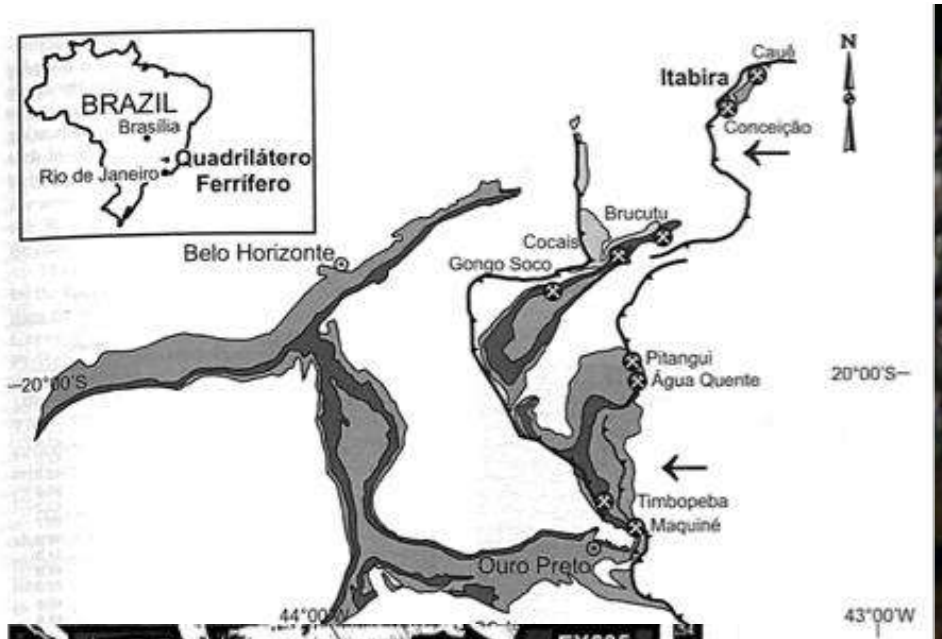


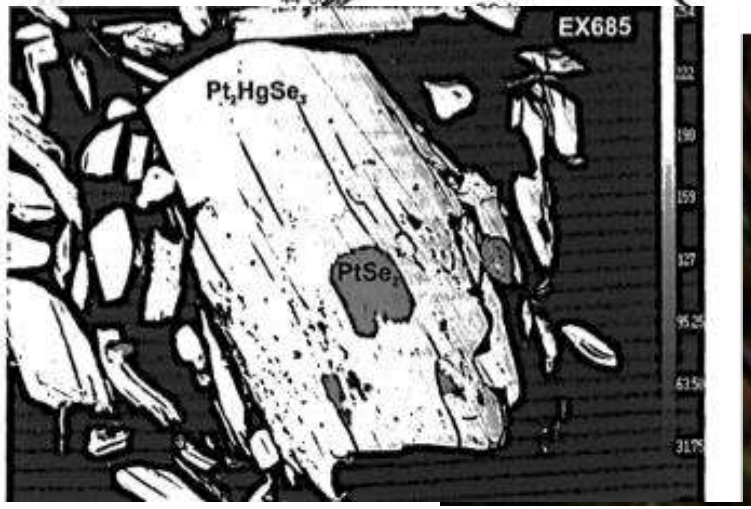




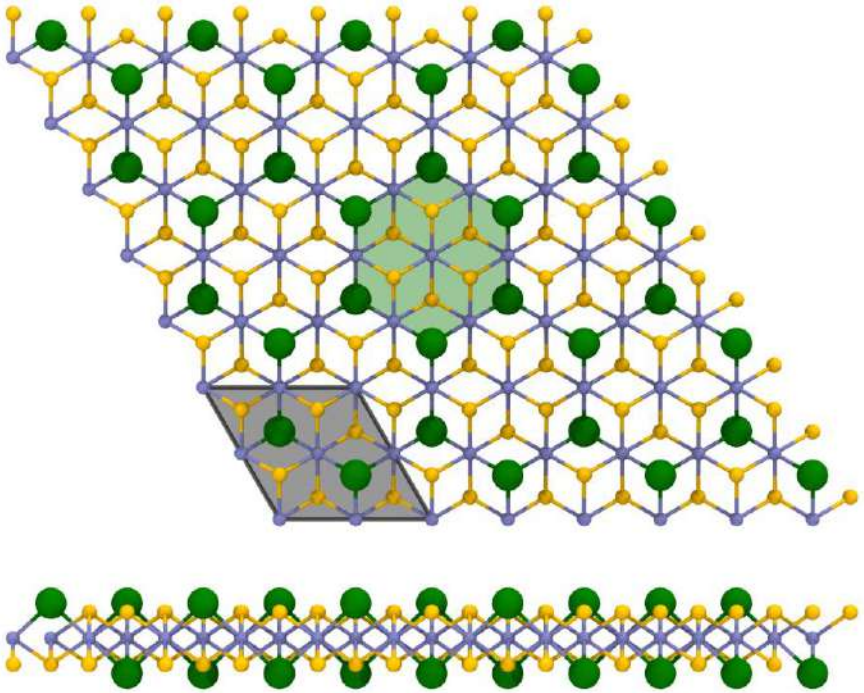
Science Advances (2019), and under review (2021)

