THE SCIENCE

MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

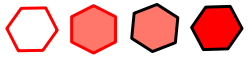
Swiss National Science Foundation

The Zeroes – taught us – Phosphorous –
We learned to like the Fire
By playing Glaciers – when a Boy –
And Tinder – guessed – by power
Of Opposite – to balance Odd –
If White – a Red – must be!
Paralysis – our Primer – dumb –
Unto Vitality – !

[Emily Dickinson, Poem 689]

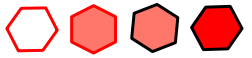
MARVEL VISION – 2011/12

1) **Accelerated design and discovery of materials** displaying novel physics or improved properties via a
2) materials' informatics platform of **database-driven, high-throughput** quantum simulations
3) **predictive accuracy** supported by advanced or innovative electronic-structure capabilities,
4) **verified and validated** thanks to code interoperability and automated benchmarking
5) **applied to materials** for energy, information-and-communication technologies, and pharmaceuticals.

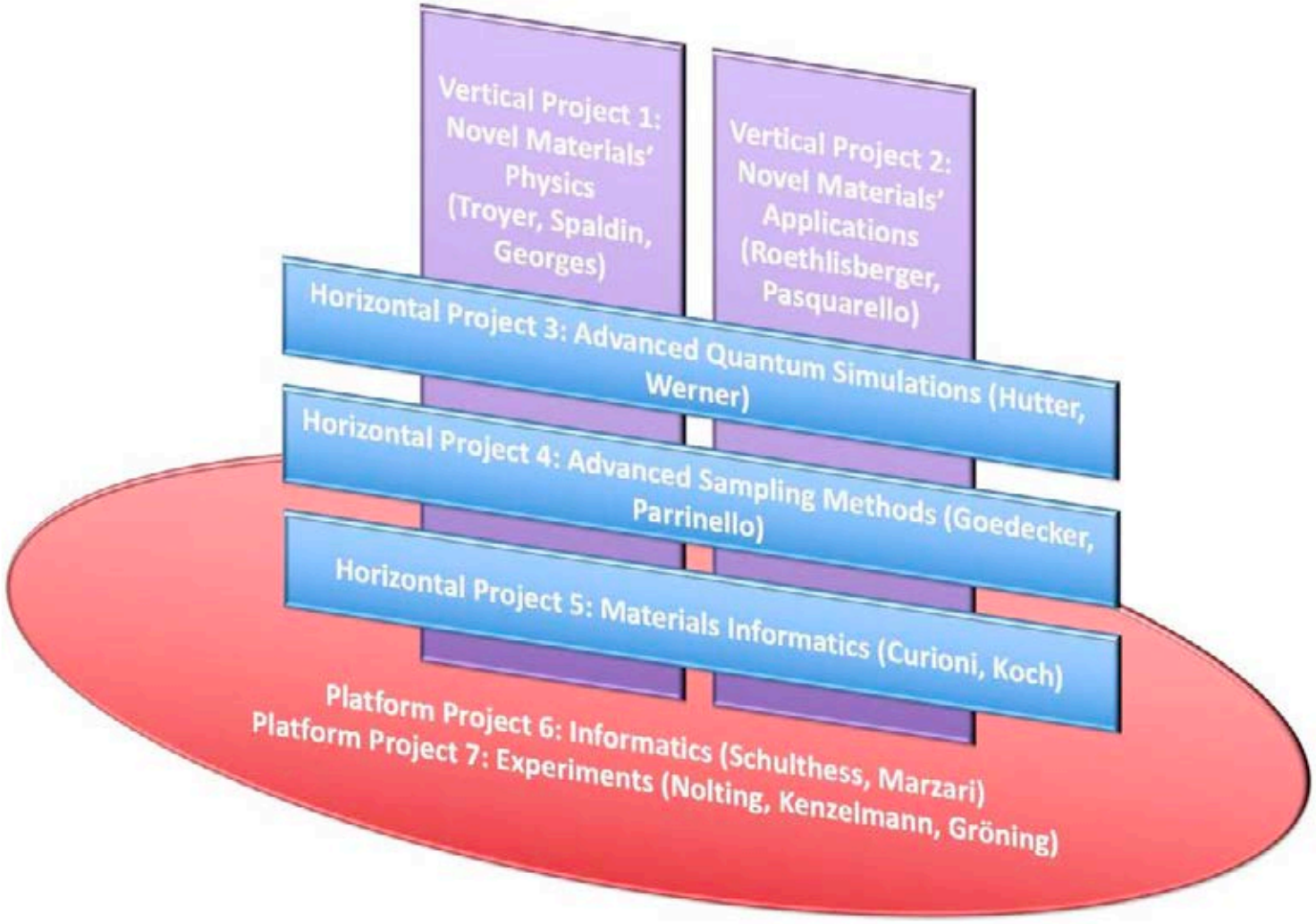


MARVEL VISION – 2011/12

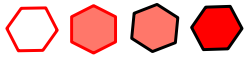
1) **the writers:** a community of **database-driven interoperable quantum engines**
2) **the library:** a **database of materials**, of materials' properties and performance, and of the results of quantum simulations, that starts with the structures of known materials, and that continuously expands
3) **the language:** a **data management system** that allows to store data heterogeneously, in its original and usually most natural format
4) **the librarian:** **the agent** that controls the quantum engines, reads the library, directs the effort to fill the library with the missing pieces, and addresses the grand challenges of the vertical materials design projects



IN THE BEGINNING IS MY END

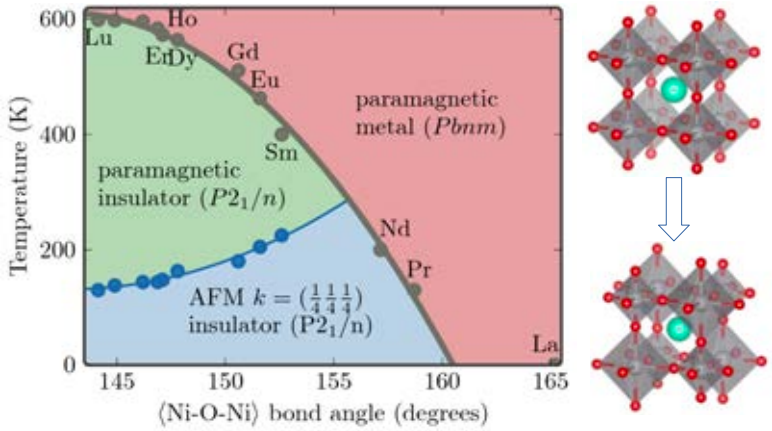


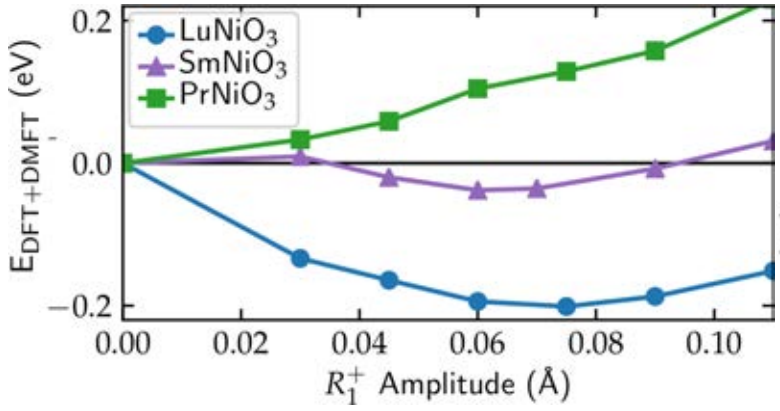
CORRELATED OXIDES

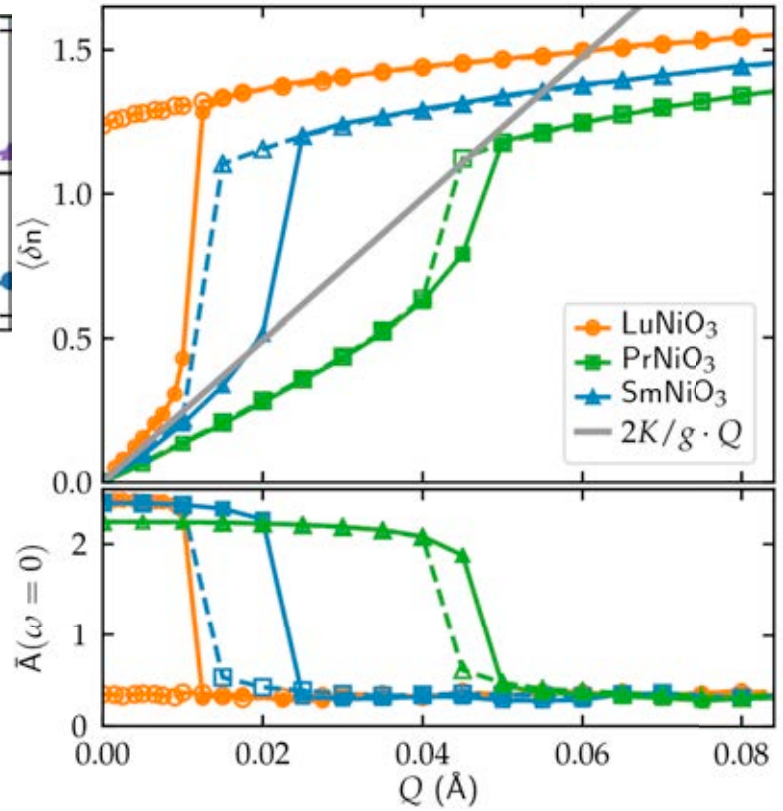


METAL-INSULATOR TRANSITION IN RARE-EARTH NICKELATES

Coupled structural and electronic metal-insulator transition in RNiO$_3$







- Established low-energy physics controlling interplay between structural distortion (Q) and electronic disproportionation (δn)

$$H = H_{\text{kin}} + H_{\text{int}} - \frac{g}{2} Q\delta n + \frac{K}{2} Q^2$$

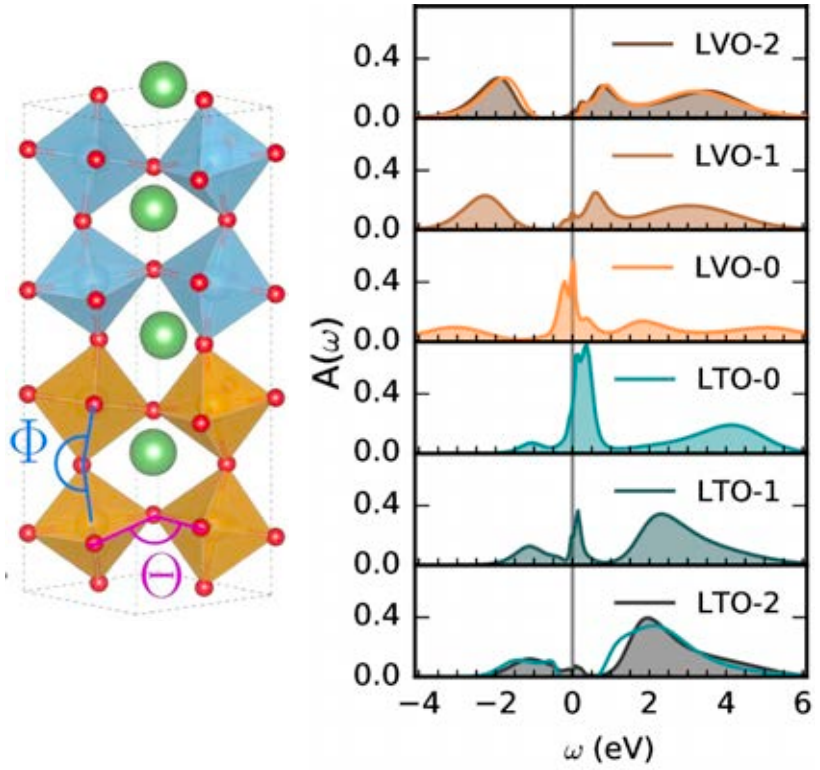
- Quantitative DFT+DMFT description of structural energetics and electronic properties across the whole series.

Subedi et al, PRB 91, 075128 (2015);
Hampel et al., npj Quantum Mater. 4, 5 (2019);
Peil et al., PRB 99, 245127 (2019).

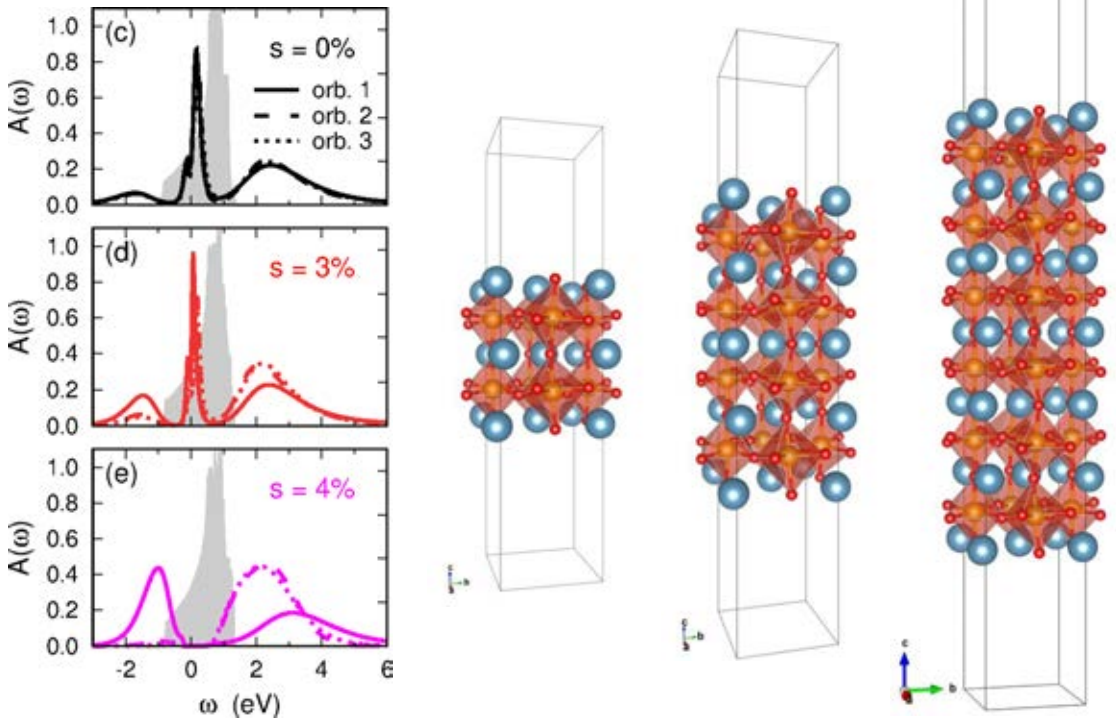
COMPLEX OXIDE HETEROSTRUCTURES

Controlling interfacial metallicity by epitaxial strain, chemistry, dimensional confinement, …

Example 1: Tunable metallic interfacial layer between two Mott insulators ($LaTiO_3/LaVO_3$):

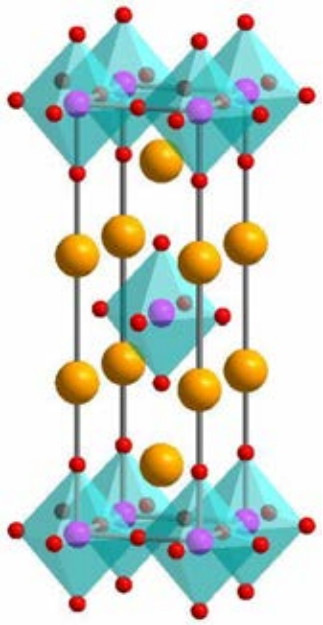


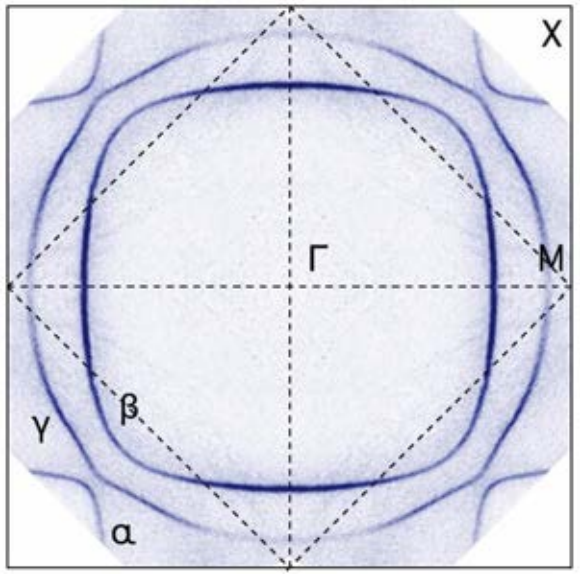
Example 2: Strain- and thickness-dependent metal-insulator transition in $CaVO_3$



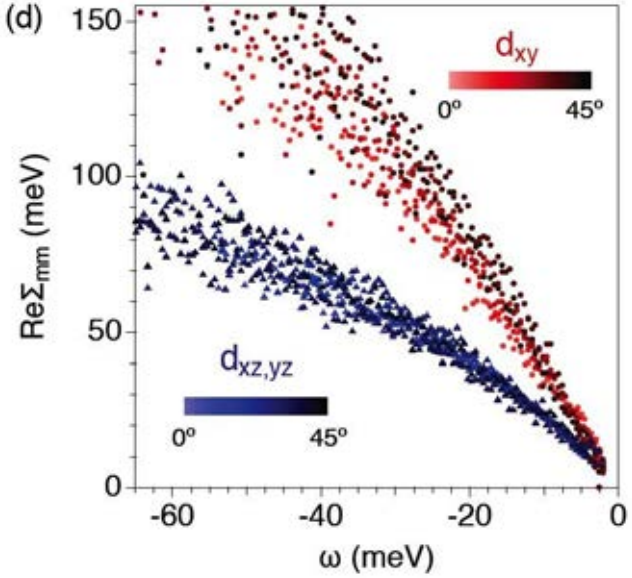
Beck et al., PRB 97, 075107 (2018)
Beck/Ederer, PR Materials 3, 095001 (2019); 4, 125002 (2020); 7, 055003 (2023).

Sr_2RuO_4: JOINT EXPT/TH AND DIRECT VALIDATION OF DMFT

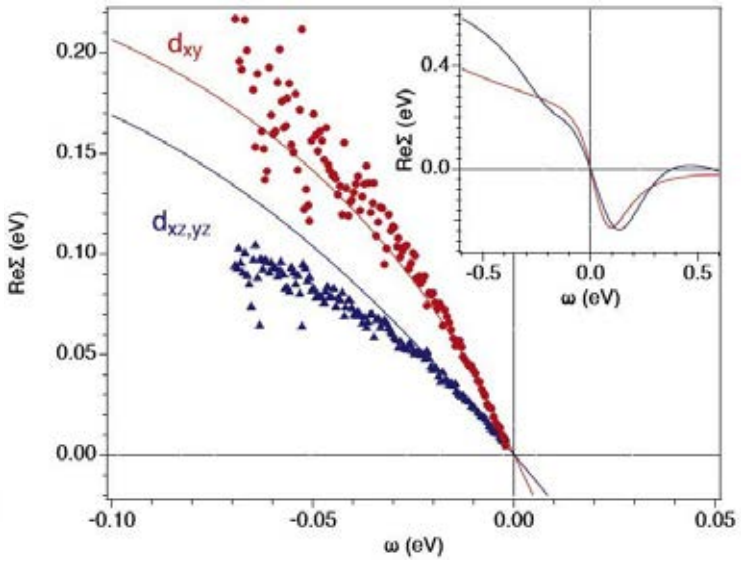




Ultra high resolution Laser-based ARPES



Direct ARPES validation of the DMFT locality assumption



Quantitative agreement between the ARPES determined self-energy and DMFT

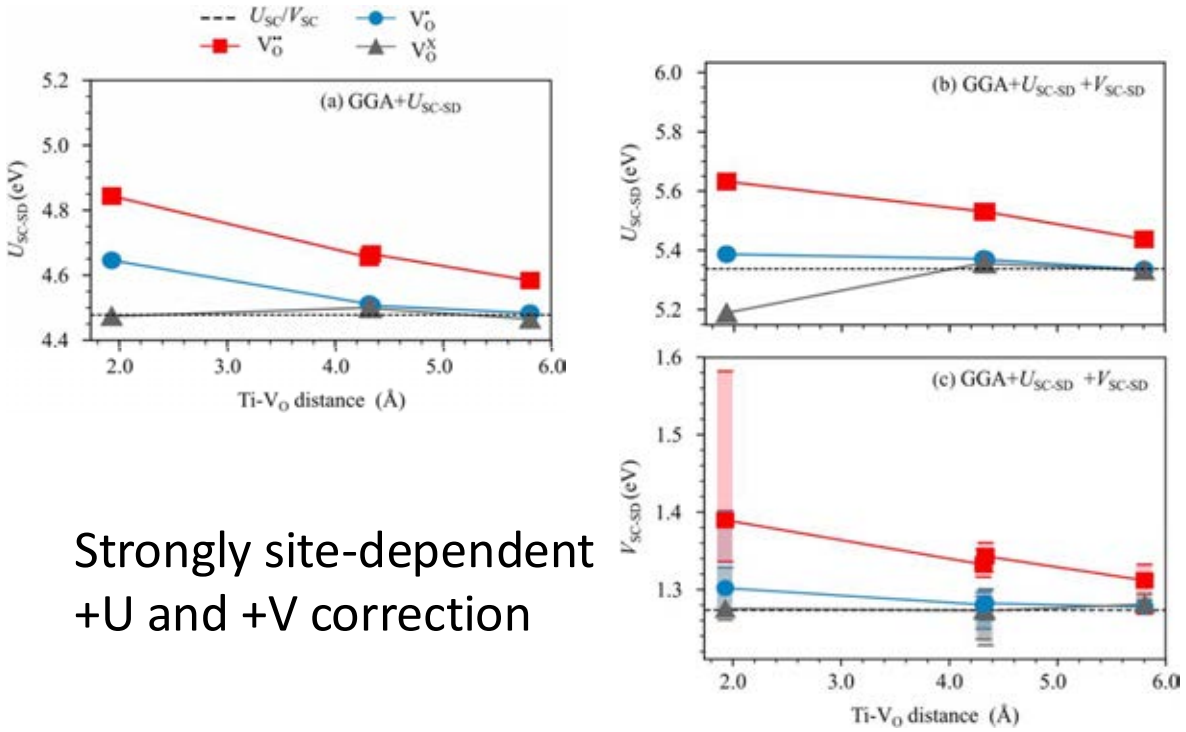
Tamai et al. Phys Rev X 9, 021048 (2019)

Sr_2RuO_4: a "drosophila"for transition-metal oxides with strong electronic correlations!

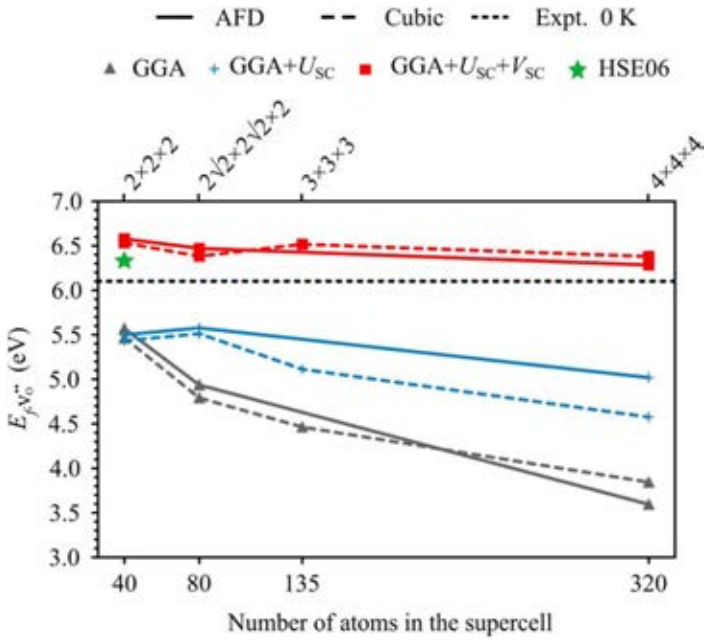
See also: A. Georges and G. Kotliar "The Hund Metal Path to Strong Electronic Correlations" Physics Today, April 2024

DFT+U+V FOR PREDICTIVE DEFECT CALCULATIONS

Oxidation states and geometries affected by defects → site-dependent Hubbard U corrections



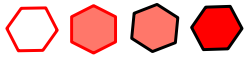
Strongly site-dependent
+U and +V correction



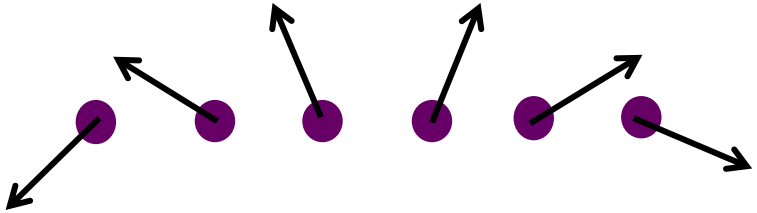
Accurate electronic structure and formation energy

Predictive defect calculations in transition-metal oxides – with semi-local functional cost

MULTIFERROIC DESIGN



MULTIFERROIC MAGNETIC SPIRAL DRIVEN BY Cu/Fe DISORDER



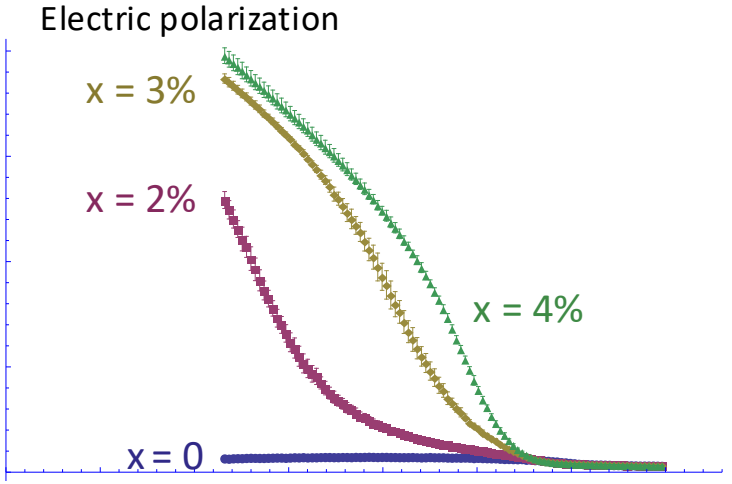
Spin spirals break inversion symmetry and cause electric polarization
Usually caused by spin frustration and so occur at low temperature
We found a new mechanism and stabilized a spin spiral at room temperature

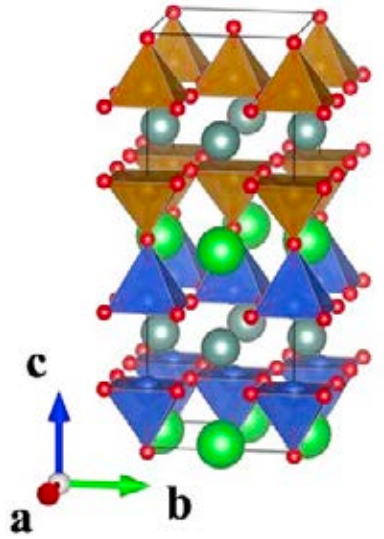
Our high-T spiral magnet multiferroic: $YBaCuFeO_5$

Theoretical predictions from DFT and Monte Carlo simulations:

The spiral is caused by competition between magnetic Cu-Cu, Fe-Fe and Cu-Fe interactions

The temperature of the spiral and hence the polarization will increase with increasing Cu / Fe disorder, x.





EXPERIMENTAL DEMOTRATION OF RT MULTIFERROIC

New magnetoelectric multiferroic has room-temperature properties frozen in

30 December 2016

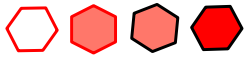
materialstoday
Connecting the materials community

PSI researchers Mickaël Morin and Marisa Medarde freeze-in the atomic arrangement of the multiferroic material YBaCuFeO5. The material is first heated in an oven to 1000°C and then dropped into a vessel filled with liquid nitrogen at a temperature of -200°C. (Photo: Paul Scherrer Institute/Markus Fischer).

M. Morin, … , N. A. Spaldin, … , M. Medarde, *Tuning magnetic spirals beyond room temperature with chemical disorder*, Nature Communications 7, 13758 (2016)

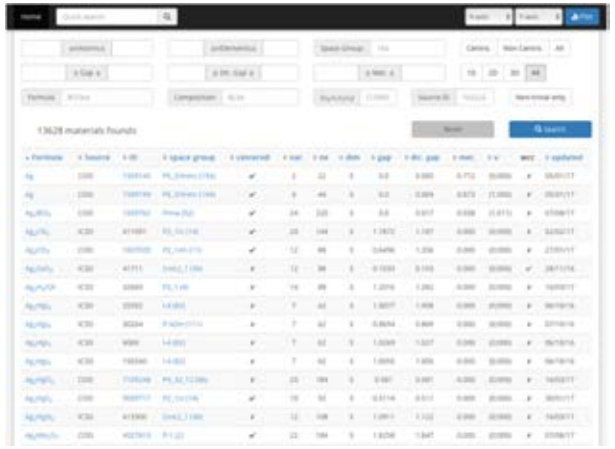
A. Scaramucci, … , M. Troyer, N. Spaldin, *Multiferroic magnetic spirals induced by random magnetic exchanges*, Physical Review X 8, 011005 (2018)

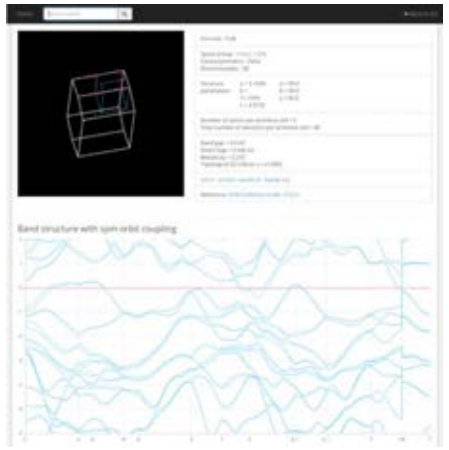
TOPOLOGICAL MATERIALS

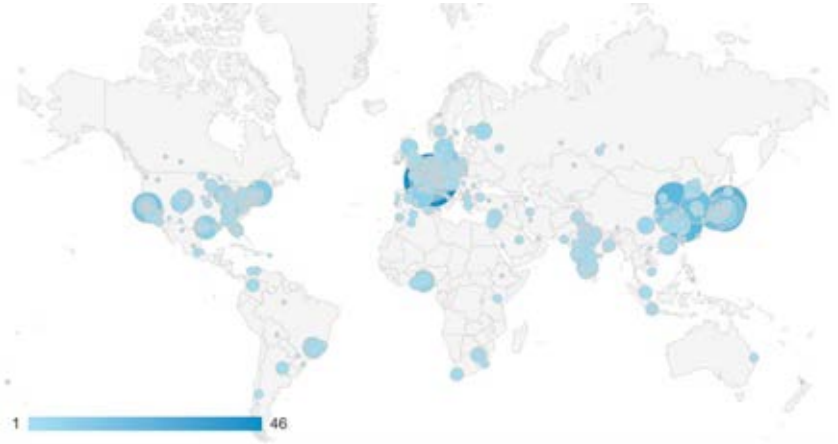


TopoMat: topological materials database

- crystal structures from ICSD and COD databases – total 108423 unique crystal structures
- currently 13628 entries ("pre-screened" materials: <20 atoms per unit cell, even number of electrons, no lanthanides)
- band structures, Z_2 indices, Wannier charge center plots (Z2Pack)
- >4000 materials with nontrivial Z_2 indices
- https://archive.materialscloud.org/record/2019.0019/v2

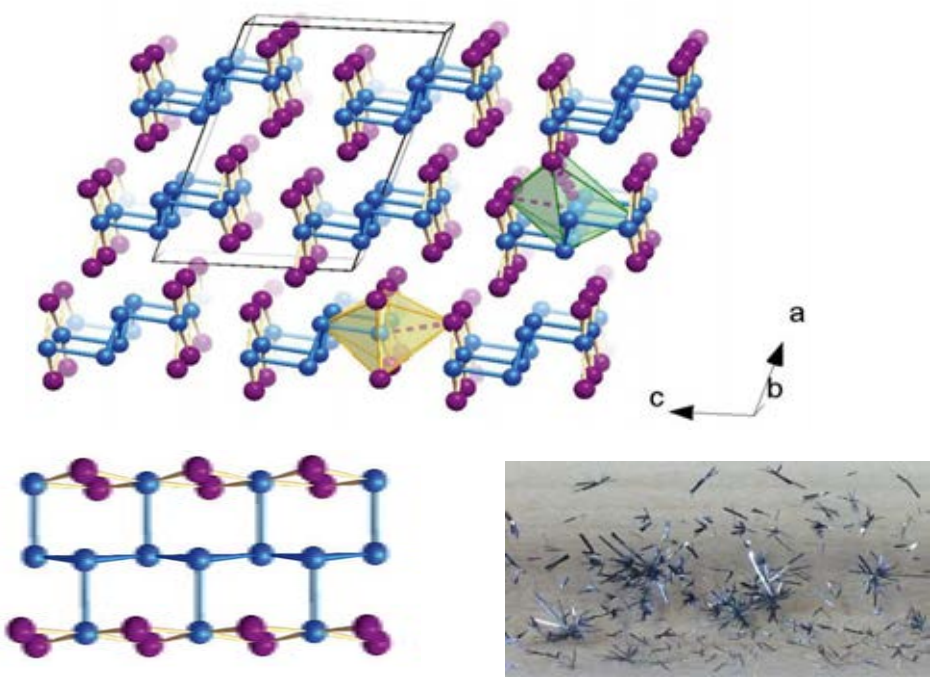






Discovery of a new topological insulator: β-Bi_4I_4

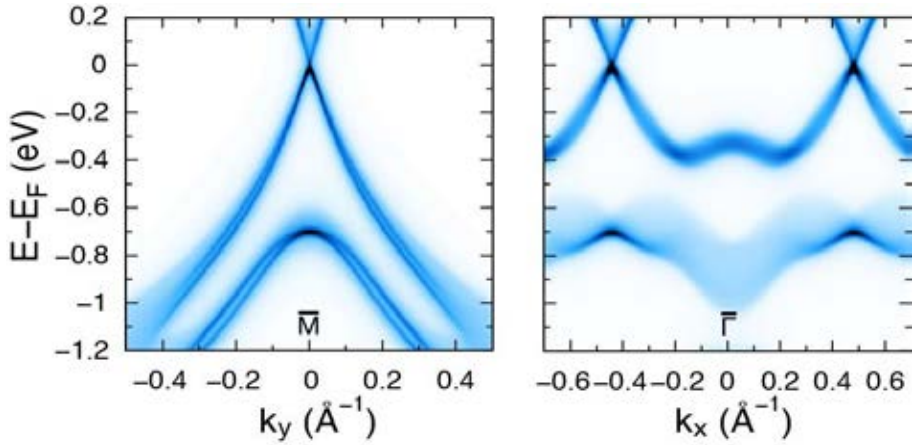
- quasi-1D crystal structure (space group C12/m1)



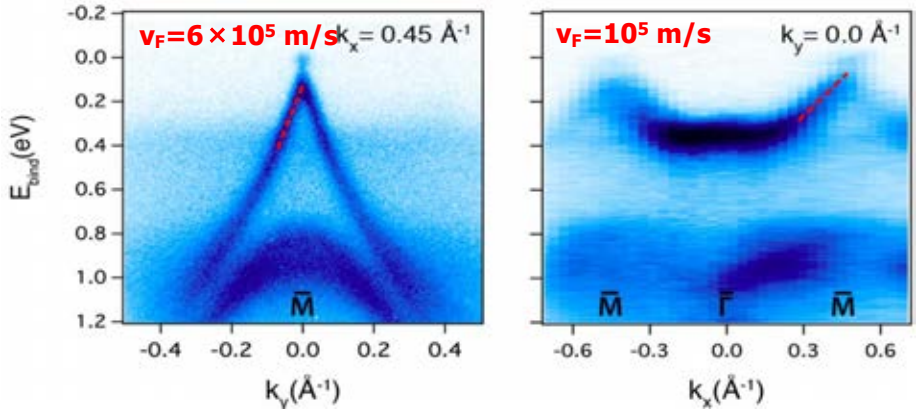
- Predicted and experimentally confirmed as Z_2 topological insulator (1;110)
- Coordinated by MARVEl theorists, with experiments done in Lausanne, Dresden, Berkeley, Moscow and Seoul

G. Autès, … O. V. Yazyev, Nature Materials 15, 154 (2016)

Theory (GW)

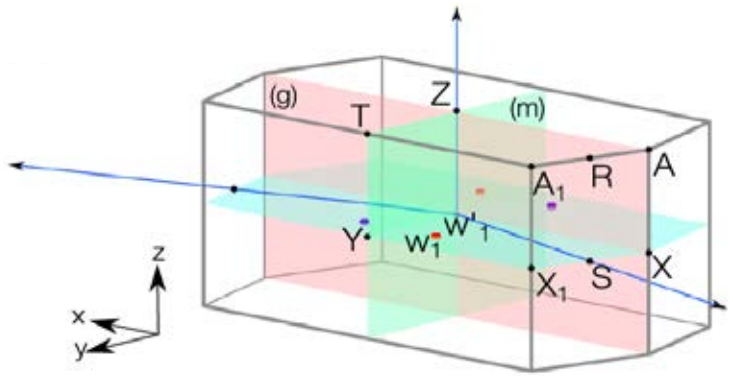


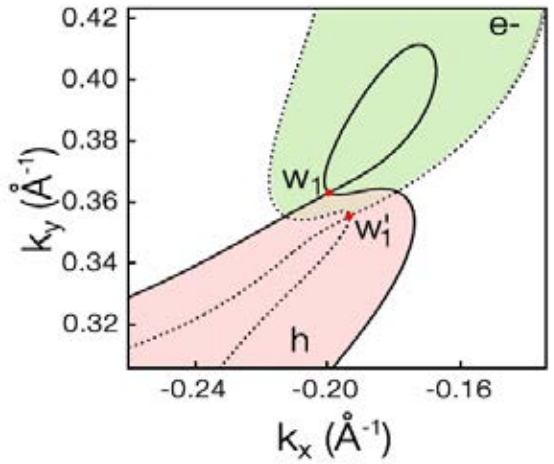
Experiments

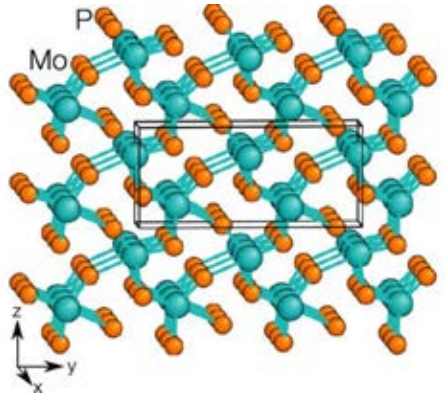


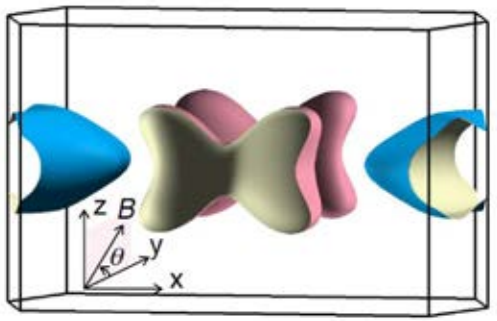
Discovery of new Weyl semimetals MoP_2 and WP_2

- Two isostructural materials MoP_2 and WP_2 first synthesized in the 60s
- Discovered with the help of the TopoMat database
- Realizes a type-II WSM phase
- Uniquely large distance in momentum space between Weyl points of opposite chirality (robust WSM)









G. Autès, D. Gresch, M Troyer, A. Soluyanov, O. V. Yazyev, Phys. Rev. Lett. 117, 066402 (2016)

- Synthesis and confirmation of the topological phase accomplished by other groups

Novel properties of MoP_2 and WP_2

- very high low-T conductivity ($\rho \approx 3$ nΩ cm at 2 K)
- residual resistivity ratios (RRR ≈ 25000) record for binary materials
- highest measured magnetoresistances (2×10^8 % at 63 T and 0.5 K, 4×10^6 % at 9 T and 2 K)
- mean free path of 0.5 mm

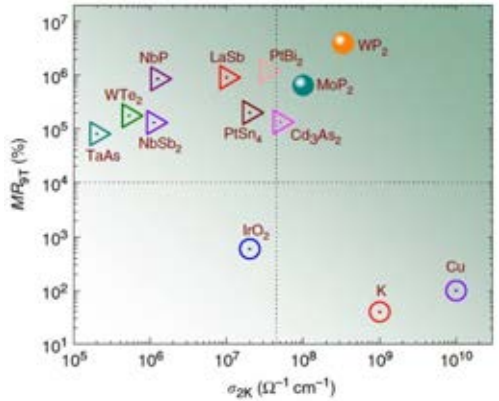
  N. Kumar et al., Nat. Commun. 8, 1642 (2017)

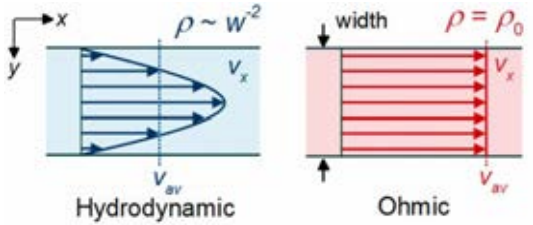
- hydrodynamic electron fluid transport below 20 K

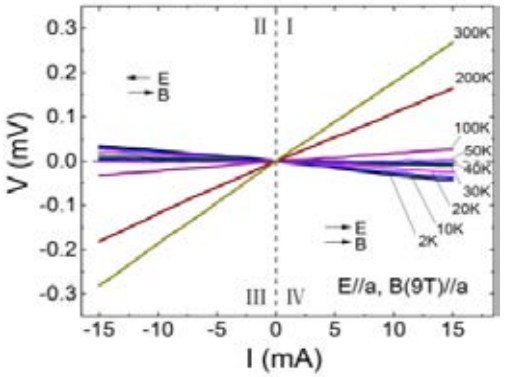
  J. Gooth et al., Nat. Commun. 9, 4093 (2018)

- "negative" resistivity (at low T and for B||E)

  Y.-Y. Lv et al., arXiv:1708.03489

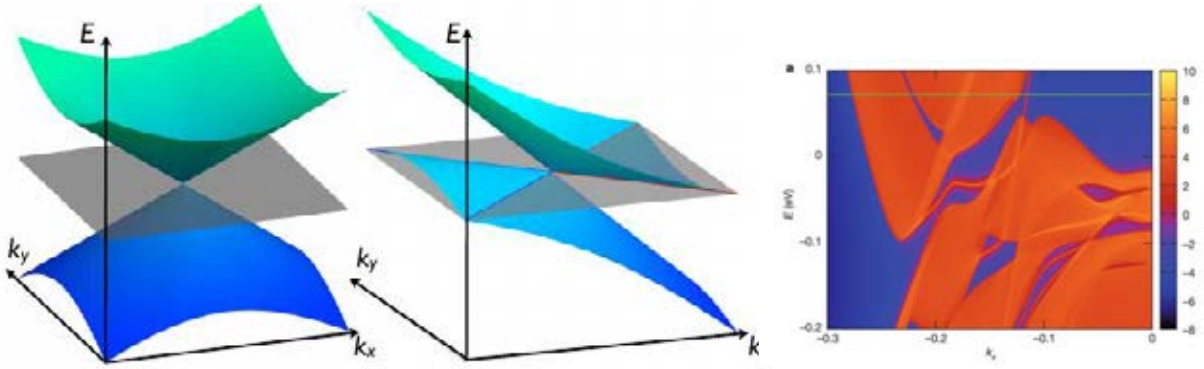






Type-II Weyl semimetal: topology inside a metal

WTe2 connected Weyl physics to electron–hole Fermi pockets



Type I Type II Topological surface states

A Weyl node can live at the touching point
of electron and hole pockets.

