

Data-driven Materials Design and Applications to Two-Dimensional Nano-systems

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Theoretical Chemistry, Technische Universität Dresden

Predictive Theory

Discovery of Neptune

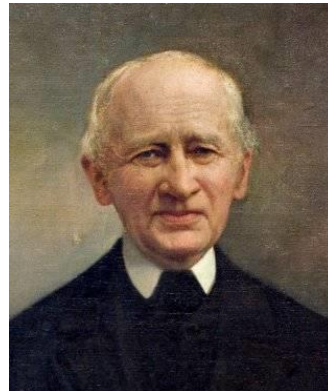


universal law of gravitation

$$\mathbf{F}_1 = \gamma \frac{m_1 m_2}{r_{12}^2} \frac{\mathbf{r}_{12}}{r_{12}} = m_1 \ddot{\mathbf{r}}_1$$



Urbain Le Verrier
(1811-1877)



Johann Gottfried Galle
(1812-1910)

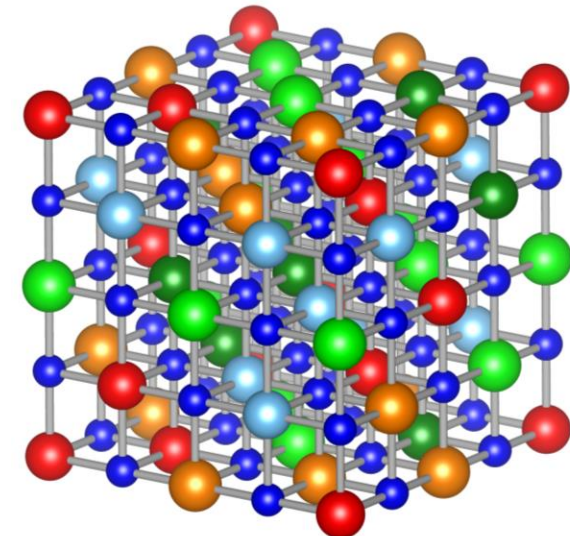
Predictive Solid-state Theory

$$\hat{H}\Psi = E\Psi$$

→ problem of $\sim 10^{23}$ interacting particles

$$E_{\text{KS}}[n] = T_s[\{\phi_i[n]\}] + V_{\text{eK}}[n] + U_{\text{H}}[n] + E_{\text{xc}}[n]$$