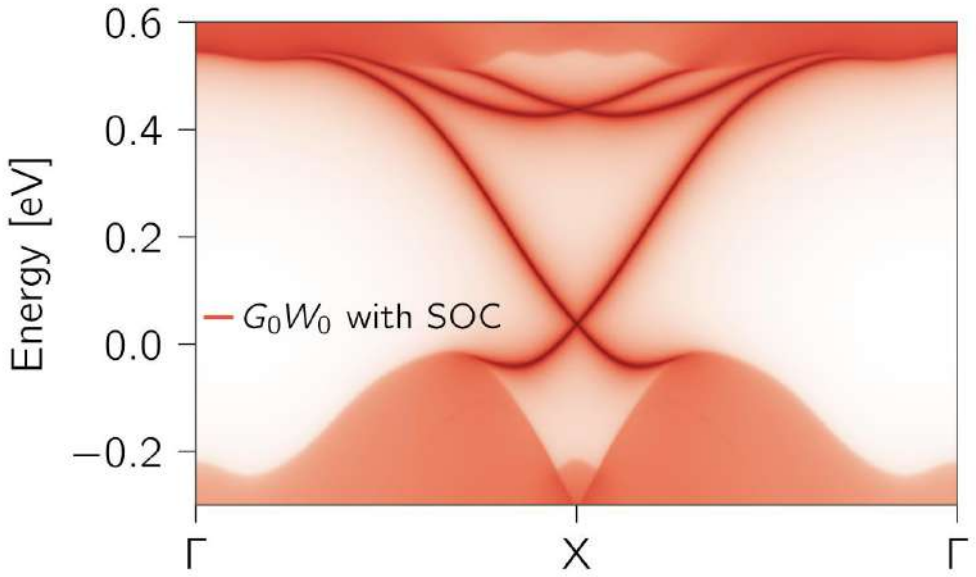
THE DISCOVERY OF JACUTINGAITE





THE DISCOVERY OF JACUTINGAITE

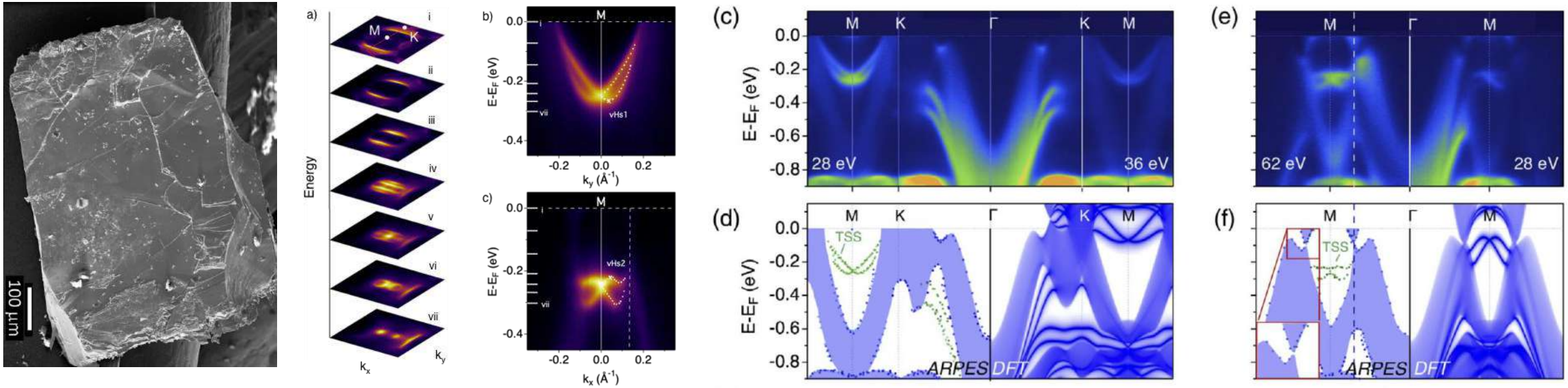




A. Marrazzo *et al.*, Phys. Rev. Lett. 120, 117701 (2018)

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

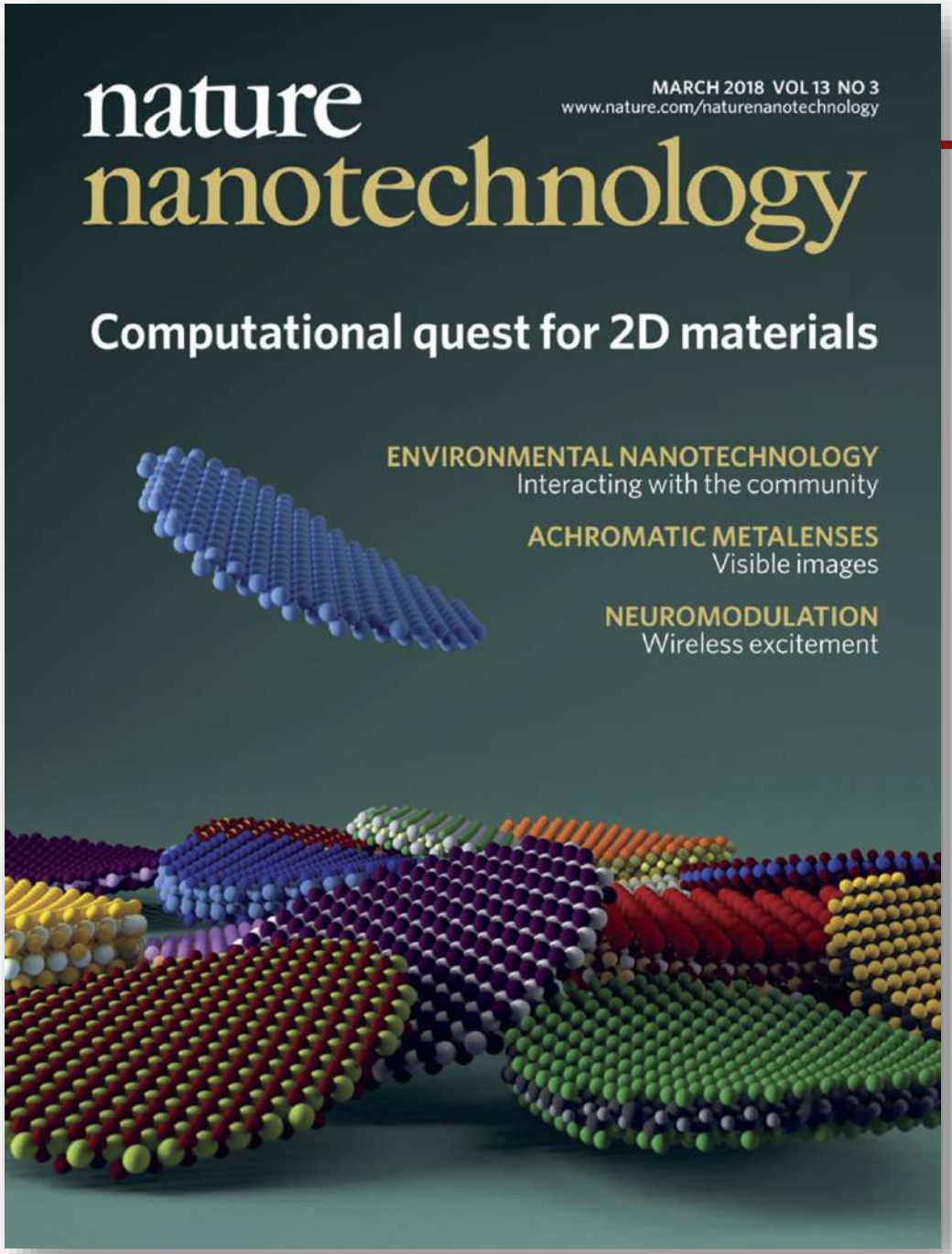
ROOM-TEMPERATURE KANE-MELE QSHI



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

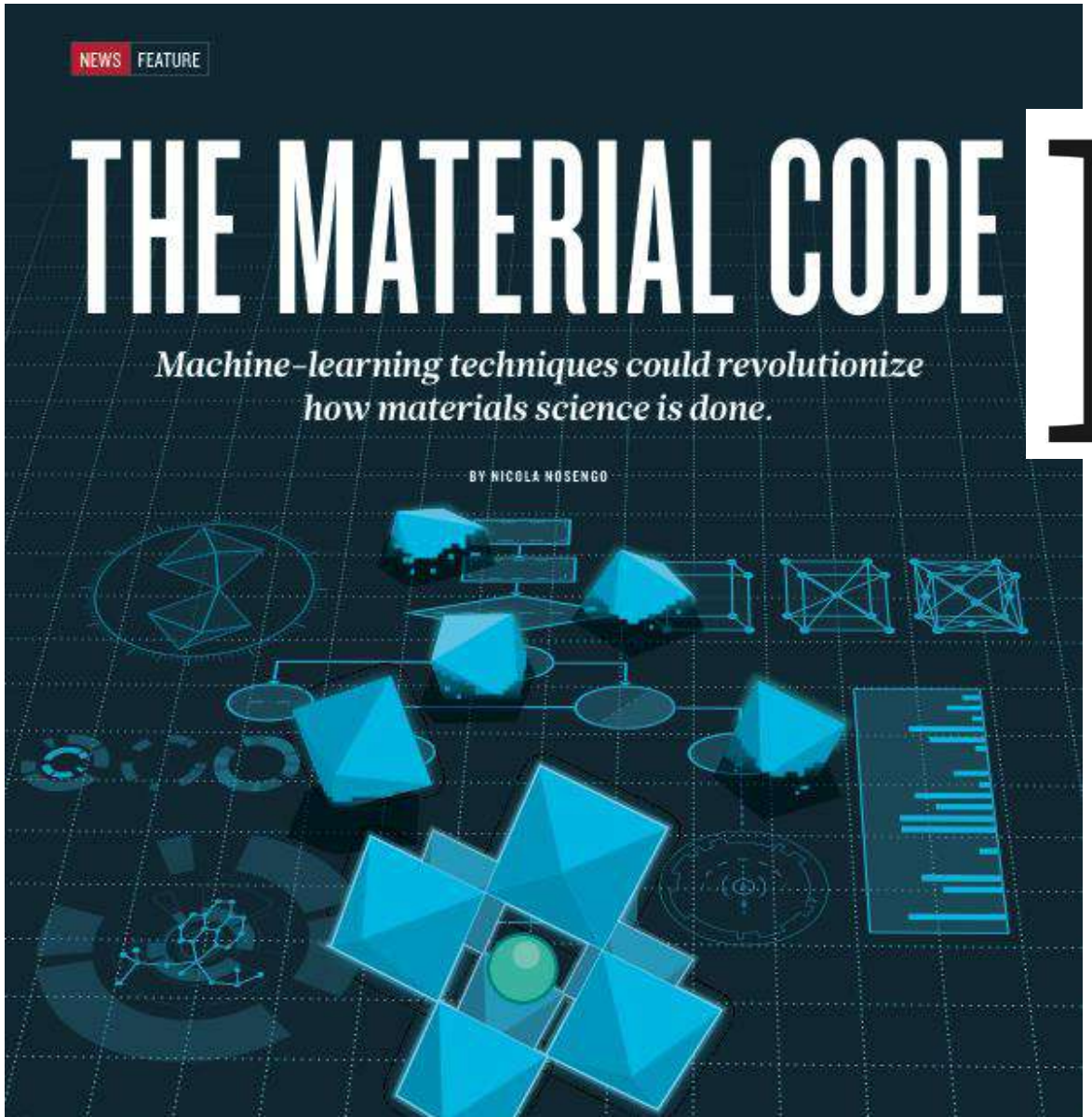
- High electron/hole mobility devices
- Topological insulators, quantum computing
- Ferromagnetic/spintronics in 2D
- Charge-density waves and superconductors
- Plasmonics, transparent conductors

3D layered parents:

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

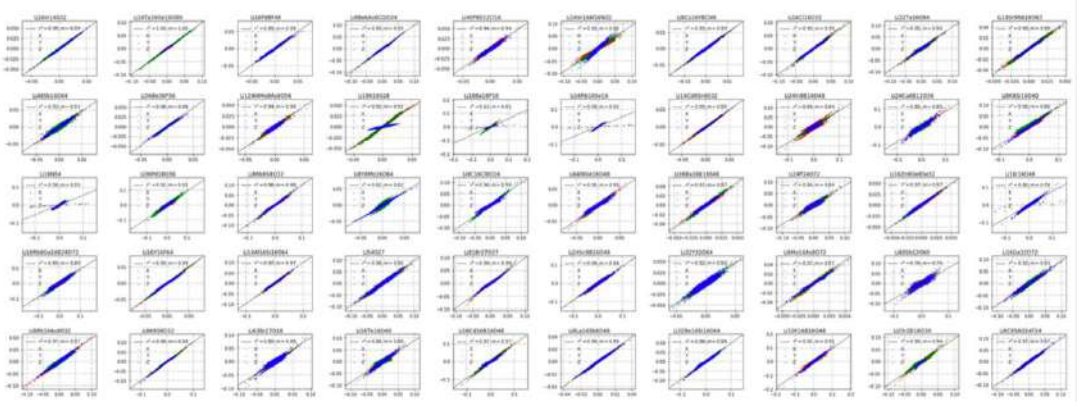
N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi and N. Marzari, Nature Nanotechnology 13, 246 (2018)