1. Lorentz-violating tilt
2. Open finite-density Fermi surface
3. Natural bridge to non-saturated magnetoresponse

Soluyanov, Gresch, Wang, Wu, Troyer, Dai & Bernevig, Nature 527, 495 (2015).

WannierTools: an open-source software for topological materials

Toolkit for topological material

Feature-rich, High Efficiency, Universal Interface

DFT software

VASP WIEN2k

Abinit QE

ABACUS PWMAT

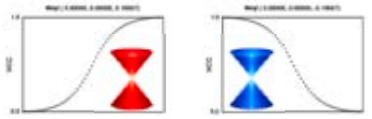
and so on

→ **Standard interface** Wannier90 →

WannierTools

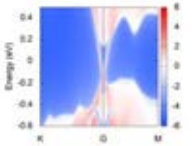
Topological classification

Chern number,
Weyl points, etc.



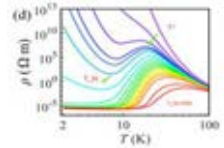
Spectroscopic response

Surface states, QPI etc.



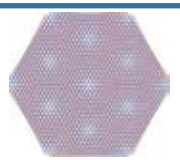
Transport response

Anomalous Hall effect,
magnetotransport.



Large scale

Moire systems, Landau level, etc.

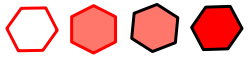


QS Wu, SN Zhang, HF Song, M Troyer, AA Soluyanov Comp. Phys. Comm. 224, 405 (2015)

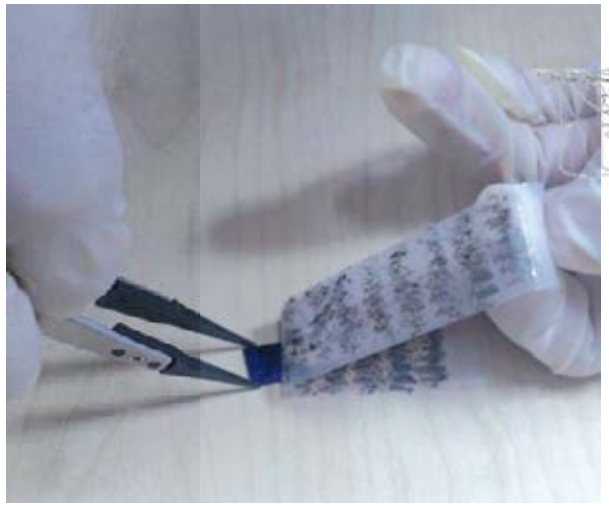
Open source: https://github.com/quanswngwu/wannier_tools

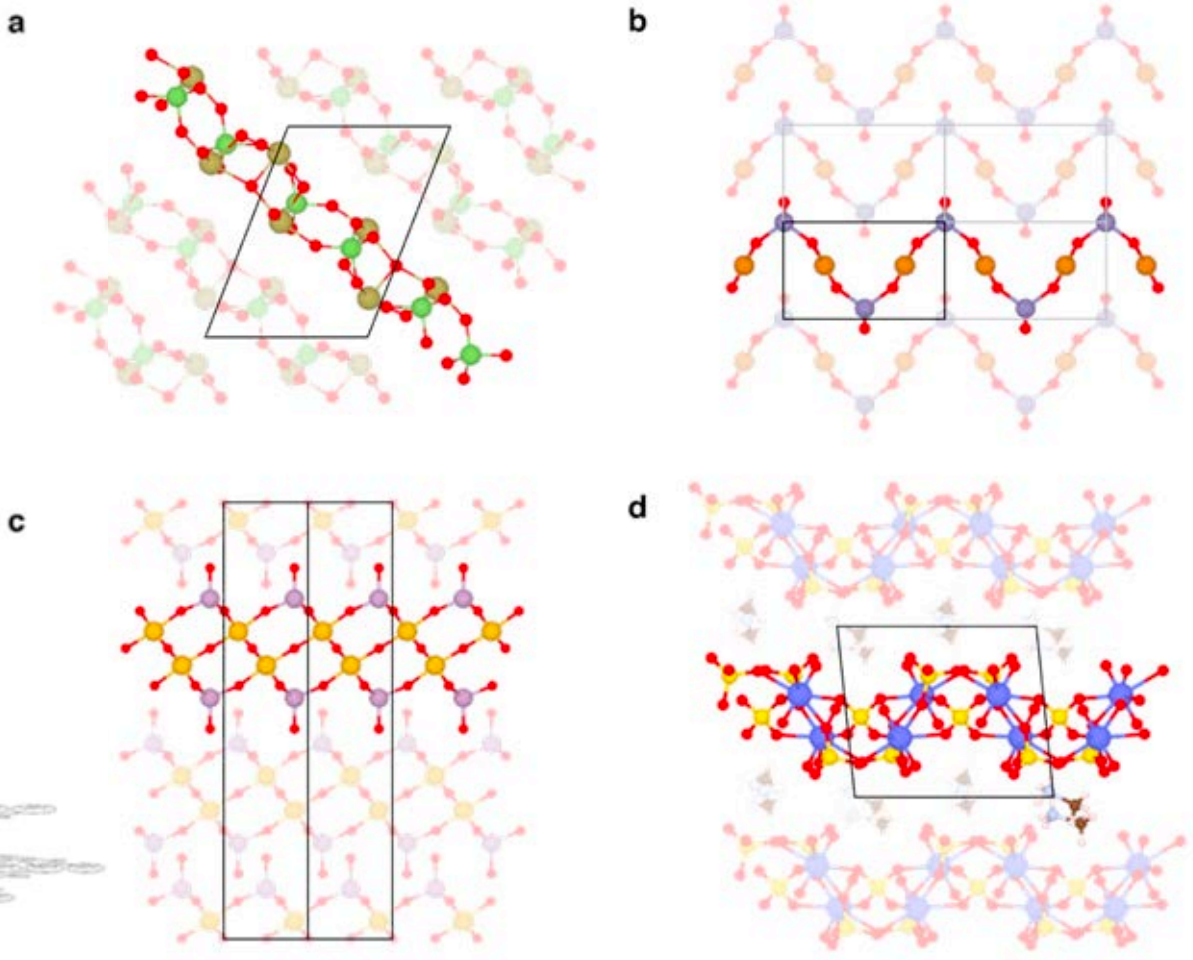
Google scholar citation: 2900+

NOVEL 2D MATERIALS



LET'S SCOTCH TAPE EVERYTHING





http://www.aiida.net

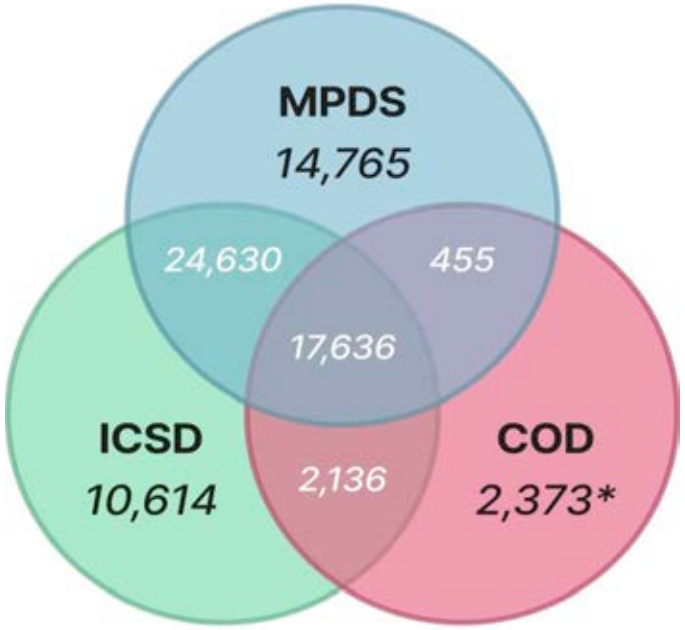
S.P. Huber *et al.*, Nature Scientific Data (2020)

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

MATERIALS CLOUD THREE-DIMENSIONAL STRUCTURE DATABASE

“SOURCE” (EXPT, PRIVATE)

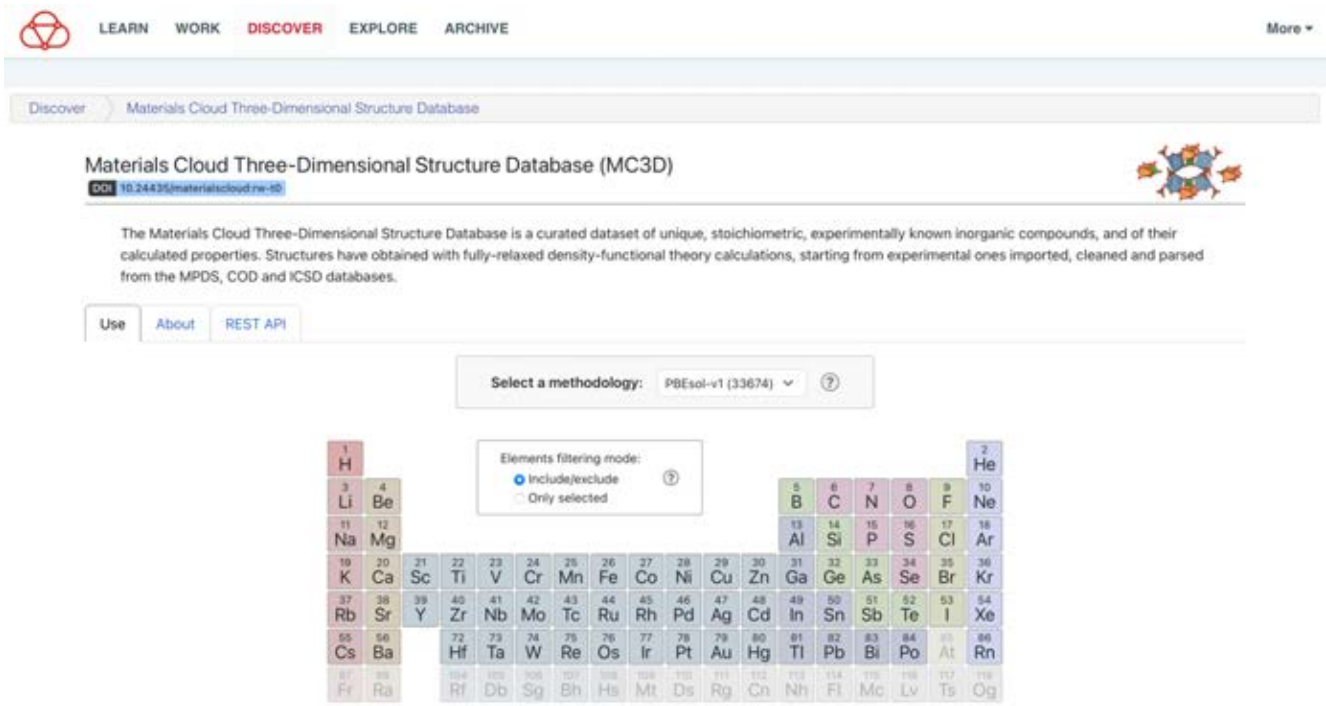
TOTAL: *72,609**



** Excluding COD structures containing hydrogen*

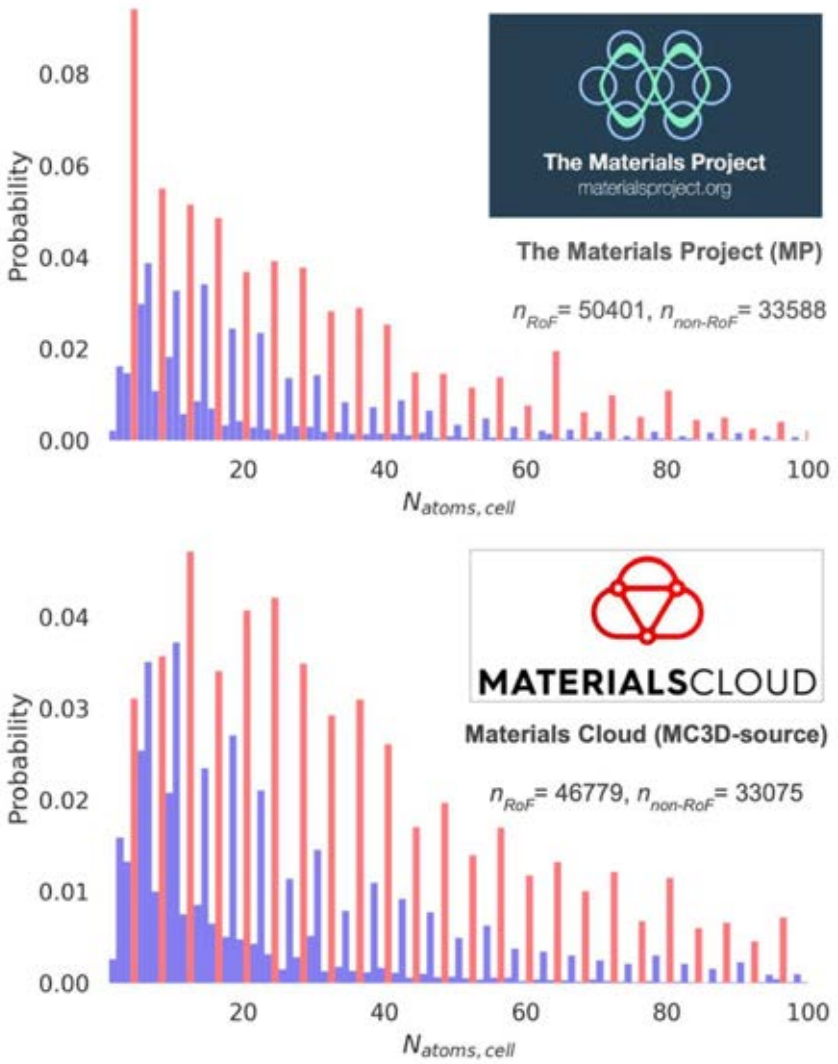
“MC3D” (COMPUTATIONAL, OPEN)

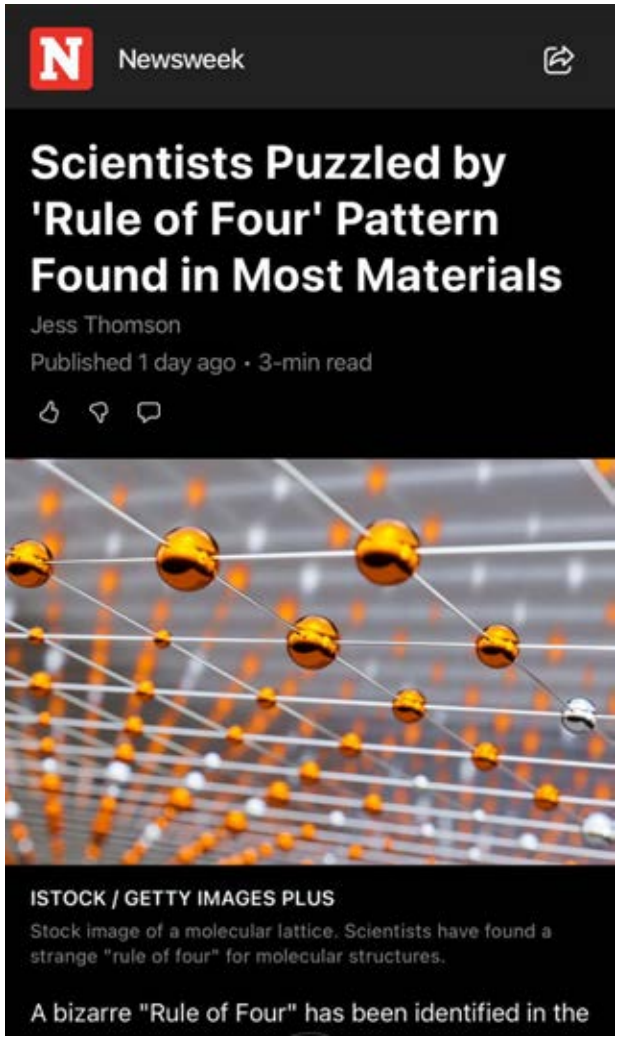
https://mc3d.materialscloud.org/



S.P. Huber, M. Bercx, N. Hörmann, M. Uhrin, N. Marzari and G. Pizzi, Digital Discovery 5, 1114 (2026)

THE RULE OF FOUR – A MARVEL INSPIRE FELLOWSHIP





E. Gazzarrini, R. K. Cersonsky, M. Bercx, C. S. Adorf, and N. Marzari, npj Comput Mater 10, 73 (2024)

Matters Arising

R. G. Palgrave, npj Comput Mater 12, 42 (2026)

E. Gazzarrini *et al.*, npj Comput Mater 12, 43 (2026)

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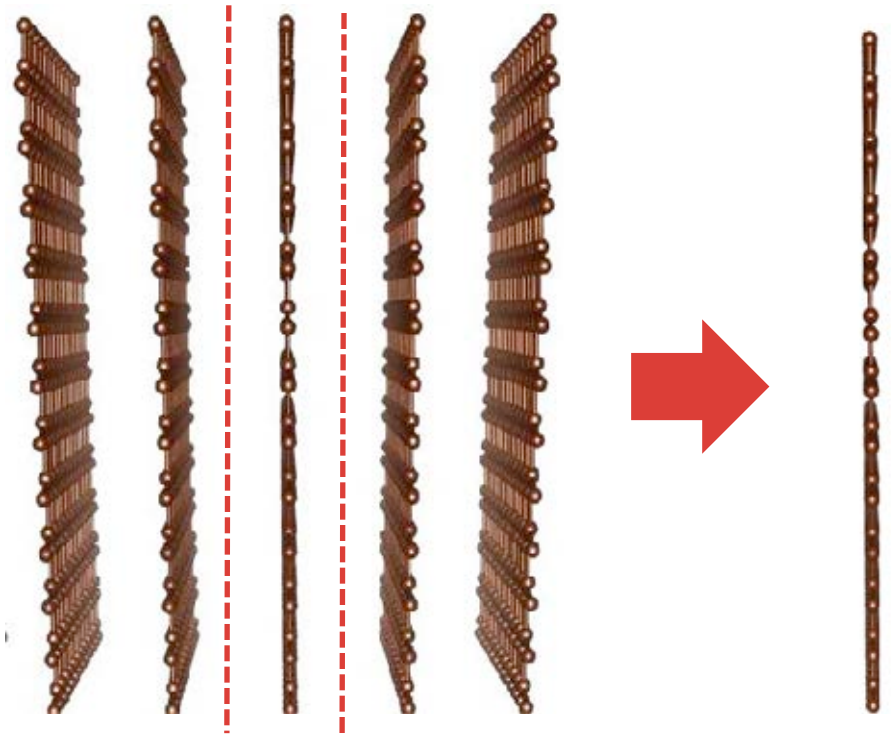
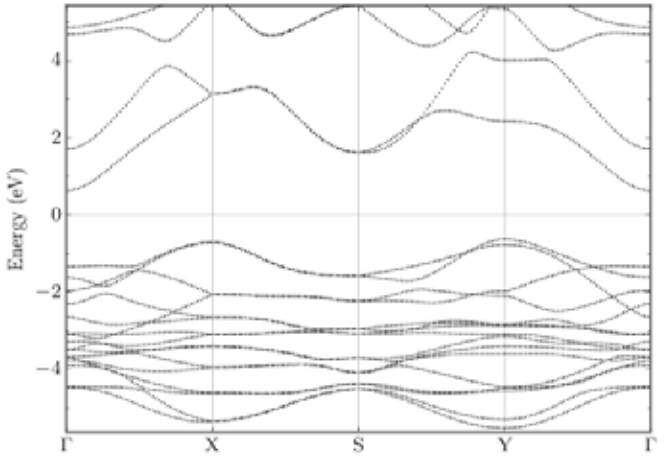
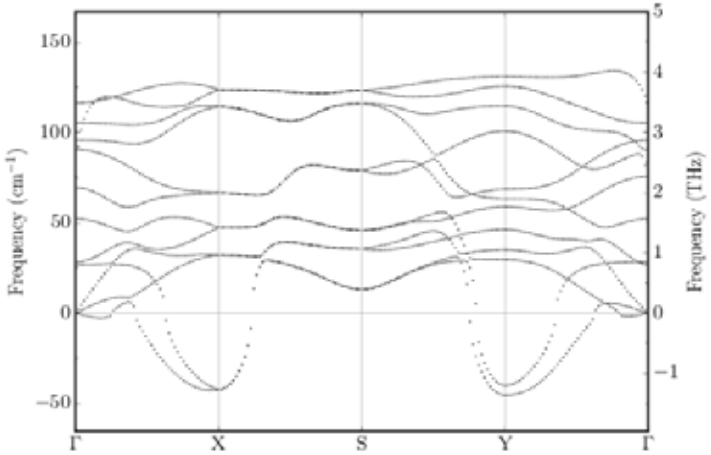
ALL AUTOMATED



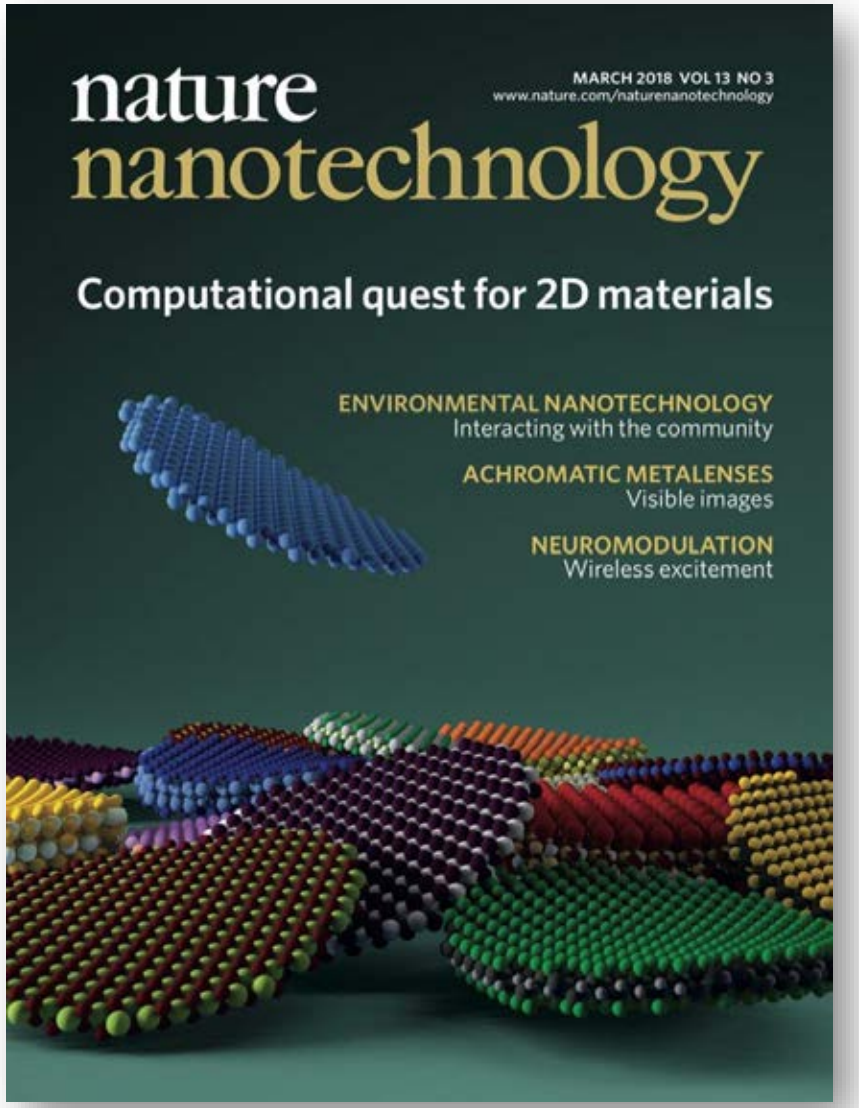
Band structures



Phonon dispersions



MC2D: 2000+ EASILY EXFOLIABLE INORGANICS



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Expansion of the Materials Cloud 2D Database

Davide Campi*, Nicolas Mounet, Marco Gibertini, Giovanni Pizzi, and Nicola Marzari*

Cite this: *ACS Nano* 2023, 17, 12, 11268−11278

Publication Date: June 13, 2023

https://doi.org/10.1021/acsnano.2c11510

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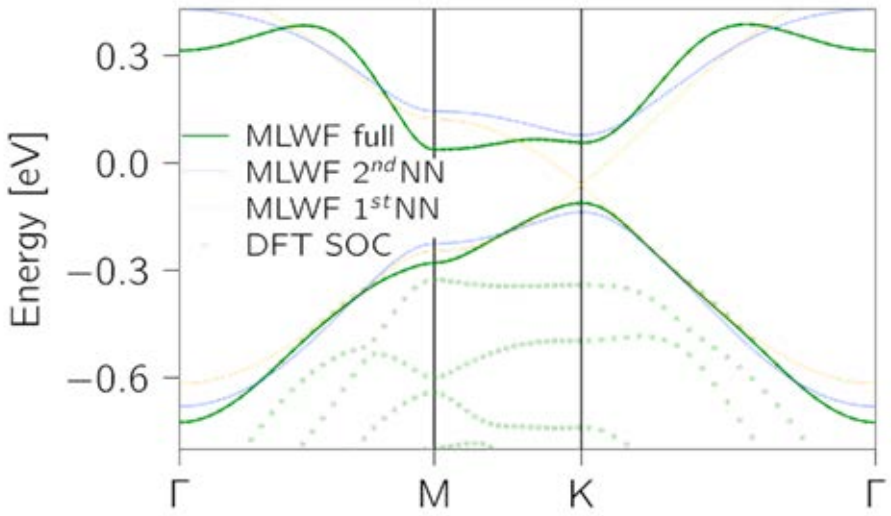
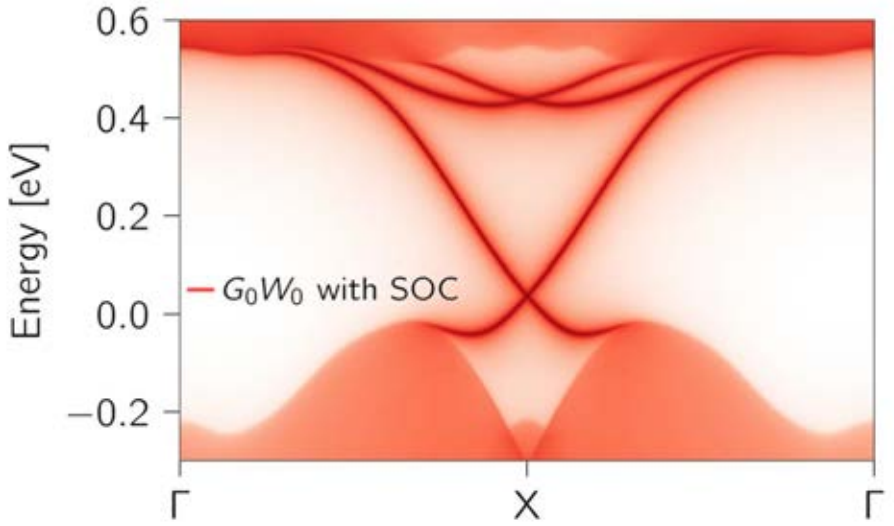
D. Campi *et al.*, ACS Nano 17, 11268 (2023)

https://mc2d.materialscloud.org/

Swiss National Science Foundation

THE DISCOVERY OF THE LARGEST-GAP KANE-MELE QSHI



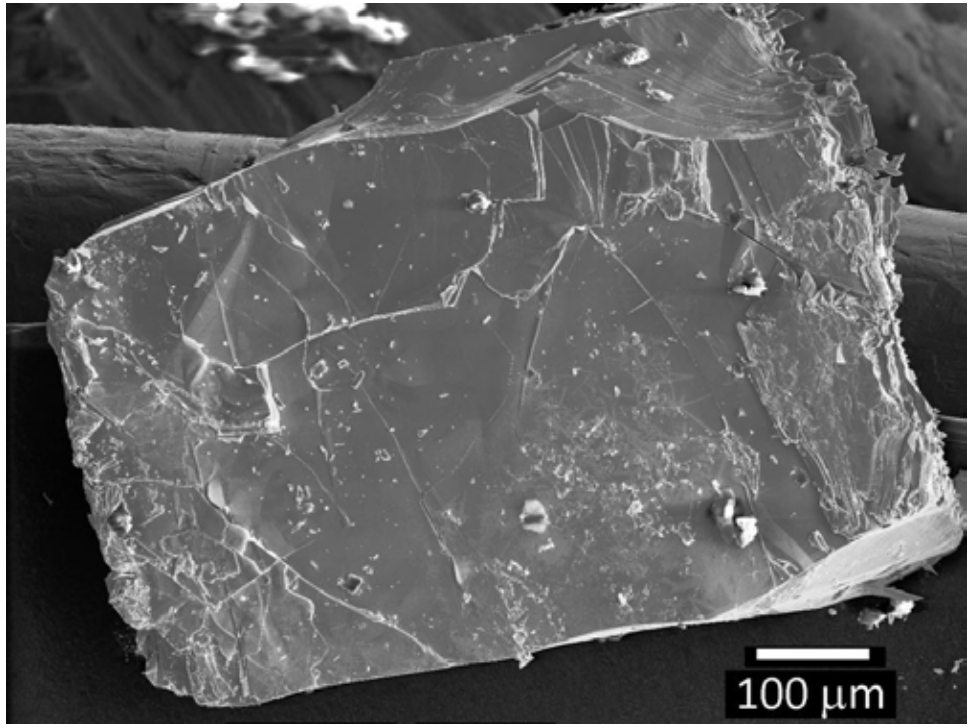


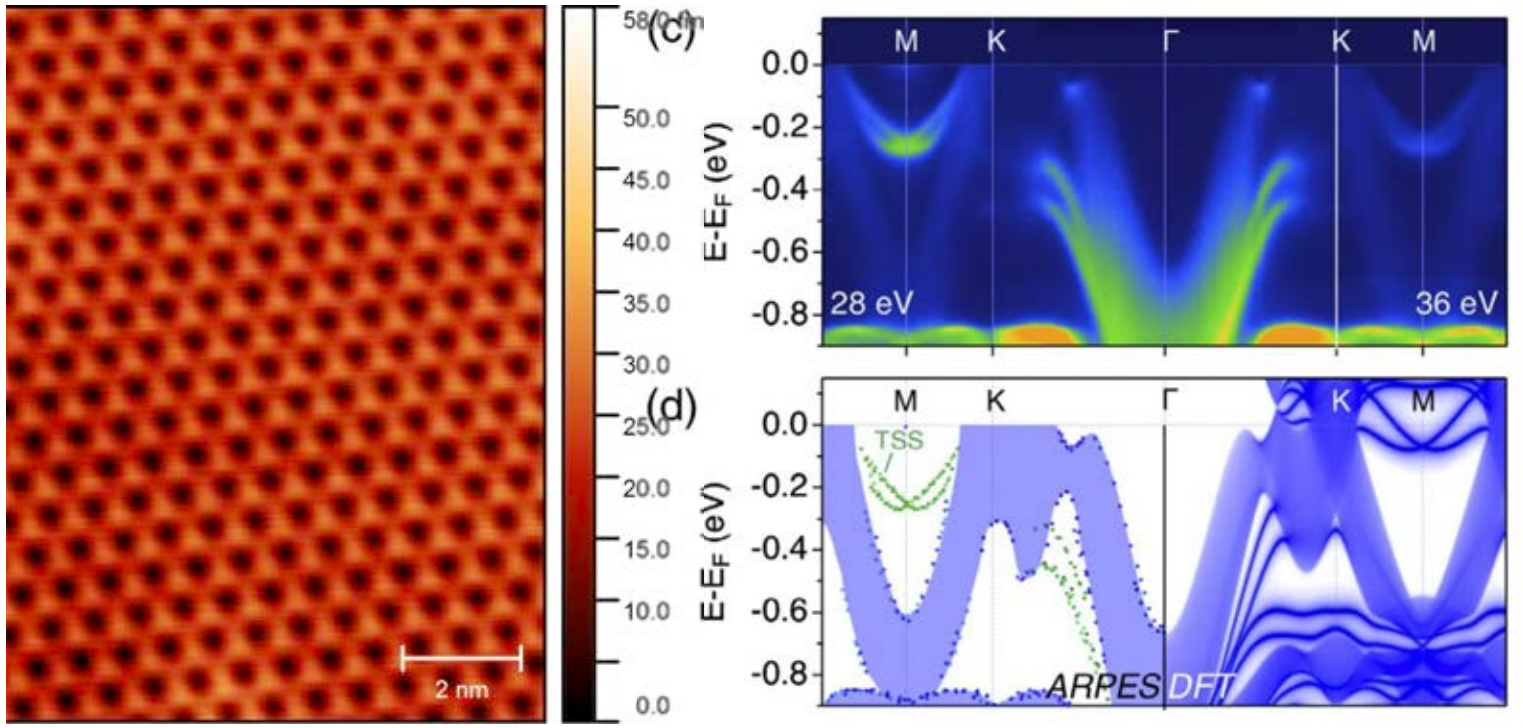
SOC due to 2nd NN hopping!

$$H = \underbrace{t \sum_{\langle ij\rangle\alpha} c^{\dagger}_{i\alpha} c_{j\alpha}}_{1^{st}\text{NN}} + \underbrace{it_2 \sum_{\langle\langle ij\rangle\rangle\alpha\beta} v_{ij} s^{z}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta}}_{\text{KM SOC}} + \underbrace{t_2' \sum_{\langle\langle ij\rangle\rangle\alpha} c^{\dagger}_{i\alpha} c_{j\alpha}}_{2^{nd}\text{NN}} + \underbrace{it_2'' \sum_{\langle\langle ij\rangle\rangle\alpha\beta} u_{ij} (\mathbf{s}\times\mathbf{d}^{0}_{ij})^{z}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta}}_{\text{in-plane SOC}},$$

Antimo Marrazzo, Marco Gibertini, Davide Campi, Nicolas Mounet, and Nicola Marzari, Phys. Rev. Lett. 120, 117701 (2018)

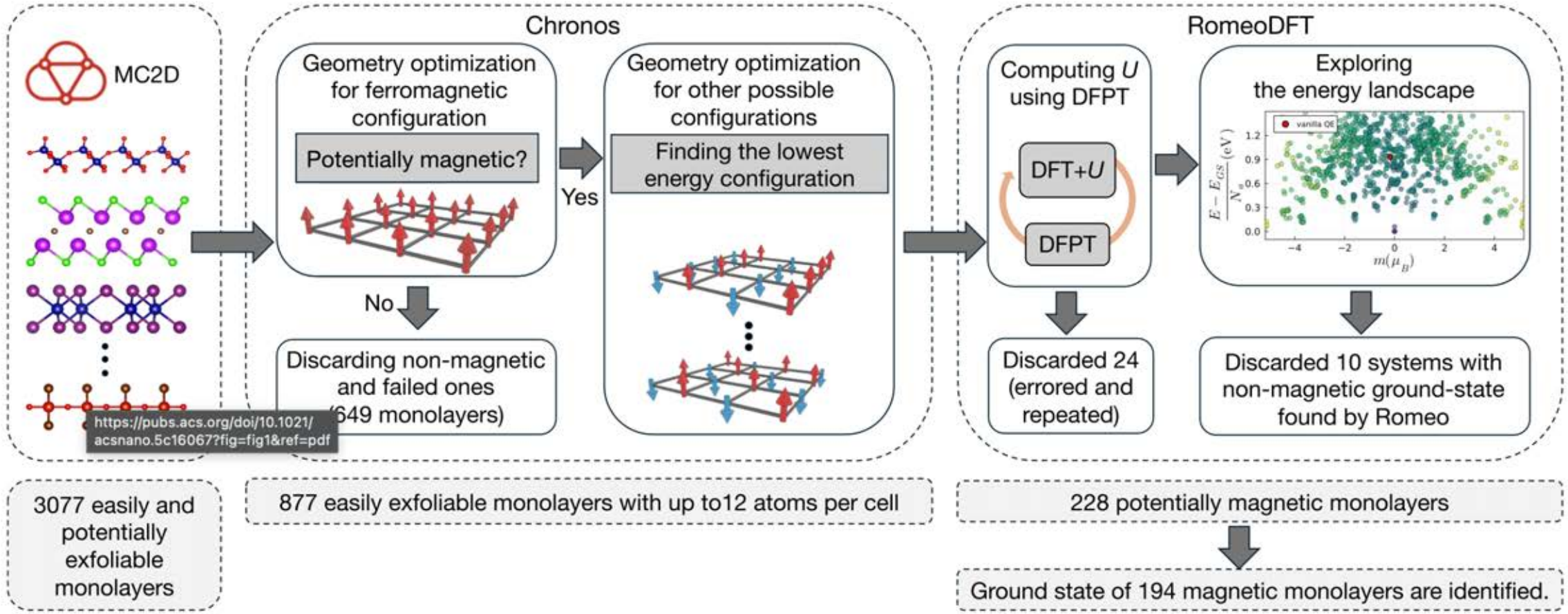
FROM PREDICTION TO SYNTHESIS TO CHARACTERIZATION