→ DFT as ultimate work horse for predictive materials discovery

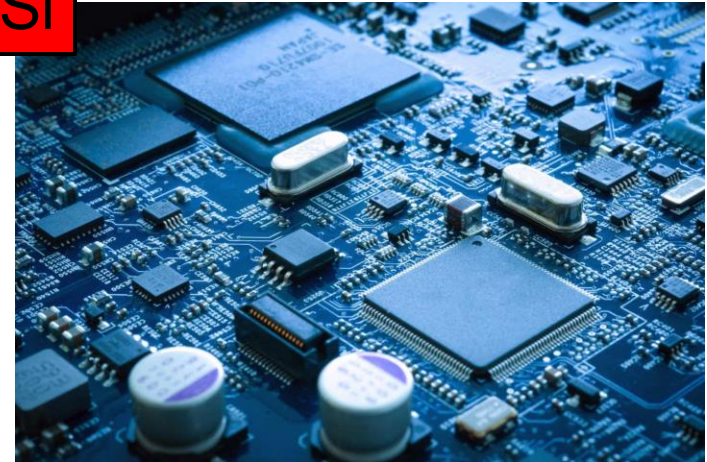


Materials, Science & Technology

Rh



Si



Li

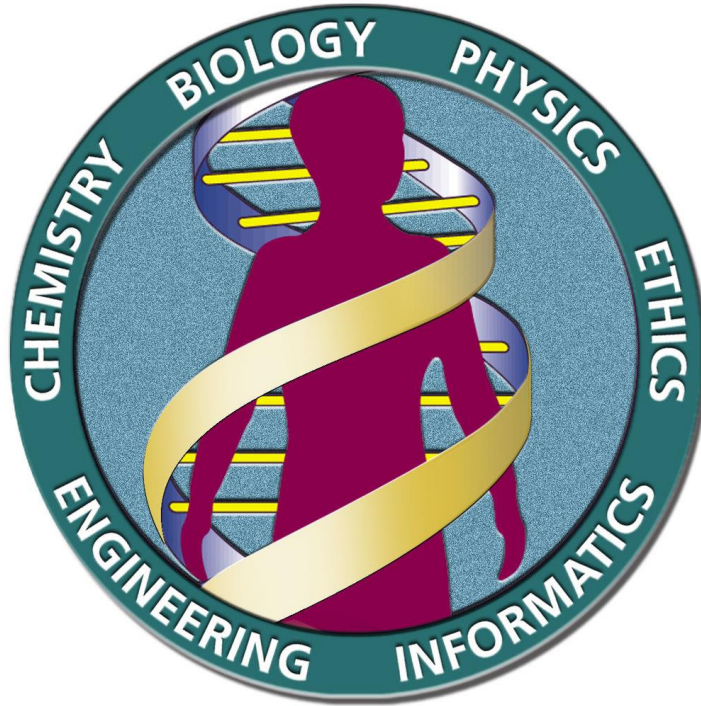


CoPt



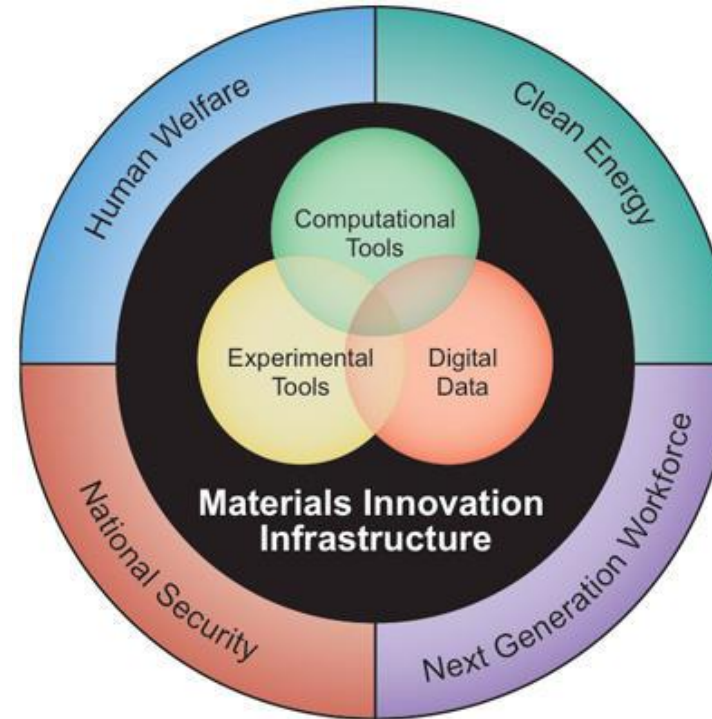
Materials Genome Initiative

Human Genome Project (1990-2003)



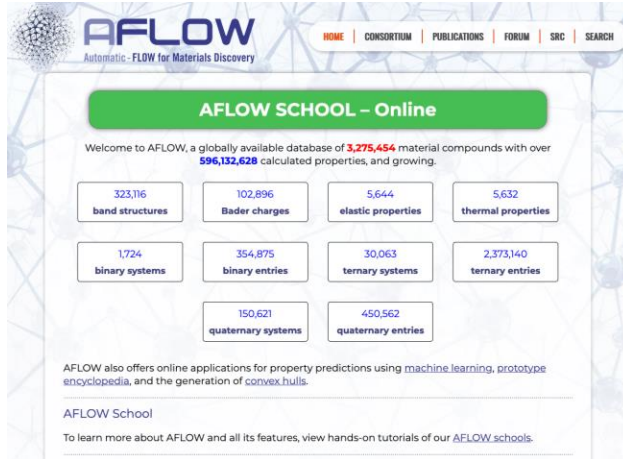
By U.S. Department of Energy, Human Genome Project -
<http://www.ornl.gov/hgmis>, Public Domain,
<https://commons.wikimedia.org/w/index.php?curid=2485616>

Materials Genome Initiative (2011)