MACHINE LEARNING AS THE GREAT ACCELERATOR

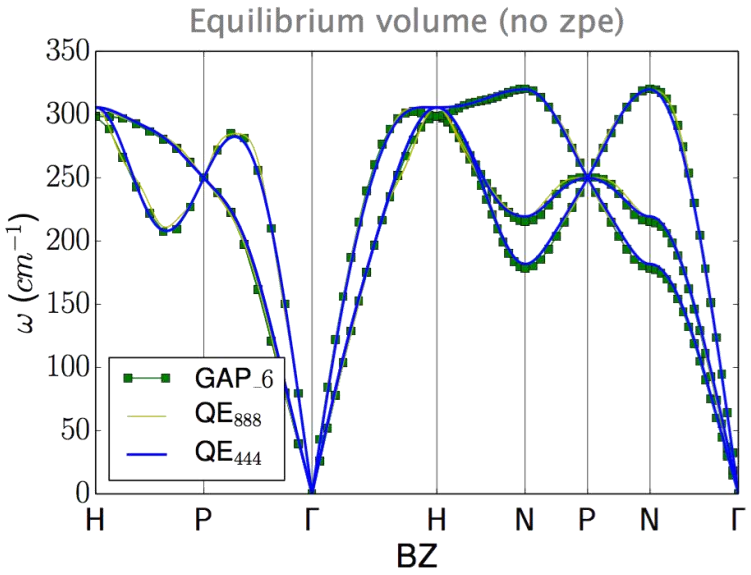


Nature, May 2016

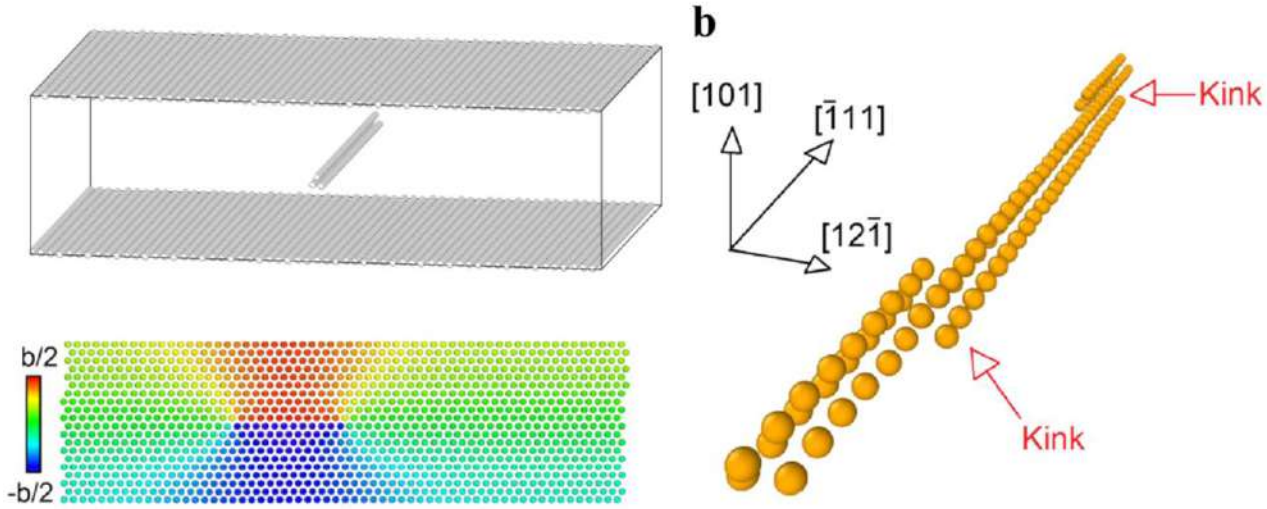
It's a strong contender for the geekiest video ever made: a close-up of a smartphone with line upon line of numbers and symbols scrolling down the screen. But when visitors stop by Nicola Marzari's office, which overlooks Lake Geneva, he can hardly wait to show it off. "It's from 2010," he says, "and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



MACHINE-LEARNING QUANTUM MECHANICS



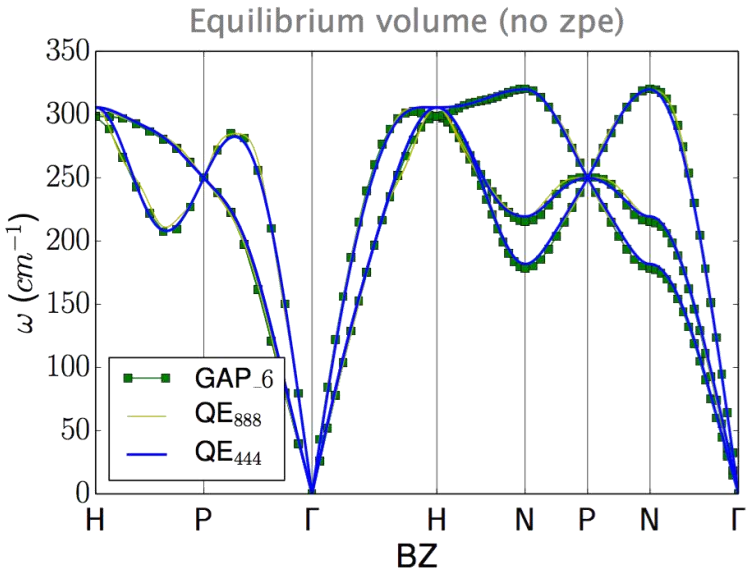
Dislocation glide by kink-pair nucleation and propagation



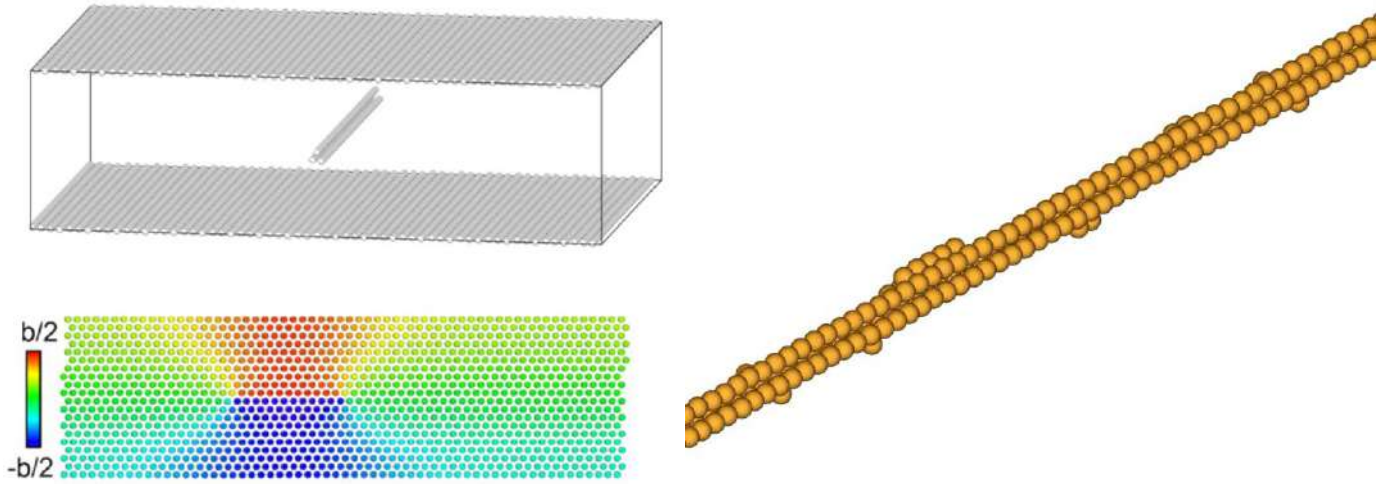
D. Dragoni, T. Duff, G. Csányi, and N. Marzari, Phys. Rev. Materials 2, 013808 (2018)