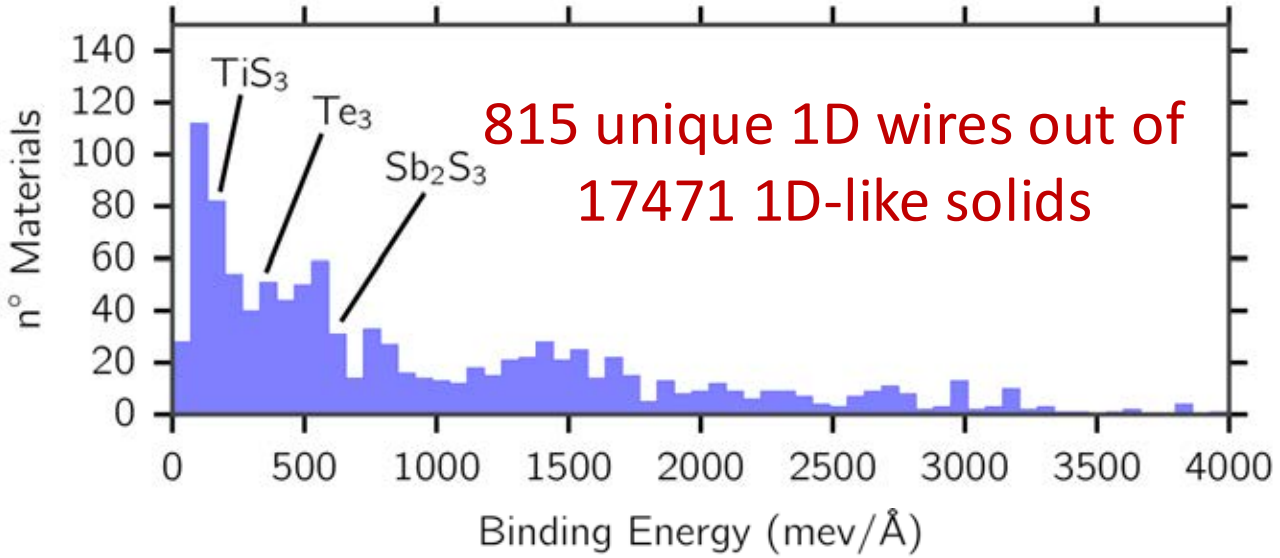
I. Cucchi, *et al.,* Phys. Rev. Lett. 124, 106402 (2020)
A. Marrazzo, N. Marzari, and M. Gibertini, Phys. Rev. Res. 2, 012063(R) (2020)

THE 2D MAGNETIC LANDSCAPE

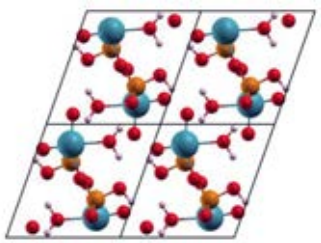


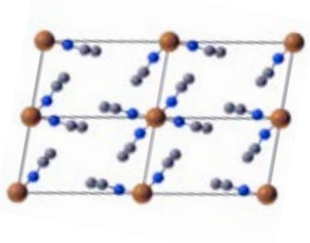
F. Haddadi, D. Campi, F. J. dos Santos, N. Mounet, L. Ponet, N. Marzari, and M. Gibertini, ACS Nano 20, 13528 (2026)

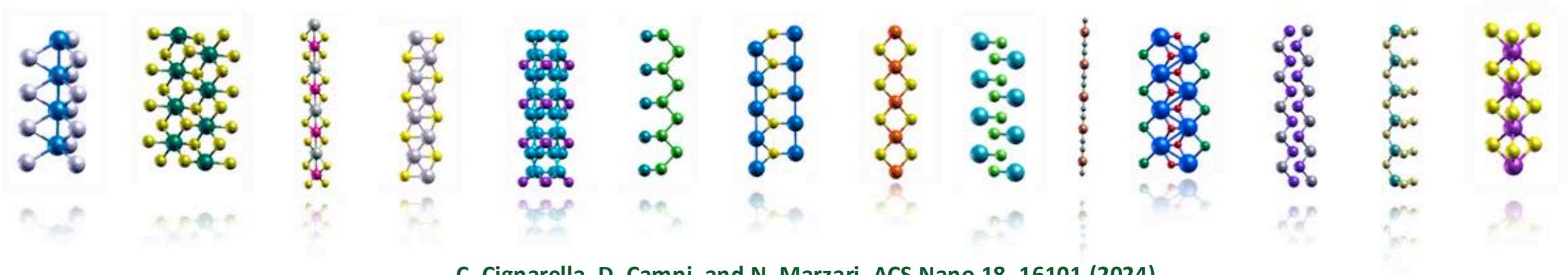
THE 1D LANDSCAPE



815 unique 1D wires out of
17471 1D-like solids

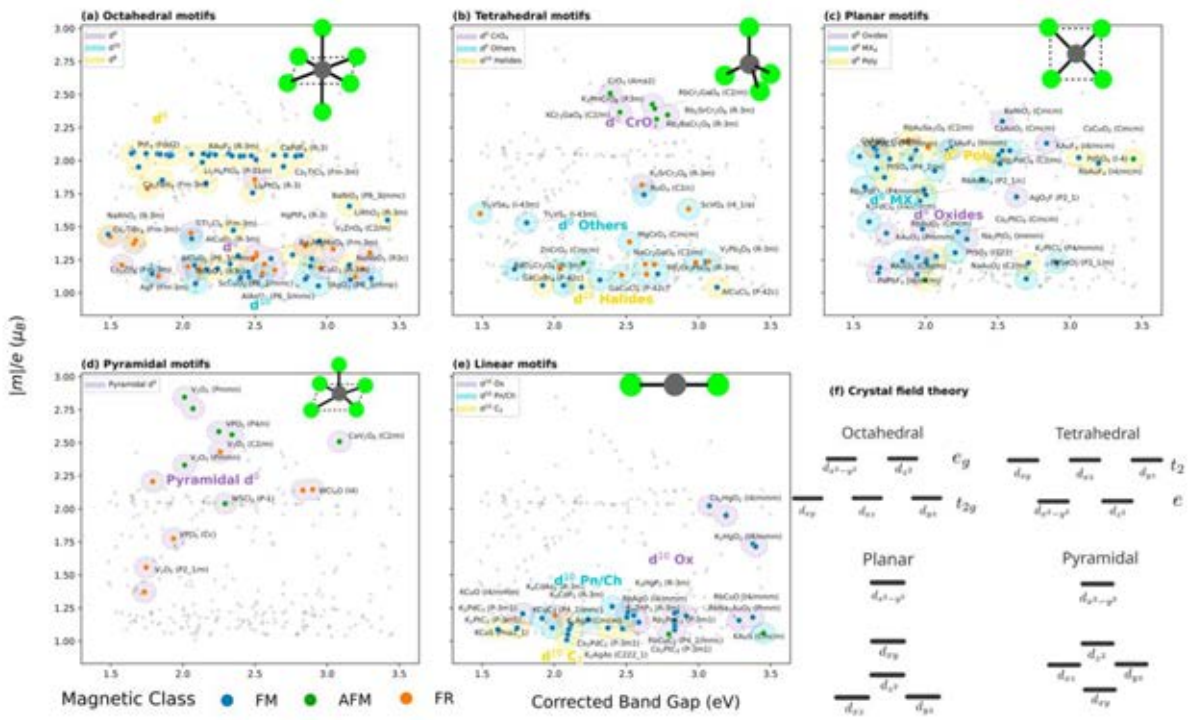


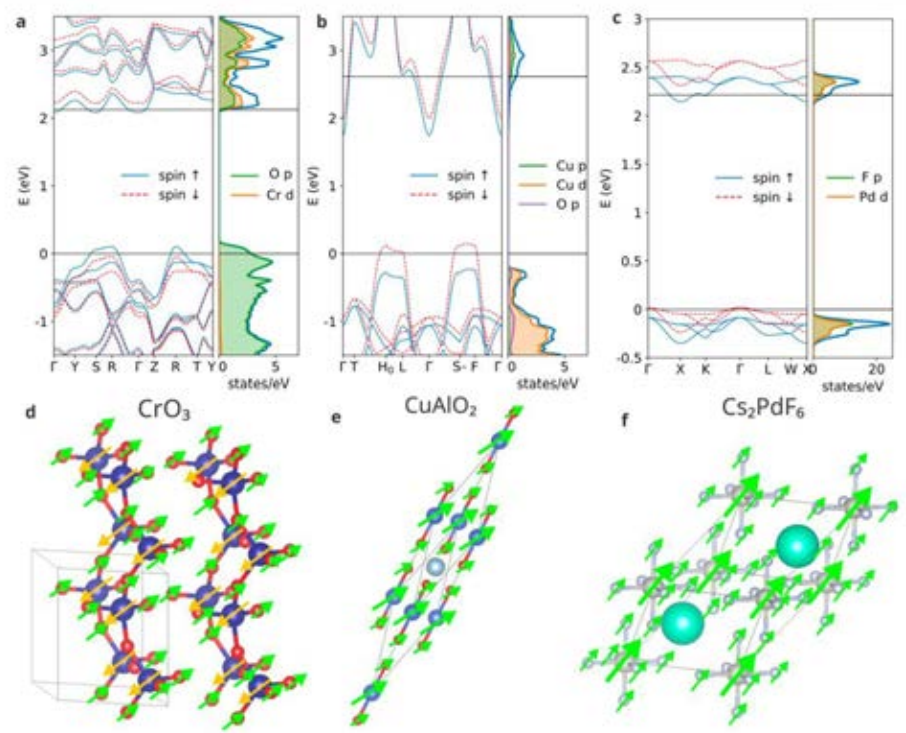




C. Cignarella, D. Campi, and N. Marzari, ACS Nano 18, 16101 (2024)
C. Cignarella, L. Bastonero, L. Monacelli, and N. Marzari, Nano Letters 25, 15919 (2025)
S. Grillo, C. Cignarella, F. Bechstedt, P. Gori, M. Palummo, D. Campi, N. Marzari, and O. Pulci, ACS Nano 20, 2664 (2026)

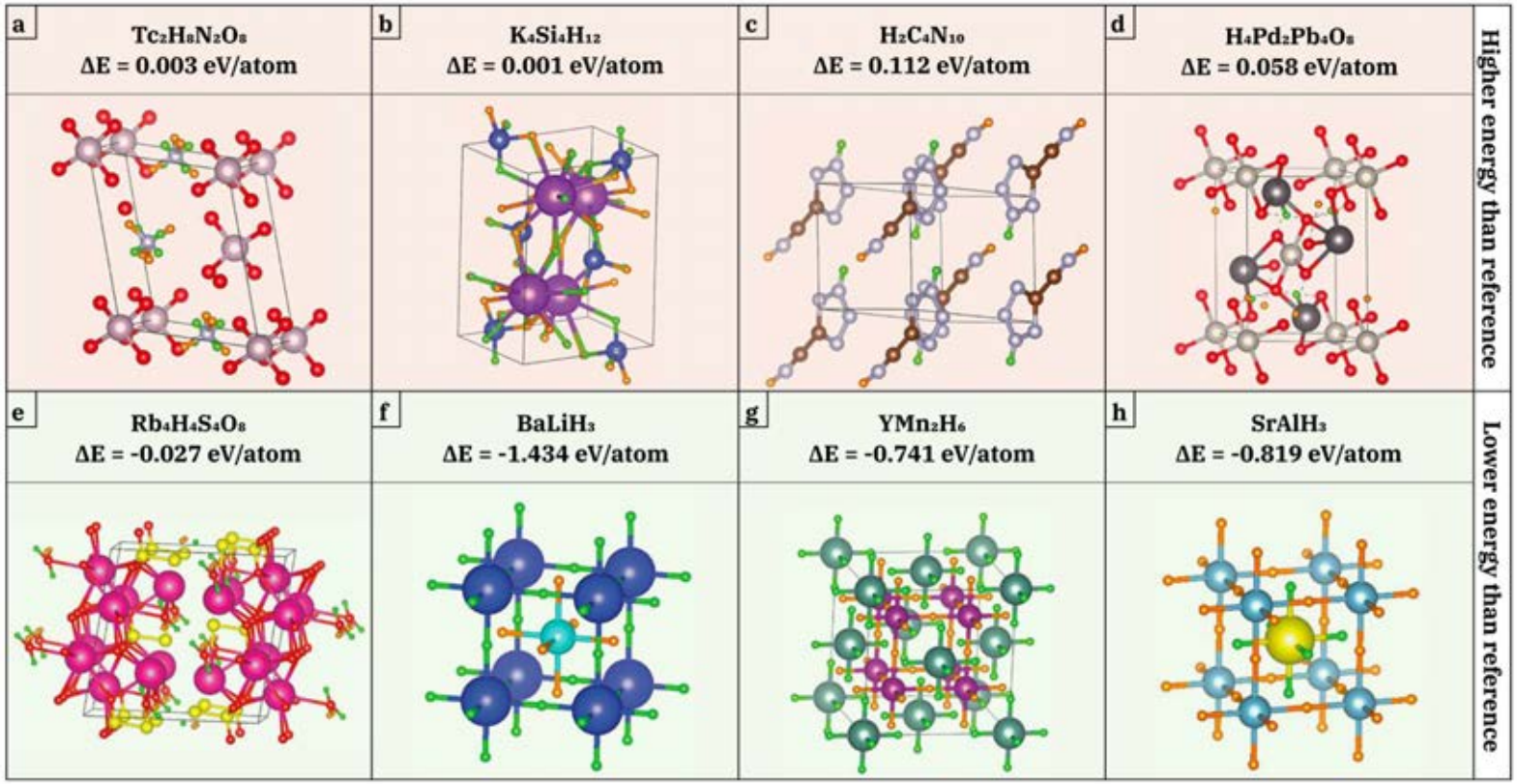
THE 3D MAGNETIC PHOTOEXCITATIONS





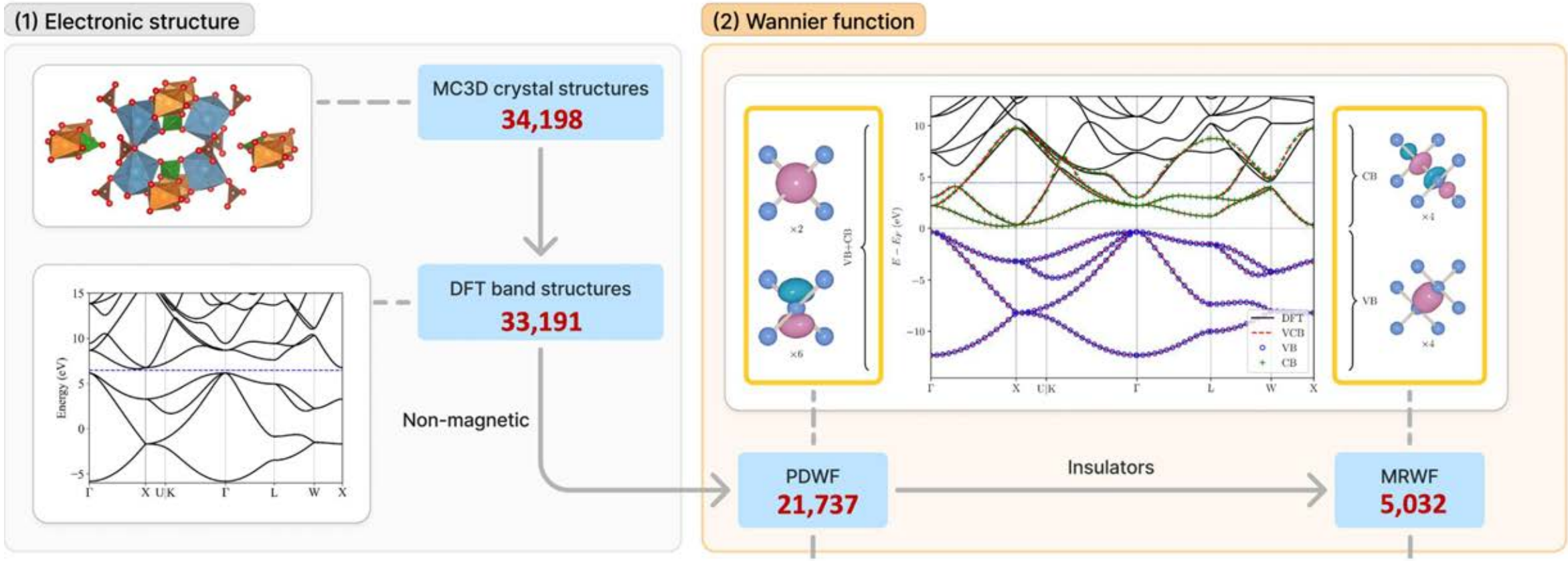
X. Zhu, J. Qiao, N. Marzari, and M. Calandra, arXiv.2606.31358 (2026)

THE MISSING HYDROGENS



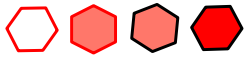
T. Reents, A. Cantarella, M. Bercx, P. Bonfà, G. Pizzi, npj Computational Materials 12, 203 (2026)

WANNIER-DRIVEN SEARCHES (2M MLWFs)



J. Qiao, G. Pizzi, and N. Marzari, *under review,* Nature Materials

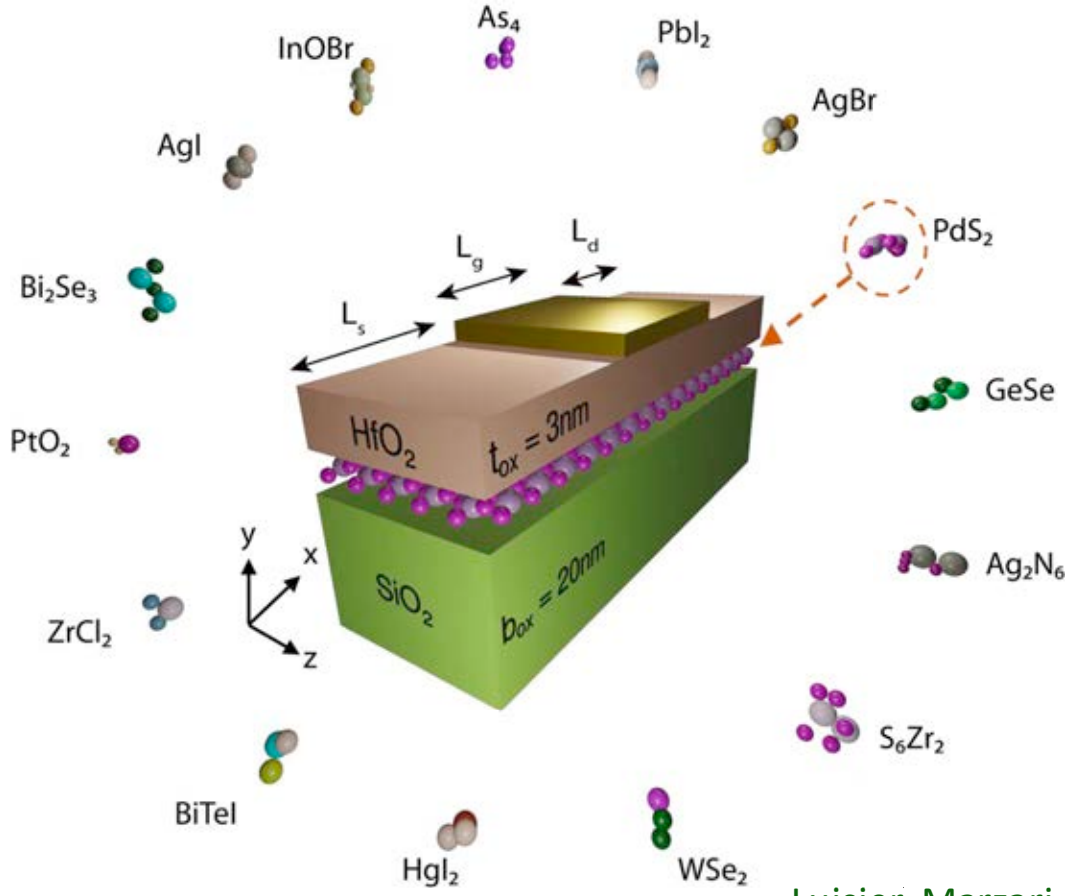
FROM 2D TO NANOELECTRONICS



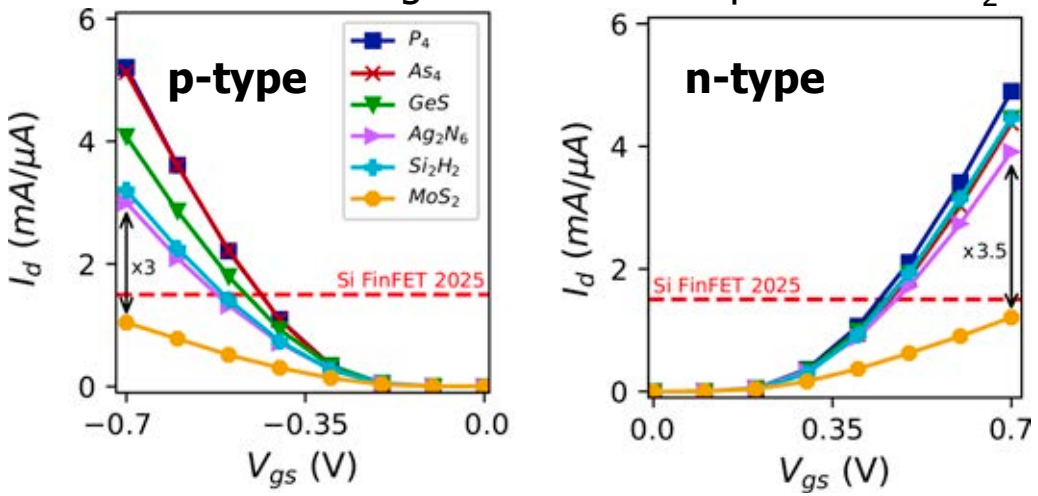
Nano-ribbon transistors with novel 2D as channel materials

Goal: beyond FinFET transistor with large ON-currents:

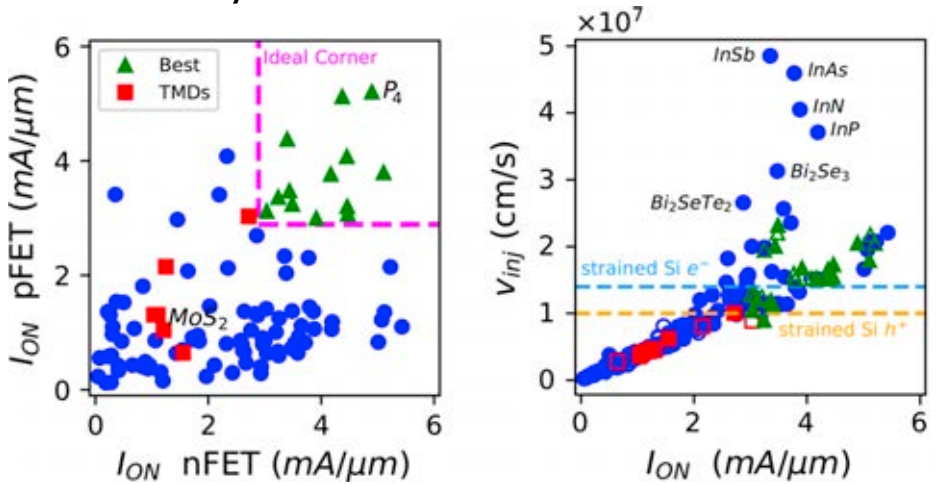
- 100 novel 2-D materials from MARVEL database investigated
- Promising candidates with higher performance than TMDCs



Five outstanding candidates compared to MoS_2



Summary of ON-state currents and velocities



Luisier, Marzari,… ACS Nano 14, 8605 (2020)

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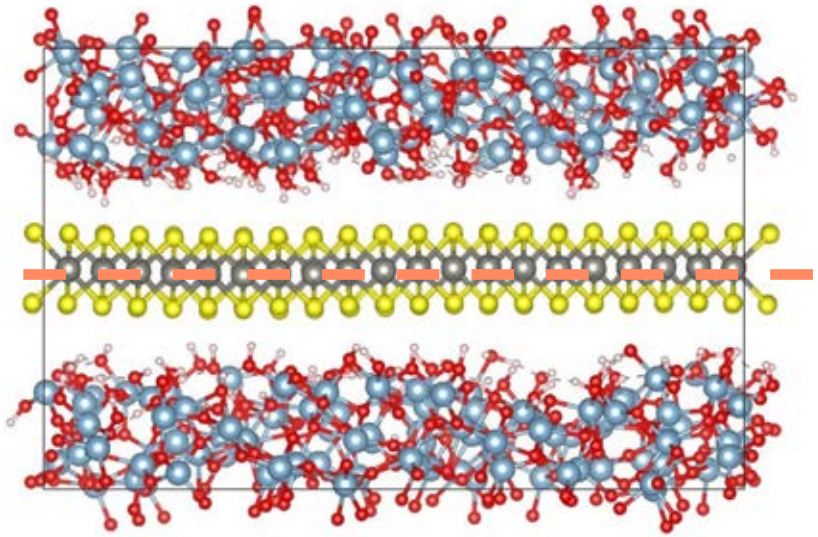
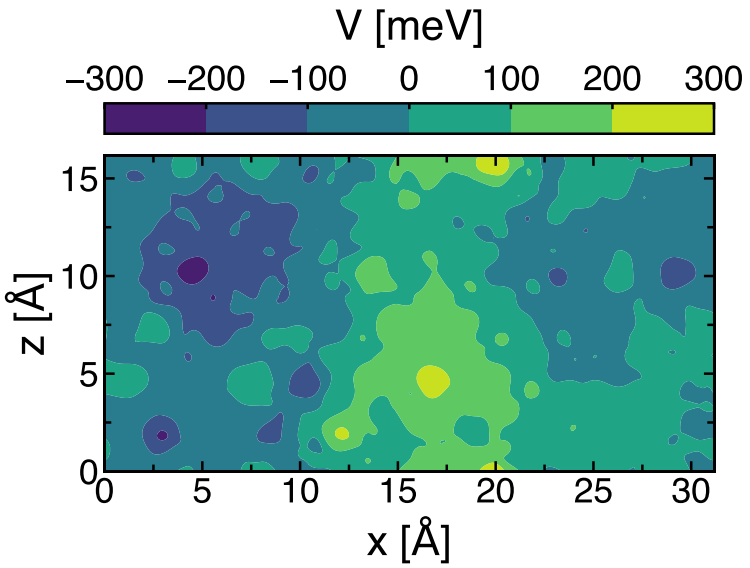
Influence of dielectric environment on the WS_2 mobility





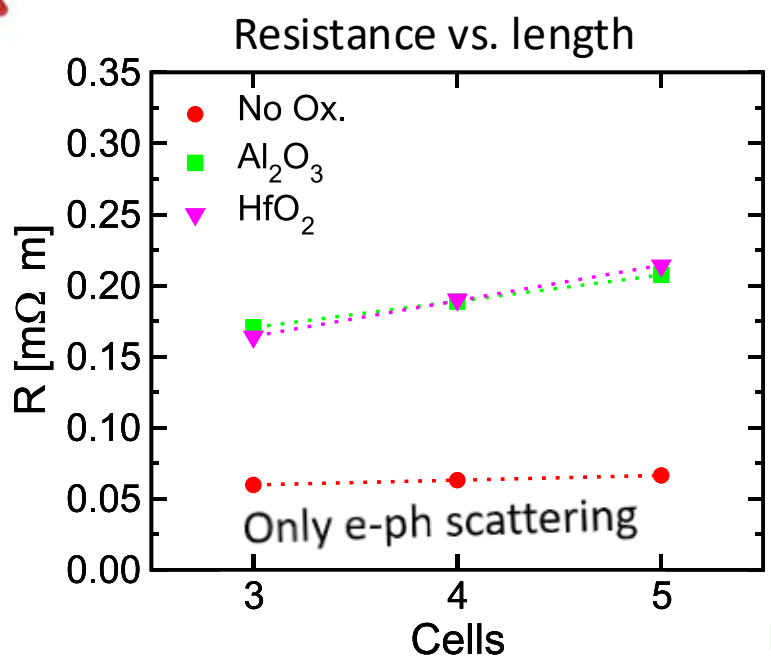
Construction of WS_2+Al_2O_3 or WS_2+HfO_2 samples with DFT and MD

Extraction of the electrostatic potential in the middle of the WS_2 layer:

- Formation of non-periodic hills and valleys with ΔE~600 meV

Calculation of the electron mobility with the dR/dL method

- Linear increase of the resistance vs. sample length
- Drastic reduction of mobility with respect to intrinsic value



dR/dL method (TLM): $\mu = \left(qn\frac{dR}{dL}\right)^{-1}$

	$n\ [cm^{-2}]$	$\mu\ [cm^2/(V \cdot s)]$
No Ox.	1.86e13	312.01
Al_2O_3	1.87e13	56.50
HfO_2	1.80e13	43.33

Luisier, … npj 2D Mat. & App. 9, 67 (2025)

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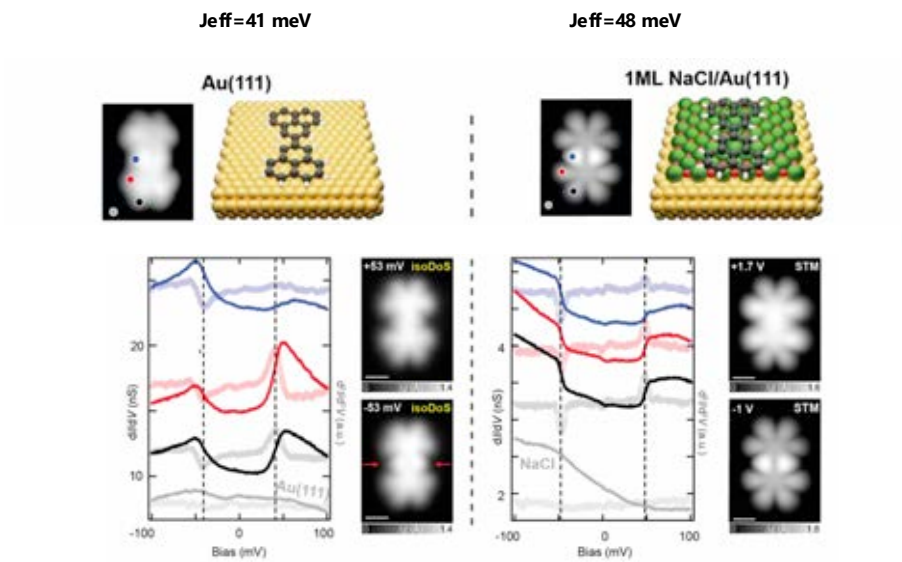
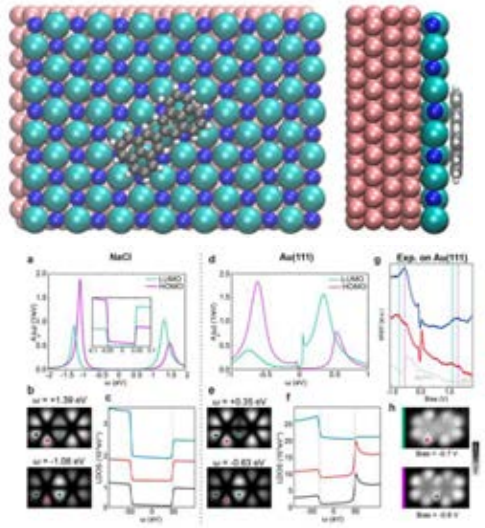
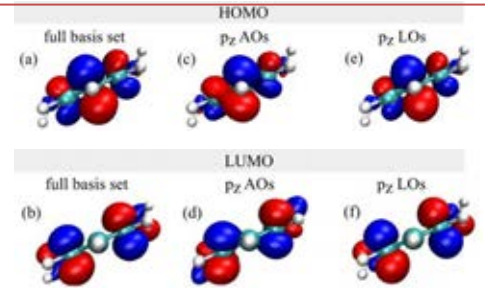
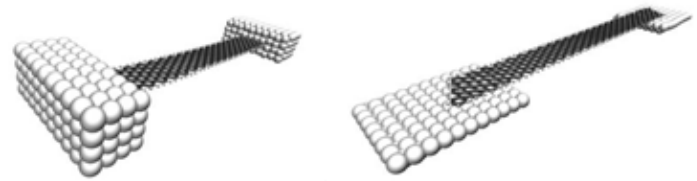
Empa : FROM ON-SURFACE SYNTHESIS TO DEVICES



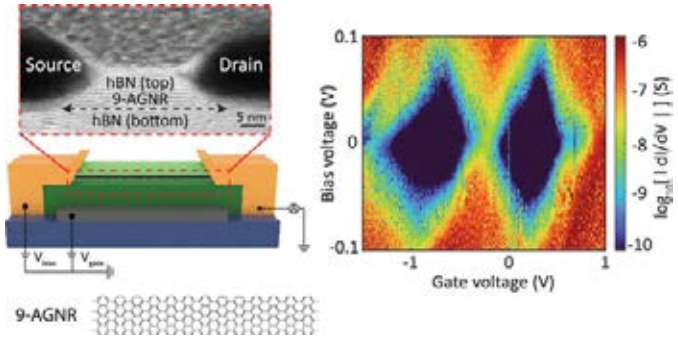


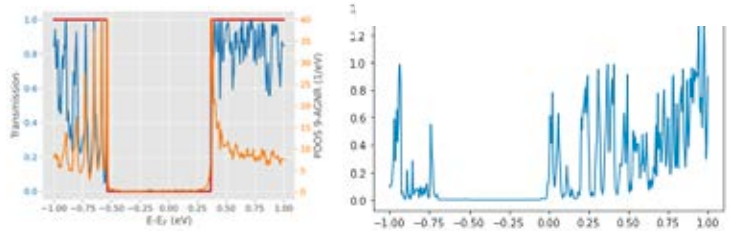
Smart local orbitals + DFT (with gate and bias potential)
+ NEGF including DMFT correlation:
modelling Coulomb diamonds in realistic systems, for example edge-contacted graphene nanoribbons

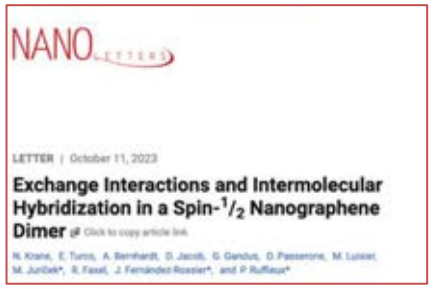


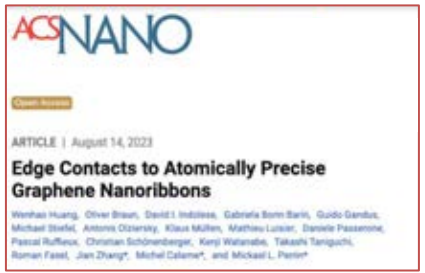


A hierarchy of theoretical methods to include surface screening and hybridization effects, from MFH through DFT and NEGF to unveil subtle inelastic transitions in organic biradicals (relevant for carbon-based quantum computing)









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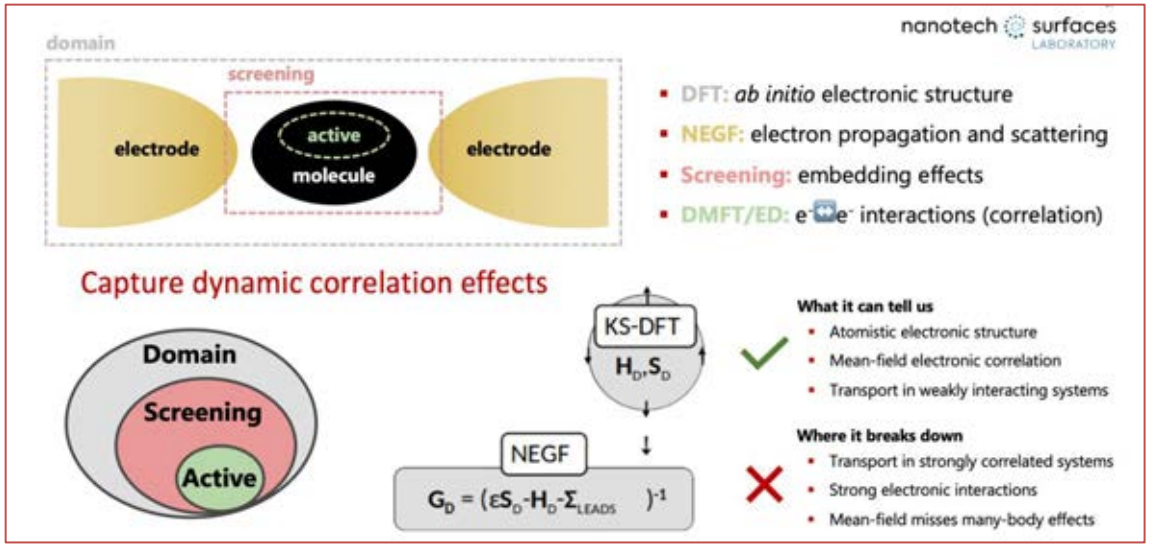
Empa : “To learn the Transport by the Pain…”



Including DMFT in the workflow

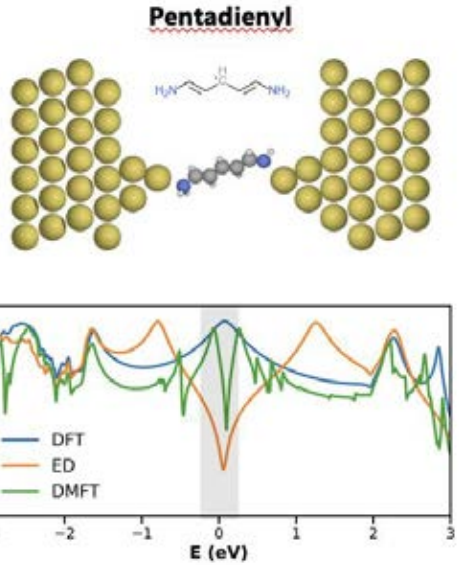
DFT: predicts near resonant transport

ED: predicts conductance suppression

- **Pros:**
  - Captures many-body effects
  - Includes both local/non-local effects
  - Exact!
- **Cons:**
  - Small systems (~20 atom limit)

DMFT: captures conductance suppression

- **Pros:**
  - Larger systems and inelastic scattering
- **Cons:**
  - No explicit non-local effects



Insight in the physics with minimal models

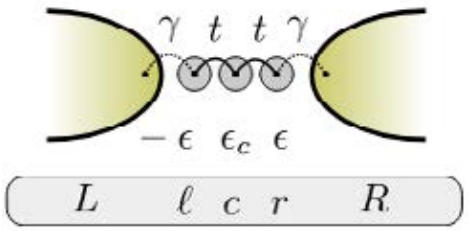
$$\mathbf{G}_D(z) = \left[z - \mathbf{H} + i\mathbf{\Gamma}_L/2 + i\mathbf{\Gamma}_R/2 - \mathbf{\Sigma}_D(z)\right]^{-1}$$

$$\mathbf{H} = \begin{pmatrix} \epsilon_\ell & t & t' \\ t & \epsilon_c & t \\ t' & t & \epsilon_r \end{pmatrix} \quad -\epsilon_\ell = \epsilon_r = \epsilon$$

$$\mathbf{\Gamma}_L = \begin{pmatrix} \Gamma & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \mathbf{\Gamma}_R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Gamma \end{pmatrix}$$

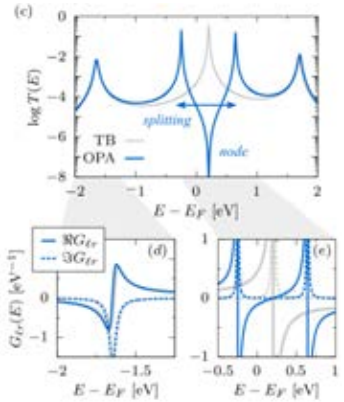
$$\mathbf{\Sigma}_D(z) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Sigma_{\mathrm{OPA}}(z) & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Sigma_{\mathrm{OPA}}(E) = \frac{a^2}{E - E_F - \epsilon_{\mathrm{res}} + i\gamma}$$



ϵ = 1.5
ϵc = 0.25
a = 0.5

Γ = 0.05
γ = 0.003
t = 0.1
t' = 0



Strongly correlated physics in organic open-shell quantum systems

G. Gandus[1,*], A. Jayaraj[2,*], D. Passerone[2], R. Stadler[3], M. Luisier[1], and A. Valli[4,5,†]

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Phys. Rev. Research **8**, 023221 – **Published 28 May, 2026**

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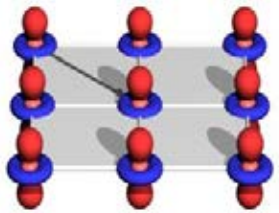
Tight-binding Hamiltonians from *ab initio* calculations for CAS/DMRG

Empa

A portfolio of localization methods for quantum science and transport

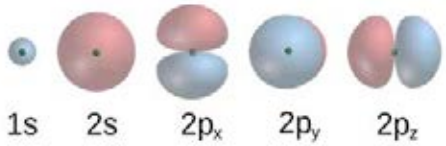
Wannier functions



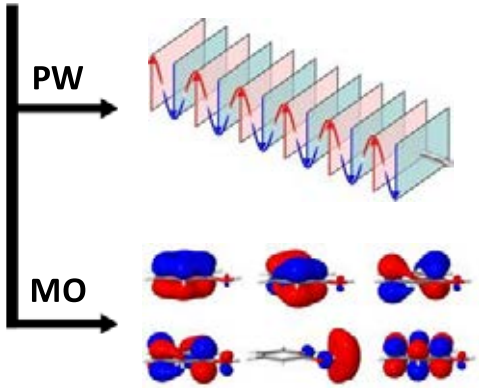
WANNIER90

or

Local orbitals (LOs)



from



PAOFLOW

QTPYT

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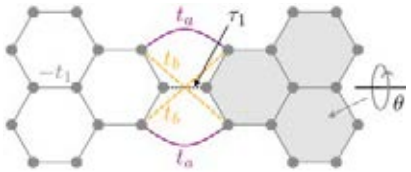
Goncalo Catarina

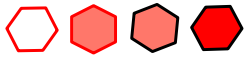


	θ = 0°		θ = 30°	
	Model	qtpyt	Model	qtpyt
t_1 (eV)	2.7	2.745	2.7	2.747
τ_1 (eV)	-2.7	-2.736	-2.338	-2.451
t_a (eV)	-0.521	-0.388	-0.336	-0.249
t_b (eV)	-0.180	-0.120	-0.185	-0.128
$2/3\|t_a - t_b\|$ (eV)	0.227	0.179	0.101	0.081
max $\Delta_{on\text{-}site}$ (eV)	0	0.658	0	0.674
$\|\max S_{ij}\|$	0	0.372	0	0.374

Hubbard treatment

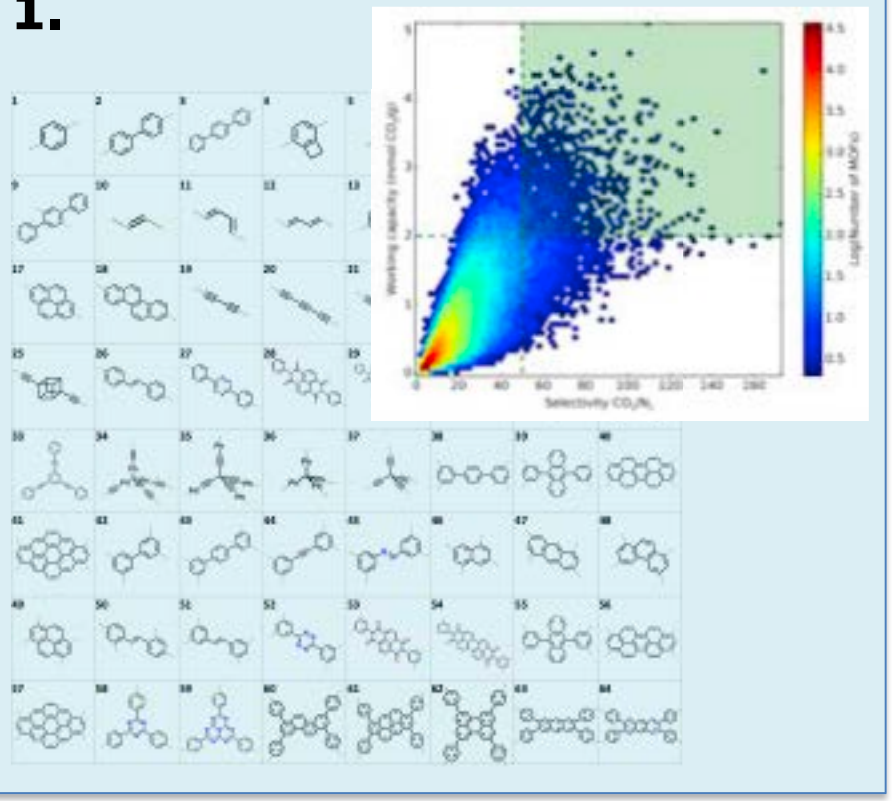
Andres Ortega Guerrero

MOFs, COFs, AND CARBON CAPTURE



AI-driven design of materials that can capture CO_2 in wet flue gasses

1.