<https://www.mgi.gov/>

Materials Genome Initiative – Databases



AFLOW
Automatic - FLOW for Materials Discovery

HOME | CONSORTIUM | PUBLICATIONS | FORUM | SRC | SEARCH

AFLOW SCHOOL – Online

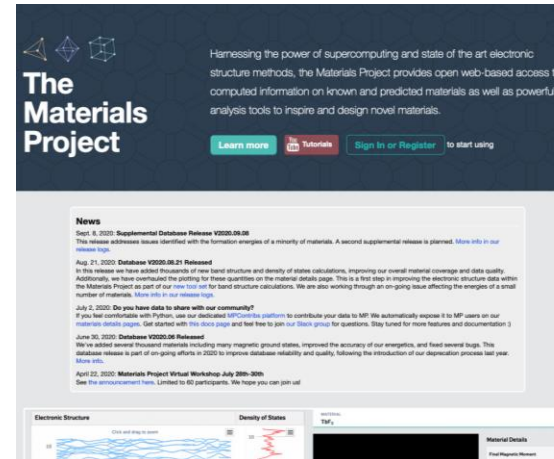
Welcome to AFLOW, a globally available database of **3,275,454** material compounds with over **596,132,628** calculated properties, and growing.

323,116 band structures	102,896 Bader charges	5,644 elastic properties	5,632 thermal properties
1,724 binary systems	354,875 binary entries	30,063 ternary systems	2,373,140 ternary entries
	150,621 quaternary systems	450,562 quaternary entries	

AFLOW also offers online applications for property predictions using [machine learning](#), [prototype encyclopedia](#), and the generation of [convex hulls](#).

AFLOW School
To learn more about AFLOW and all its features, view hands-on tutorials of our [AFLOW schools](#).

<http://aflow.org/>



The Materials Project

Harnessing the power of supercomputing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Learn more](#) [Tutorials](#) [Sign in or Register](#) to start using

News

Sept 8, 2020 **Supplemental Database Release V2020.09.08**
This release addresses issues identified with the formation energies of a minority of materials. A second supplemental release is planned. [More info in our release log](#)

Aug. 21, 2020 **Database V2020.08.21 Released**
In this release we have added thousands of new band structure and density of states calculations, improving our overall material coverage and data quality. Additionally, we have overhauled the plotting for these quantities on the material details page. This is a first step in improving the electronic structure data within the Materials Project as part of our new tool set for band structure calculations. We are also working through an on-going issue affecting the energies of a small number of materials. [More info in our release log](#)

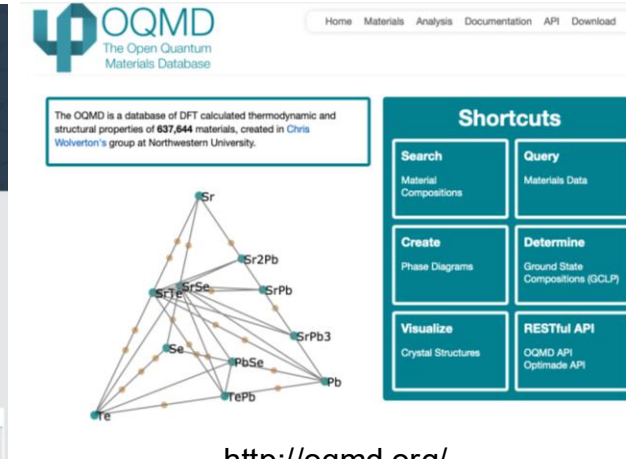
July 2, 2020 **Do you have data to share with our community?**
If you feel comfortable with Python, use our dedicated [MPContribs platform](#) to contribute your data to MP! We automatically receive it to MP users on our [material details page](#). Get started with [this doc page](#) and feel free to join our [Slack group](#) for questions. Stay tuned for more features and documentation!

June 30, 2020 **Database V2020.06 Released**
We've added several thousand materials including many magnetic ground states, improved the accuracy of our energetics, and fixed several bugs. This database release is part of on-going efforts in 2020 to improve database reliability and quality, following the introduction of our deprecation process last year. [More info](#)

April 22, 2020 **Materials Project Virtual Workshop July 20th-30th**
See the [announcement here](#). Limited to 60 participants. We hope you can join us!