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

MACHINE-LEARNING QUANTUM MECHANICS



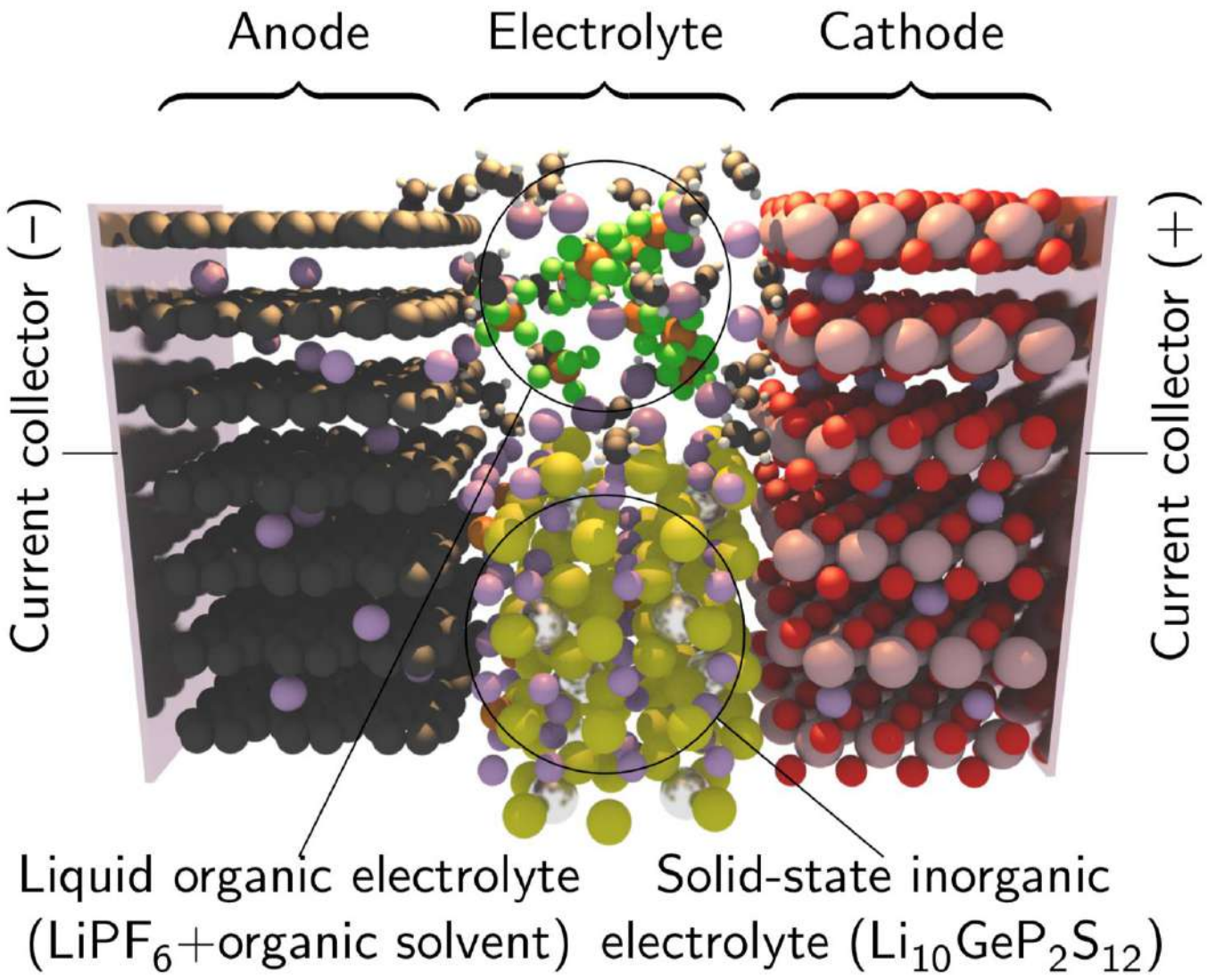
Dislocation glide by kink-pair nucleation and propagation



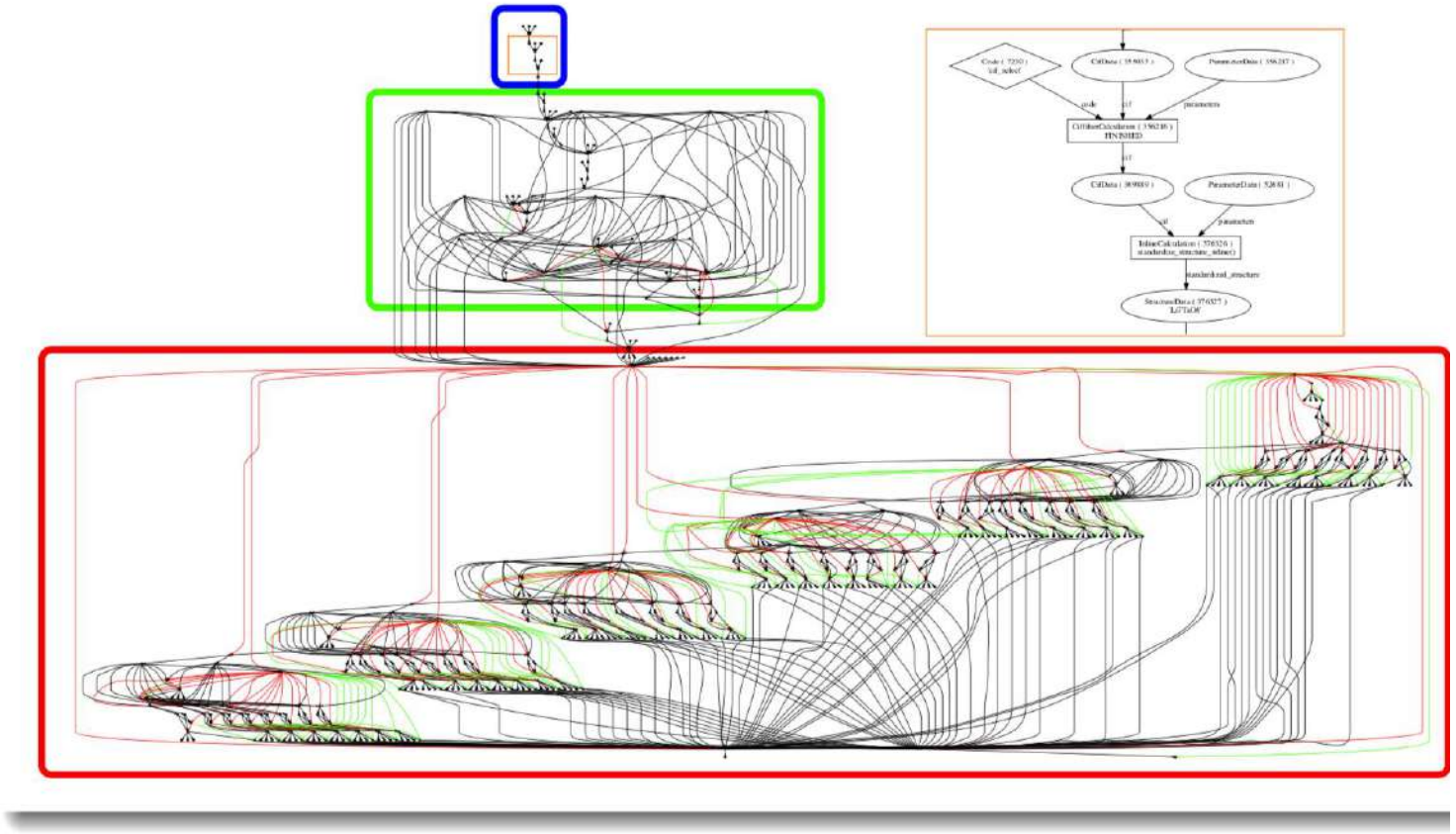
D. Dragoni, T. Duff, G. Csányi, and N. Marzari, Phys. Rev. Materials 2, 013808 (2018)