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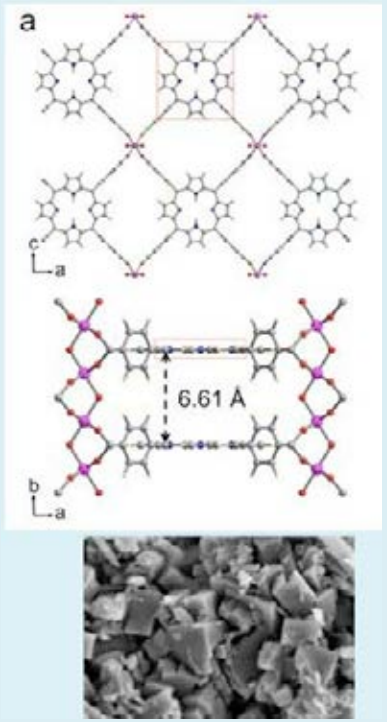
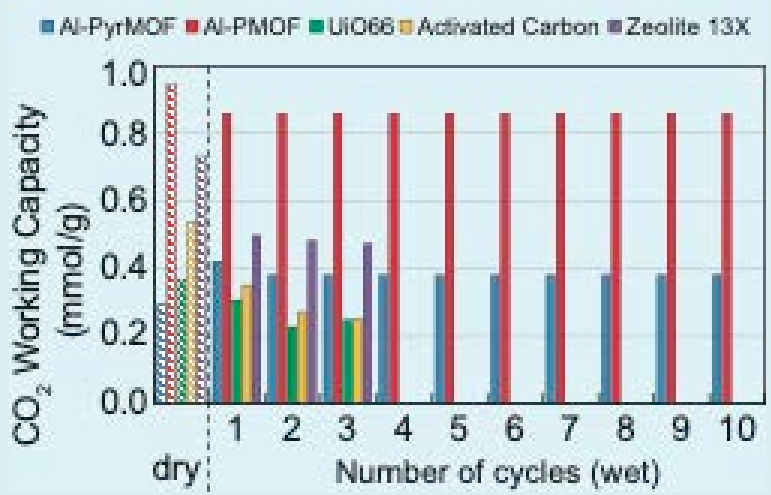


1. **Generate and screen a library of 300’000 MOFs for separating wet flue gasses**
2. **Identify the “adsorbaphore” and synthesize materials with an adsorbaphore**
3. **Testing and comparing against commercial materials**

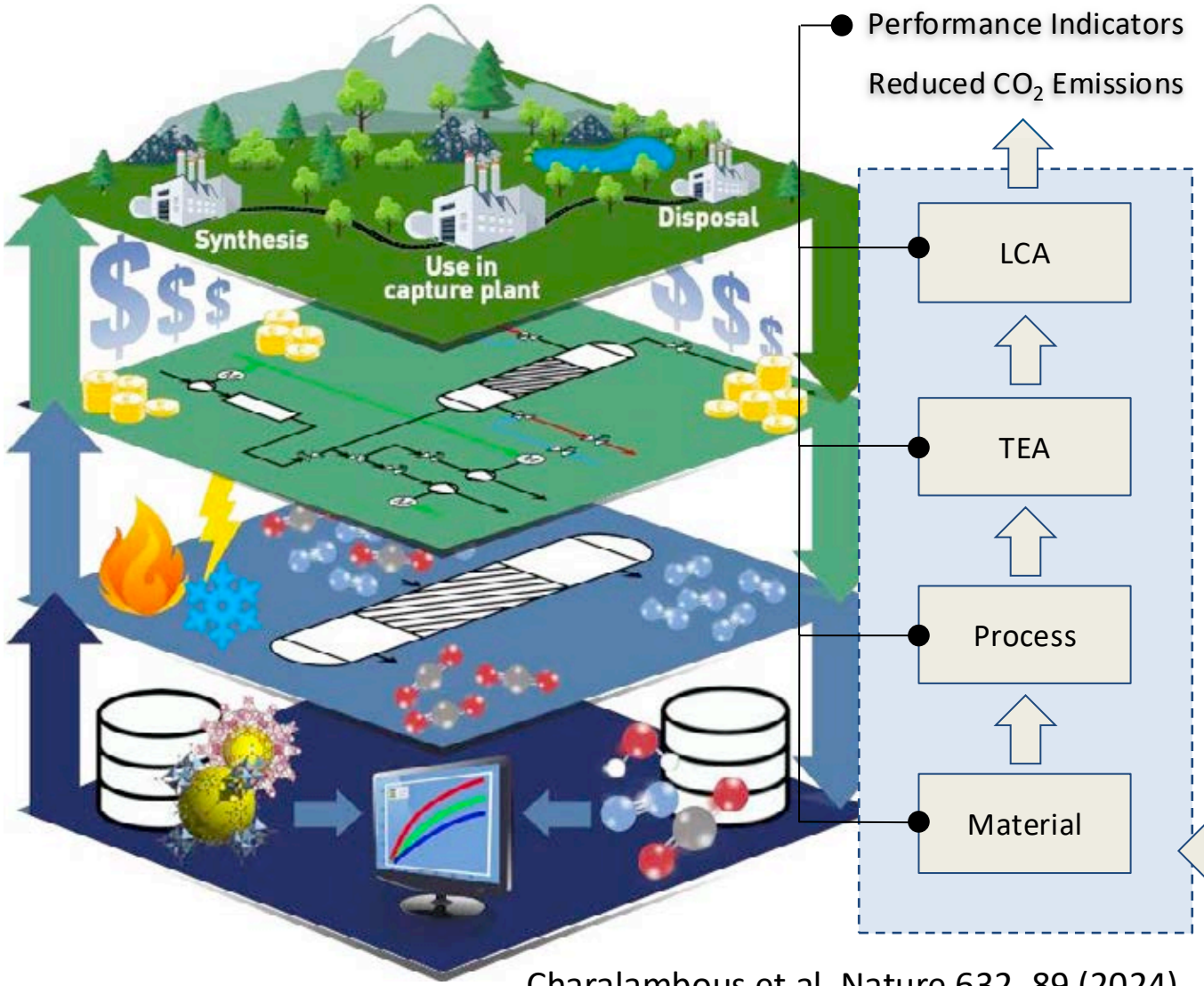
3.



P. G. Boyd et al, *Data-driven design of metal–organic frameworks for wet flue gas CO2 capture,* **Nature** 576 (7786), 253 (2019) doi.org/10.1038/s41586-019-1798-7

Swiss National Science Foundation

A holistic platform for accelerating sorbent-based carbon capture .



Performance Indicators

Reduced CO_2 Emissions

LCA

TEA

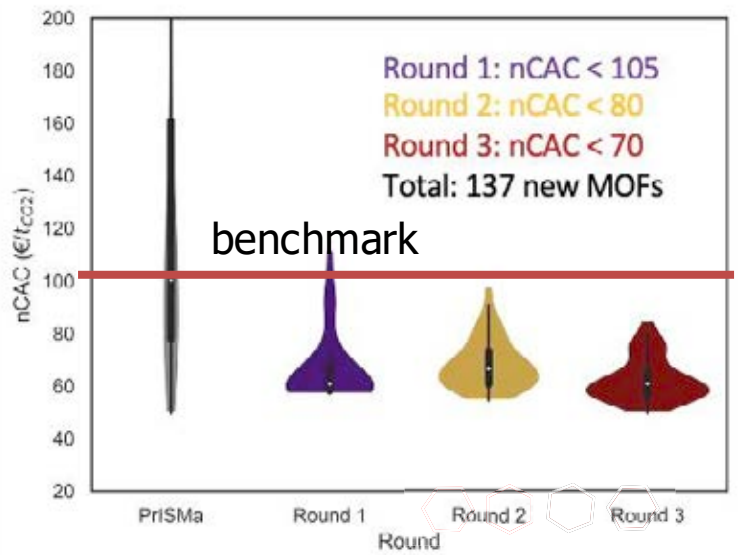
Process

Material

Evaluate the performance of a material in a carbon capture process: (nCAC- net carbon avoidance cost)

1. **Materials**: predict the properties for process design
2. **Design of a carbon capture process:** for a given source of CO_2 and sink of CO_2 in
3. **Techno-economics;** prediction of the cost to capture a ton of CO_2
4. **Life-cycle assessment:** calculations of the indirect emissions and impact on the environment

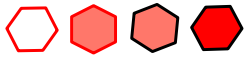
AI-driven design: > 135 new MOFs outperform the benchmark



Charalambous et al, Nature 632, 89 (2024)

Swiss National Science Foundation

PHOTOVOLTAICS AND CATALYSTS

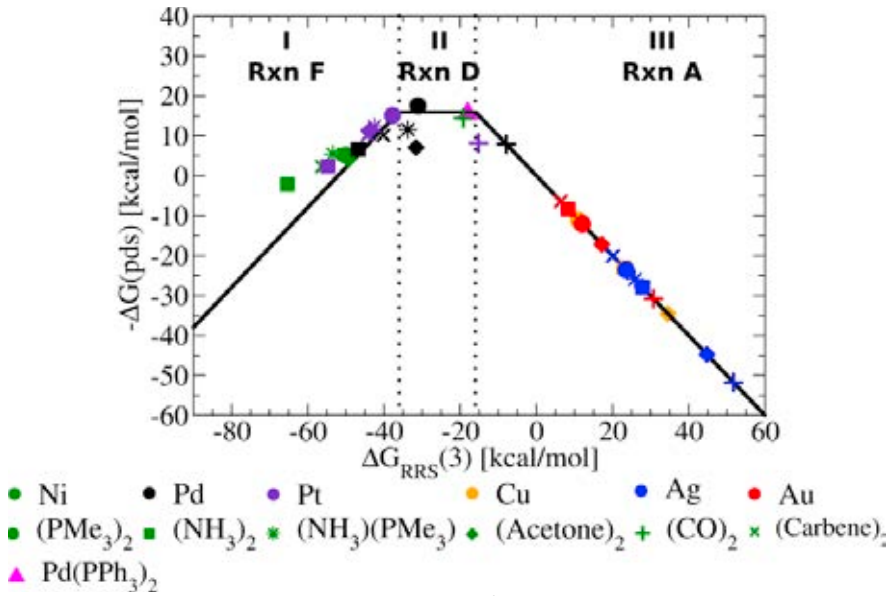


Navigating catalyst landscapes

Concept of volcano plots

first extension to homogeneous catalysis

The Suzuki-Miyaura Volcano



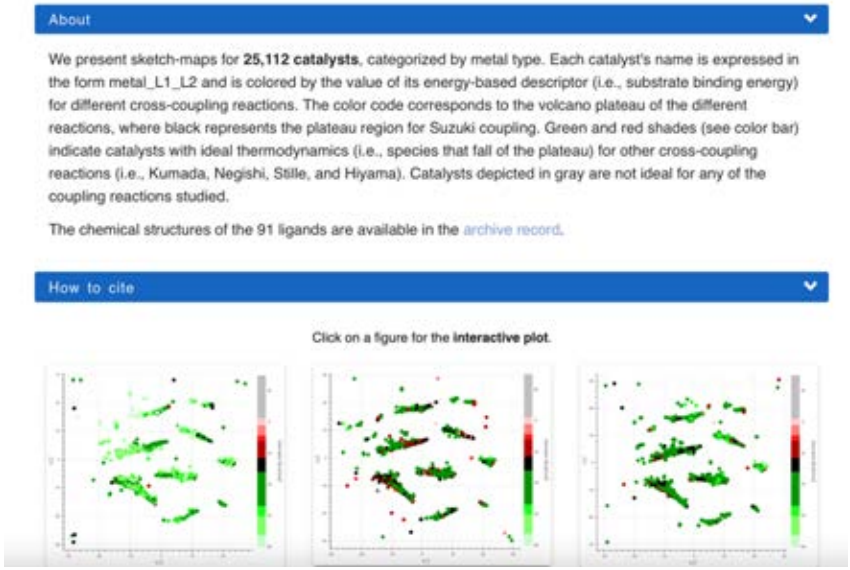
Chem. Sci. 2015, 6, 6754.

In agreement with experiment:

- Plots identify **highly** catalytically **active** regions.

Scaling up

from a handful of systems to data

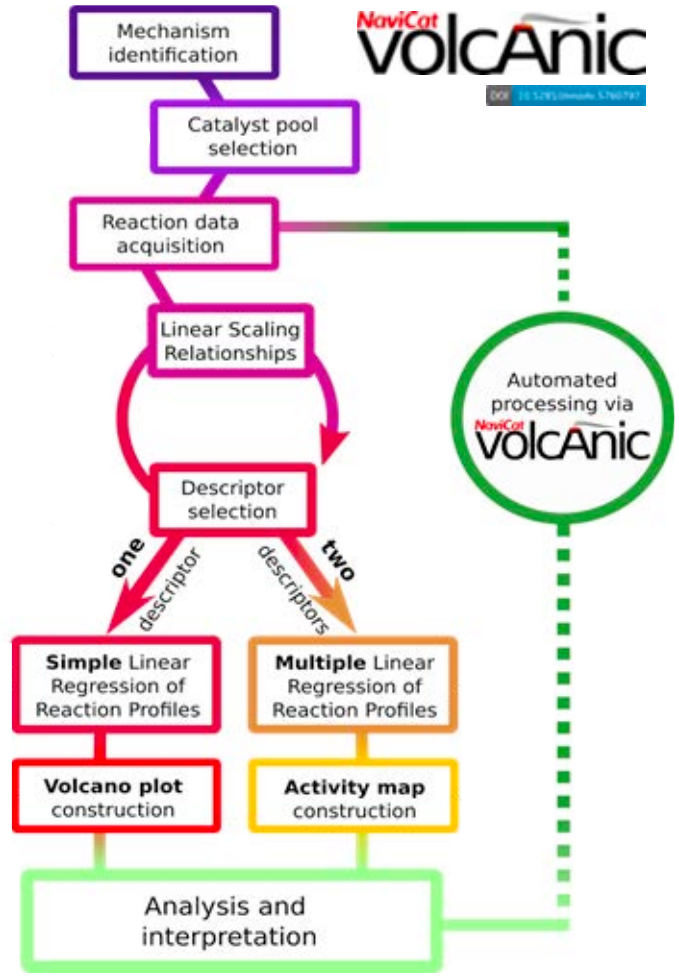


Chem. Sci. 2018, 9, 7069.

MATERIALSCLOUD

25 papers, 1.353 citations.

Automated tools

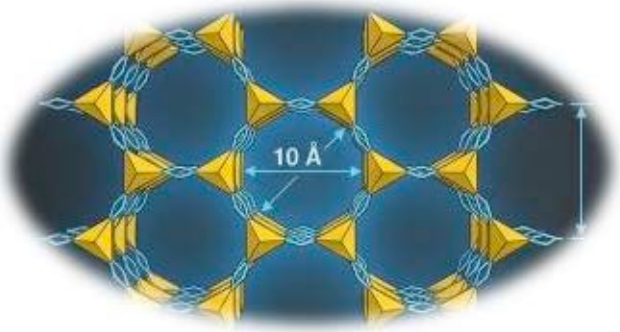


Nat. Protoc., 2022, 17, 2550.

Swiss National Science Foundation

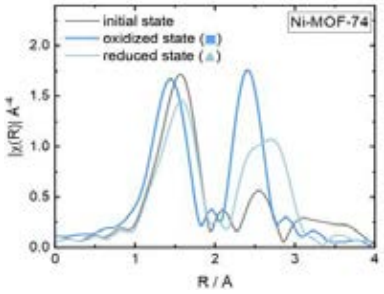
Ni-MOF electrocatalyst for water electrolysis: The paradox

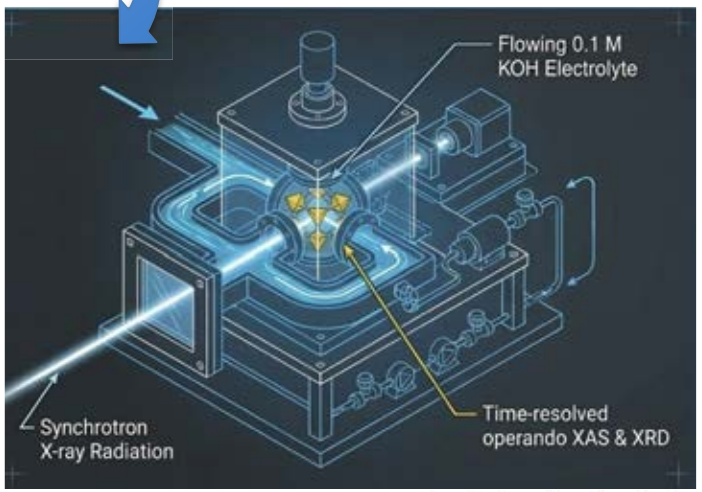
Crystalline Ni-MOF:
High surface area,
precise tunable nodes



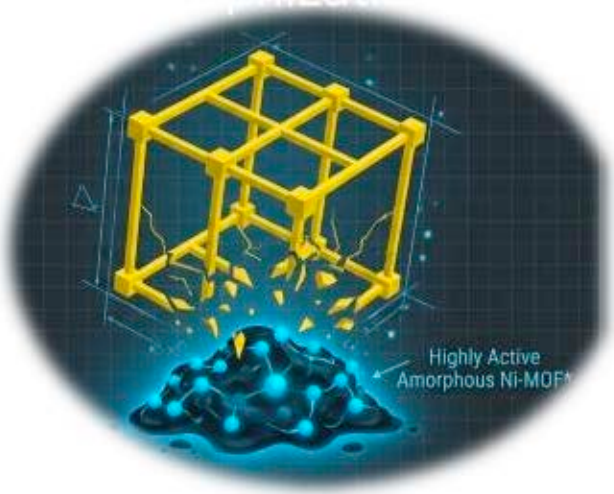
Are MOFs actually stable during anodic oxidation reaction of water electrolysis?
Why their performance improve with operation?

Operando EXAFS



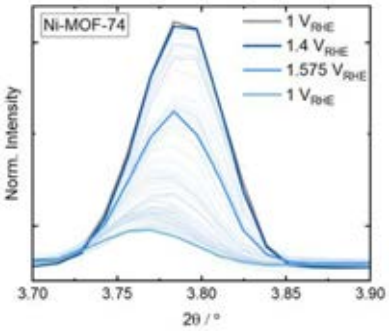


OER performance is generated by the destruction of the framework, yielding a highly active, amorphous Ni-MOF*.



The pristine Ni-MOF catalyst is not the active catalyst; the engineered crystal structure irreversible collapse during water splitting, enhancing catalyst performance

Operando XRD



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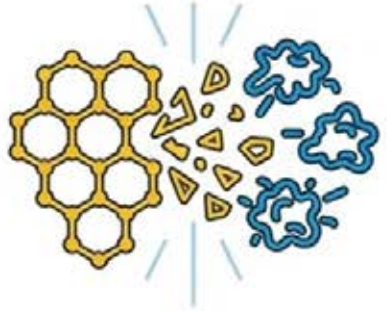
From Crystal to Catalyst: Ni-Metal Organic Compounds (Ni-MOC)

Irreversible transformation of Ni-MOF

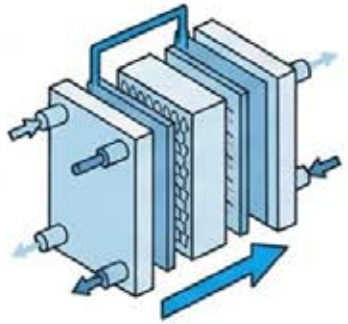


MOF-74 derives its exceptional OER activity not from its crystalline framework, but from irreversible amorphization into dynamic NiOOH-like clusters.

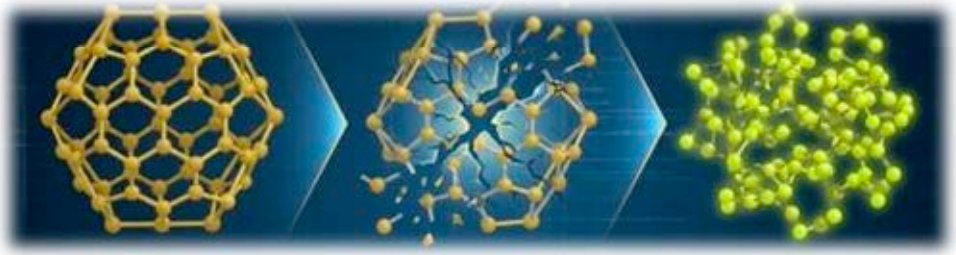
Direct synthesis of the active phase: Ni-MOC

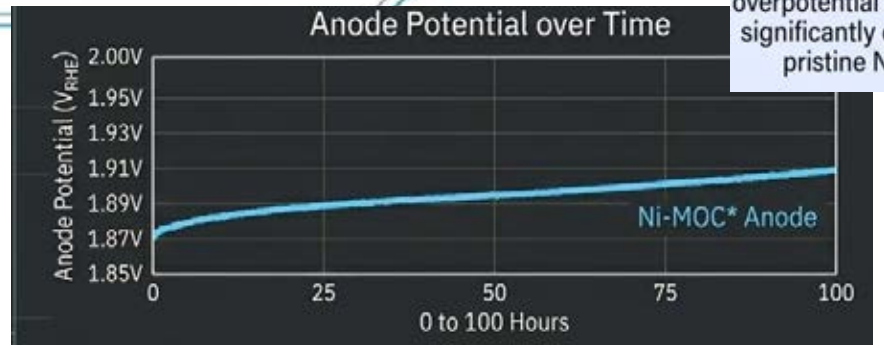
Bypassing high-temperature crystal synthesis to directly precipitate the amorphous phase (Ni-MOC*) yields vastly superior initial activity and radically lowers production complexity

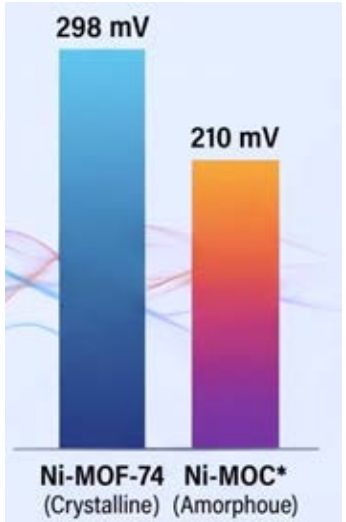
Device validation



Ni-MOC* provides a highly scalable, robust non-noble metal anode solution, proven stable over 100 hours of continuous AEM water electrolysis at 500 mA cm^{-2}.







Enhanced Catalytic Efficiency

Ni-MOC* exhibits an overpotential of only 210 mV, significantly outperforming pristine Ni-MOF-74.

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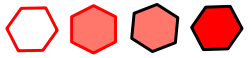
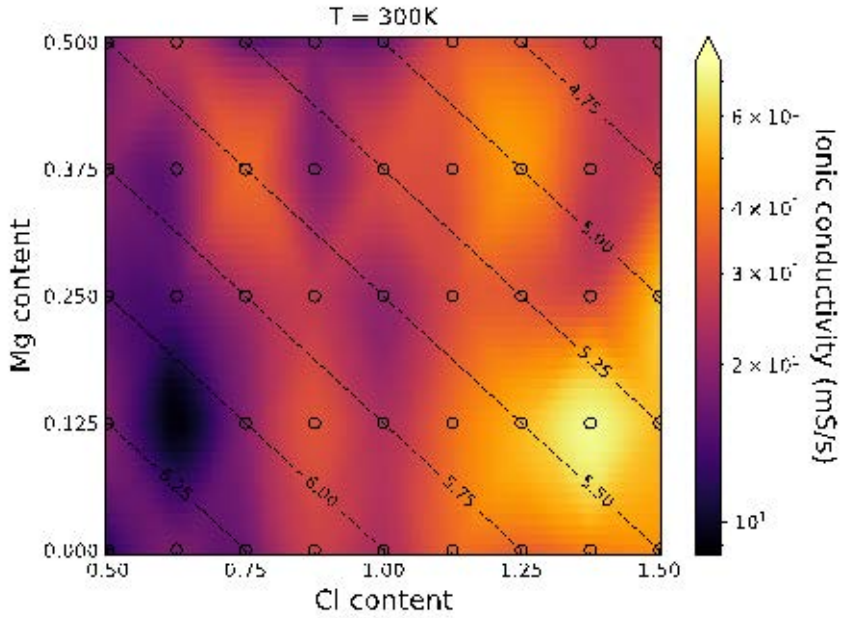
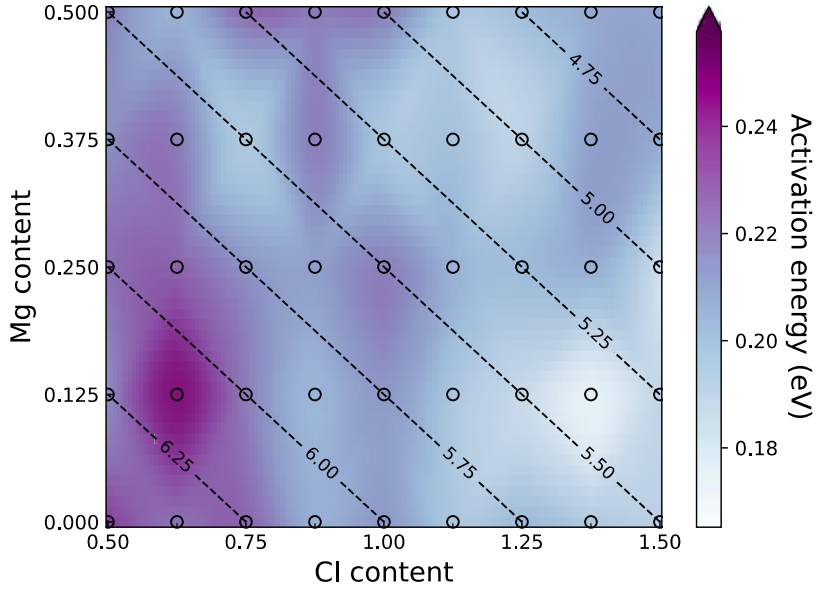
BATTERY MATERIALS



OPTIMAL DOPING IN SOLID-STATE BATTERIES





- The region with the highest ionic conductivity corresponds to high Cl and low Mg content.
- These results were confirmed by experiments, and two patents granted.


(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
(19) World Intellectual Property Organization
International Bureau
(43) International Publication Date
22 June 2023 (22.06.2023)
WIPO | PCT
(10) International Publication Number
WO 2023/110697 A1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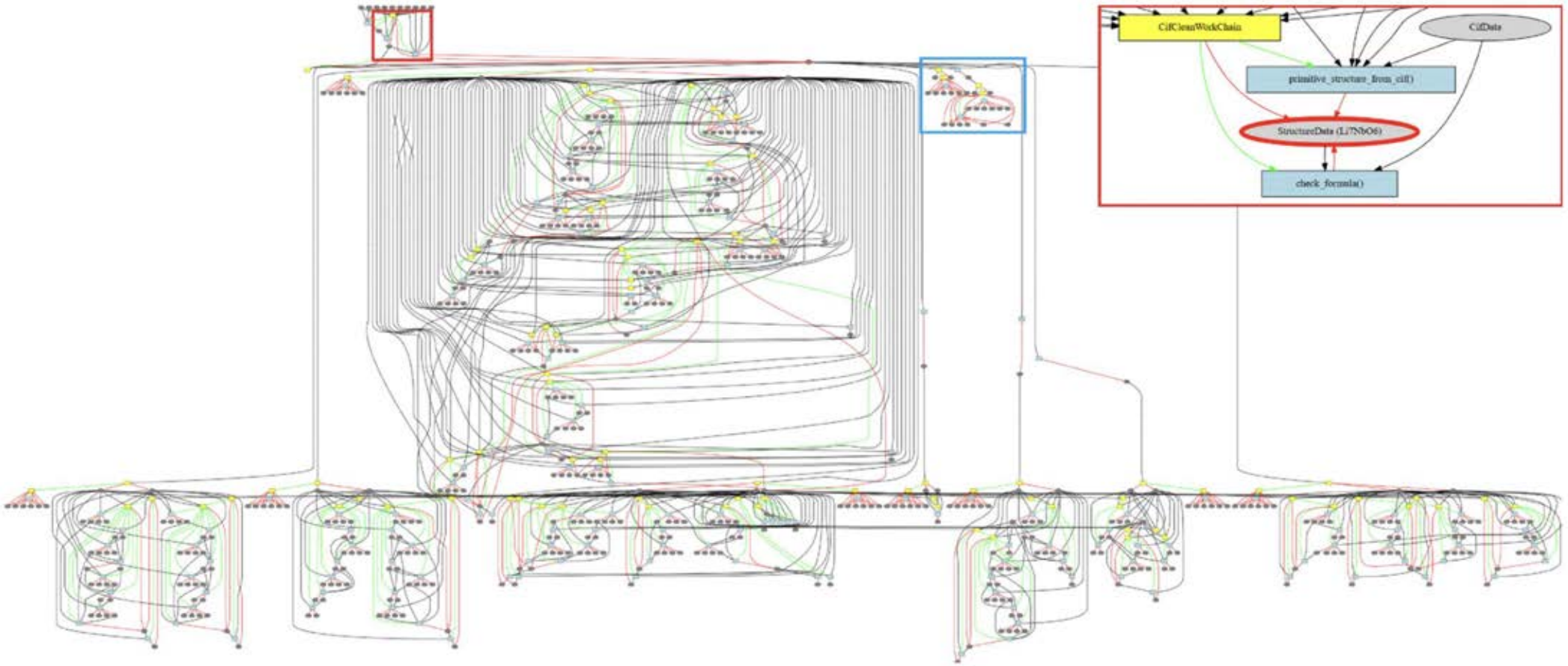
(19) World Intellectual Property Organization
International Bureau
(43) International Publication Date
22 June 2023 (22.06.2023)
WIPO | PCT
(10) International Publication Number
WO 2023/111083 A1

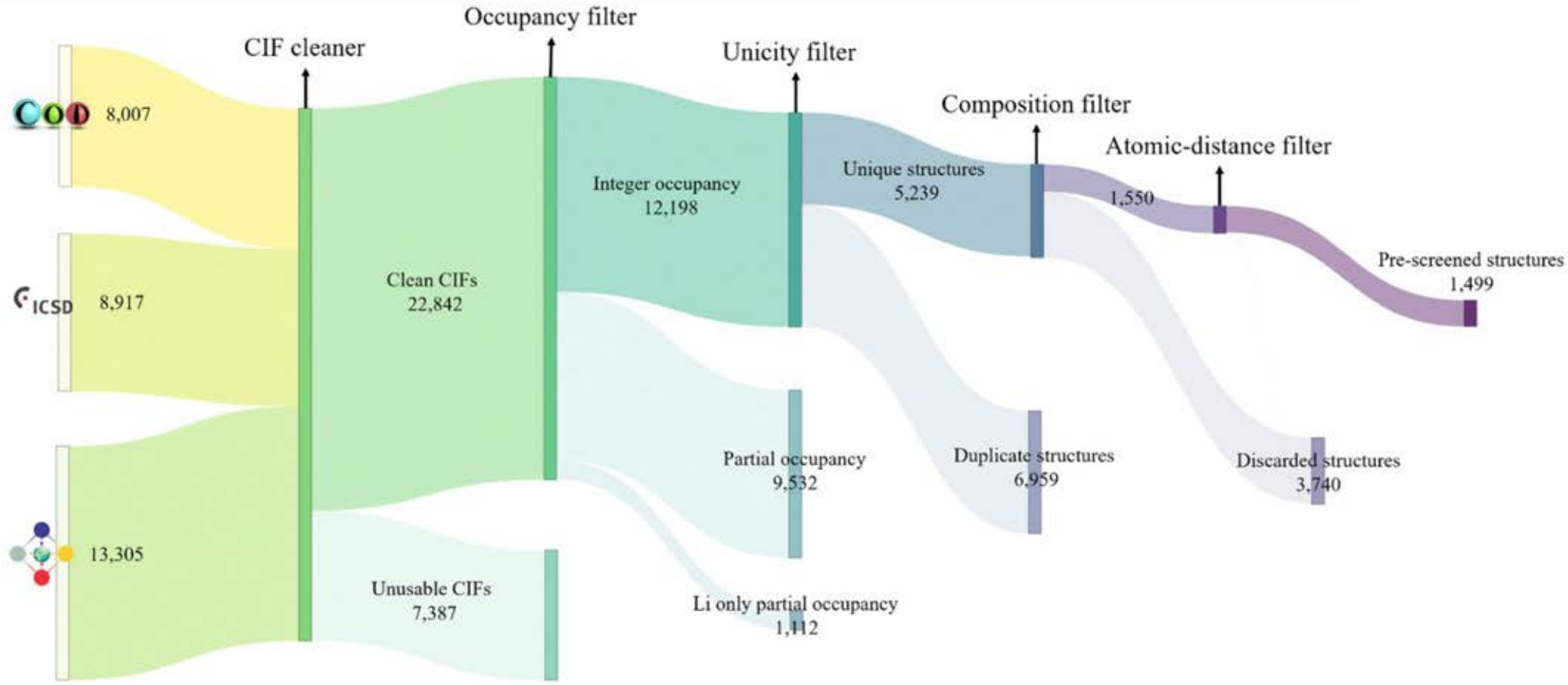
S.Muy, Solvay team, and N. Marzari, Chemistry of Materials 37, 2395 (2025)

HIGH-THROUGHPUT SCREENING OF ALL LI-ION MATERIALS



L. Kahle, A. Marcolongo, and N. Marzari, Energy Environ. Sci. 13, 928 (2020).
T. S. Thalur, L. Ercole, and N. Marzari, Energy Environ. Sci. 19, 3214 (2026)

SOLID-STATE LI-ION CONDUCTORS



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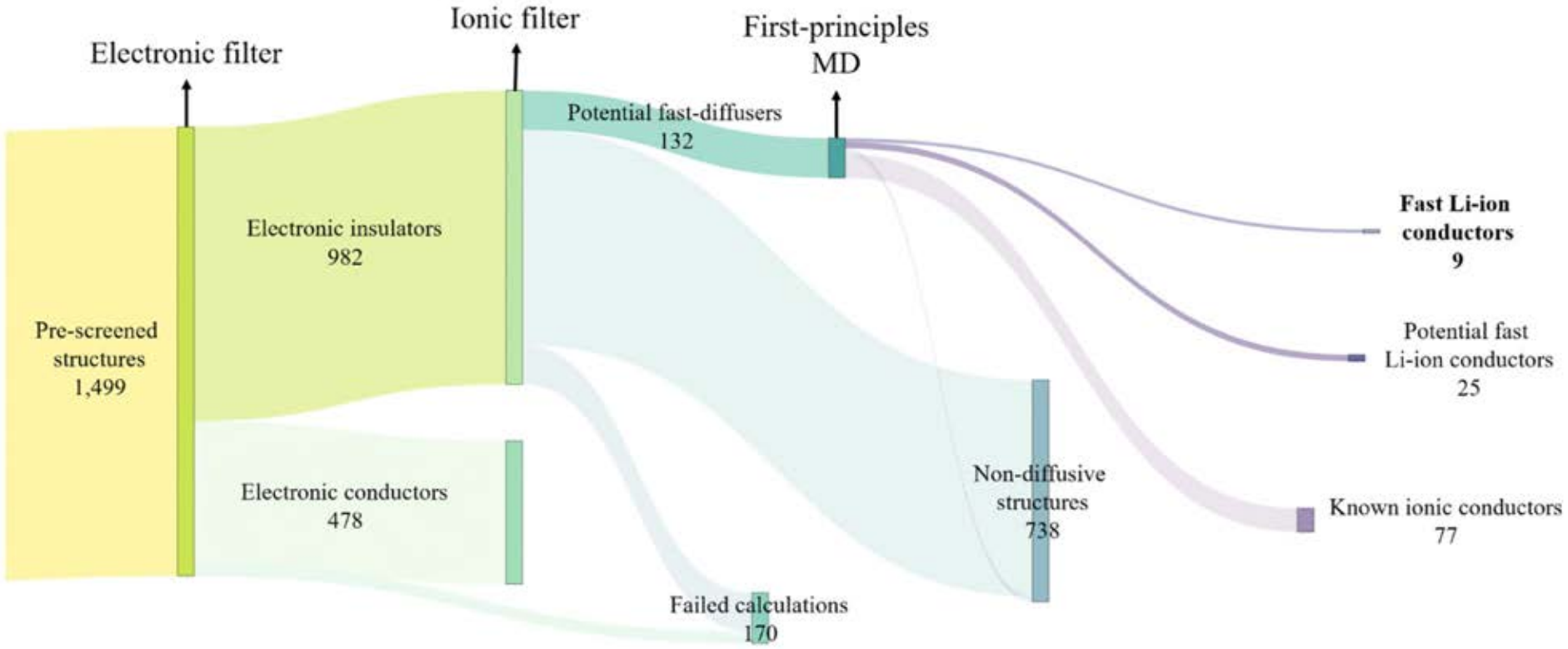
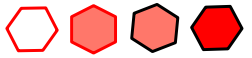
SOLID-STATE LI-ION CONDUCTORS