Electronic Structure Density of States

<https://materialsproject.org/>



OQMD
The Open Quantum Materials Database

Home Materials Analysis Documentation API Download

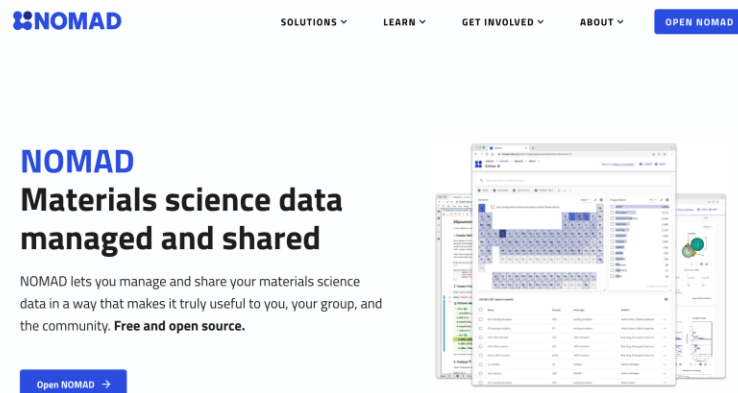
The OQMD is a database of DFT calculated thermodynamic and structural properties of **637,644** materials, created in Chris Wolverton's group at Northwestern University.

Shortcuts

Search Material Compositions	Query Materials Data
Create Phase Diagrams	Determine Ground State Compositions (GCLP)
Visualize Crystal Structures	RESTful API OQMD API Optimade API

<http://oqmd.org/>

...



NOMAD

SOLUTIONS ▾ LEARN ▾ GET INVOLVED ▾ ABOUT ▾ [OPEN NOMAD](#)

NOMAD
Materials science data managed and shared

NOMAD lets you manage and share your materials science data in a way that makes it truly useful to you, your group, and the community. **Free and open source.**

[Open NOMAD →](#)

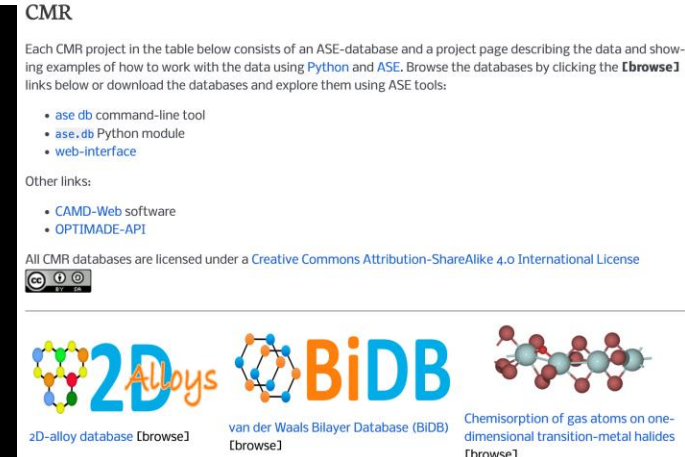
<https://nomad-lab.eu/nomad-lab/>



MATERIALSCLOUD

LEARN WORK DISCOVER EXPLORE ARCHIVE

<https://www.materialscloud.org/>



CMR

Each CMR project in the table below consists of an ASE-database and a project page describing the data and showing examples of how to work with the data using [Python](#) and [ASE](#). Browse the databases by clicking the [\[browse\]](#) links below or download the databases and explore them using ASE tools:

- [ase db](#) command-line tool
- [ase.db](#) Python module
- [web-interface](#)

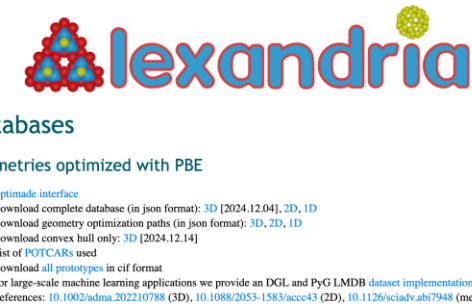
Other links:

- [CAMD-Web](#) software
- [OPTIMADE-API](#)

All CMR databases are licensed under a [Creative Commons Attribution-ShareAlike 4.0 International License](#)