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

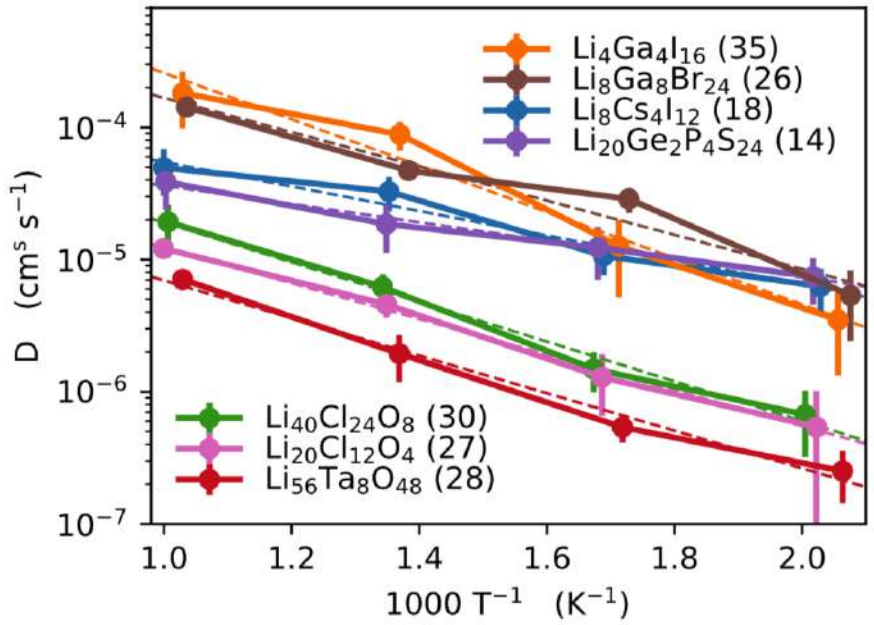
ALL SOLID-STATE BATTERIES



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

MATERIALS CLOUD

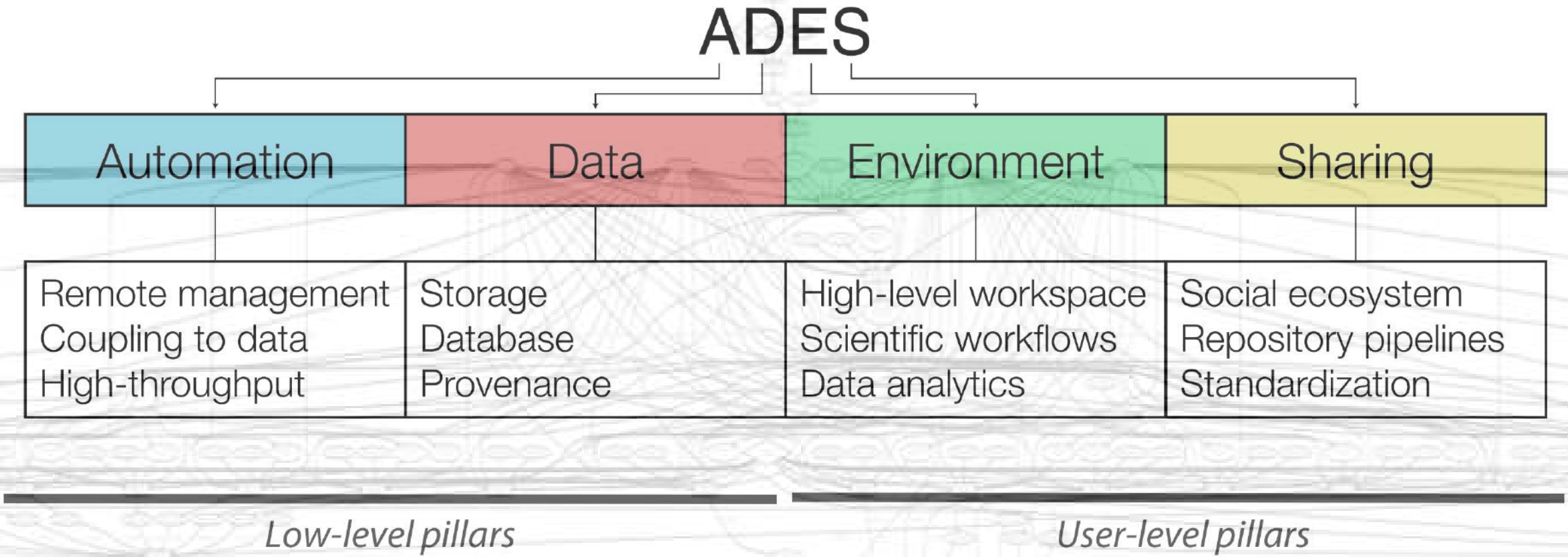
Automation **Data** **Environment** **Sharing**

AiiDA

http://www.aiida.net

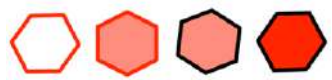
S.P. Huber *et al.*, Nature Scientific Data (2020)

ADES MODEL FOR COMPUTATIONAL SCIENCE

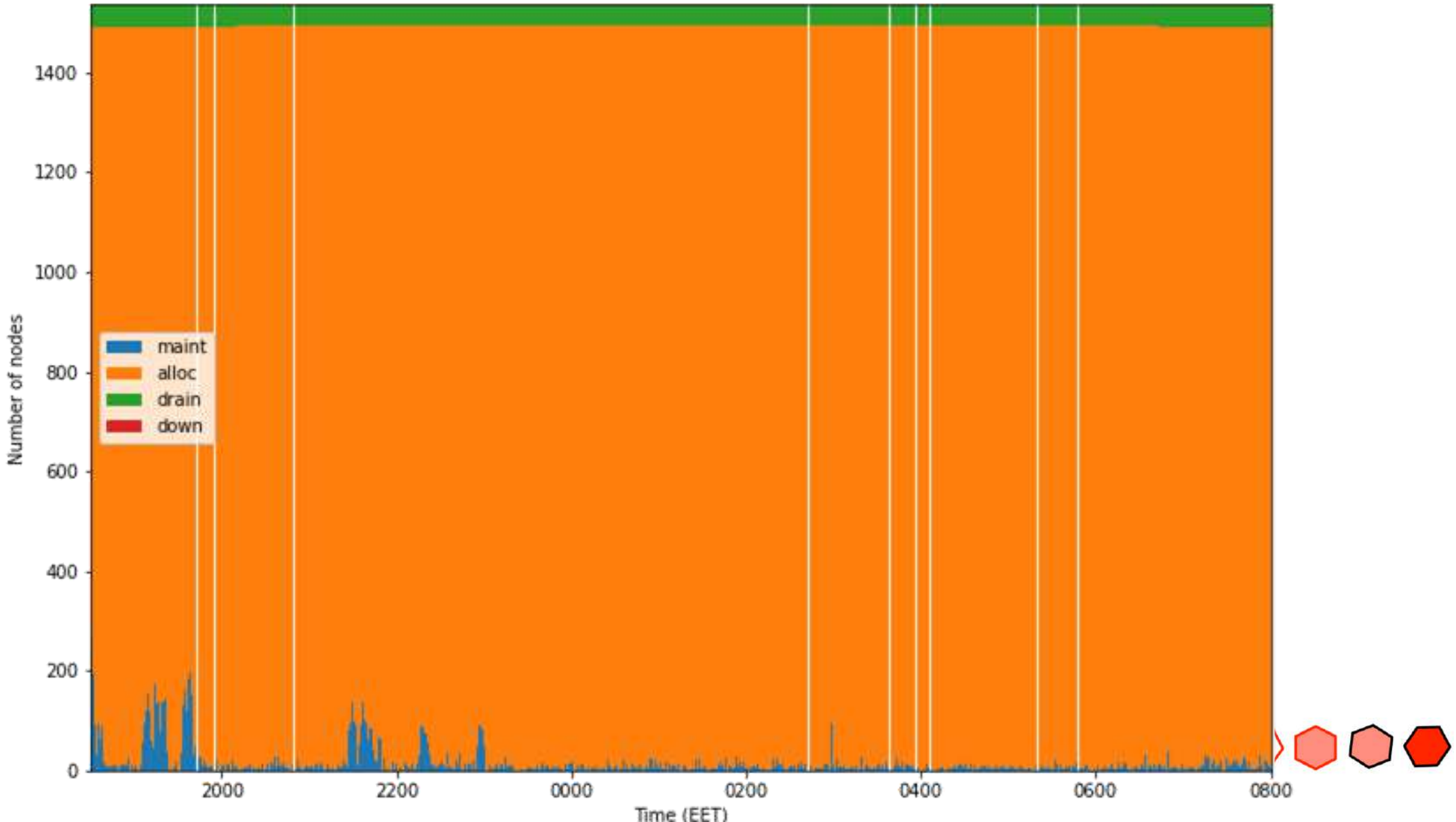


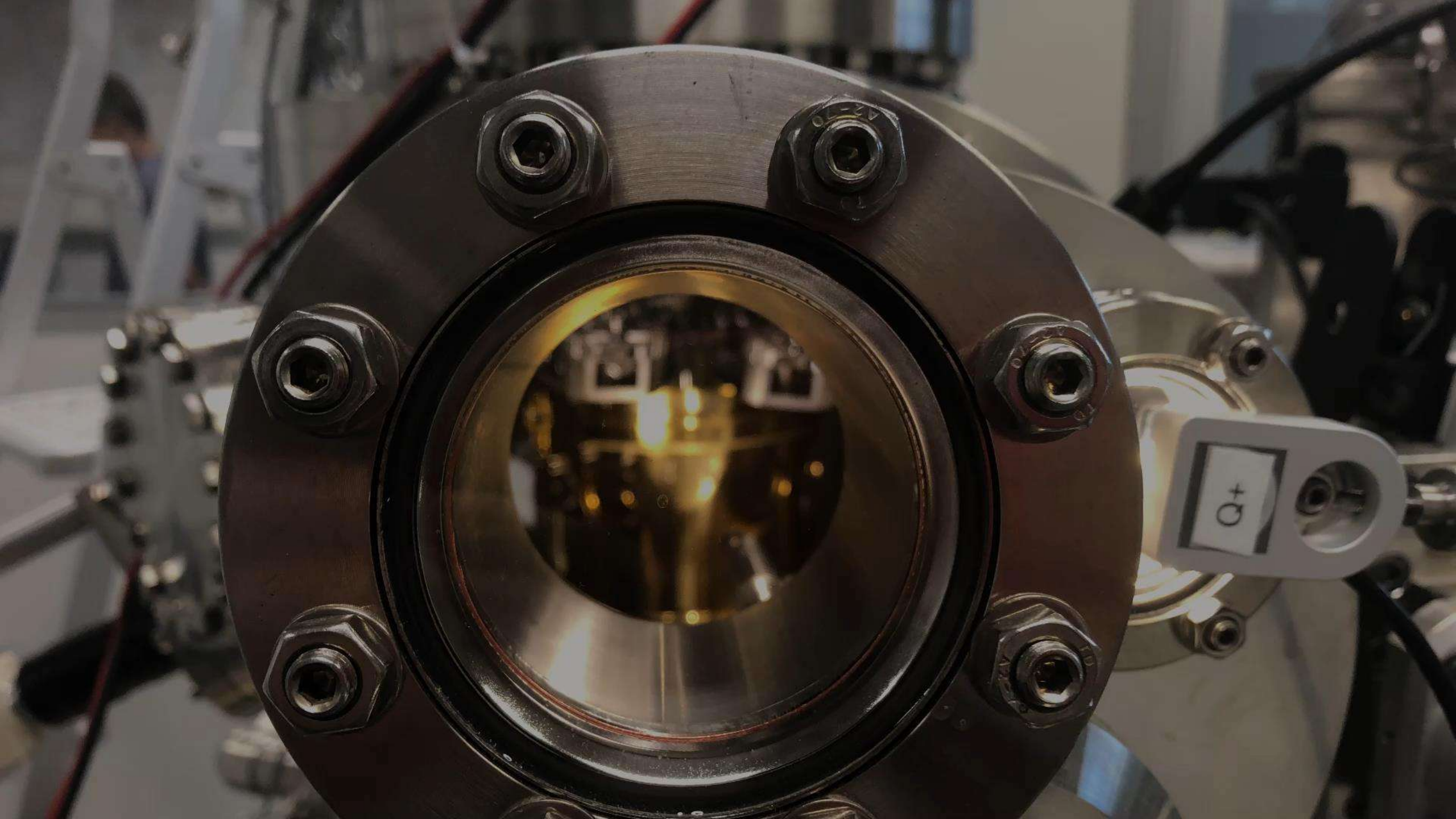
S.P. Huber *et al.*, Nature Scientific Data (2020)