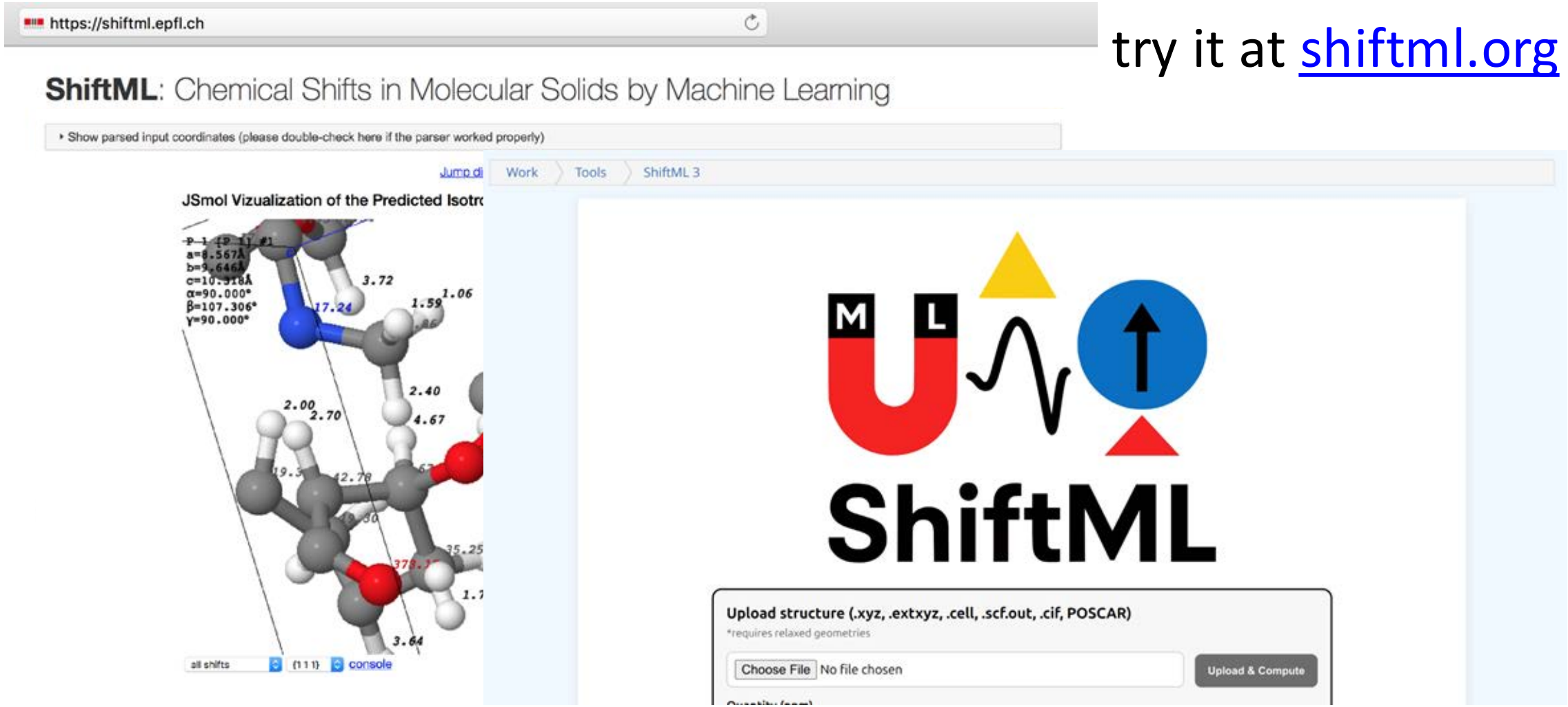
Structure	Database
Li_4CO_4	ICSD
$LiCsI_2$	ICSD
Li_3CsBr_4	ICSD
$Li_3Cs_2Br_5$	ICSD
Li_7NbO_6	MPDS
$Li_3Cs_2I_5$	ICSD
$LiCs_3Cl_4$	ICSD
$Li_4Mo_3O_8$	MPDS
Li_5NaN_2	ICSD
$Li_1Ga_1I_4$	ICSD
$Li_1Ga_1Br_3$	ICSD
$Li_2Cs_1I_3$	ICSD
$Li_{10}Ge_1P_2S_{12}$	—
$Li_5Cl_3O_1$	ICSD
$Li_5Cl_3O_1$	ICSD
$Li_7Ta_1O_6$	ICSD

L. Kahle, A. Marcolongo, and N. Marzari, Energy Environ. Sci. 13, 928 (2020).
T. S. Thalur, L. Ercole, and N. Marzari, Energy Environ. Sci. 19, 3214 (2026)

MOLECULAR CRYSTALS AND NMR CRYSTALLOGRAPHY



MACHINE LEARNING OF CHEMICAL SHIFTS IN MOLECULAR SOLIDS

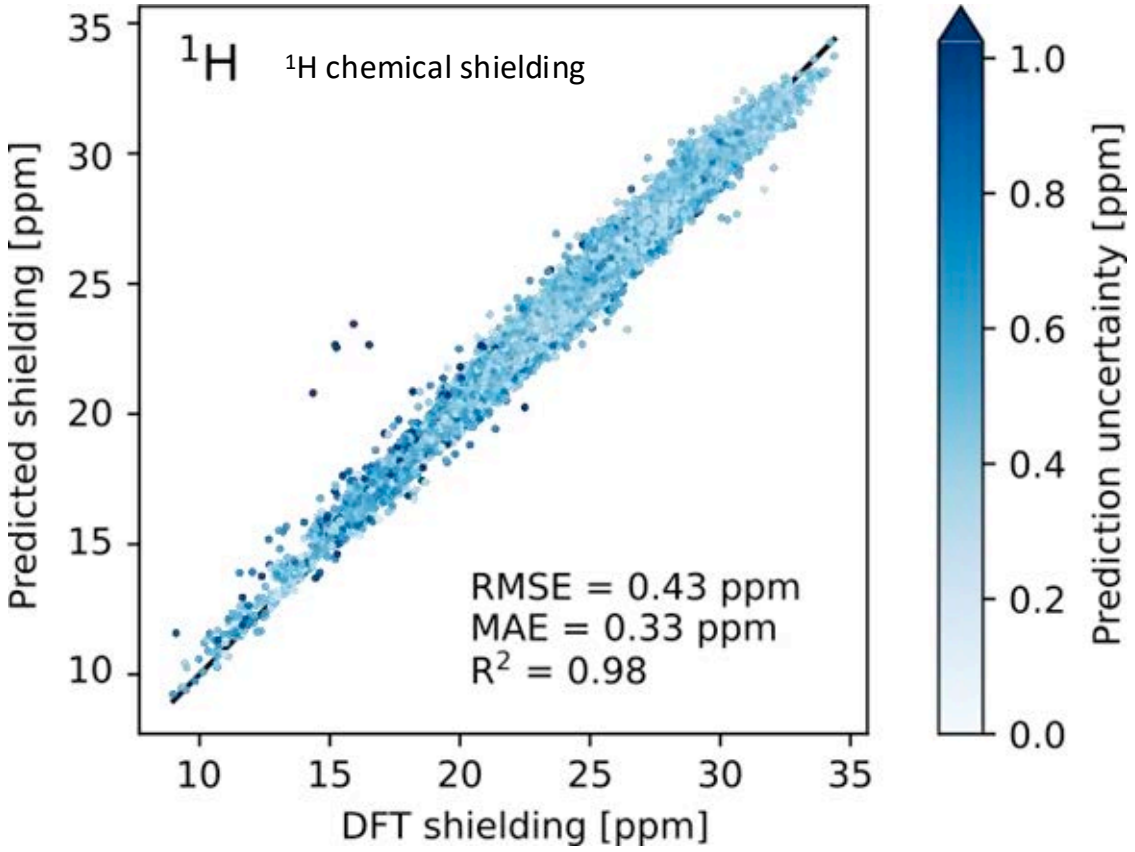


try it at shiftml.org

Paruzzo, Hofstetter, Musil, De, Ceriotti, Emsley, Nature Comm. **9**, 4501 (2018)

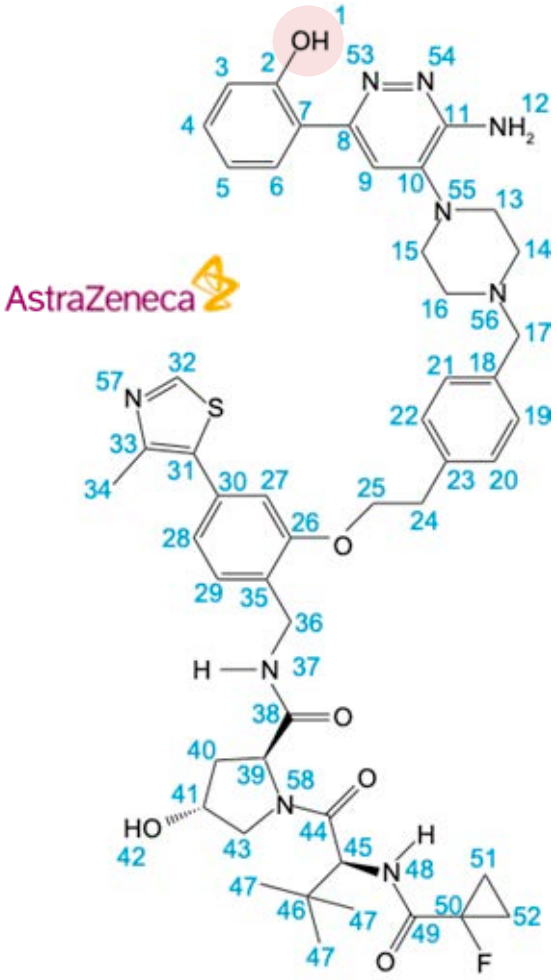
NOW VERY COMPREHENSIVE

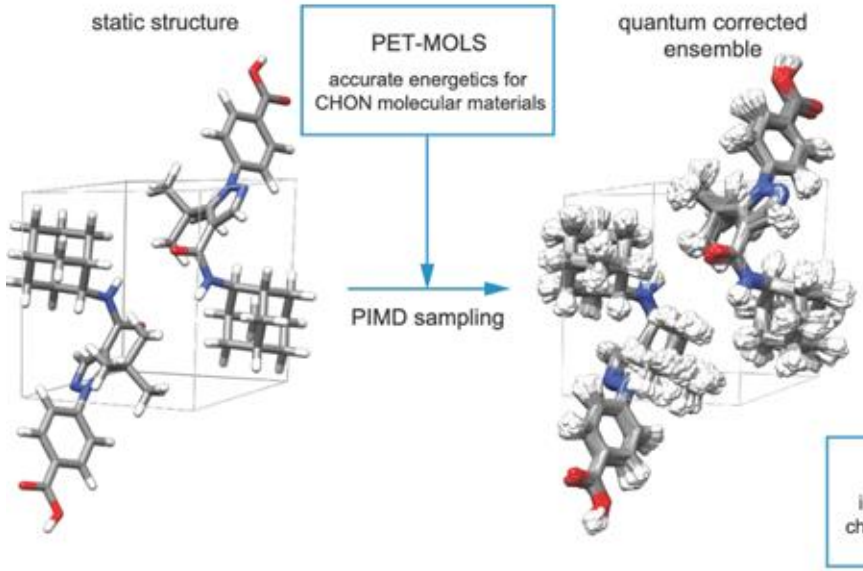
- 12 elements (H, C, N, O, S, P, F, Cl, K, Mg, Na, Ca)
- Full tensor including anisotropy
- 10,593 training crystal structures
- DFT-optimised + MD structures
- Built-in uncertainty quantification
- GNN / PET model

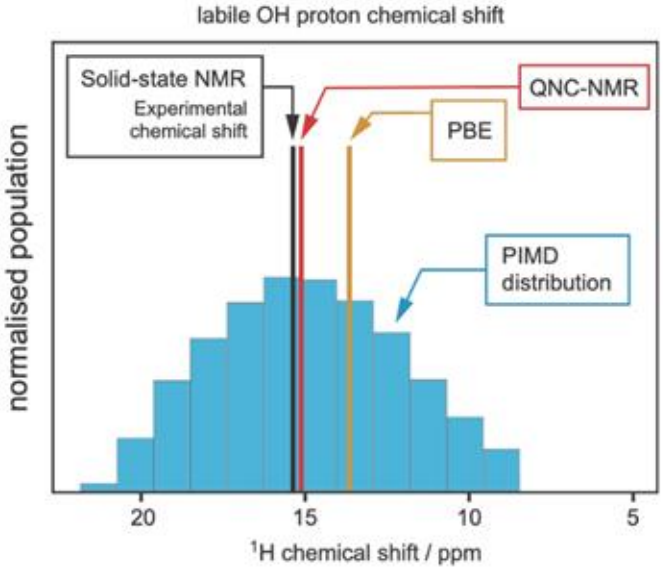


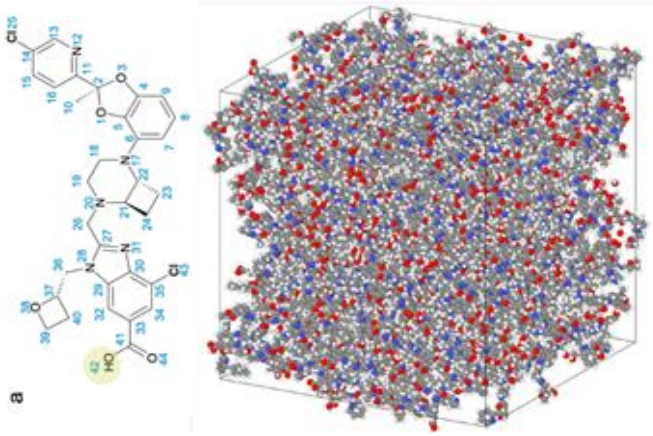
Paruzzo, Hofstetter, Musil, De, Ceriotti, Emsley, Nat. Commun. 9, 4501 (2018)
Cordova, Engel, Stefaniuk, Paruzzo, Hofstetter, Ceriotti, Emsley, J. Phys. Chem. C. 126, 16710–16720 (2022)
Kellner, Holmes, Rodriguez-Madrid, Viscosi, Zhang, Emsley, Ceriotti, J. Phys. Chem. Lett. 16, 8714 (2025)

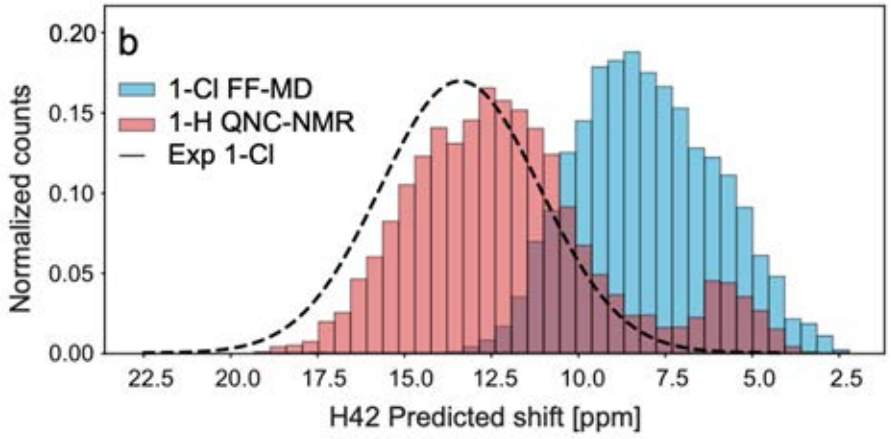
CHARACTERIZATION OF H BONDS, INCLUDING QUANTUM EFFECTS











Torodii et al., Nature Comm. 16, 9694 (2025)

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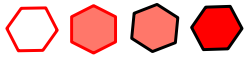
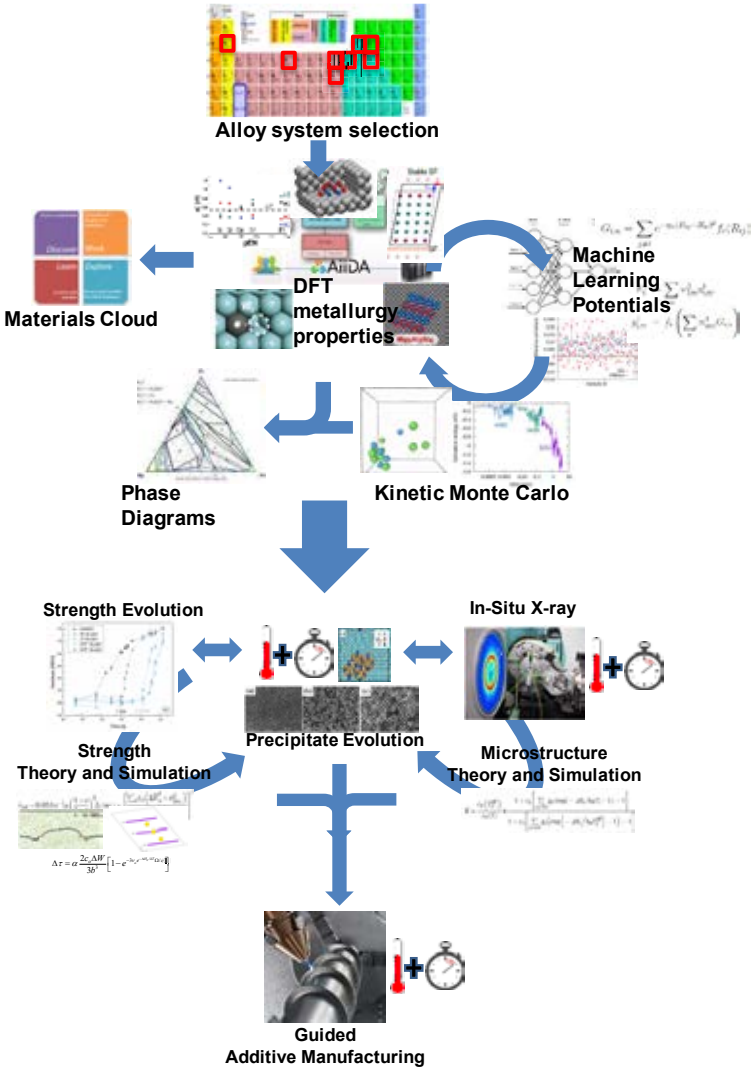
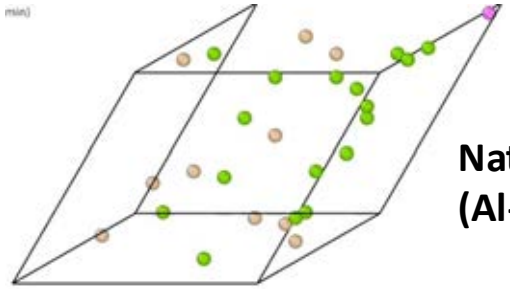
COMPLEX ALLOYS AND ADDITIVE MANUFACTURING



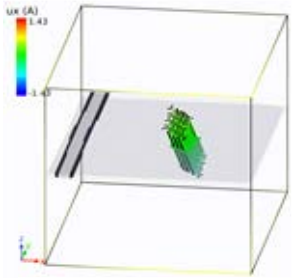
Design and discovery of complex alloys



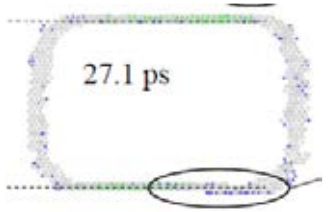
Lightweight Alloys:
DFT-trained ML potentials for Al-Mg-Si-Cu-Zn alloys



Natural aging in Al-Mg-Si (Al-6xxx)

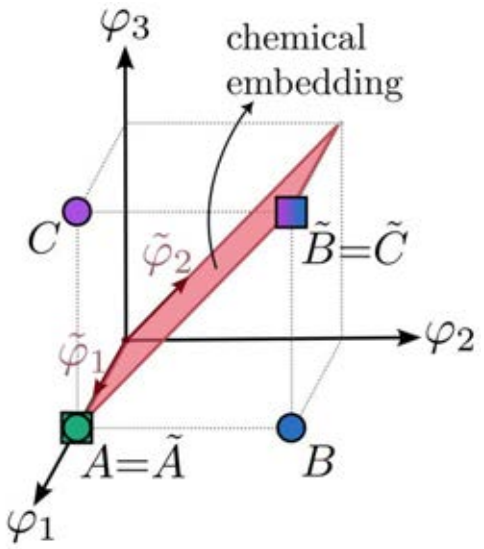


Peak-aged strengthening (Al-6xxx)



Mechanism of prismatic slip in Mg

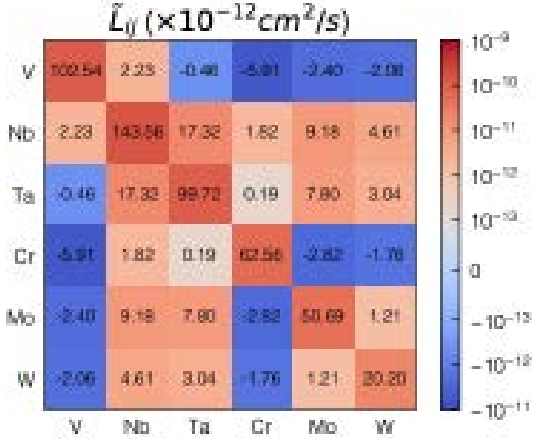
COMPUTATIONAL TOOLS FOR MODELING COMPLEX ALLOYS



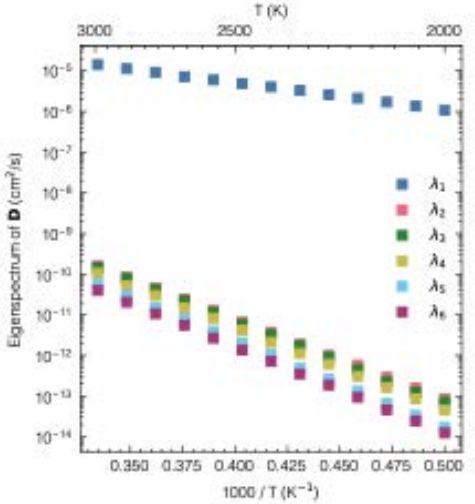
***embedded* cluster expansions** for predicting thermodynamic and kinetic properties of *high-entropy alloys*

Finite-temperature **diffusion constants of high-entropy alloys** from electronic structure calculations

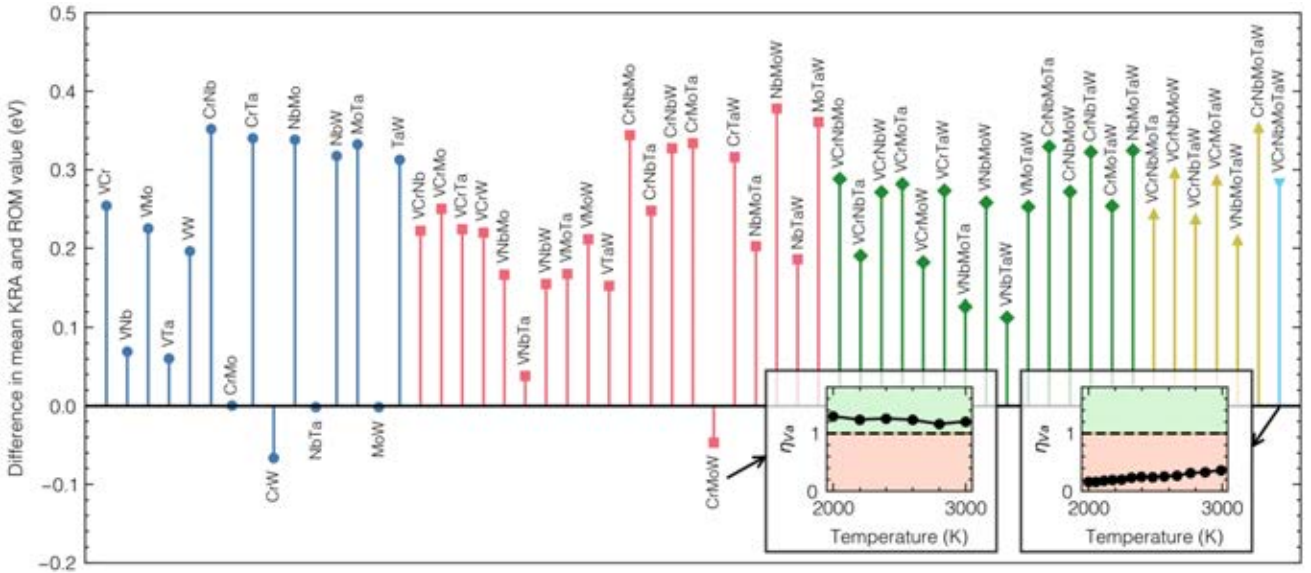
Onsager mobilities



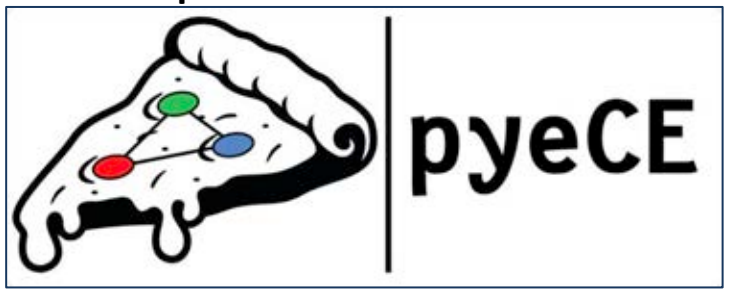
Eigenspectrum of D



Elucidate **origins of sluggish diffusion** and *screen* for fast/slow diffusion



Open-Source Software



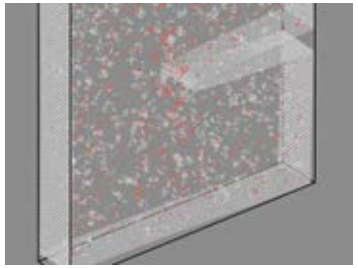
github.com/epfl-mades/pyece

Swiss National Science Foundation

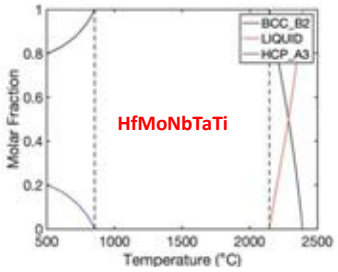
Theory-driven design, fabrication and testing of ductile refractory alloys

Computational design of strong and ductile "High-Entropy" Refractory Alloys

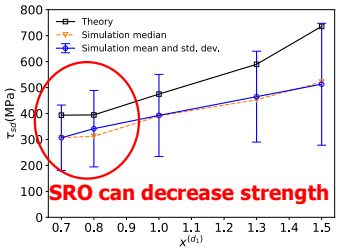
Experimental fabrication, validation and testing



New mechanism of ductility in BCC alloys



Phase behavior



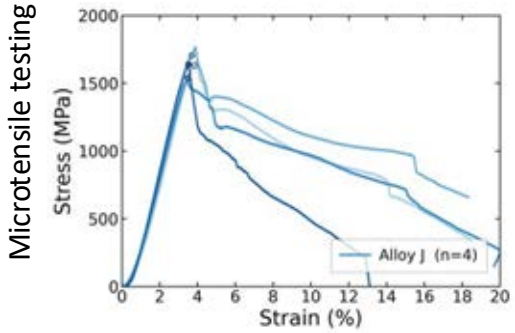
Effect of Short-range Order on Strength

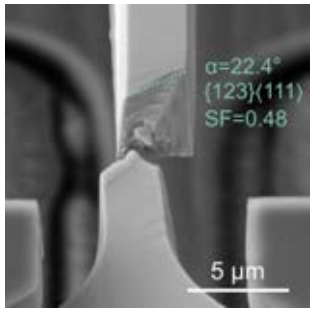
Alloy	r_a	r_a^*	ρ	VEC	r_a/ρ	T^*	T_m
$Hf_{25}Mo_{25}Nb_{25}Ti_{25}$	1.66	0.56	9.46	4.75	176.10	812	2028
$Hf_{20}Mo_{15}Nb_{30}Ti_{35}$	1.11	0.27	8.60	4.60	129.71	831	2011
$Hf_{15}Mo_{20}Nb_{35}Ti_{30}$	1.13	0.29	8.19	4.65	137.70	710	2054
$Hf_{20}Mo_{15}Nb_{35}Ti_{30}$	1.14	0.29	8.79	4.65	129.56	855	2045
$Hf_{15}Mo_{20}Nb_{30}Ti_{35}$	1.15	0.30	8.38	4.70	137.45	735	2098
$Hf_{20}Mo_{15}Nb_{40}Ti_{25}$	1.16	0.30	8.98	4.70	129.27	880	2073

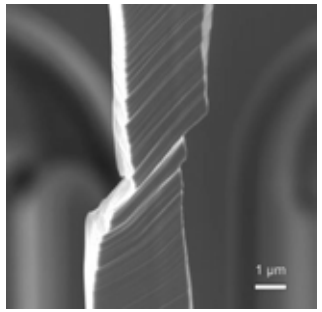
Multi-property alloy design

Hf-Mo-Nb-Ti alloy

Ductile alloy at **room temperature**



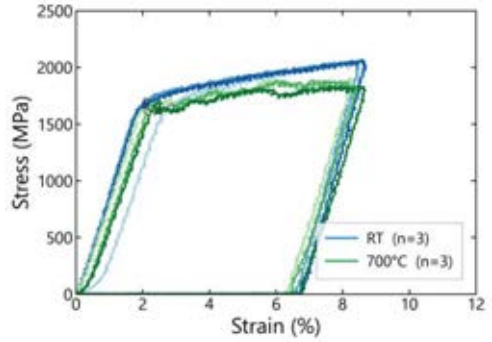




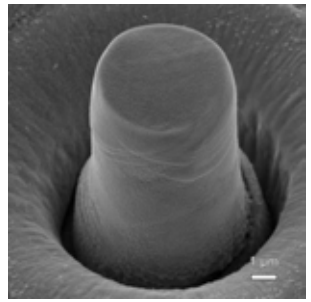
Strong at **high temperatures**

RT: 800 MPa

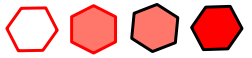
700°C: 777 MPa



700 C

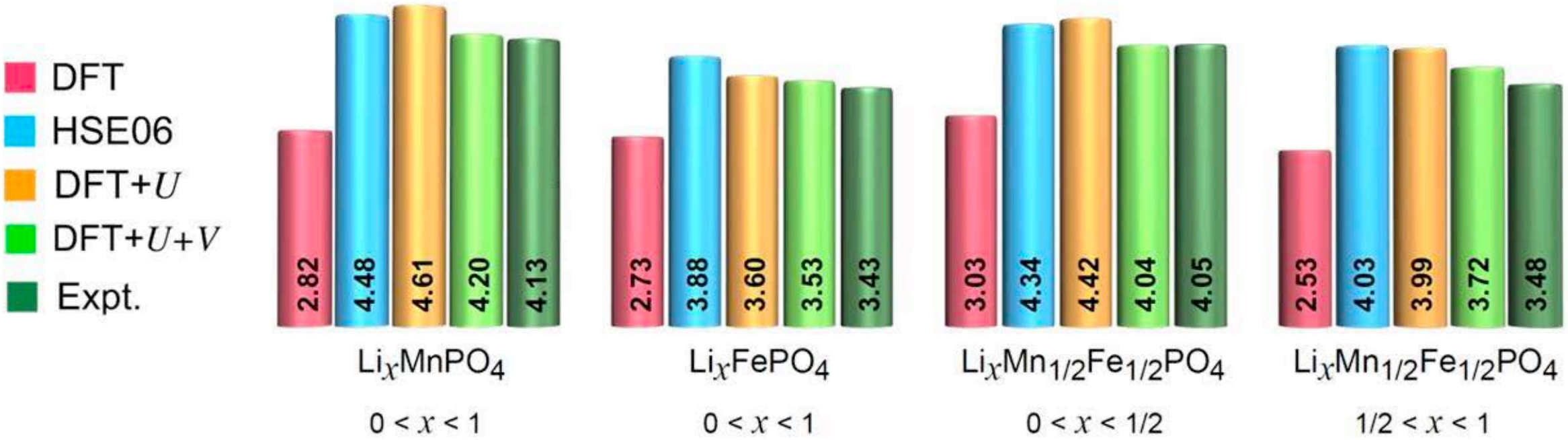


PREDICTIVE ACCURACY: THE FUNCTIONAL ROUTE



LITHIUM INTERCALATION VOLTAGES

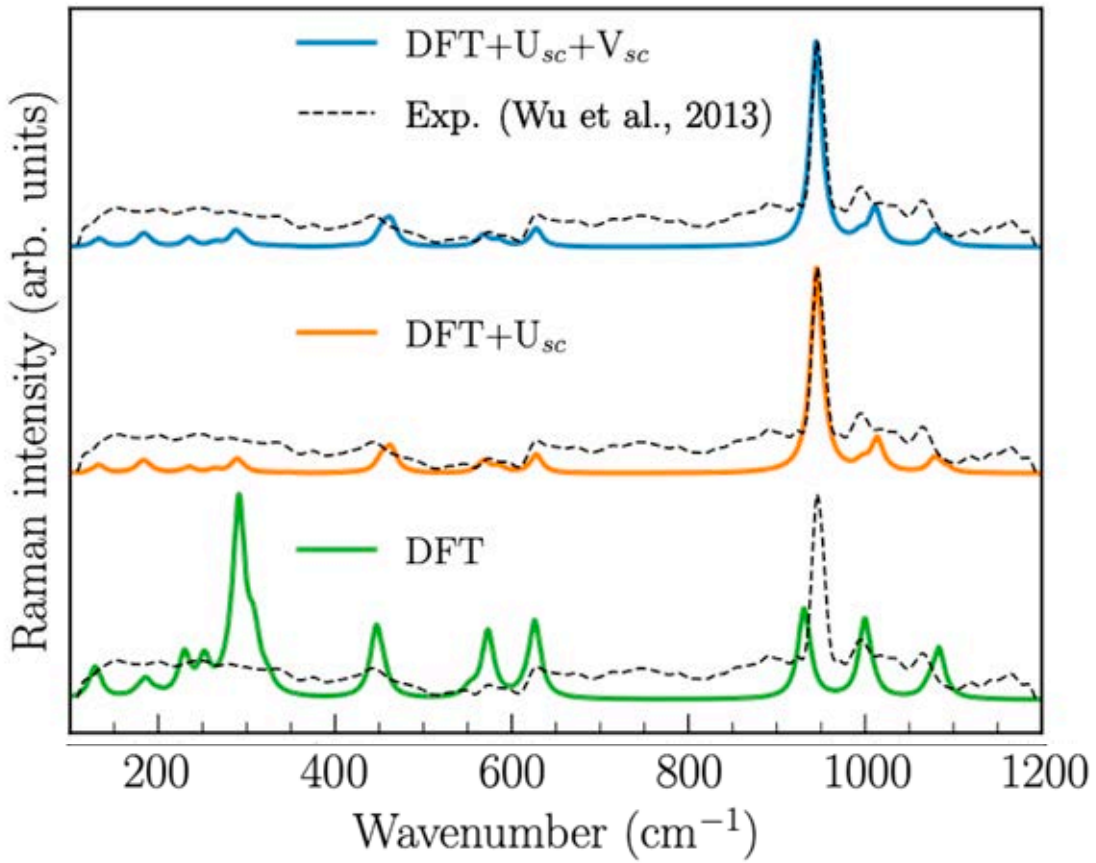
$$\Phi = -\frac{E(\mathrm{Li}_{x_2}\mathrm{S}) - E(\mathrm{Li}_{x_1}\mathrm{S}) - (x_2 - x_1)E(\mathrm{Li})}{(x_2 - x_1)e}$$



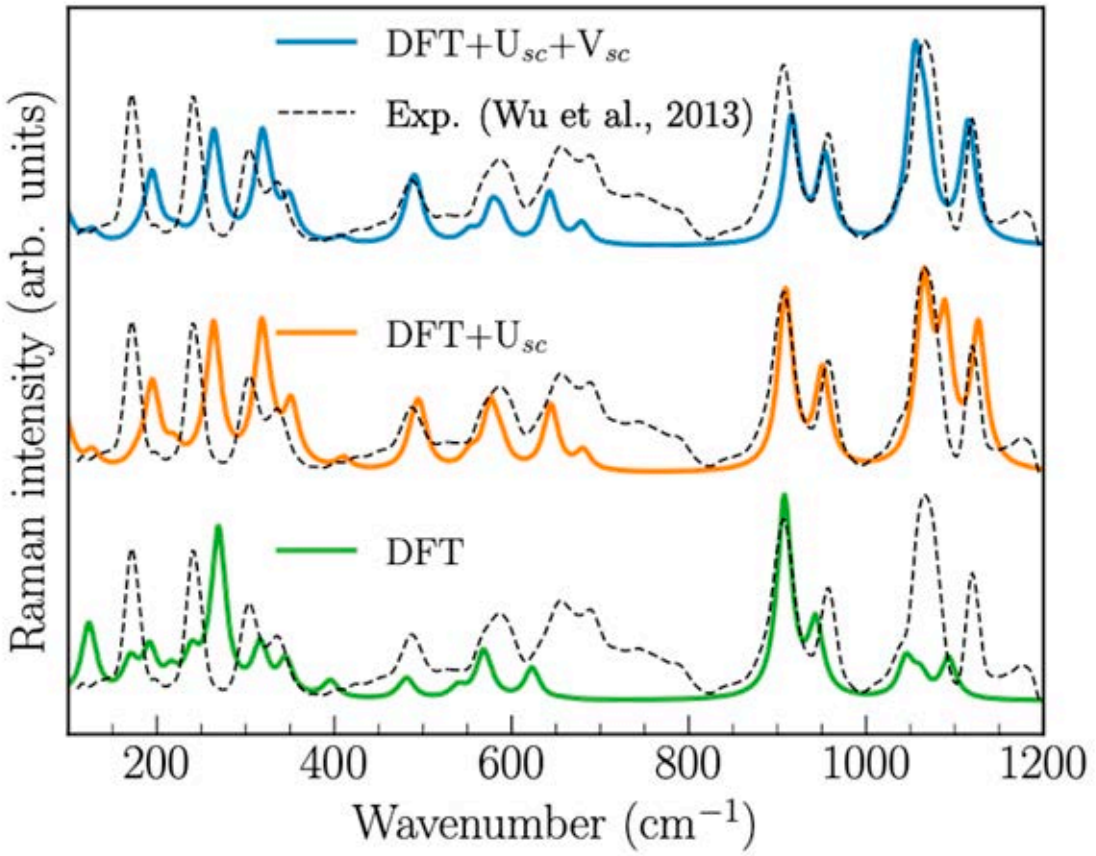
M. Cococcioni and N. Marzari, Phys. Rev. Materials 3, 033801 (2019)
I. Timrov, F. Aquilante, M. Cococcioni, and N. Marzari, Phys. Rev. X Energy 1, 033003 (2022)

AUTOMATED VIBRATIONAL SPECTROSCOPIES

$LiFePO_4$



$FePO_4$

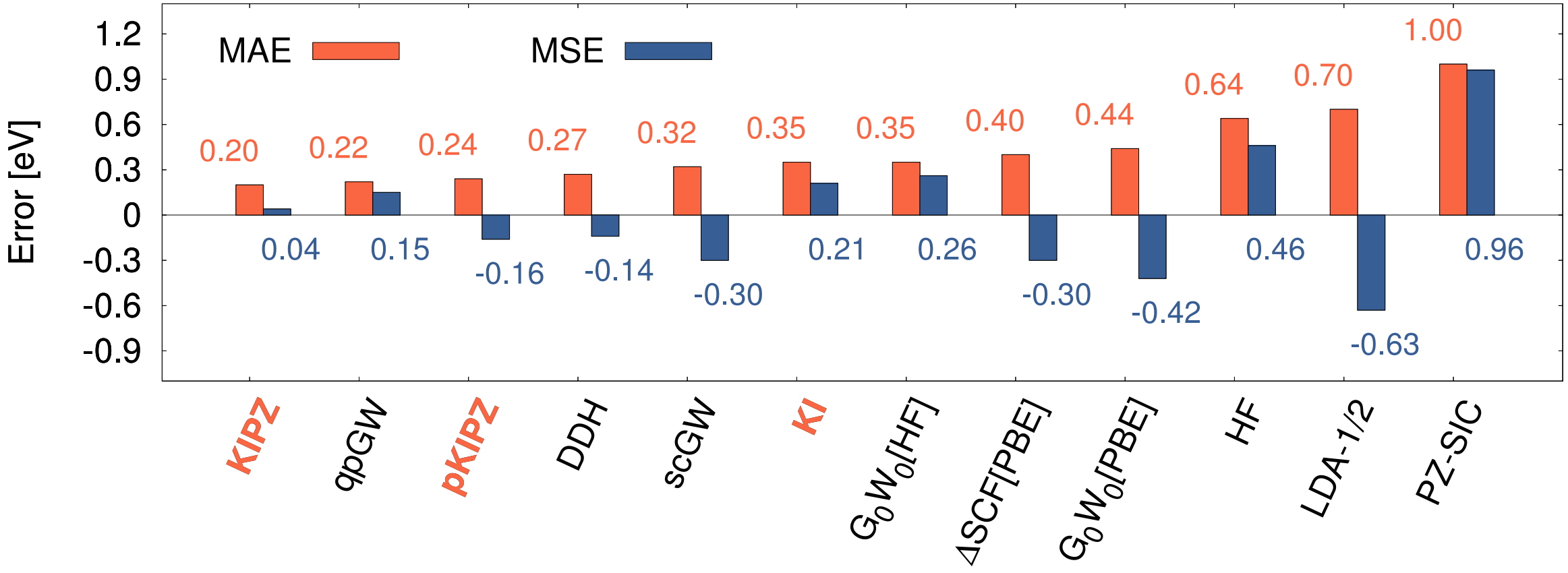


AiiDA

L. Bastonero and N. Marzari, npj Computational Materials 10, 55 (2024)

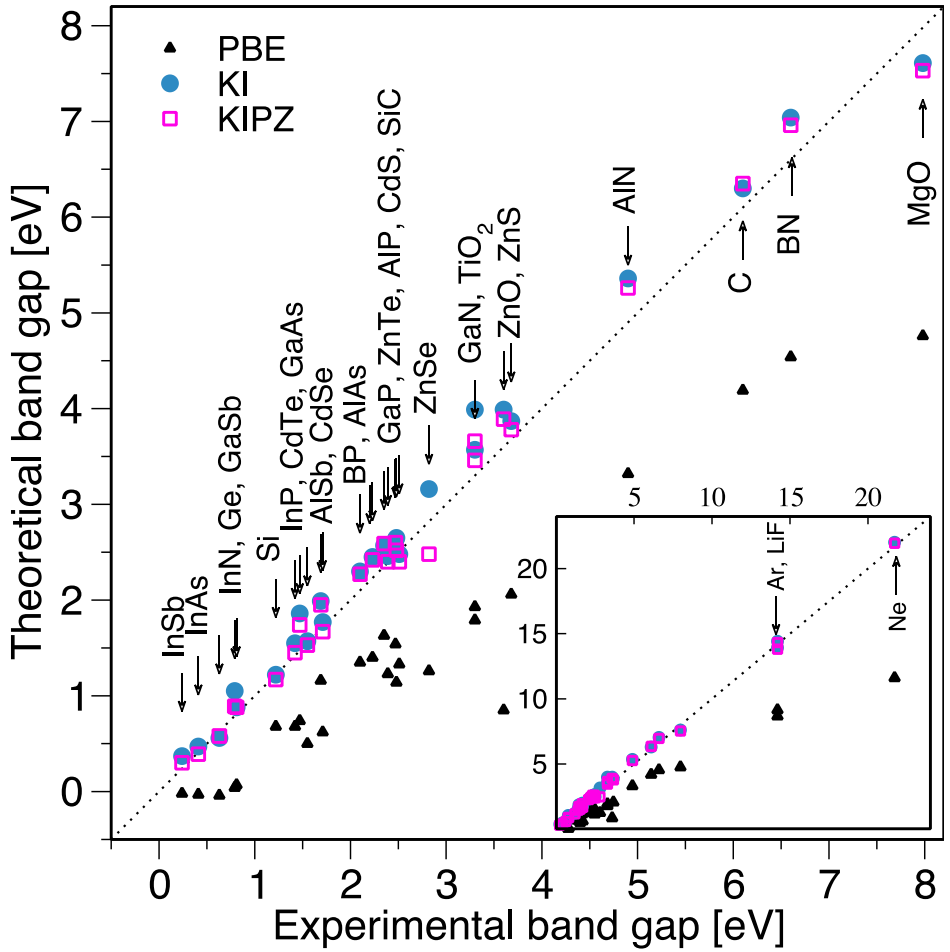
Swiss National Science Foundation

KOOPMANS: FUNCTIONALS FOR EXCITATIONS (MOLECULES)