[2D-alloy database](#) [\[browse\]](#) [BiDB](#) [\[browse\]](#) [Chemisorption of gas atoms on one-dimensional transition-metal halides](#) [\[browse\]](#)

<https://cmr.fysik.dtu.dk/>



Alexandria

Databases

Geometries optimized with PBE

- [Optimade interface](#)
- Download complete database (in json format): [3D](#) [2024.12.04], [2D](#), [1D](#)
- Download geometry optimization paths (in json format): [3D](#), [2D](#), [1D](#)
- Download convex hull only: [3D](#) [2024.12.14]
- List of POTCARs used
- Download all [prototypes](#) in cif format
- For large-scale machine learning applications we provide an DGL and PyG [LMDb dataset implementation](#)
- References: [10.1002/adma.202210788](#) (3D), [10.1088/2053-1583/acce43](#) (2D), [10.1126/sciadv.abi7948](#) (method)

Geometries optimized with PBEsol

- [Optimade interface](#)
- Download complete database (in json format): [PBEsol](#), [SCAN](#)
- Download geometry optimization paths (in json format): [PBEsol](#)
- Download convex hull only: [PBEsol](#), [SCAN](#)
- List of POTCARs used
- Download [phonon](#) and [electron-phonon](#) data calculated with Quantum Espresso
- Download [phonon](#) and [electron-phonon](#) data for 2D compounds calculated with Quantum Espresso
- References: [10.1038/s41597-022-01177-w](#) (ground-state), [10.1002/adfm.202404043](#) (phonons)

<https://alexandria.icams.rub.de/>

Outline

1. The AFLOW Database and Software

- AFLOW Apps and search functionality

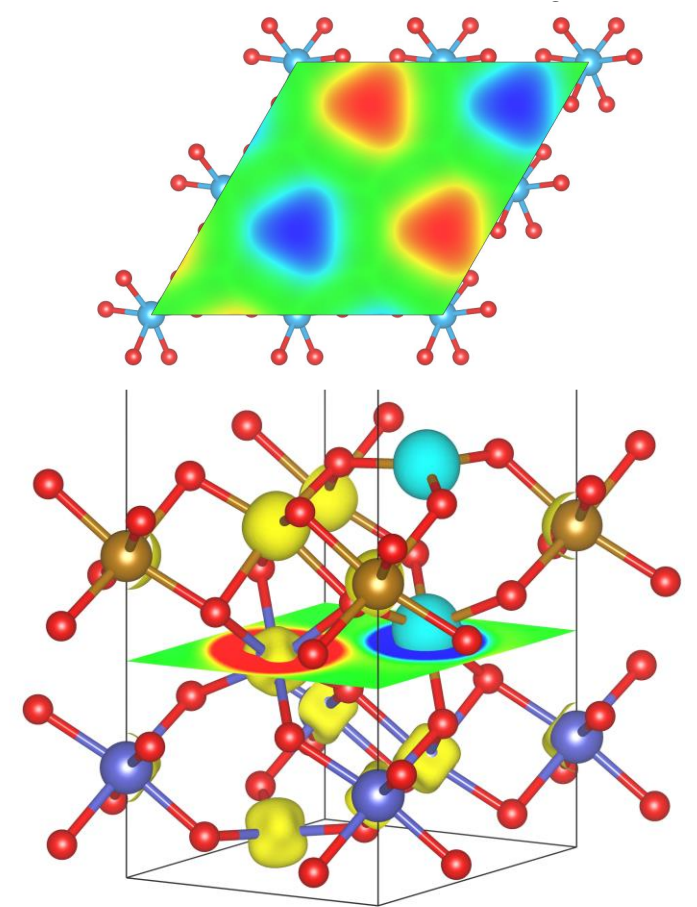
2. Data-driven Quest for Non-vdW 2D Materials