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

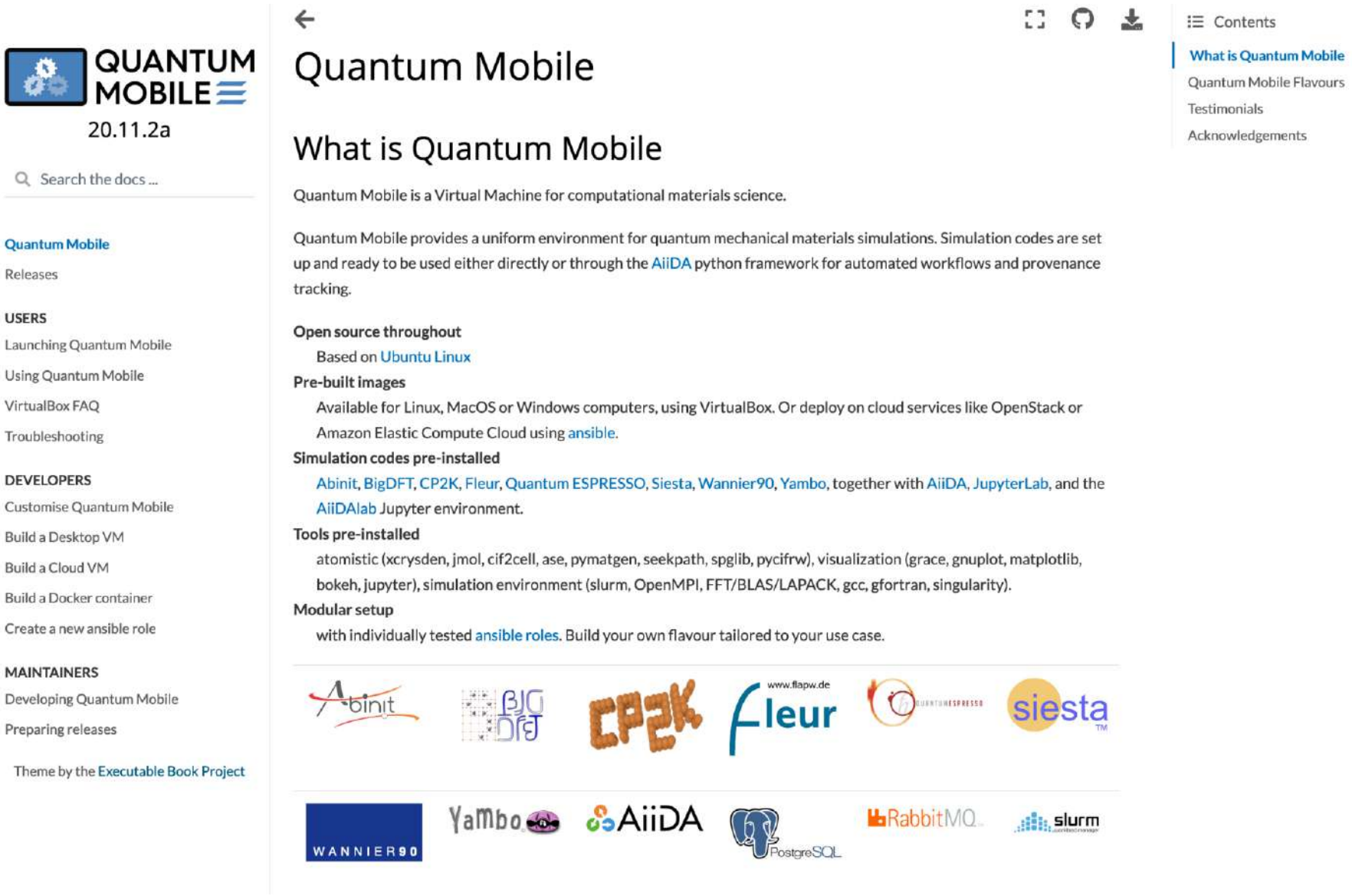


LUMI-C HERO RUN





READY TO GO IN THE QUANTUM MOBILE



COMMON WORKFLOWS

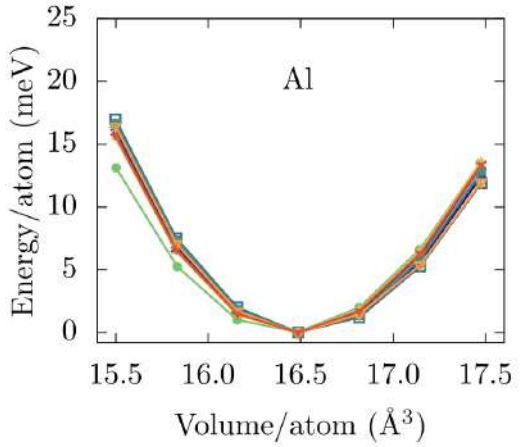
ARTICLE OPEN

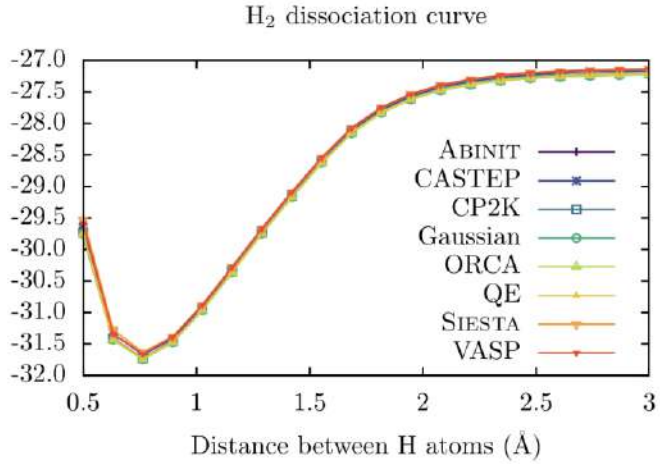
Check for updates

Common workflows for computing material properties using different quantum engines

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

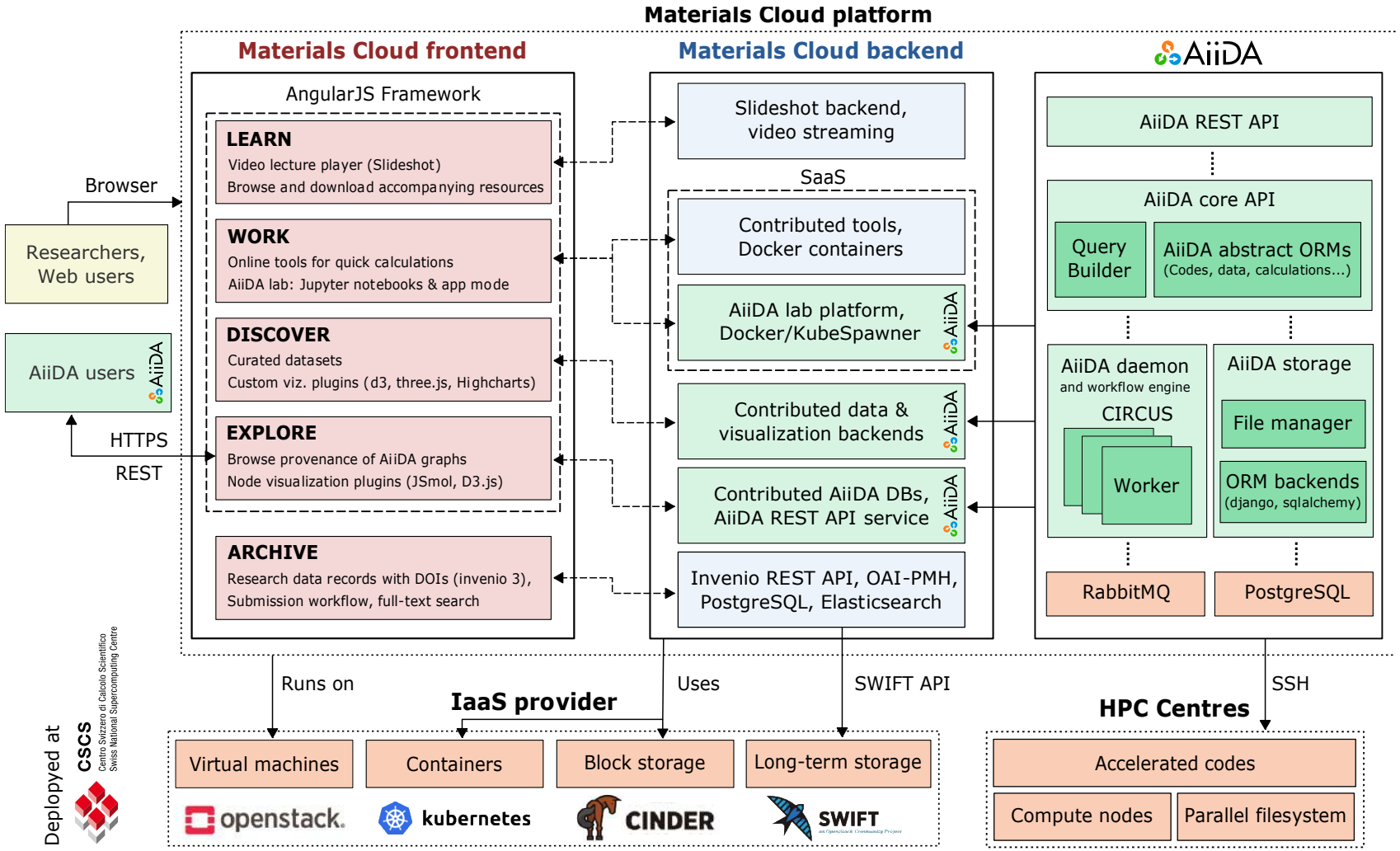
```
$ aiida-common-workflows launch eos siesta --structure=Al --protocol=precise
```





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

MATERIALS CLOUD



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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

Discover curated data sets

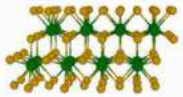
Add DISCOVER section

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

Standard solid-state pseudopotentials (SSSP)

DOI 10.24435/materialscloud:2018.0001/v3

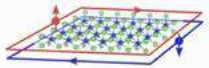
Authors: Gianluca Prandini, Antimo Marrazzo, Ivano E. Castelli, Nicolas Mounet & Nicola Marzari
Description: A Standard Solid State Pseudopotentials (SSSP) library optimized for precision and efficiency.