N. Colonna, N.L. Nguyen, A. Ferretti, and N. Marzari, JCTC 15, 1905 (2019)

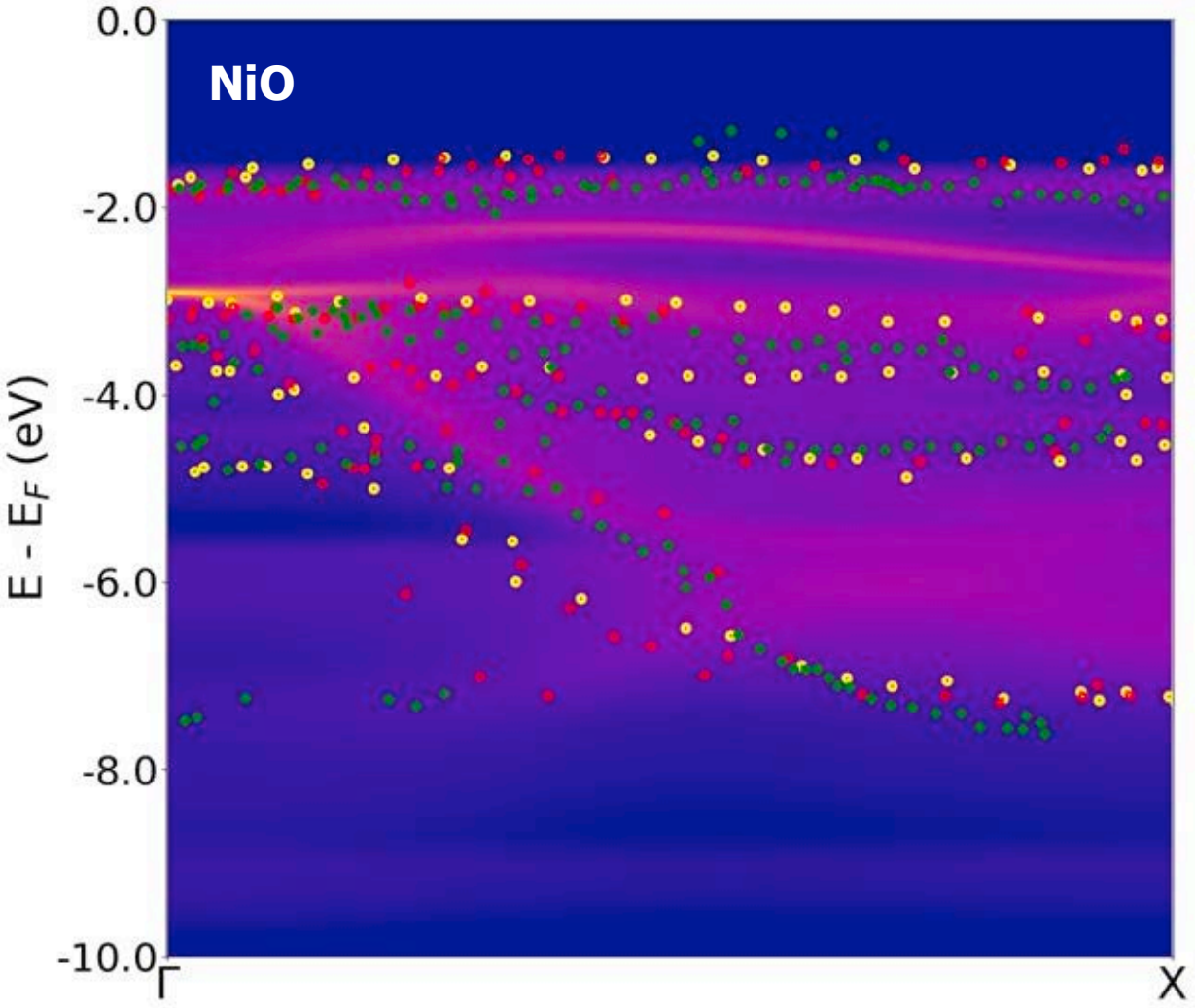
KOOPMANS: FUNCTIONALS FOR EXCITATIONS (SOLIDS)

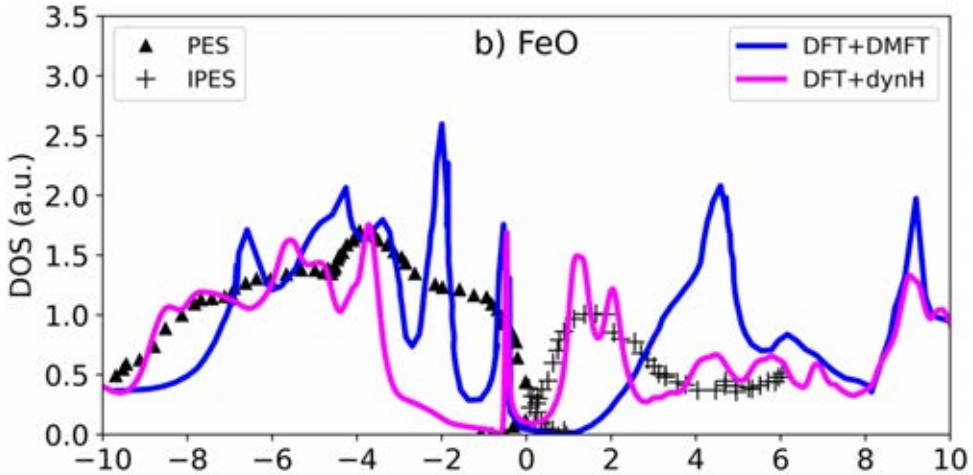


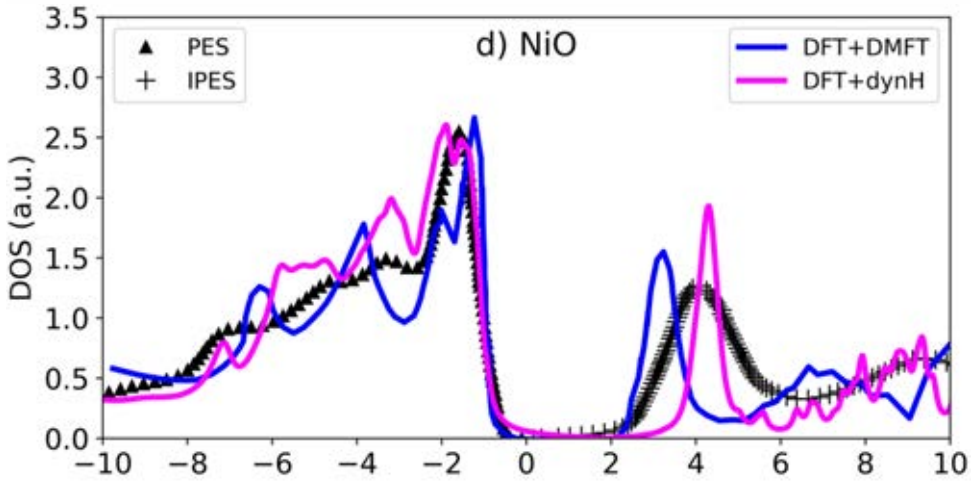
MAE (eV)	Gap	IP
PBE	2.54	1.09
G_0W_0	0.56	0.39
QSGW	0.18	0.49
KI	0.27	0.19
KIPZ	0.22	0.21

N. L. Nguyen, N. Colonna, A. Ferretti, and N. Marzari, PRX 8, 021051 (2018)

dynH: FUNCTIONALS FOR CORRELATIONS

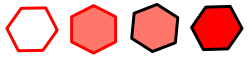






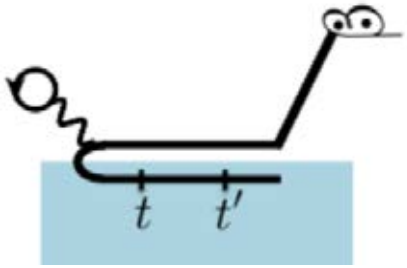
M. Caserta, T. Chiarotti, M. Vanzini, and N. Marzari, arXiv:2503.10893 (2025)

PREDICTIVE ACCURACY: THE MANY-BODY ROUTE

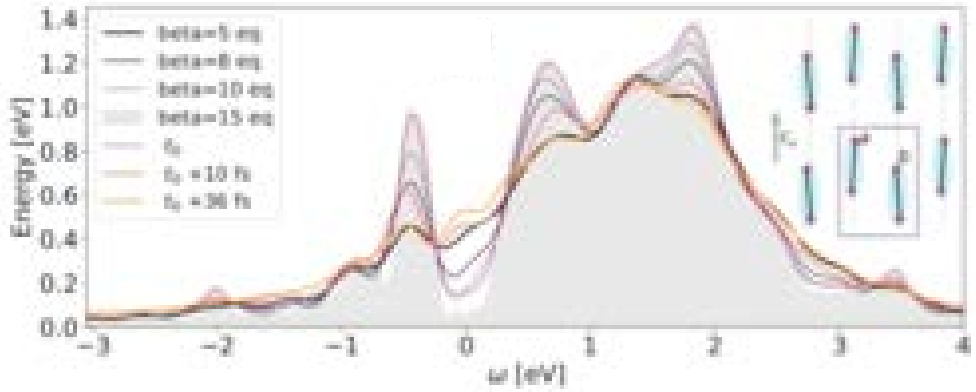


Nonequilibrium electronic structure methods

- Development of software libraries for efficient nonequilibrium Green's function calculations:
  - NESSi — M. Schueler et al., Comp. Phys. Comm. (2020)
  - NESSi2.0 — F. Kuenzel et al., arXiv (2026)



- Ab-initio calculations based on nonequilibrium (GW+)DMFT: Photo-induced dynamics in
  - $1T$-TaS_2 — F. Petocchi et al., PRB (2023)
  - VO_2 — J. Chen et al., PRB (2024)
  - Ta_2NiSe_5 — J. Chen et al., arXiv (2026)

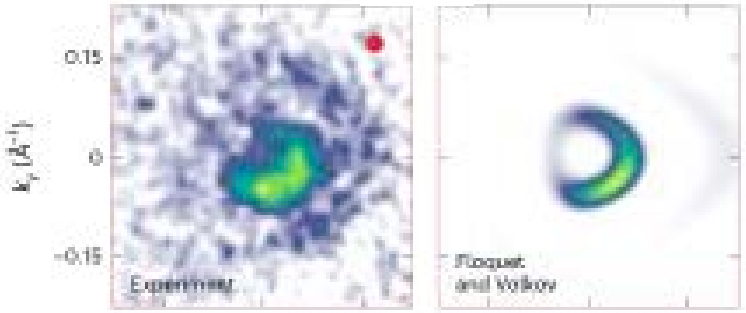


Nonequilibrium electronic structure methods

- Ab initio simulations of time-resolved ARPES:

M. Merboldt, M. Schüler et al., Nat. Phys. (2025)

Code based on Wannier ecosystem
Open-source code release until end of 2026



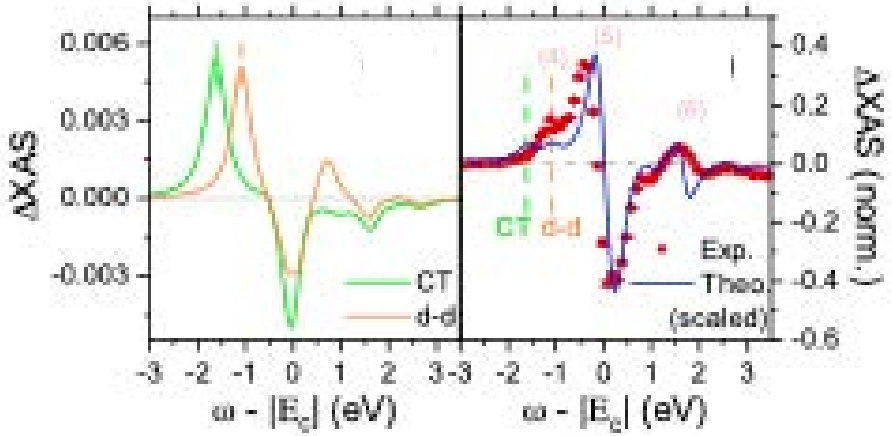
- Nonequilibrium DMFT formalisms for core-level spectroscopies:
  - XAS
  - RIXS

P. Werner et al., PRB (2023)

Lojewski et al., PRB (2024)

M. Eckstein et al., PRB (2020)

P. Werner et al., EPL (2021)

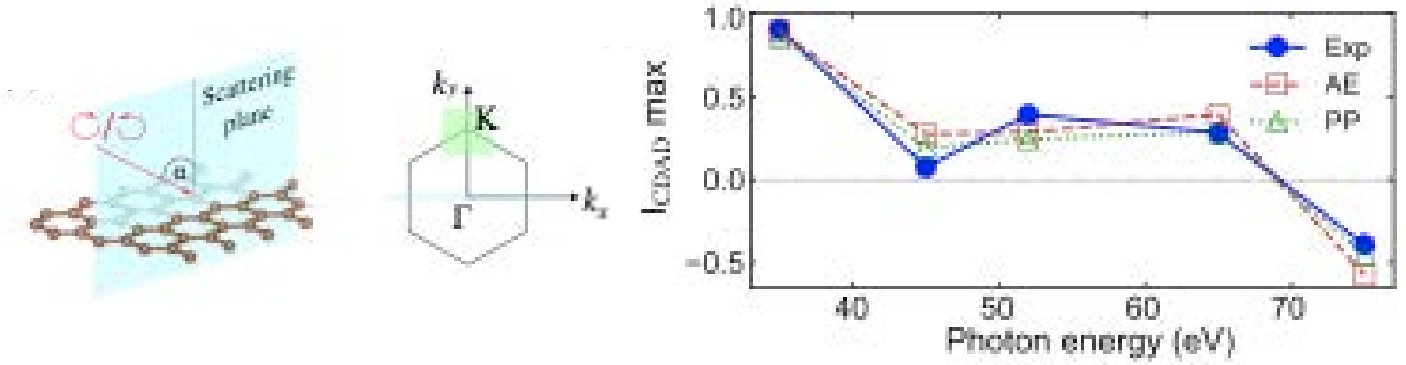


ARPES from first principles

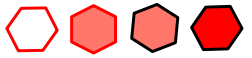
- Development of ab initio ARPES code on top of plane-wave DFT codes
  - Accurate simulation of ARPES
  - Release of open-source code PESKIT this year

Parusa et al. (2026)

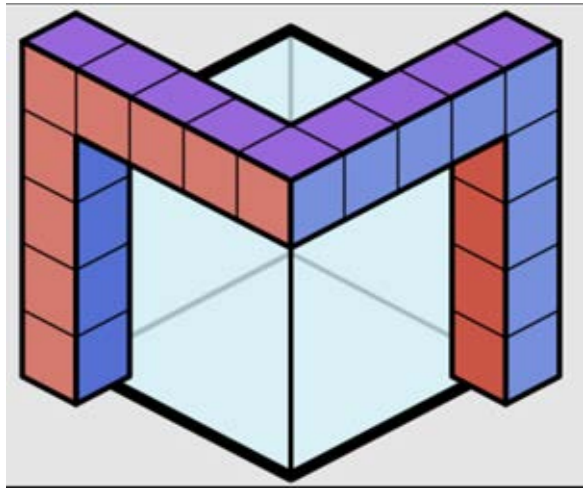
Circular dichroism in ARPES: graphene



ATOMISTIC MACHINE LEARNING AS A SCIENTIFIC PLATFORM

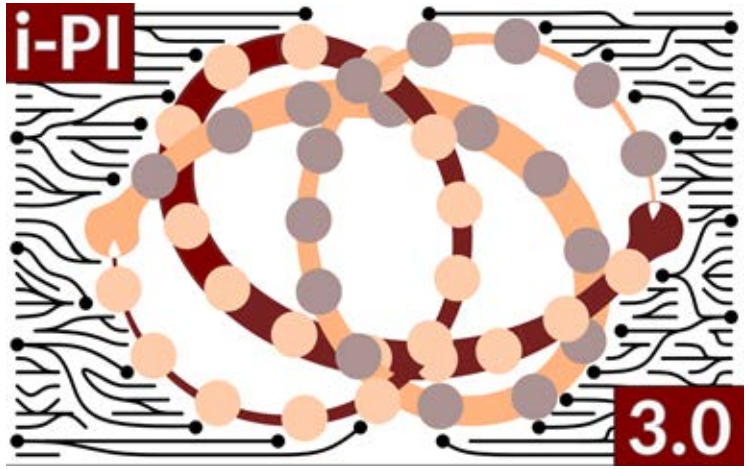


AN OPEN SW STACK FOR ATOMISTIC MACHINE LEARNING



metatensor/metatomic/metatrain
Bigi, “et al.”, Fraux, arXiv (2025)

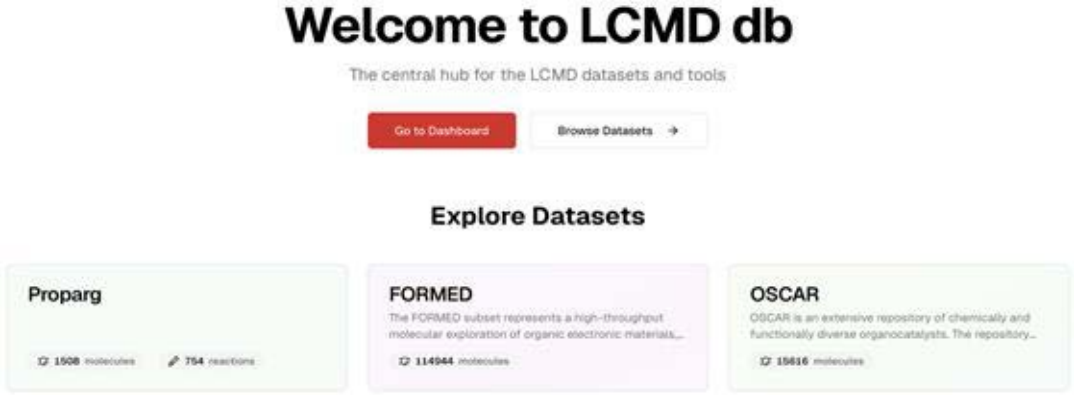
chemiscope.org 1.0



i-PI 3.0 Litman *et al.* JCP (2024)t

torch-pme
Huguenin *et al.* JCP (2025)

Q-stack
Briling *et al.* Zenodo (2025)

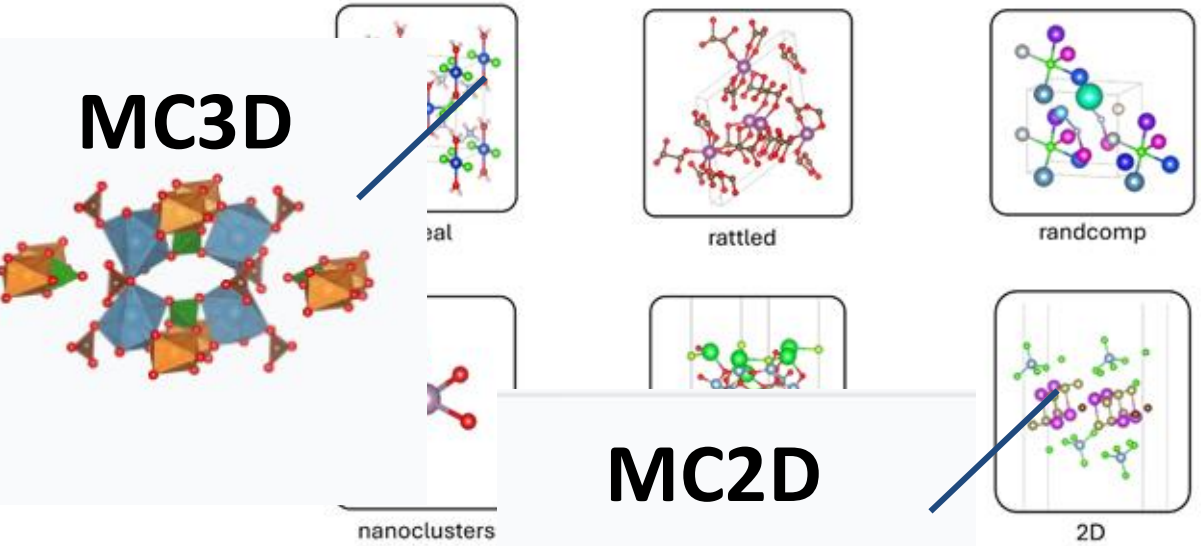


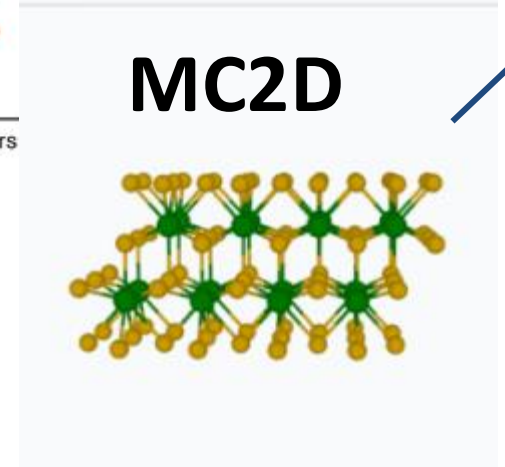
LCDM-db **What You Can Do**
Graux *et al.* GitHub (2026)

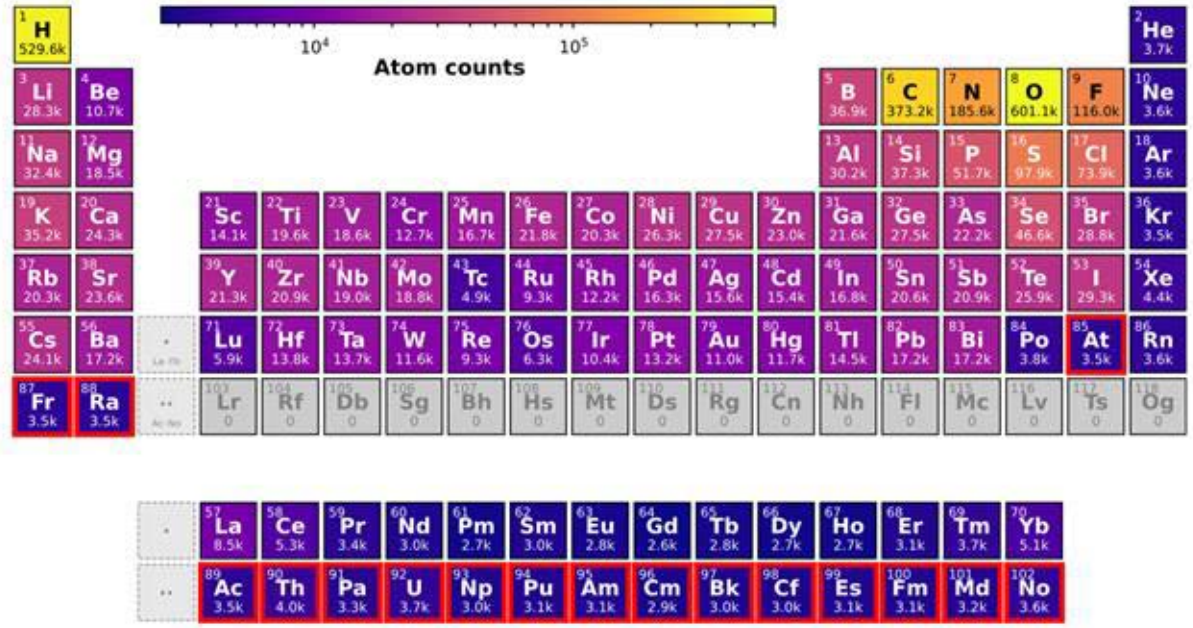
Swiss National Science Foundation

MC3D AND MC2D GOING FOR MASSIVE ATOMIC DIVERSITY

- Training of universal MLIP requires diversity
- Building on materialscloud datasets, to cover the full periodic table







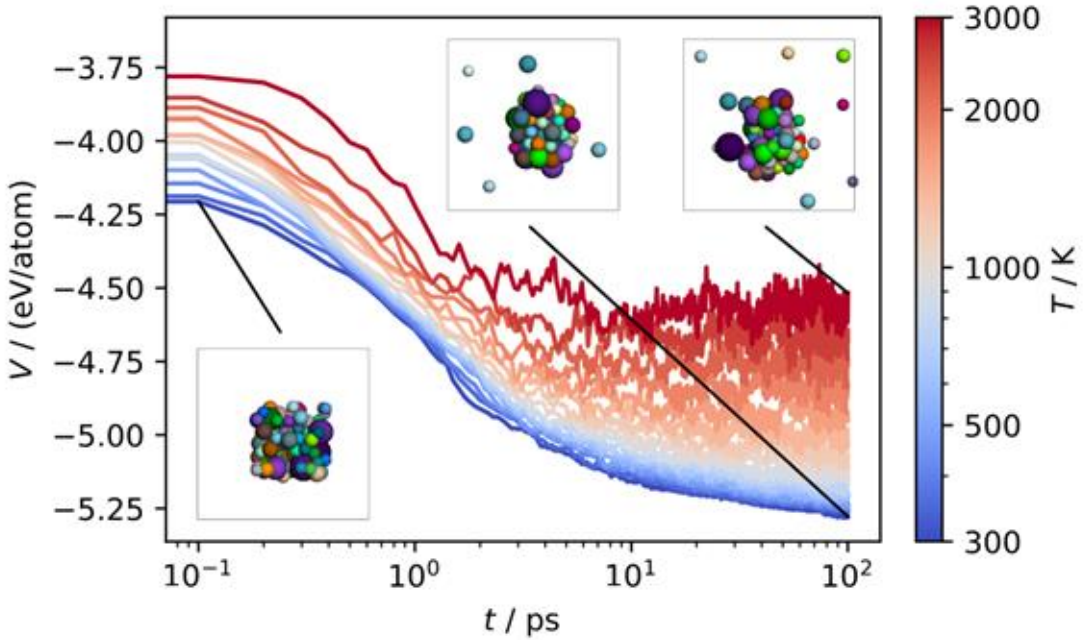
MAD 1.0
Mazitov et al. Sci. Data (2025)

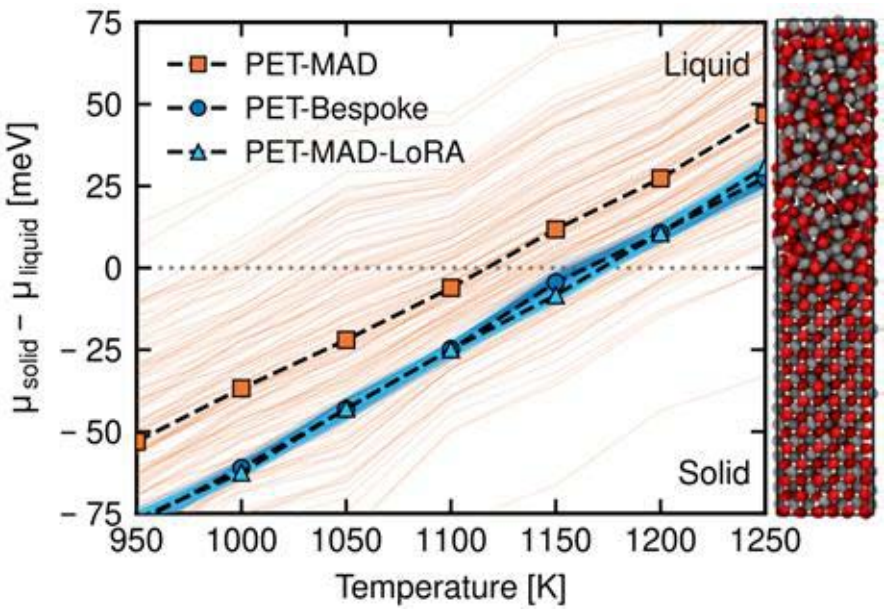
MAD 2.0 (WIP)
Malosso et al. arXiv (2026)

Swiss National Science Foundation

PET-MAD, A FAST, ACCURATE AND ROBUST UNCONSTRAINED MLIP

- Transformer based architecture learns symmetry from data
- Can simulate anything with a half-life of a day or more
- Usable, often without fine-tuning, to power materials discovery

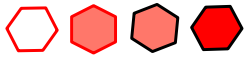




http://peterspackman.github.io/mlip.cpp/

PET-MAD **Mazitov et al. Nature Comm. 2025**

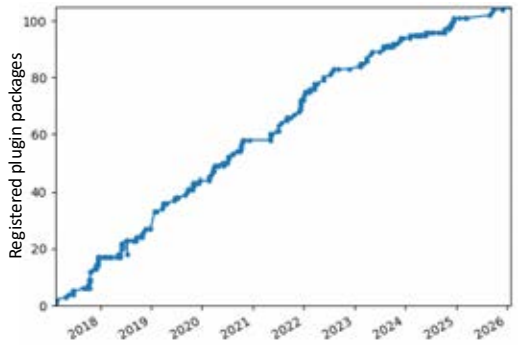
THE DIGITAL INFRASTRUCTURE BACKBONE – AiiDA, EXASCALE READINESS, COMMON WORKFLOWS, AND VERIFICATION



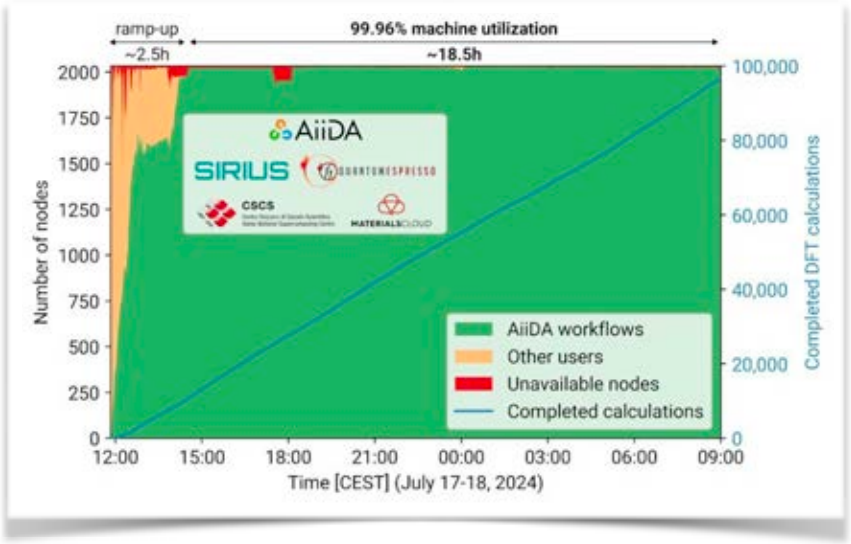
AiiDA: community-driven, exascale-ready,

Creating a community of researchers, towards accessible and common workflows

https://aiida.net/plugin-registry/



Lively community of AiiDA plugin and workflow developers



"Hero run" (Jul 2024)

Record 99.96% machine utilization for ~20 hours

Full CSCS Alps machine: 2033 NVIDIA Grace Hopper nodes, 8132 GPUs + 585,504 CPU cores
19,000+ inorganic compounds computed overnight

COMMON WORKFLOWS

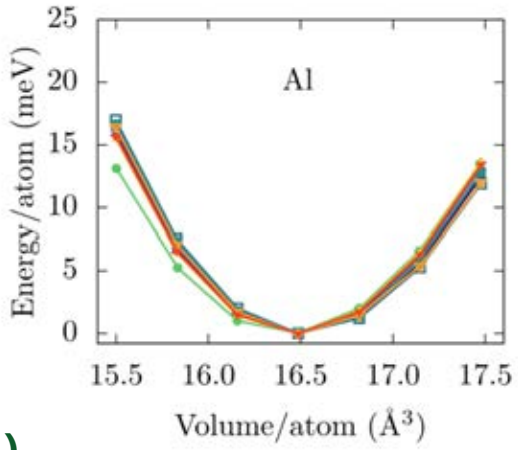
ARTICLE OPEN

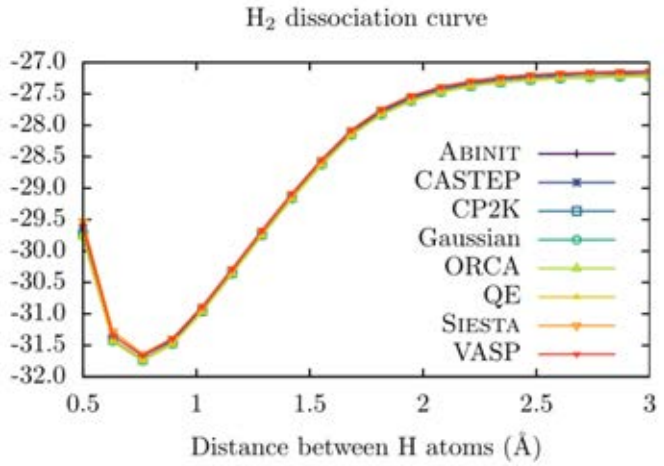
Check for updates

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

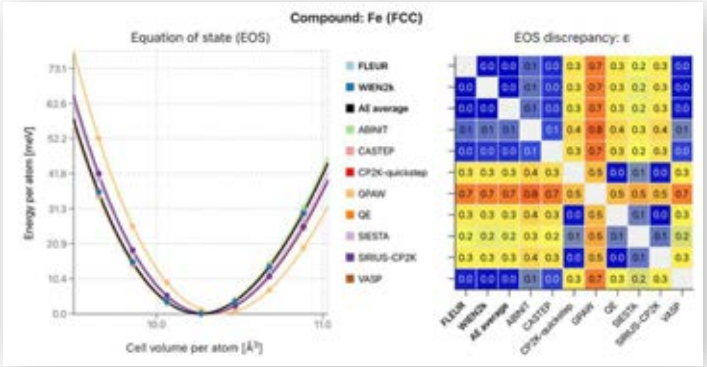




S. Huber *et al.*, npj Computational Materials 7, 136 (2021)

VALIDATE METHODS AND DATASETS

- First-principles methods widely used, but **can we trust their precision?**
- First verification effort only in 2016 [1]; **now complete** [2]:
  - Diverse chemical environments, reproducible workflows
  - High-quality all-electron (AE) reference dataset (960 equations of state)
  - Cross-verification involving 11 DFT codes
- **Relevance** of verification efforts:
  - **Reference datasets** for more accurate simulations, crucial to **trust** results
  - **Delivered improved pseudos** now available in VASP, CASTEP, SSSP, PseudoDojo, …
  - Currently used in **Bayesian optimization of improved pseudos**



K. Lejaeghere et al., Science 351, aad3000 (2016)
E. Bosoni et al., Nat. Rev. Phys. 6, 45 (2024)

https://acwf-verification.materialscloud.org

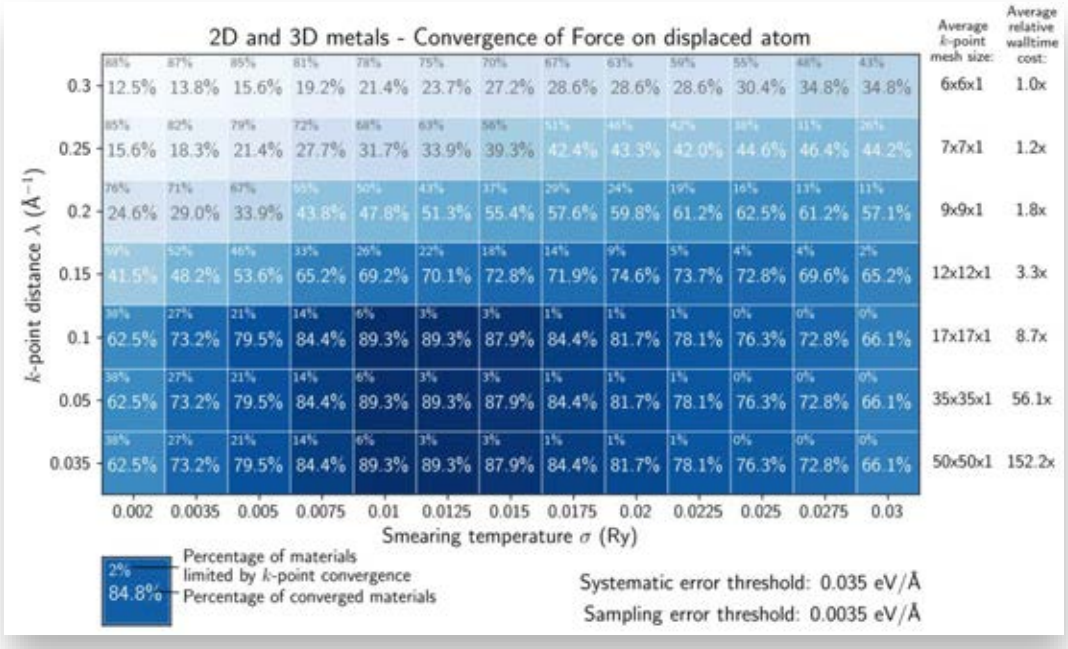
Verified pseudopotentials and protocols for DFT simulations

Standard Solid-State Pseudopotentials

SSSP 2.0 https://sssp.materialscloud.org

Standard Solid-State Protocols SSSPr

B. de Miranda Nascimento et al., Accurate and efficient protocols for high-throughput first-principles materials simulations. npj Comput Mater (2026).