- Search criterion
- Exfoliation energies and properties

3. Magnetic State Control via Hydrogenation

- Surface Passivation
- Magnetic state switching

AFLOW
Automatic - FLOW for Materials Discovery



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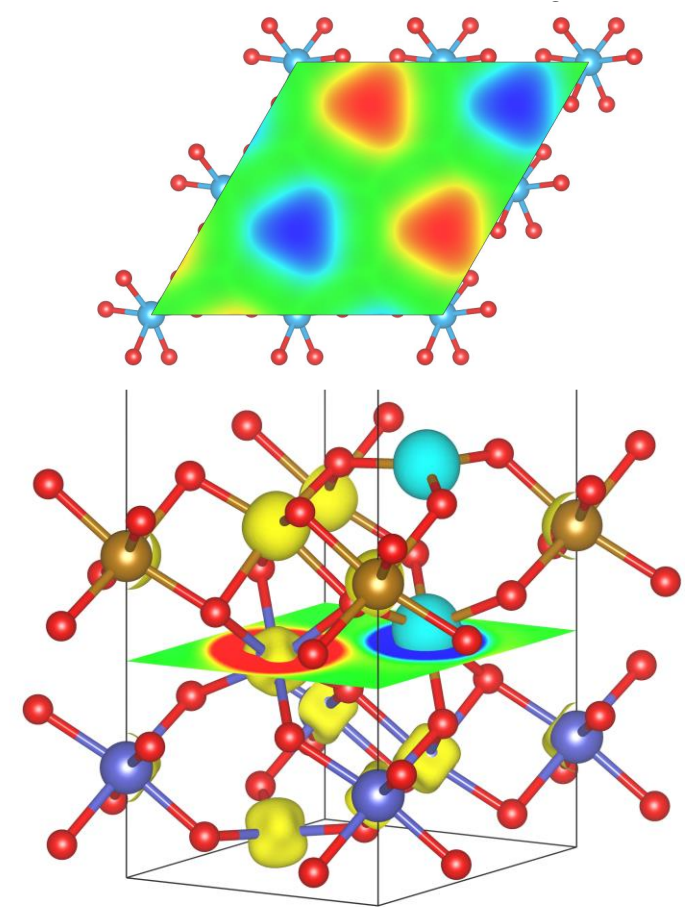
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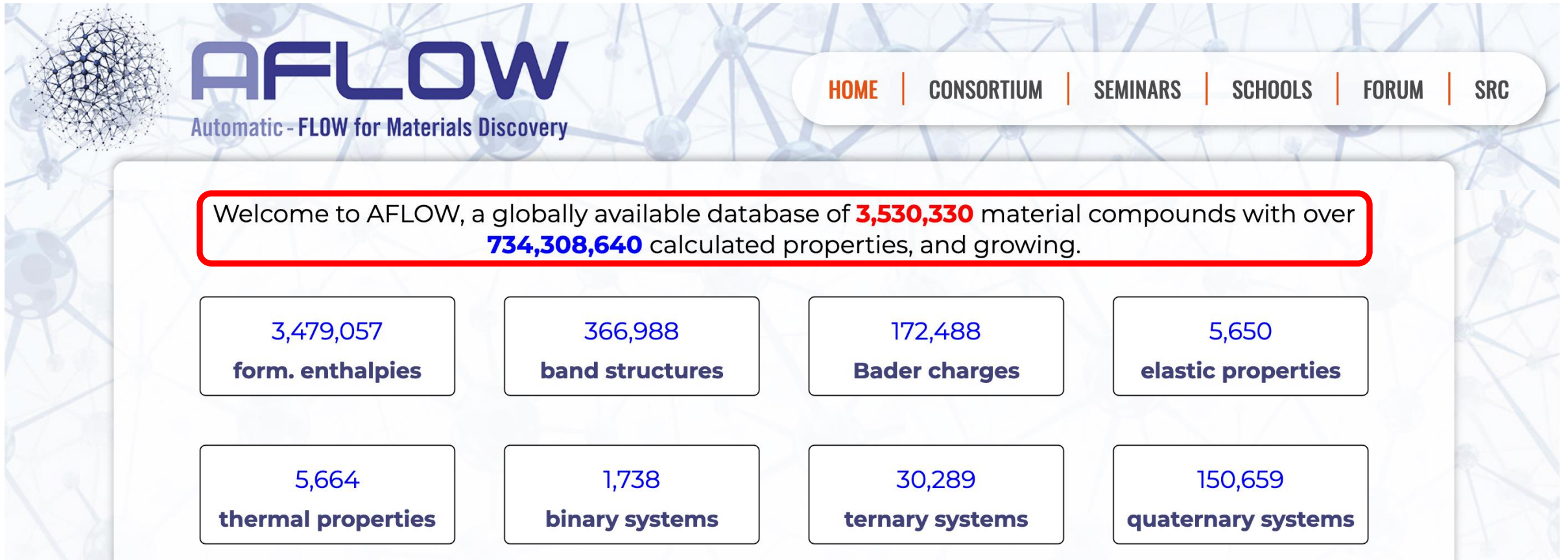
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AFLOW
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AFLOW Database & Software: aflow.org