2D structures and layered materials

DOI 10.24435/materialscloud:2017.0008/v2

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



2D topological insulators

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

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, Ella 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

Nicola 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

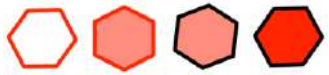
DOI 10.24435/materialscloud:5q-jt

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 ...

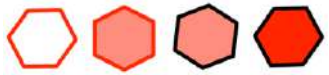
Latest version: v8
Publication date: Feb 24, 2021

LET’S BROADEN THE HORIZON

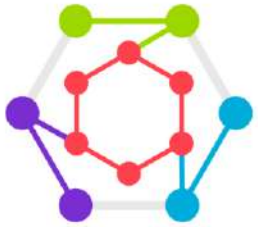


THE BEZOS MANDATE: EXTERNALIZABLE SERVICE INTERFACES

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



OPTIMADE

Open Databases Integration for Materials Design

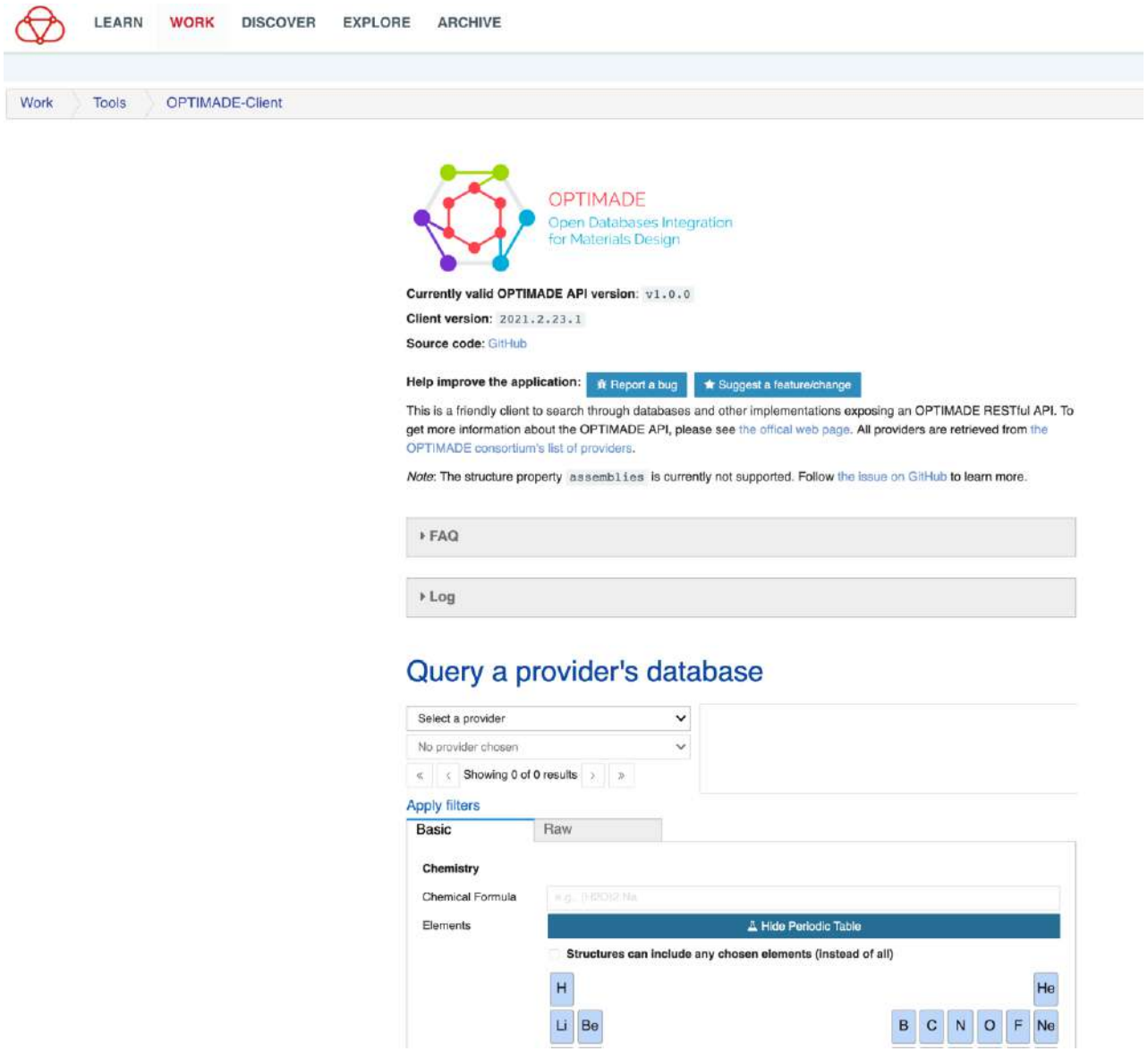
About | Documentation | Specification | Contributors | Wiki | GitHub | Forum

About us

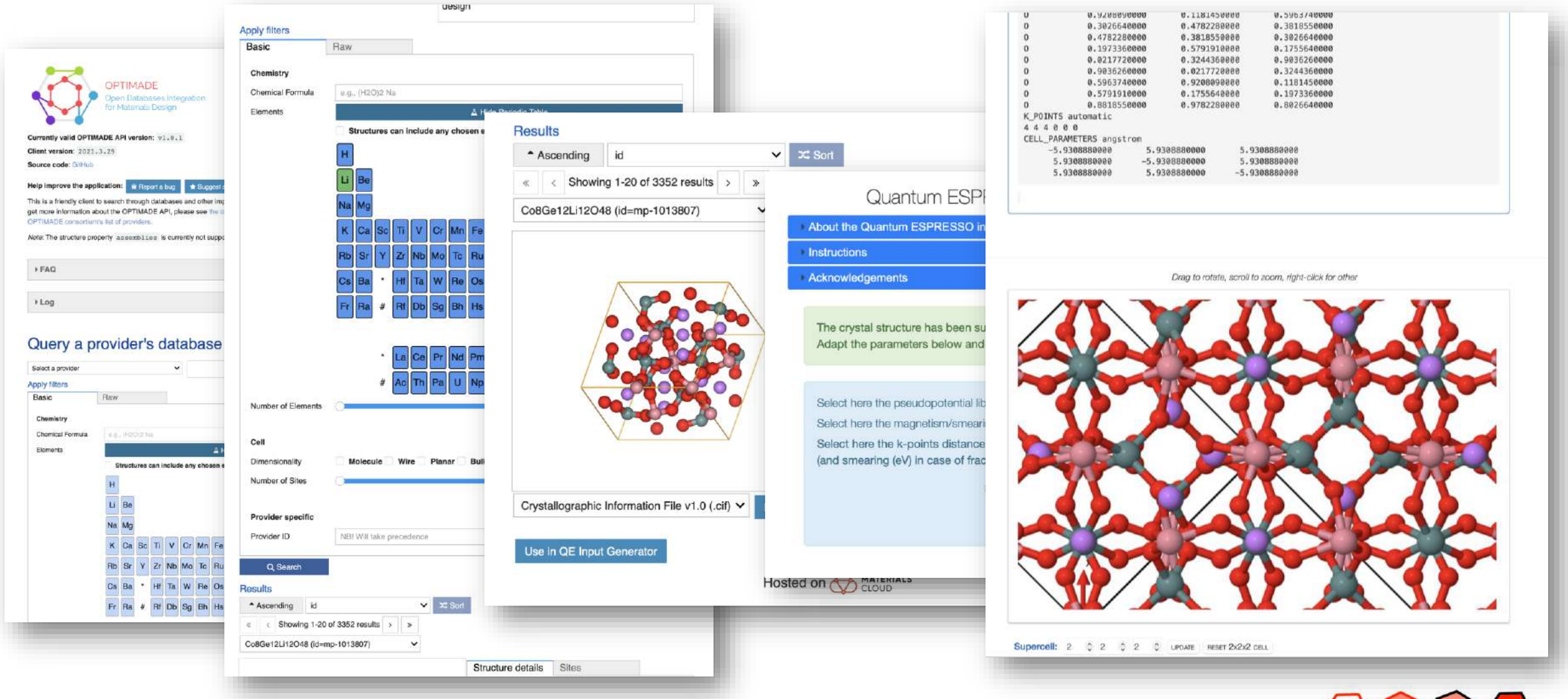
Designing new materials suitable for specific applications is a long, complex, and costly process. Researchers think of new ideas based on intuition and experience. Their synthesis and evaluation require a tremendous amount of trial and error. In the last few years, there has been a major game change 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 (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
- ...