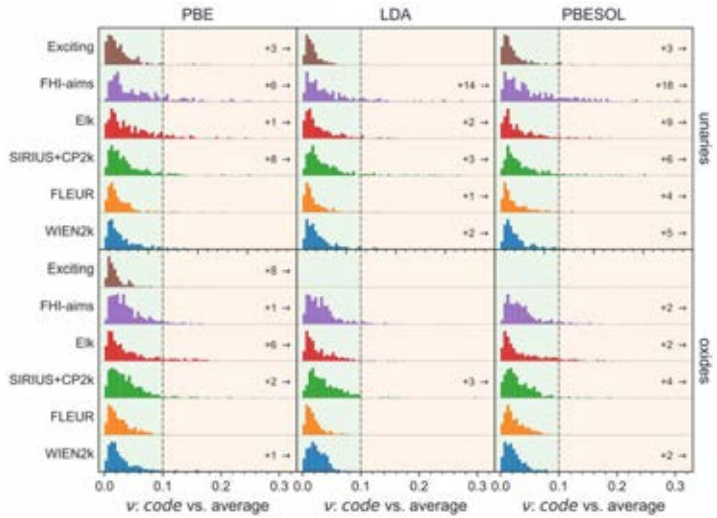


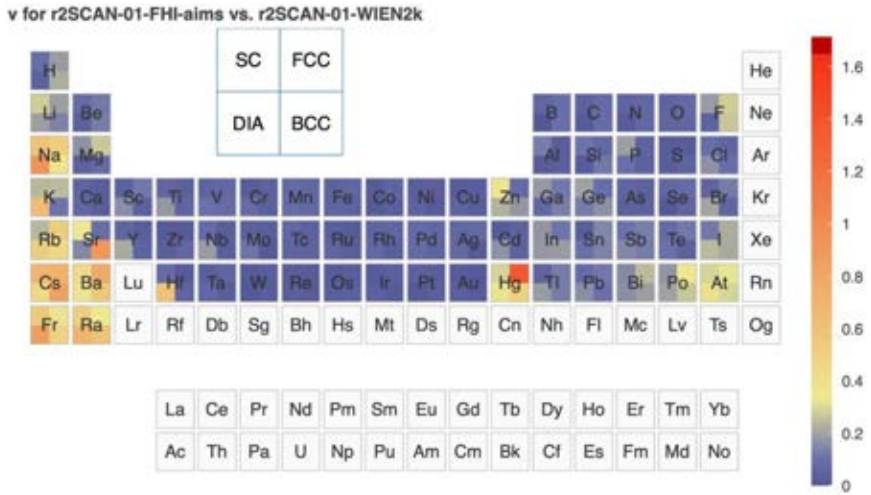
The AiiDAlab
Quantum ESPRESSO App

Current extension: magnetism, more codes and functionals

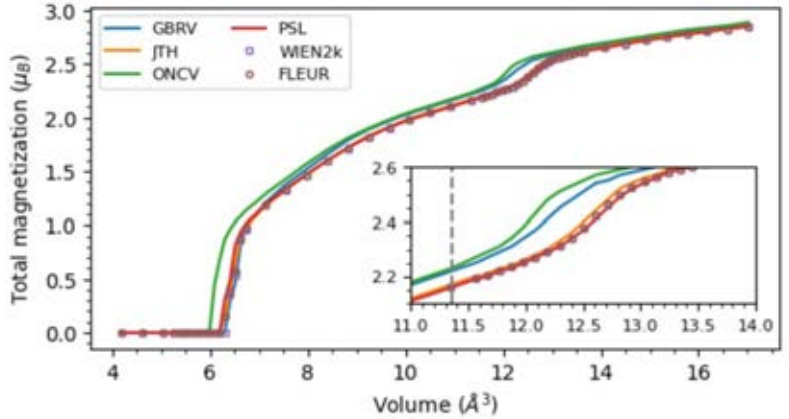
Goal: most accurate reference dataset today to assess and improve pseudopotentials

- **More functionals** (PBE, LDA, PBEsol, and r2SCAN01) and **more all-electron codes** (six; three for r2SCAN01)





- **Including magnetism**

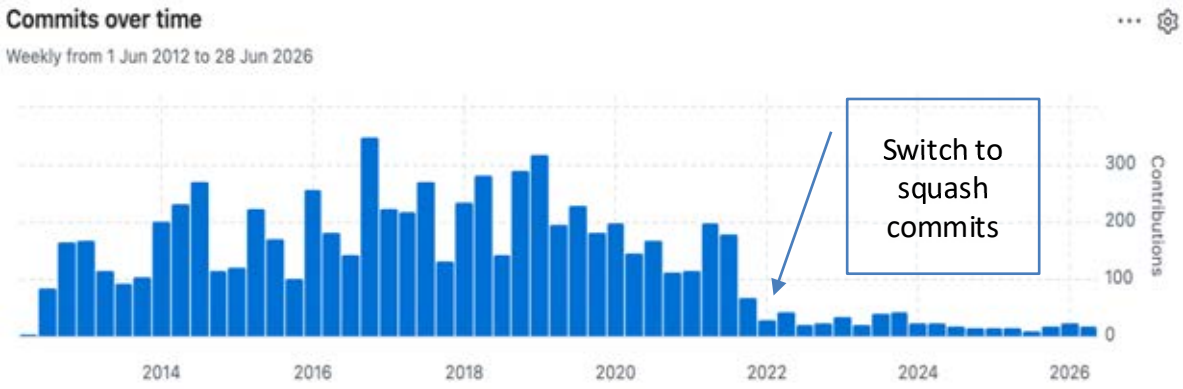


Swiss National Science Foundation

SIRIUS ELECTRONIC-STRUCTURE LIBRARY

SIRIUS

is a domain specific library for pseudopotential plane wave (PP-PW) and full potential linearized augmented plane wave (FP-LAPW) methods. It is written in C++20 with MPI, OpenMP and CUDA/ROCm programming models.



MARVEL sponsored work:

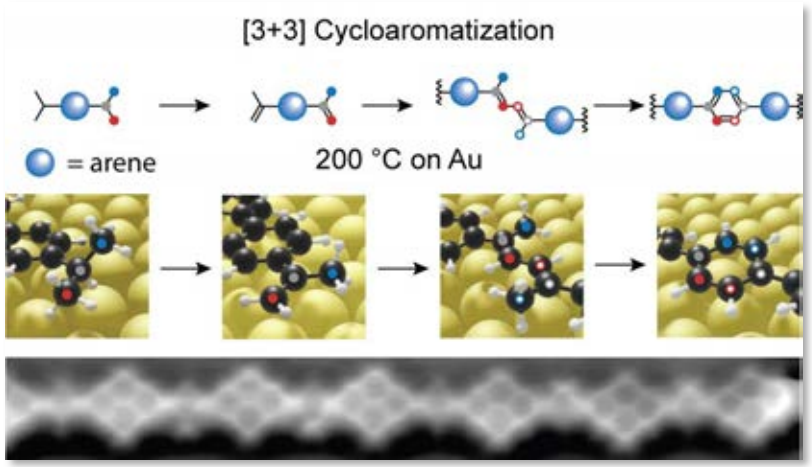
- Full support of plane-wave method with US, NC and PAW pseudopotentials
- DFT+U and DFT+U+V methods
- Spin-orbit correction
- Evaluation of forces and stress tensor
- Development of NLCG library for Sirius to support direct wave-function optimization methods
- High-accuracy LAPW calculations with CP2K/Sirius

Swiss National Science Foundation

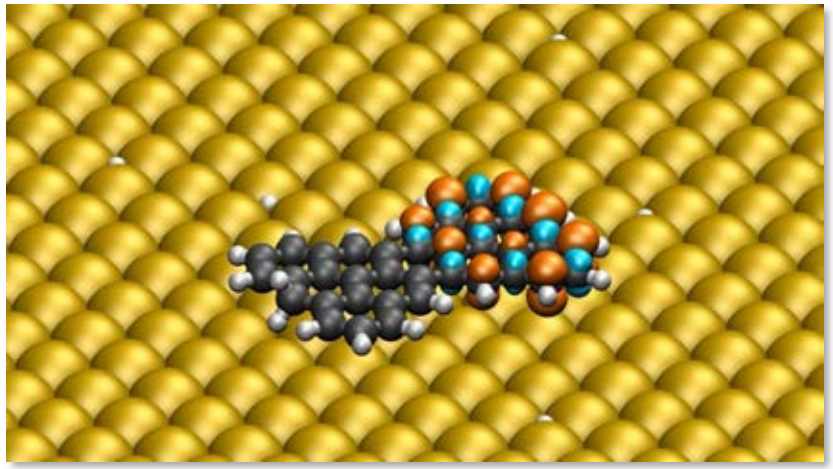
AiiDA/AiiDAlab AND MATERIALS CLOUD AS A SCIENTIFIC HIGHLIGHT

FROM COMPLEX SIMULATIONS TO SCIENTIFIC INSIGHT

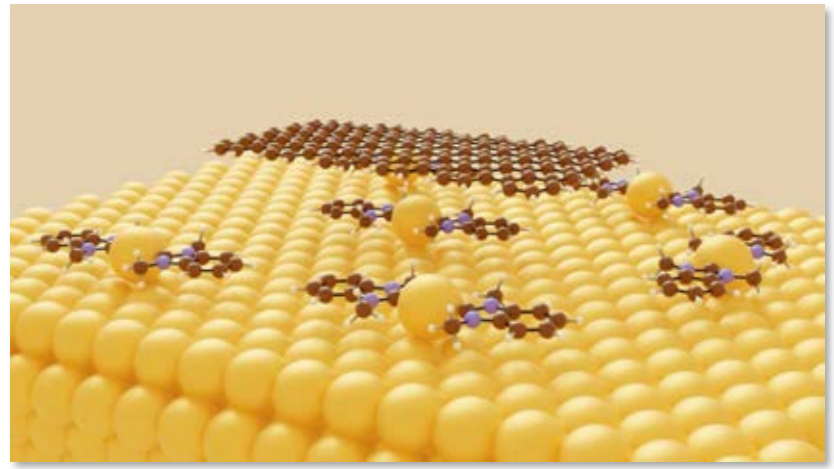
AiiDAlab made advanced simulations accessible to a broader community, including experimental researchers, enabling discovery of new materials, interpretation and prediction of experimental results



Discovering new on-surface synthesis pathways
Simulation-assisted interpretation of reaction pathways
A. Kinikar *et al. Nat. Synth.* (2022)



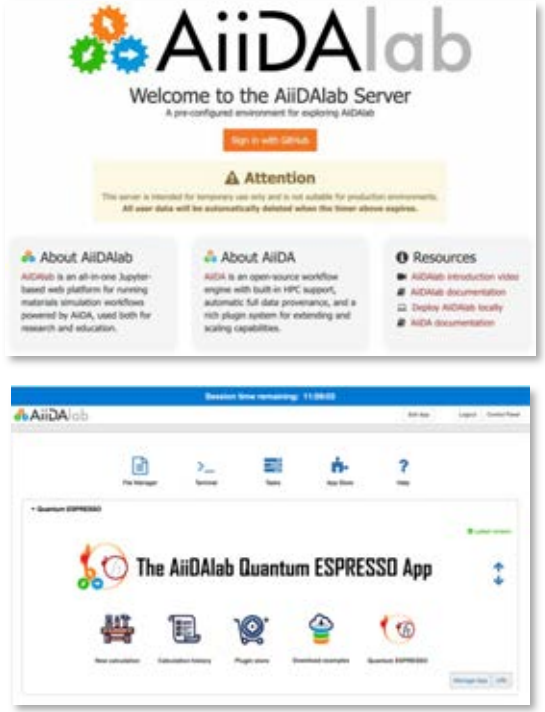
Understanding spin physics in magnetic carbon nanostructures
Revealing the underlying magnetic interactions
C. Zhao *et al. Phys. Rev. Lett.* (2024)



Understanding intercalation mechanisms for substrate decoupling
Rationalizing the success and failure of different intercalating species
D. Lüthi *et al. to be submitted* (2026)

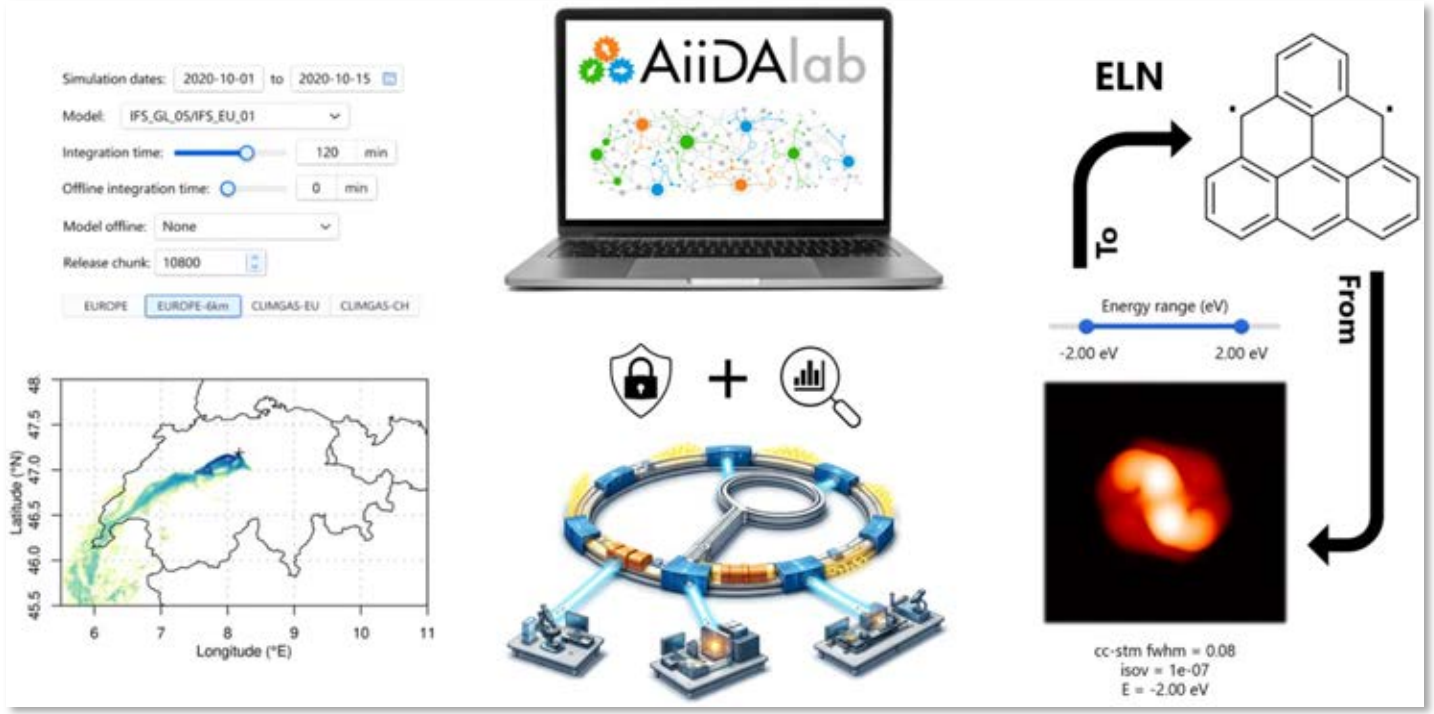
FROM HIDDEN COMPLEXITY TO SHARED UNDERSTANDING

AiiDAlab enables immediate hands-on access to realistic simulations while exposing the underlying theory step by step.
Dissemination of these solutions has promoted their adoption beyond materials science, toward interoperable digital laboratories.



Immediate hands-on access

Users can simulate realistic test cases from the first session. Theory is not hidden: Parameters, and physical meaning remain visible and can be explored step by step.

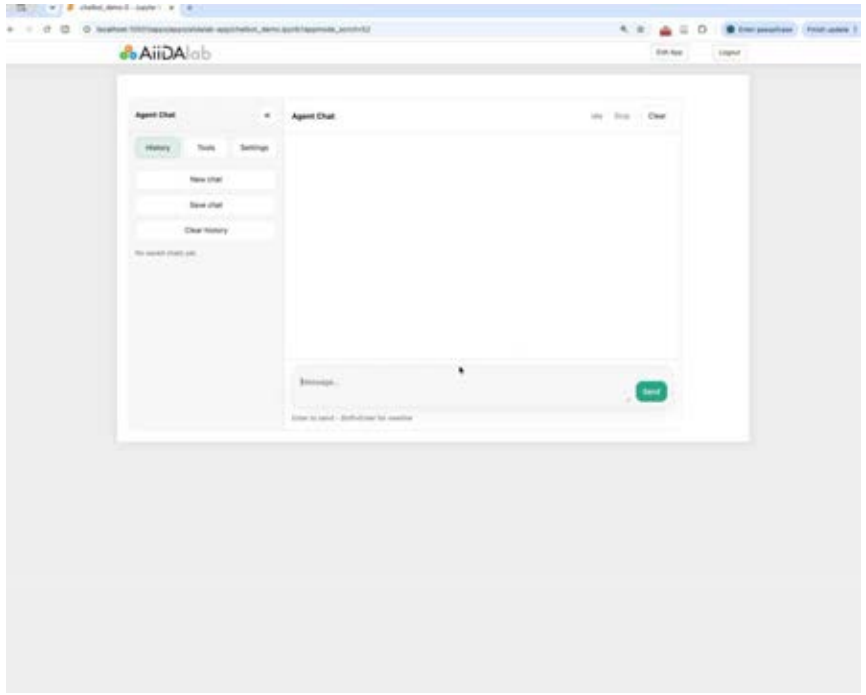


A model for digital laboratories

The same interoperable solutions support new research fields and link simulations with experiments.

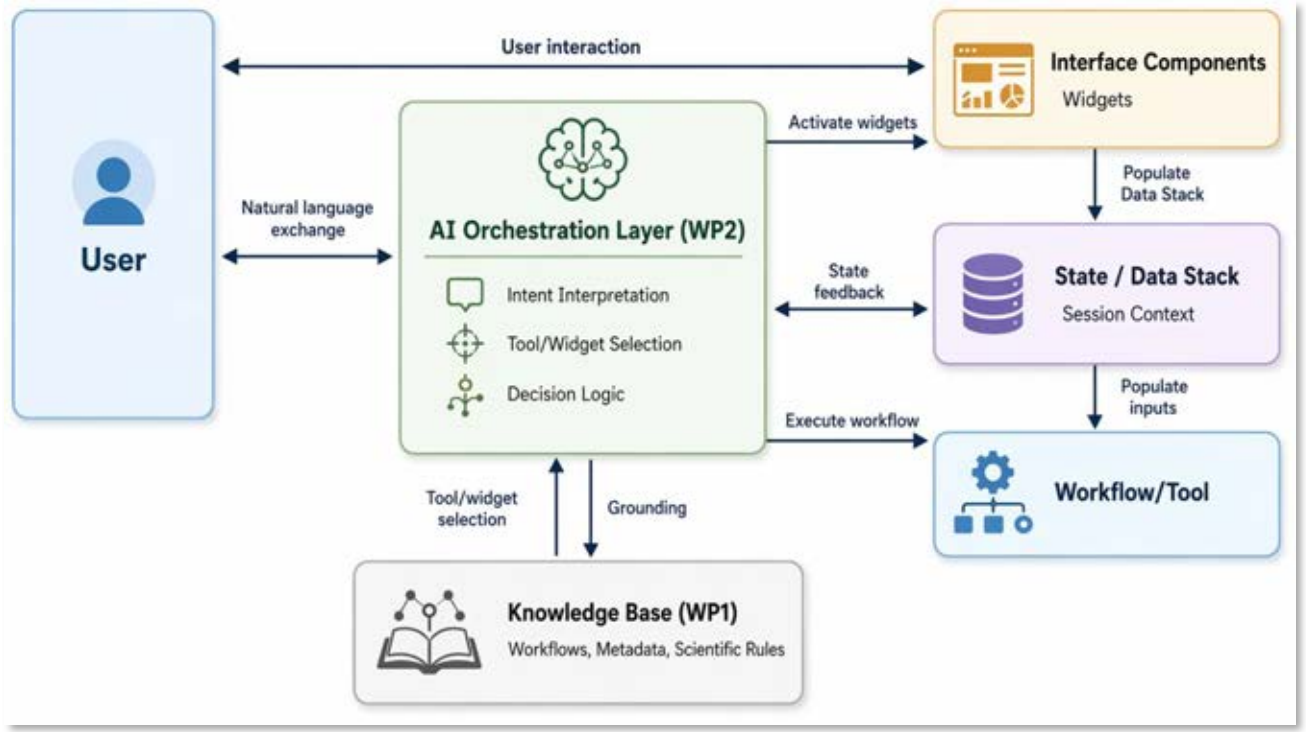
FROM DUMB INTERFACES TO GUIDED DISCOVERY

Deterministic workflows remain the trusted execution layer, while AI agents help users move from a scientific question to the right protocol, tools, and interfaces needed to prepare a simulation.



Start from the scientific question

The user expresses the problem in natural language and receives guided access to the relevant simulation setup.



AI agents facilitate discovery and adoption

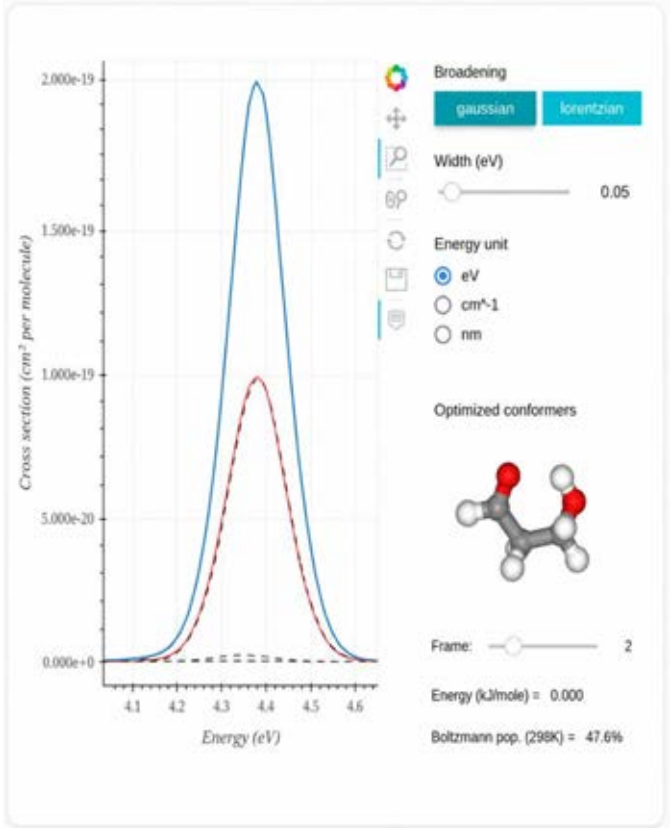
Agents expose the best tools and interfaces, while deterministic workflows preserve robustness, provenance, and reproducibility.

Swiss National Science Foundation

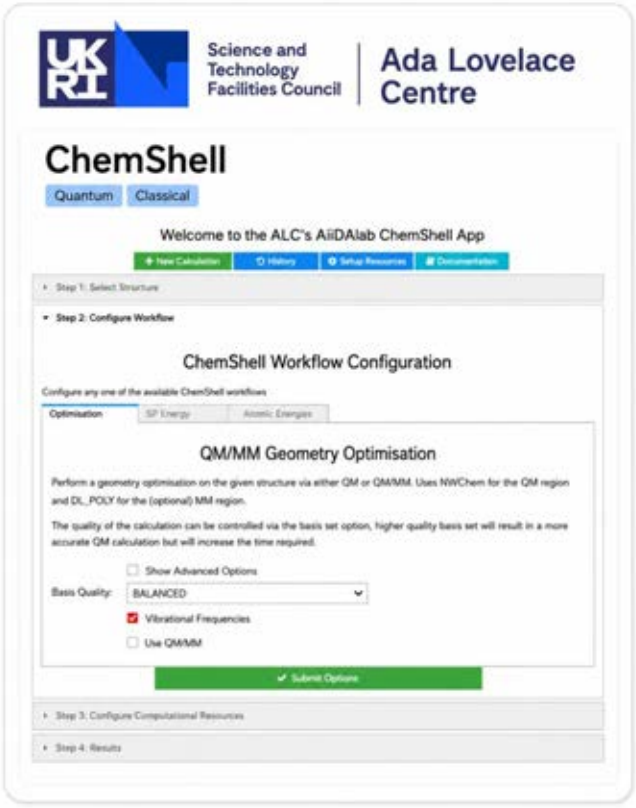
FROM THE ALPS TO THE WIDER SHORES

AiiDAlab solutions developed in MARVEL are being adopted beyond Switzerland

Built in MARVEL
Deployed at PSI and Empa, adopted beyond computational materials science



Centre for computational Chemistry (Bristol)
Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds

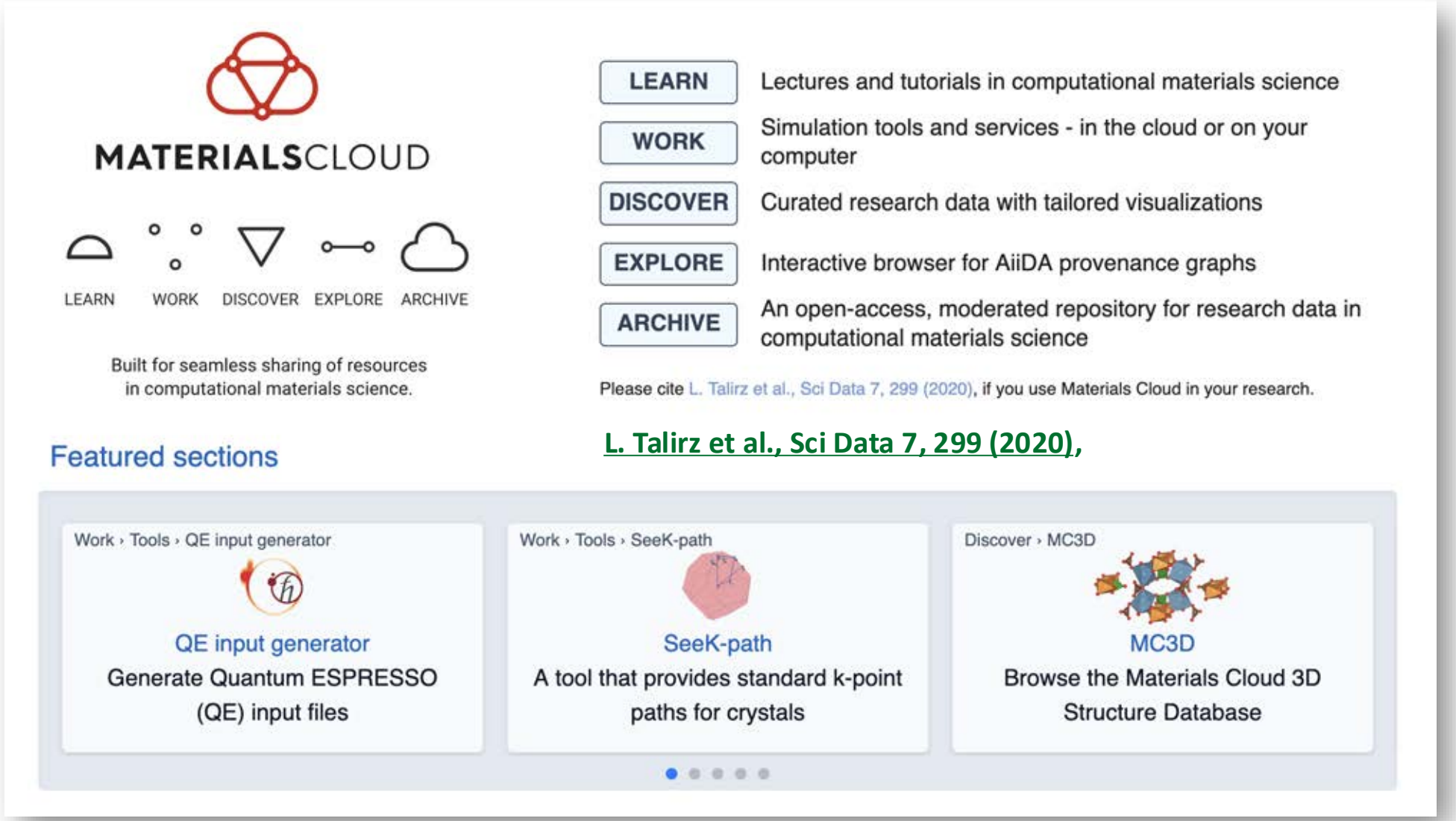


Science and Technology Facility Council
Multiscale Chemical modeling

A. Yakutovich et al. Digital Discovery (2026)

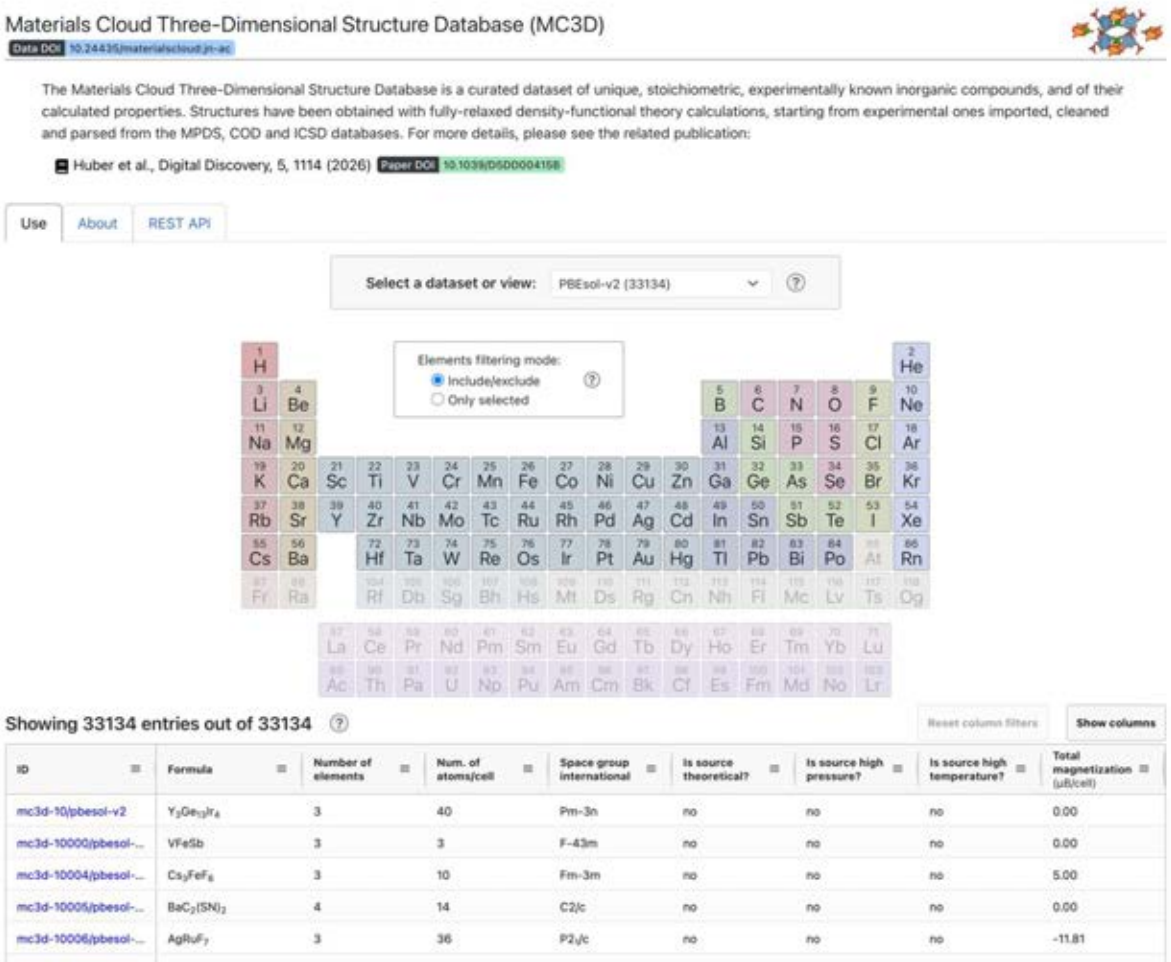
Swiss National Science Foundation

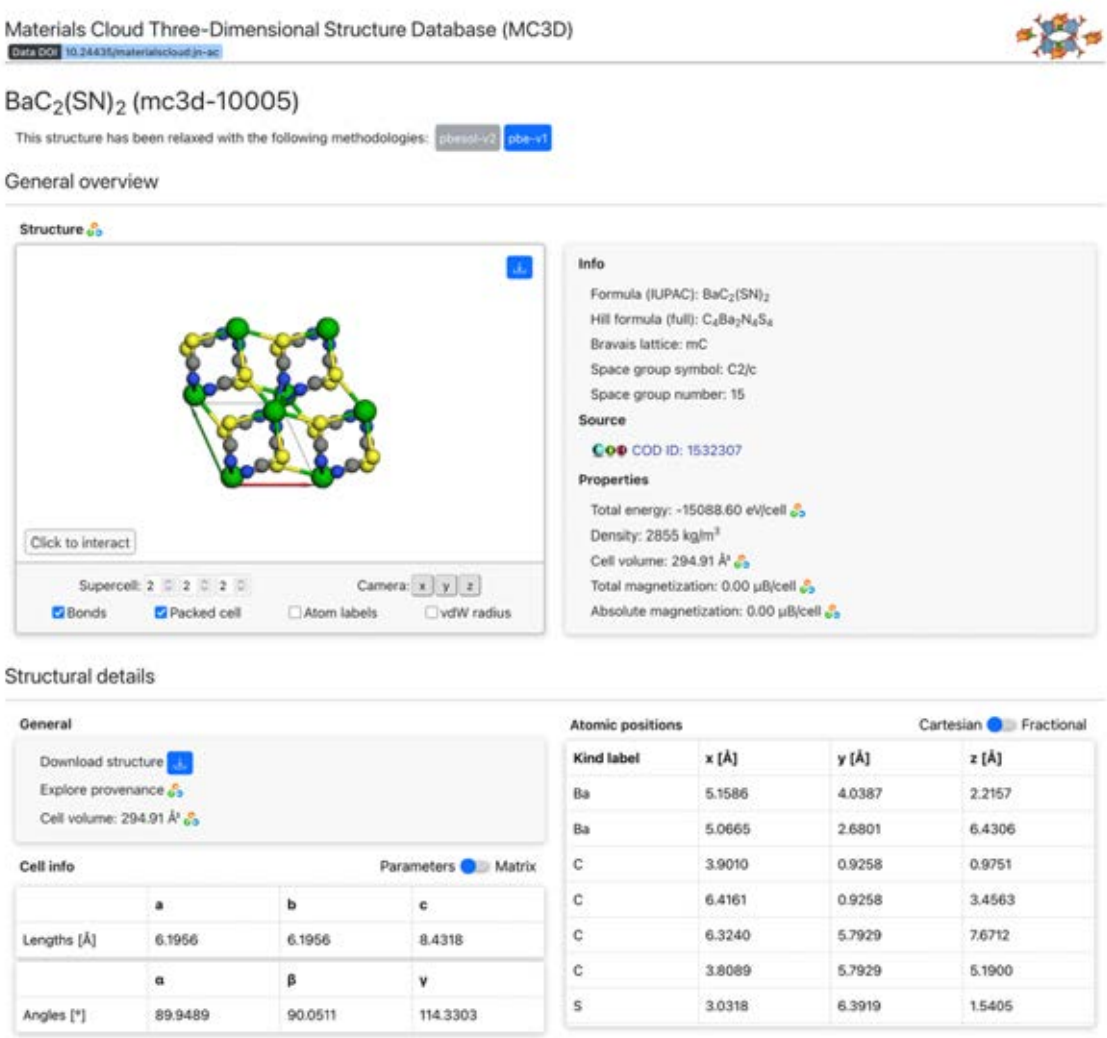
THE MATERIALS CLOUD AS THE FRONT-END DISSEMINATION



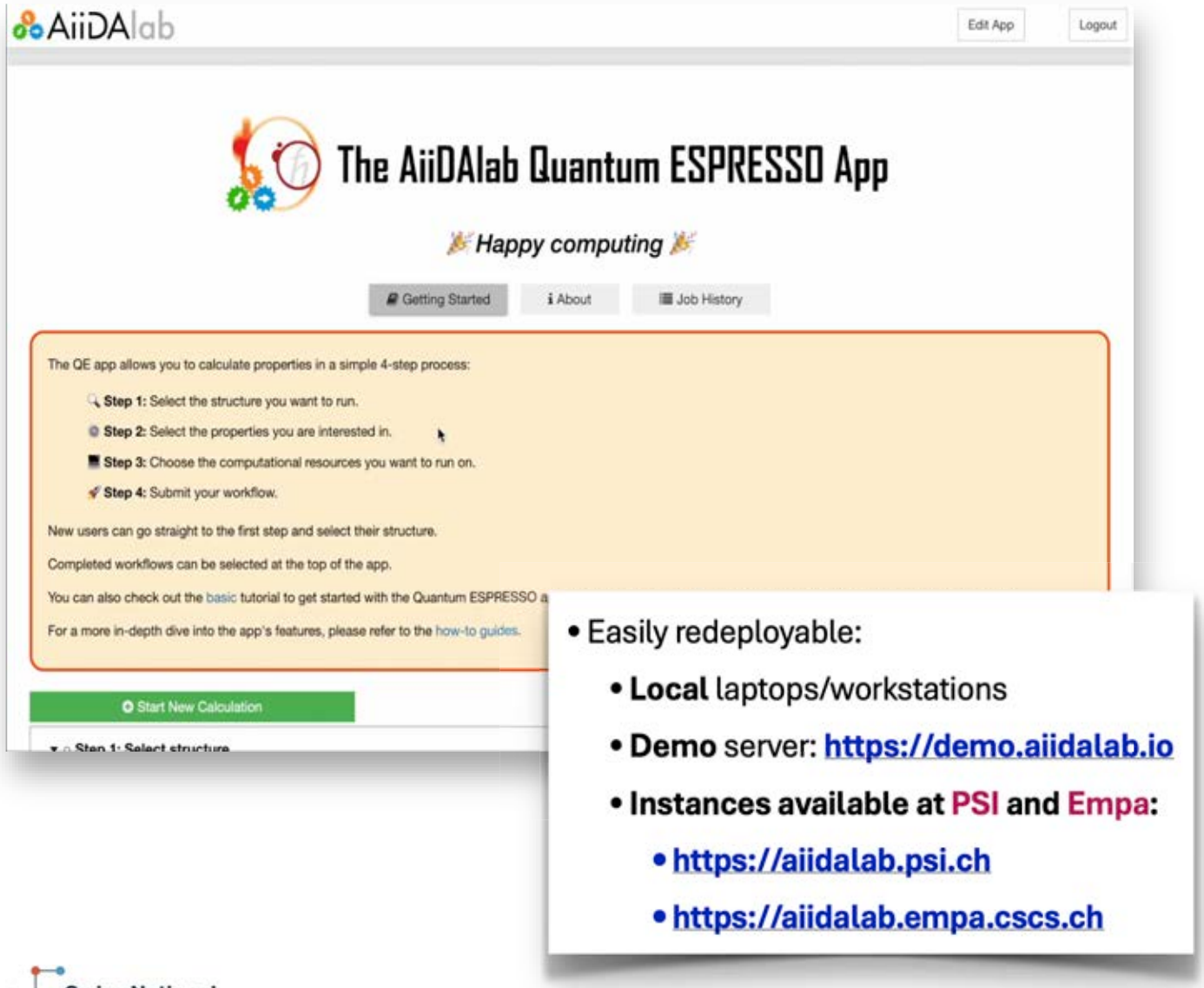
L. Talirz et al., Sci Data 7, 299 (2020),