The screenshot shows the AFLOW website homepage. At the top left is the AFLOW logo with the tagline "Automatic - FLOW for Materials Discovery". To the right is a navigation bar with links: HOME, CONSORTIUM, SEMINARS, SCHOOLS, FORUM, and SRC. Below the navigation bar is a large white box with a red border containing a welcome message. Underneath this are eight boxes arranged in two rows, each displaying a numerical value and a property name. The background of the website features a blue molecular structure pattern.

AFLOW
Automatic - FLOW for Materials Discovery

HOME | CONSORTIUM | SEMINARS | SCHOOLS | FORUM | SRC

Welcome to AFLOW, a globally available database of **3,530,330** material compounds with over **734,308,640** calculated properties, and growing.

3,479,057 form. enthalpies	366,988 band structures	172,488 Bader charges	5,650 elastic properties
5,664 thermal properties	1,738 binary systems	30,289 ternary systems	150,659 quaternary systems

Duke
UNIVERSITY

S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012); S. Curtarolo *et al.*, Comput. Mater. Sci. **58** 227 (2012);
M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023);
C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023);
S. Divilov *et al.*, High Entropy Alloys & Materials **3**, 178 (2025)

UNTERSTÜTZT VON / SUPPORTED BY



Alexander von
HUMBOLDT
STIFTUNG

AFLOW Software & Apps at aflow.org

AFLOW

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S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012)

- written in C++ utilizing VASP as density functional theory program
- AFLOW standard for:
 - *k*-point sets
 - plane wave cutoffs
 - PAW data sets ...

C. E. Calderon *et al.*, Comput. Mater. Sci. **108**, 233 (2015)



G. Kresse and J. Hafner, Phys. Rev. B **49**, 14251 (1994)

G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996)

G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15 (1996)

MendeLIB search



AFLOW database search application

AFLOW-online



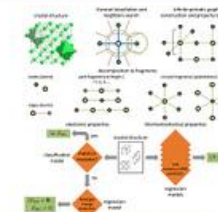
Online interface for AFLOW's symmetry, structure comparison, CCE, POCC, and other functionality

Prototype encyclopedia



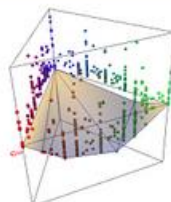
The AFLOW Prototype Encyclopedia with over 1,100 prototypes

AFLOW-ML



Machine Learning application for the PLMF, MDF, and ASC model

AFLOW-CHULL



Convex HULL application for thermodynamic stability and synthesizability

REST-API Docs

AFLOW
REST-API WIKI

Documentation for the AFLOW REST-API

➤ the AFLOW software is structured into purpose dedicated, fully interoperable modules

AFLOW.org Search Page



AFLOW

Automatic - FLOW for Materials Discovery

[HOME](#) | [CONSORTIUM](#) | [PUBLICATIONS](#) | [FORUM](#) | [SRC](#) | [SEARCH](#)

✕

ICSD only

All AFLOW

Search

(60379 entries)