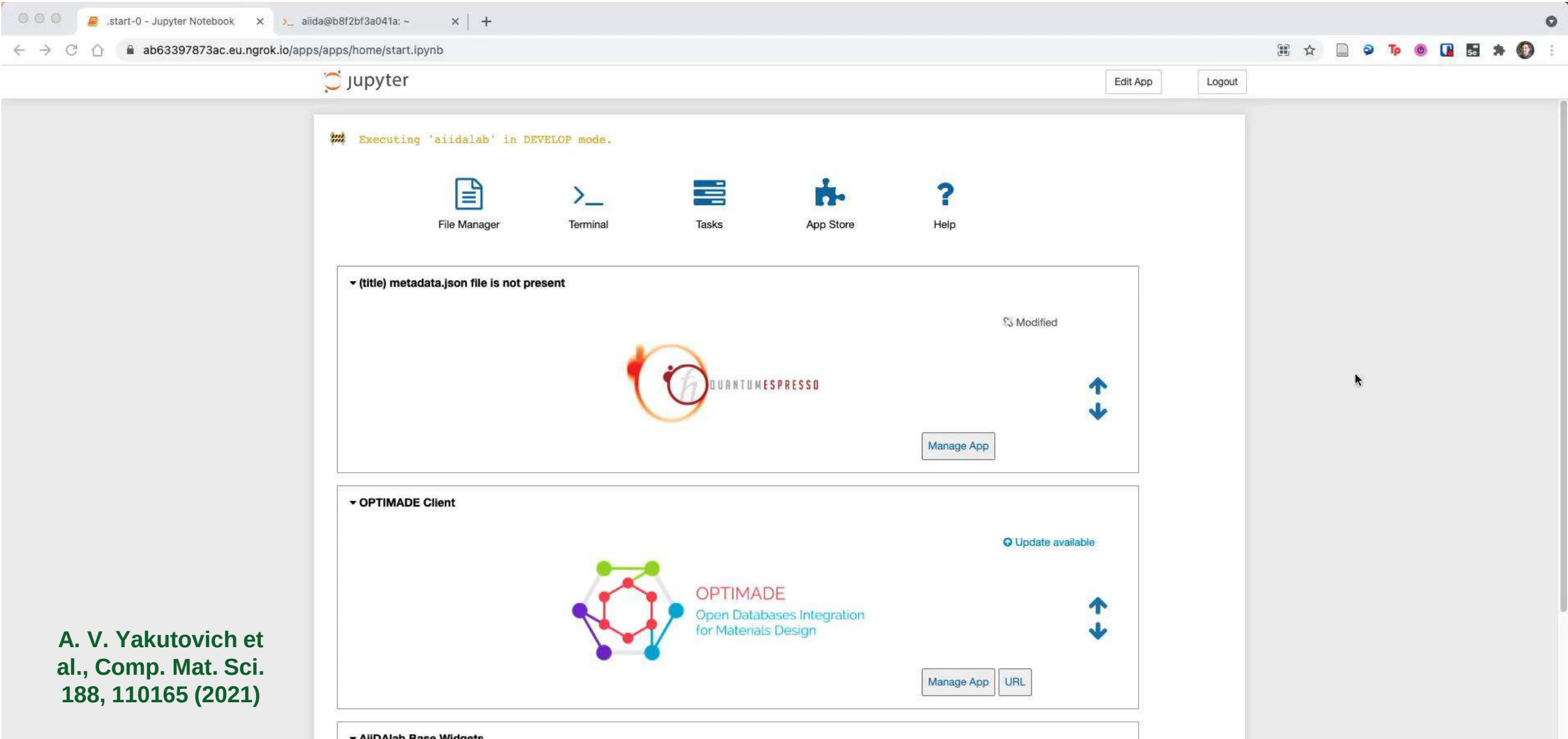
The **Open Databases Integration for Materials Design** (OPTIMADE) consortium aims to make materials databases interoperational by developing a common REST API.



IN ACTION: OPTIMADE UNIVERSAL REST API

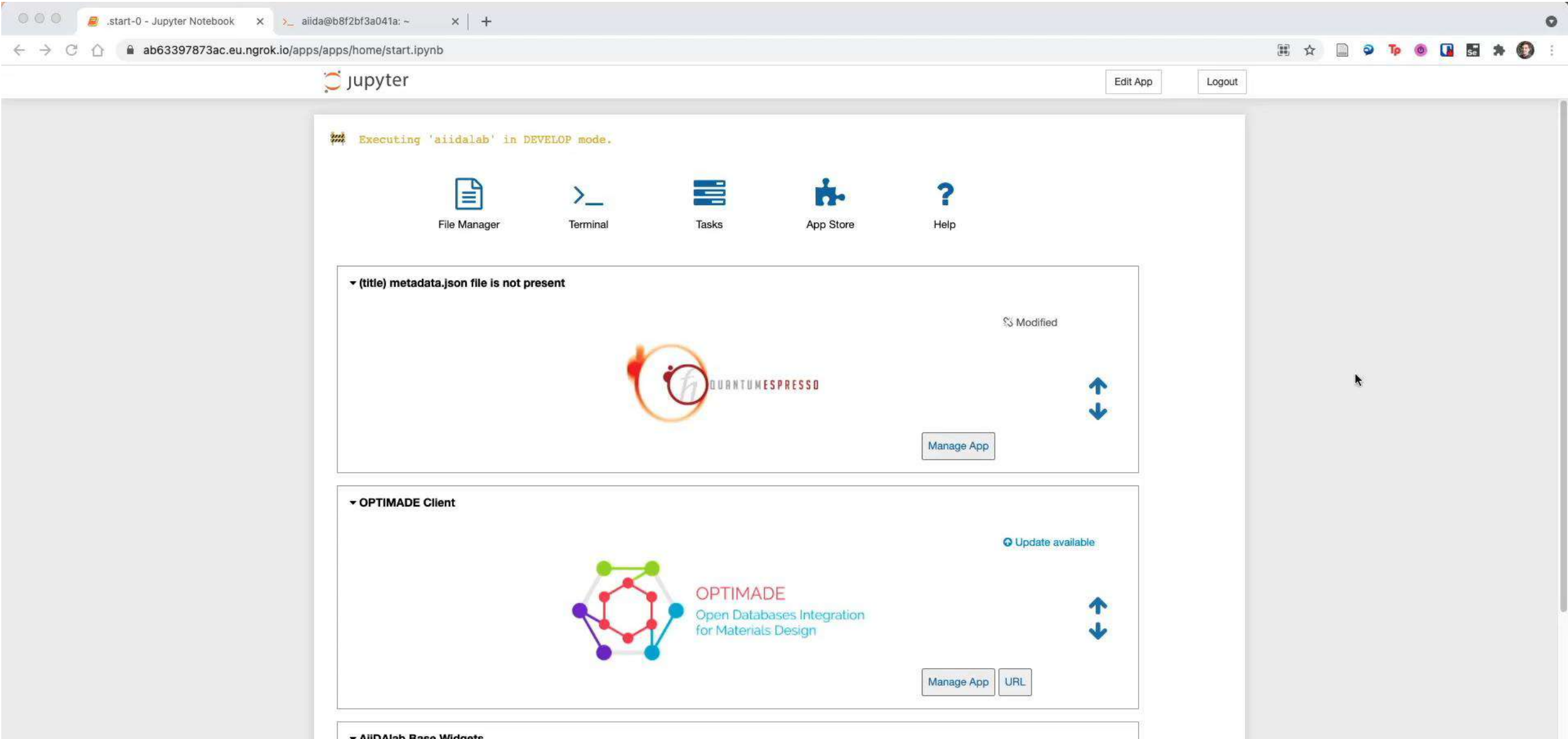


QUANTUM-AS-A-SERVICE – AiiDAlab deployment



A. V. Yakutovich et al., Comp. Mat. Sci. 188, 110165 (2021)

QUANTUM-AS-A-SERVICE – AiiDAlab deployment



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**

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REVIEW ARTICLE | INSIGHT
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nature materials

Electronic-structure methods for materials design

Nicola Marzari[1]✉, Andrea Ferretti[2] and Chris Wolverton[3]

The accuracy and efficiency of electronic-structure methods to understand, predict and design the properties of materials has driven a new paradigm in research. Simulations can greatly accelerate the identification, characterization and optimization of materials, with this acceleration driven by continuous progress in theory, algorithms and hardware, and by adaptation of concepts and tools from computer science. Nevertheless, the capability to identify and characterize materials relies on the predictive accuracy of the underlying physical descriptions, and on the ability to capture the complexity of realistic systems. We provide here an overview of electronic-structure methods, of their application to the prediction of materials properties, and of the different strategies employed towards the broader goals of materials design and discovery.

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http://www.aiida.net
http://www.materialscloud.org

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https://www.big-map.eu

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Related projects:
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H2020 European Materials Modelling Council
H2020 Marketplace
H2020 Intersect
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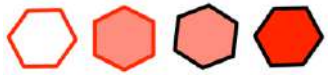

"Things were done very differently on the farm when I was your age, Kenny."