EXPLORING MATERIALS

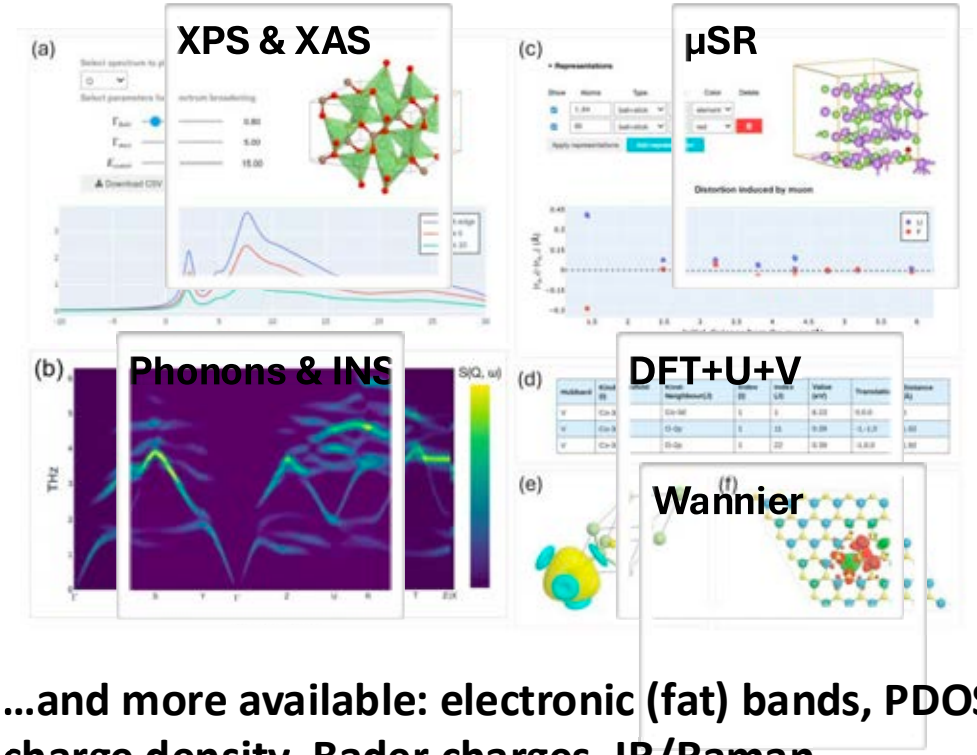




THE QE APP

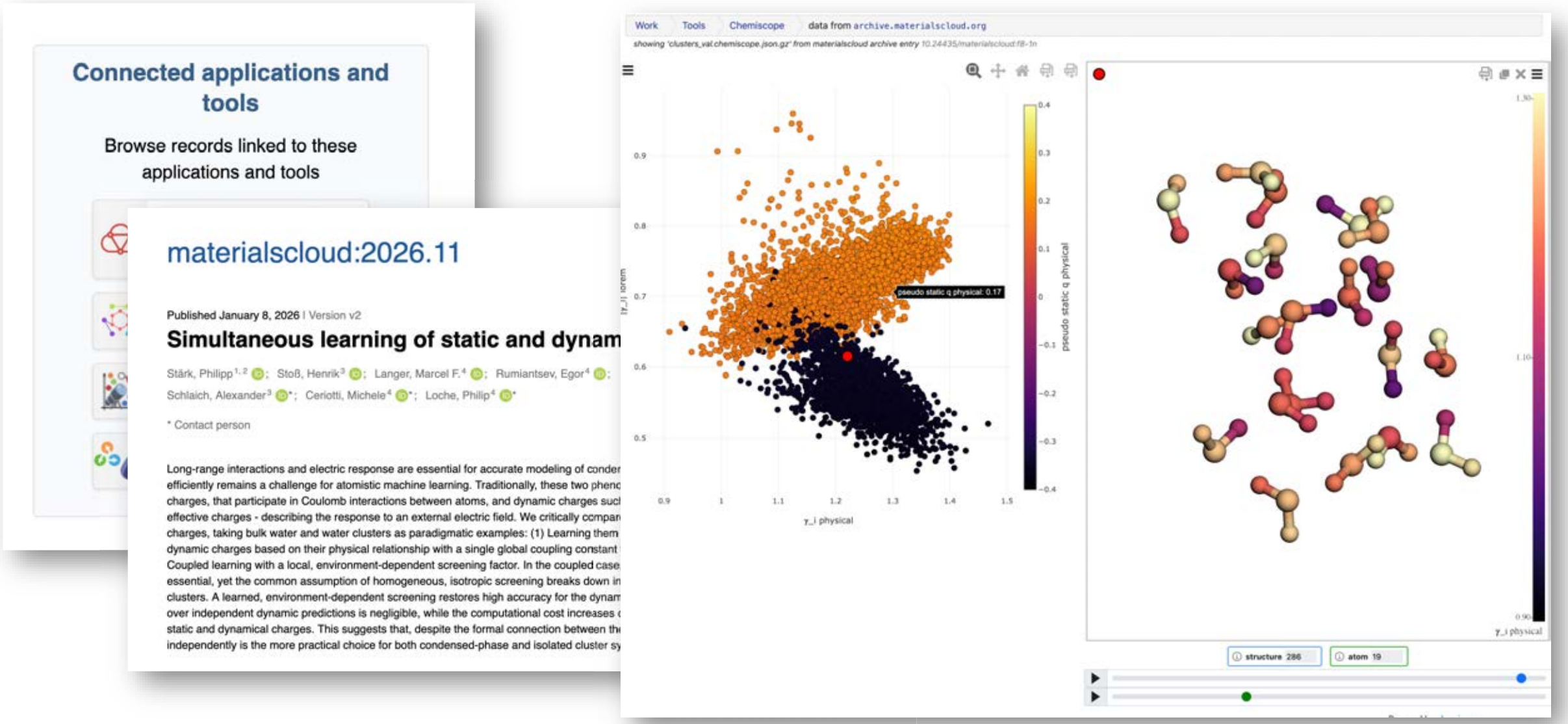


Plugin interface to integrate robust workflows

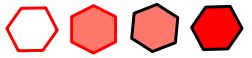


…and more available: electronic (fat) bands, PDOS, charge density, Bader charges, IR/Raman

HANDHSAKING ON THE CLOUD

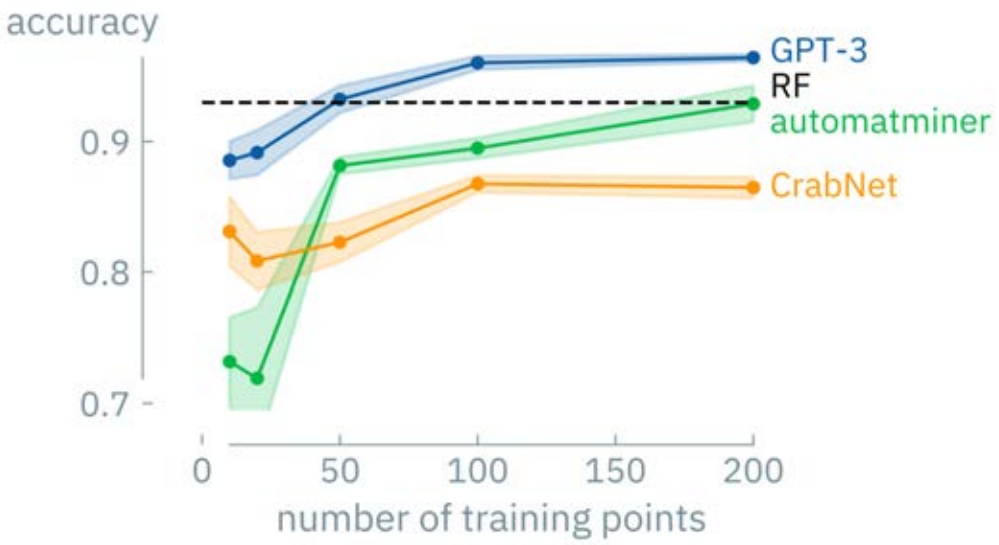


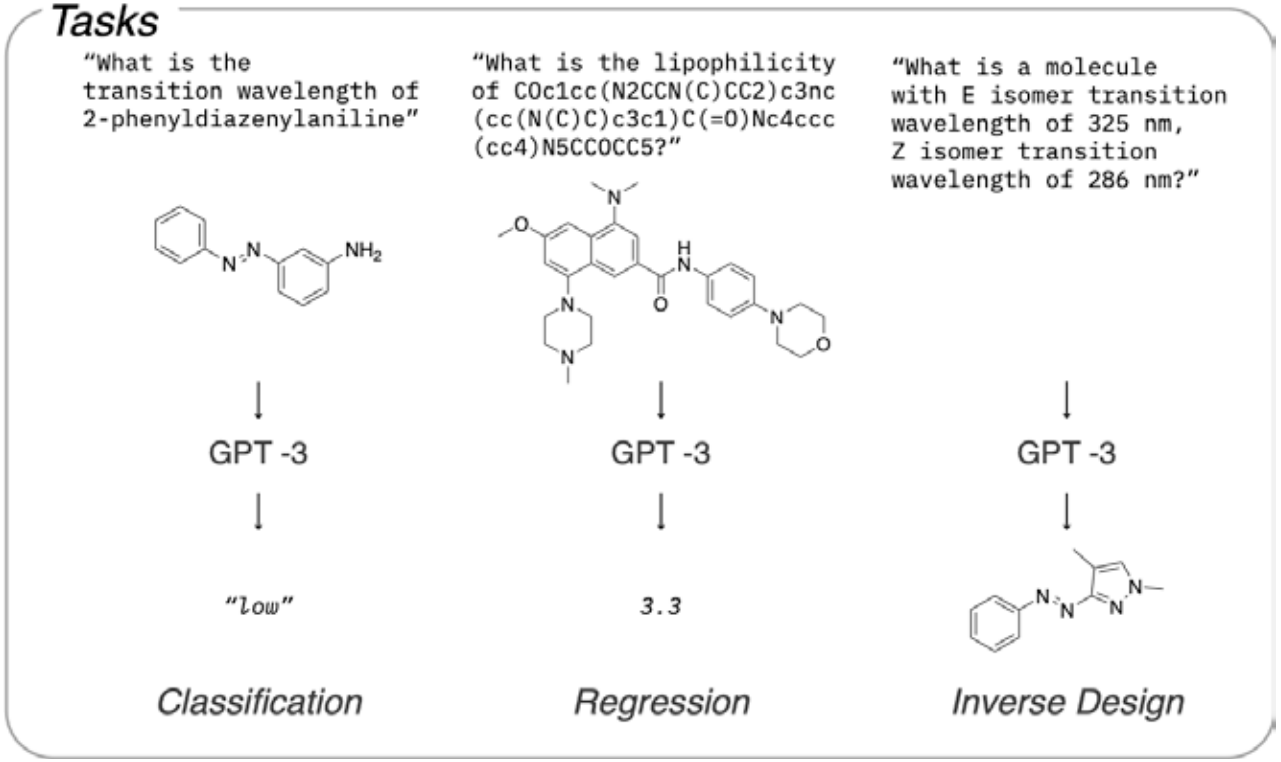
THE FRONTIERS: AI, ROBOTICS, QUANTUM



LLMs FOR PREDICTIVE CHEMISTRY

- First demonstration of finetuning of LLMs for chemical tasks



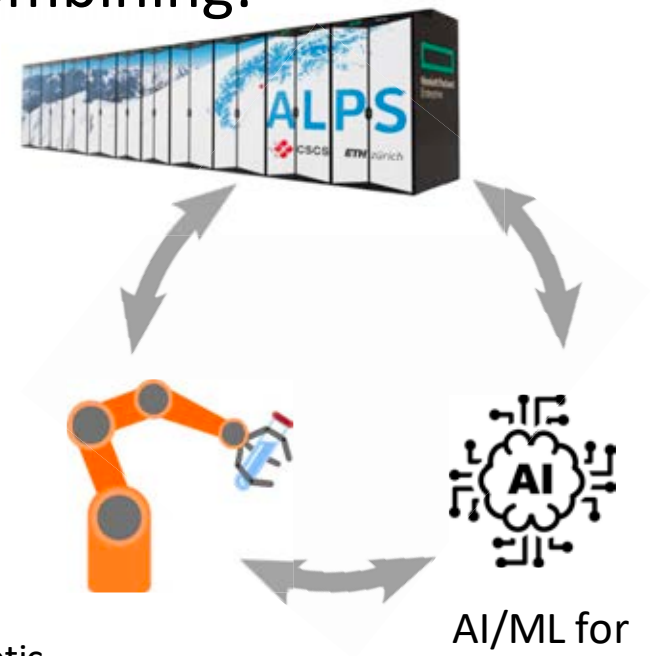


Jablonka, K. M., Schwaller, P., Ortega-Guerrero, A. & Smit, B. Leveraging large language models for predictive chemistry. *Nat Mach Intell* 6, 161–169 (2024).

“FAIR-by-design” self-driving laboratories

- Future of computational materials science: fully digital, combining:

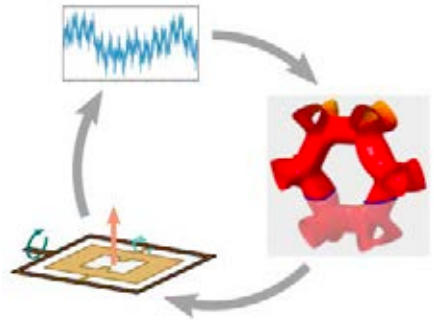
Automated simulations via robust workflows



Robotic experiments

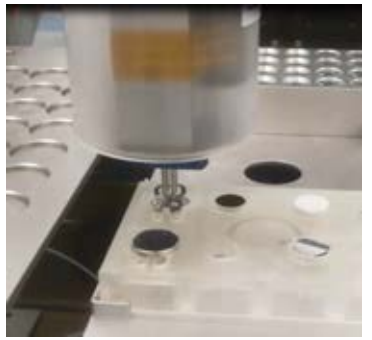
AI/ML for autonomous decisions

- Ongoing projects



Accurate Fermi surface mapping (Shubnikov-de Haas)

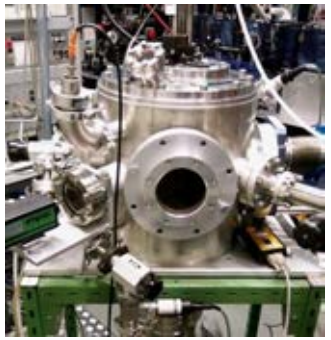
With Philip Moll (MPG, Germany)



Battery assembly and testing

With Corsin Battaglia (Empa), BIG-MAP, …

P. Kraus, .., GP, **J. Mater. Chem. A 12**, 10773 (2024)

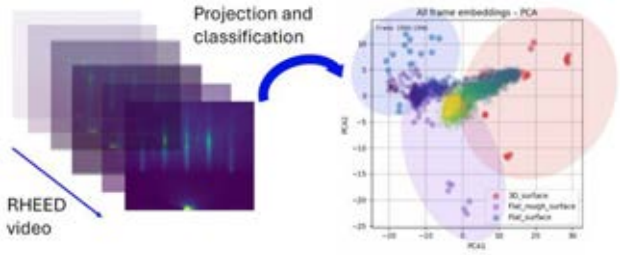


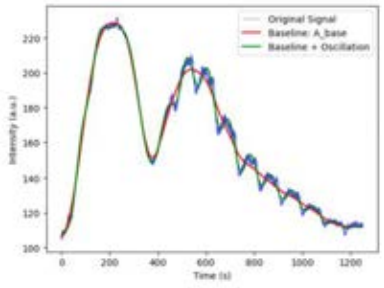
Pulsed laser deposition for autonomous crystal growth

With N. Shepelin (PSI)

Toward autonomous labs: examples

Automatic scoring of pulsed-laser depositions toward self-driving labs



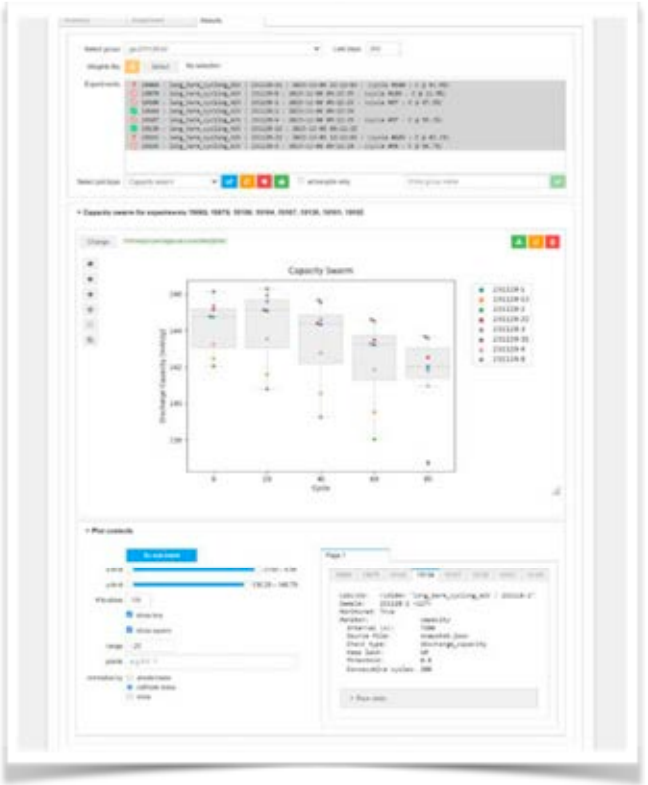


Per-frame pattern score + **Oscillation score**

AI-driven RHEED **pattern featurization** with pre-trained ViT DINOv2 **similarity-based soft-classification** for growth regime identification

AiiDA/AiiDAlab orchestration of battery experiments toward autonomous battery optimization

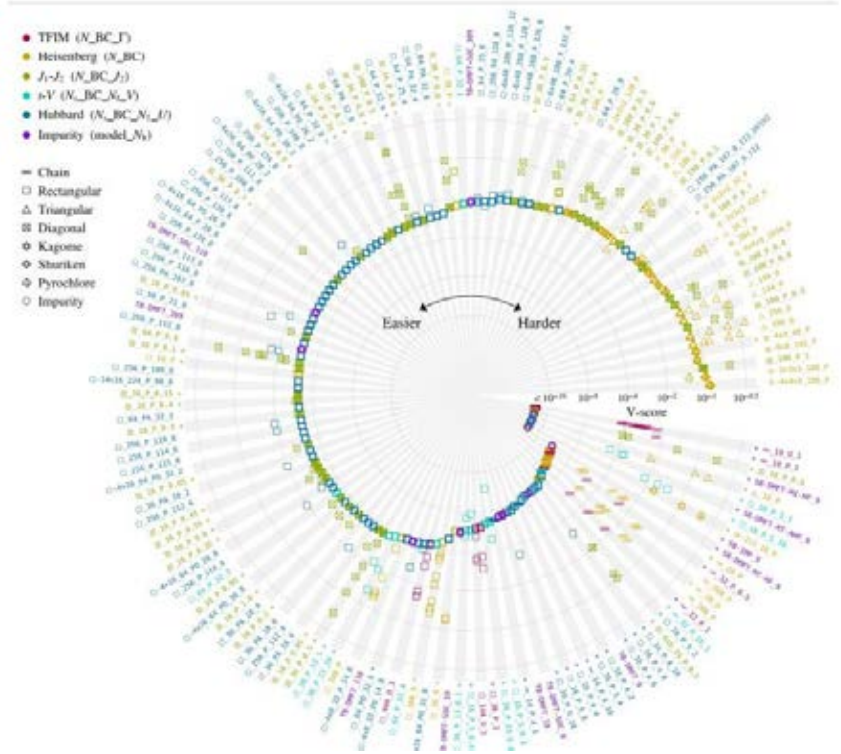
- Collaboration with Battaglia's lab (Empa)
- AiiDAlab GUI: batch experiment submission + data analysis



Quantum algorithms for materials

MARVEL moved the question from "can quantum computers help?" to "where is the advantage target, quantitatively?"

V-score map from the Science benchmark



The benchmark turns "quantum usefulness" into a falsifiable target: accuracy is judged against the best variational classical methods, not against exact diagonalization only.

1 **A quantitative hardness scale**

Energy and variance define a standardized V-score for many-body ground states, including cases where exact solutions are unavailable.

2 **A sharper map of hard regimes**

Many standard spin problems are already easy for classical ansaetze; frustrated models and 2D/3D lattice fermions still show large V-scores.

3 **Implication for materials**

Near-term quantum devices should be tested only on validated niches: frustrated magnets, correlated fermionic subspaces, and real-time dynamics.

MARVEL outcome

A community paper [Science 386, 296 (2024)] and open VarBench resource that make claims of quantum advantage testable.

D. Wu et al., *Variational benchmarks for quantum many-body problems,* Science 386, 296-301 (2024)
VarBench: github.com/varbench/varbench.

Quantum materials workflows: hybrid, embedded, and dynamics-first

The practical path is targeted quantum kernels inside classical workflows, not a standalone quantum chemistry solver.

1	2	3
IBM ZURICH / UZH	IBM / EPFL	EPFL
Active-space embedding	Dynamical correlations	Continuous-space ansaetze
Periodic range-separated DFT defines a fragment Hamiltonian; VQE / qEOM estimate local spectra. Demonstrated on the neutral oxygen vacancy in MgO.	Circuit-differentiation protocols compute retarded Green functions and spectra, benchmarked on Heisenberg and Fermi-Hubbard models under realistic noise.	First-quantized hybrid quantum-classical wave functions avoid basis-set discretization and add trainable many-body backflow correlations.

Phase-III quantum question

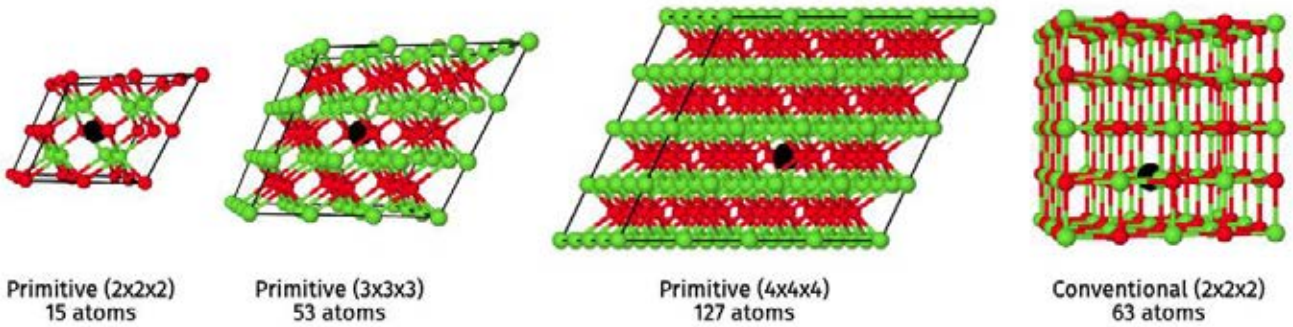
Which embedded materials observables remain hard after the strongest classical baselines, and can quantum hardware deliver them at useful accuracy and cost?

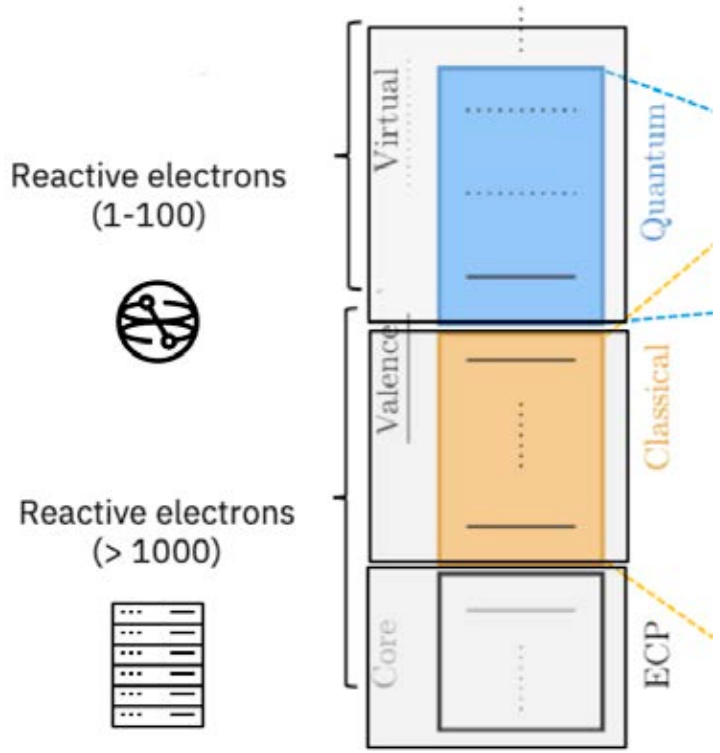
S. Piccinelli, F. Tacchino, I. Tavernelli, G. Carleo, "A circuit-differentiation framework for Green's functions on quantum computers," Quantum 10, 2060 (2026)

S. Battaglia et al., "A general framework for active space embedding methods with applications in quantum computing," npj Comput. Mater. 10, 297 (2024)

F. Metz, G. Pescia, G. Carleo, "Simulating continuous-space systems with quantum-classical wave functions," arXiv:2409.06415 (2024)

REALISTIC MATERIALS

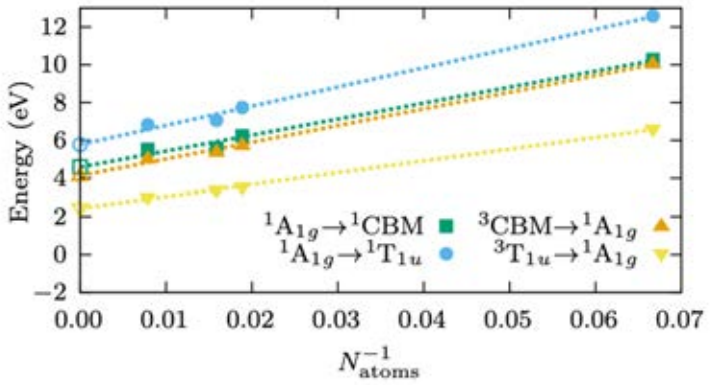




- Optical properties of the neutral oxygen vacancy in magnesium oxide.
- Multi-scale description crucial for a reliable description of the material.

cell	N_{atoms}^{-1}	${}^3\text{T}_{1u} \rightarrow {}^1\text{A}_{1g}$	${}^3\text{CBM} \rightarrow {}^1\text{A}_{1g}$
p 2x2x2	0.067	6.59	10.05
p 3x3x3	0.019	3.54	5.74
c 2x2x2	0.016	3.38	5.38
p 4x4x4	0.008	3.02	5.02
$\rightarrow \infty$	$\rightarrow 0.0$	2.44	4.14

Exp: 2.3 eV



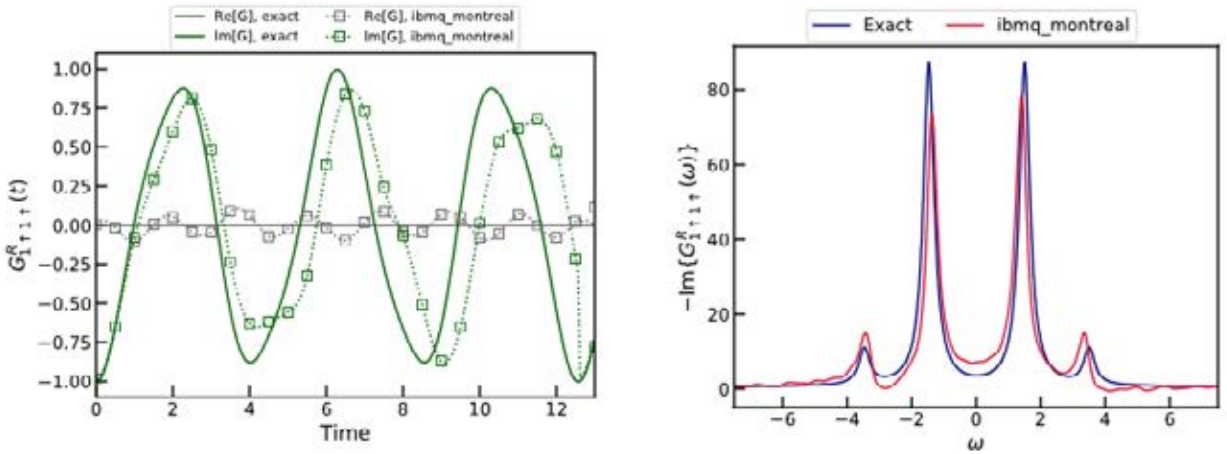
S. Battaglia, M. Rossmannek, V. Rybkin, I. Tavernelli, J. Hutter npj Comput. Mater. 10, 297 (2024)

GREEN'S FUNCTIONS

Single-particle Green's function (time domain)

$$G^R_{\alpha\beta}(t) = -i\theta(t)\langle\psi_0|\{\hat{c}_\alpha(t), \hat{c}^\dagger_\beta(0)\}|\psi_0\rangle$$

VQE + (variational) quantum time evolution



2-site Fermi-Hubbard model

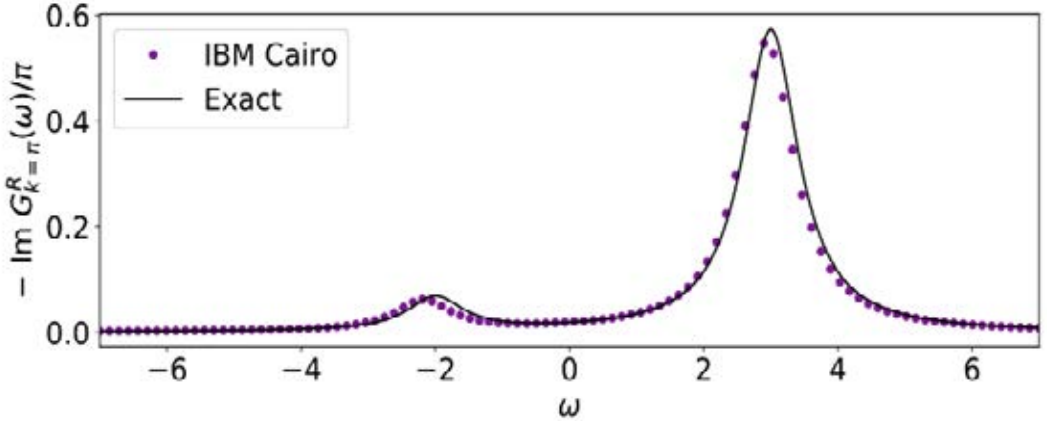
F. Libbi et al., Phys. Rev. Research 4, 043038 (2022)

Lehmann representation (frequency domain)

$$\tilde{G}^R_\alpha(\omega) = \sum_n \left(\frac{\left|\langle E_n^{N+1}|\hat{c}^\dagger_\alpha|\psi_0\rangle\right|^2}{\omega + E_0^N - E_n^{N+1} + i\eta} + \frac{\left|\langle E_n^{N-1}|\hat{c}_\alpha|\psi_0\rangle\right|^2}{\omega - E_0^N + E_n^{N-1} + i\eta} \right)$$

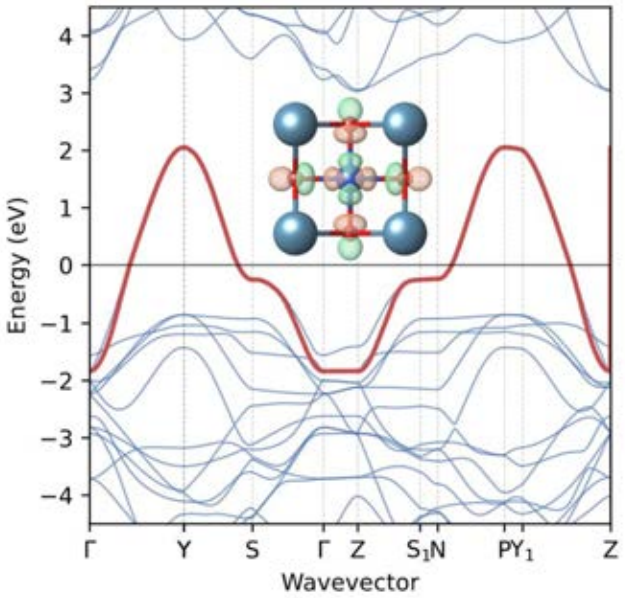
VQE + excited states methods (qEOM)

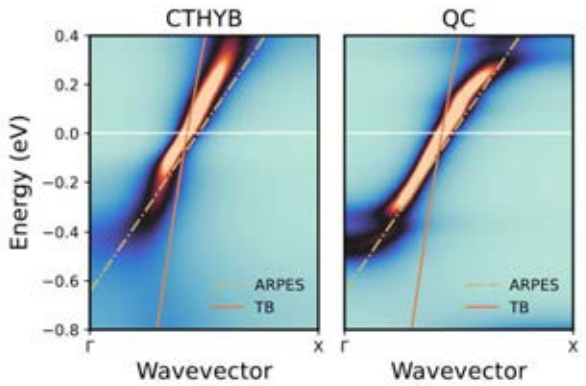
2-site Fermi-Hubbard model

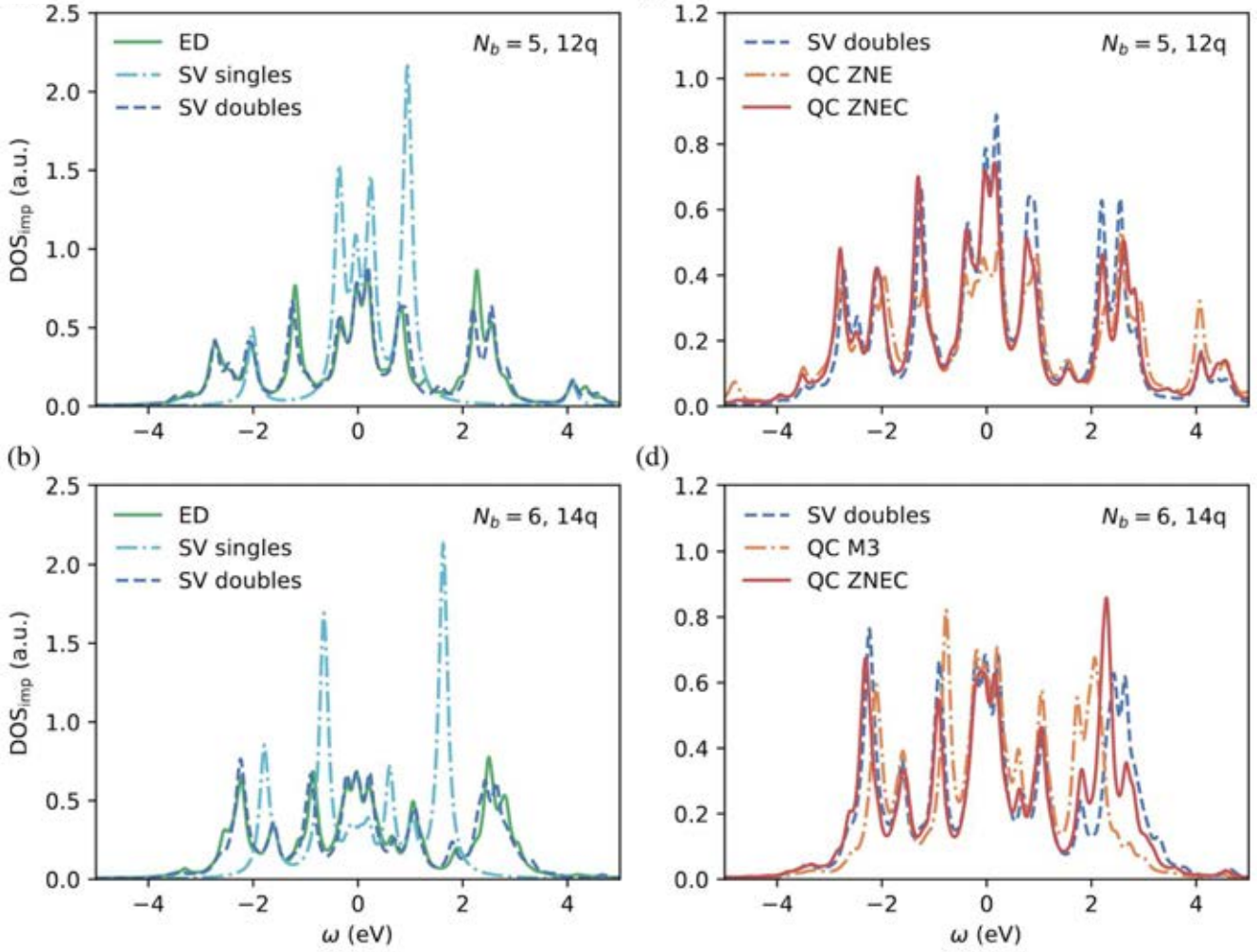


J. Rizzo et al., Phys. Rev. Research 4, 043011 (2022)

FROM GREEN'S FUNCTIONS TO DMFT



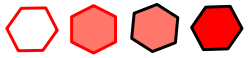




BOSCH

Swiss National Science Foundation

WHAT NEXT?



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

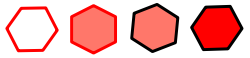
1) PREDICTIVE ACCURACY

2) REALISTIC COMPLEXITY

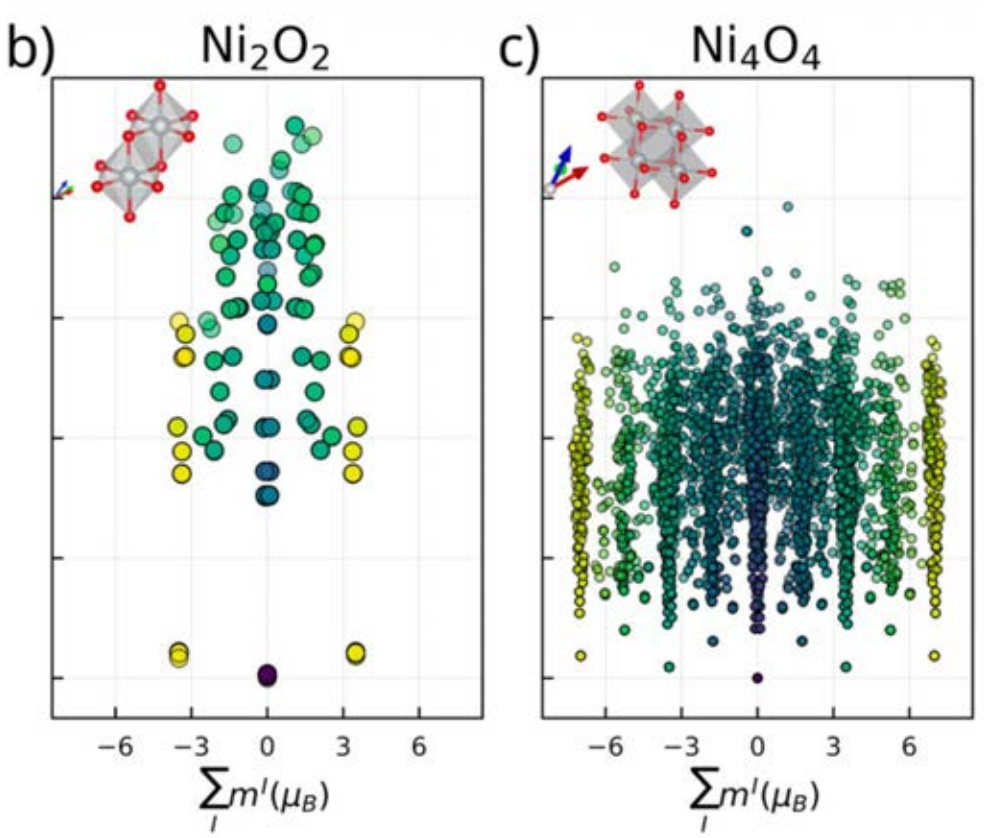
3) MATERIALS INFORMATICS

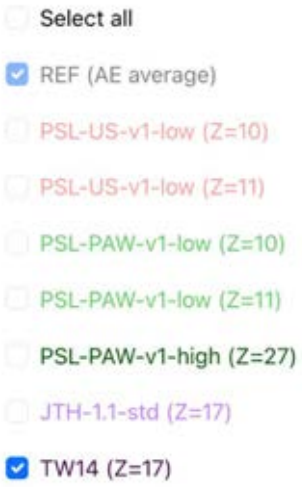
ACCURACY STILL THE HARDEST

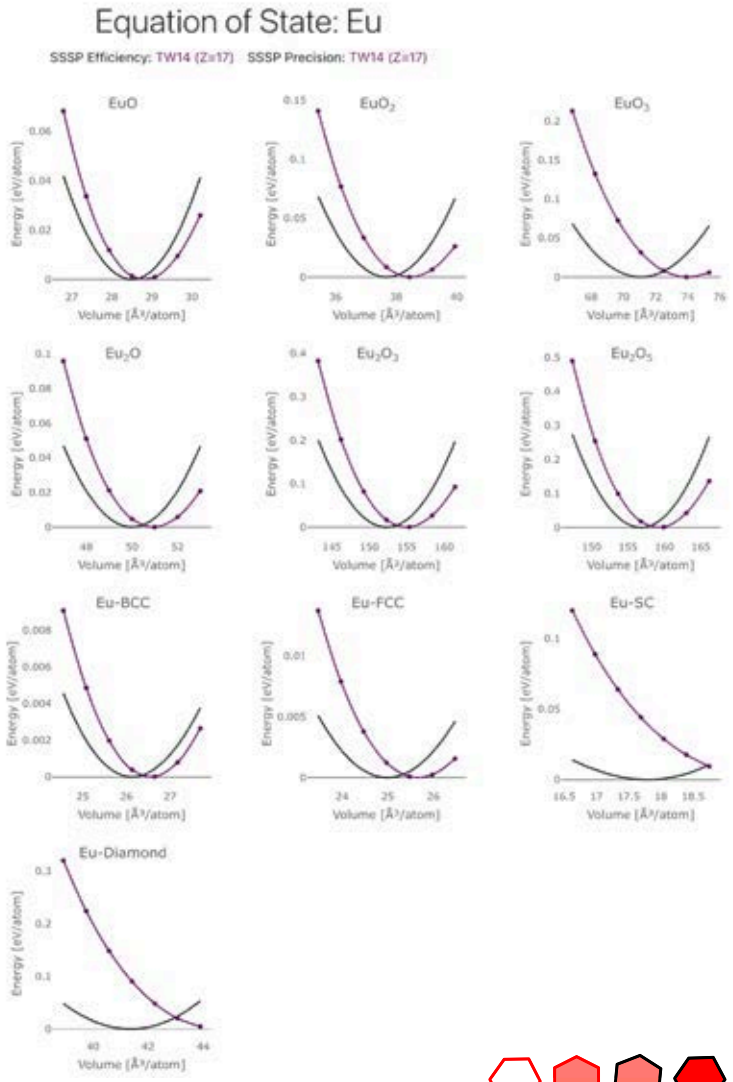
1) Cannot combine DFT with DFT+U+V; hybrids less accurate and much more expensive
2) Landscape of magnetic materials
3) Lanthanides and actinides
4) Strong on-site correlations



MAGNETIC LANDSCAPE, PSEUDOPOTENTIALS







L. Ponet, E. Di Lucente, and N. Marzari,
The energy landscape of magnetic materials,
npj Comput Mater 10, 151 (2024)

Swiss National Science Foundation