Display

Property Filters

1

H

Hydrogen

3

Li

Lithium

4

Be

Beryllium

11

Na

Sodium

12

Mg

Magnesium

19

K

Potassium

20

Ca

Calcium

21

Sc

Scandium

22

Ti

Titanium

23

V

Vanadium

24

Cr

Chromium

25

Mn

Manganese

26

Fe

Iron

27

Co

Cobalt

28

Ni

Nickel

29

Cu

Copper

30

Zn

Zinc

31

Ga

Gallium

32

Ge

Germanium

33

As

Arsenic

34

Se

Selenium

35

Br

Bromine

36

Kr

Krypton

37

Rb

Rubidium

38

Sr

Strontium

39

Y

Yttrium

40

Zr

Zirconium

41

Nb

Niobium

42

Mo

Molybdenum

43

Tc

Technetium

44

Ru

Ruthenium

45

Rh

Rhodium

46

Pd

Palladium

47

Ag

Silver

48

Cd

Cadmium

49

In

Indium

50

Sn

Tin

51

Sb

Antimony

52

Te

Tellurium

53

I

Iodine

54

Xe

Xenon

55

Cs

Cesium

56

Ba

Barium

57 - 71

*

Lanthanides

72

Hf

Hafnium

73

Ta

Tantalum

74

W

Tungsten

75

Re

Rhenium

76

Os

Osmium

77

Ir

Iridium

78

Pt

Platinum

79

Au

Gold

80

Hg

Mercury

81

Tl

Thallium

82

Pb

Lead

83

Bi

Bismuth

84

Po

Polonium

85

At

Astatine

86

Rn

Radon

57

La

Lanthanum

58

Ce

Cerium

59

Pr

Praseodymium

60

Nd

Neodymium

61

Pm

Promethium

62

Sm

Samarium

63

Eu

Europium

64

Gd

Gadolinium

65

Tb

Terbium

66

Dy

Dysprosium

67

Ho

Holmium

68

Er

Erbium

69

Tm

Thulium

70

Yb

Ytterbium

71

Lu

Lutetium

and

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or

xor

(

)

of species

=

2

He

Helium

5

B

Boron

6

C

Carbon

7

N

Nitrogen

8

O

Oxygen

9

F

Fluorine

10

Ne

Neon

13

Al

Aluminum

14

Si

Silicon

15

P

Phosphorus

16

S

Sulfur

17

Cl

Chlorine

18

Ar

Argon









Center for Autonomous Materials Design, Materials Science, Duke University

Outline

1. The AFLOW Database and Software

- AFLOW Apps and search functionality

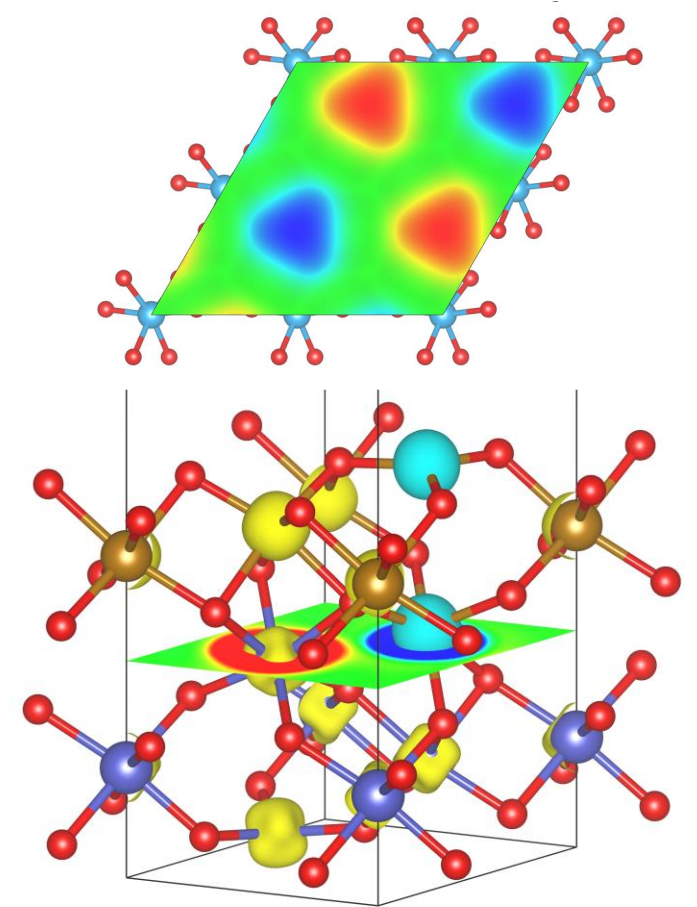
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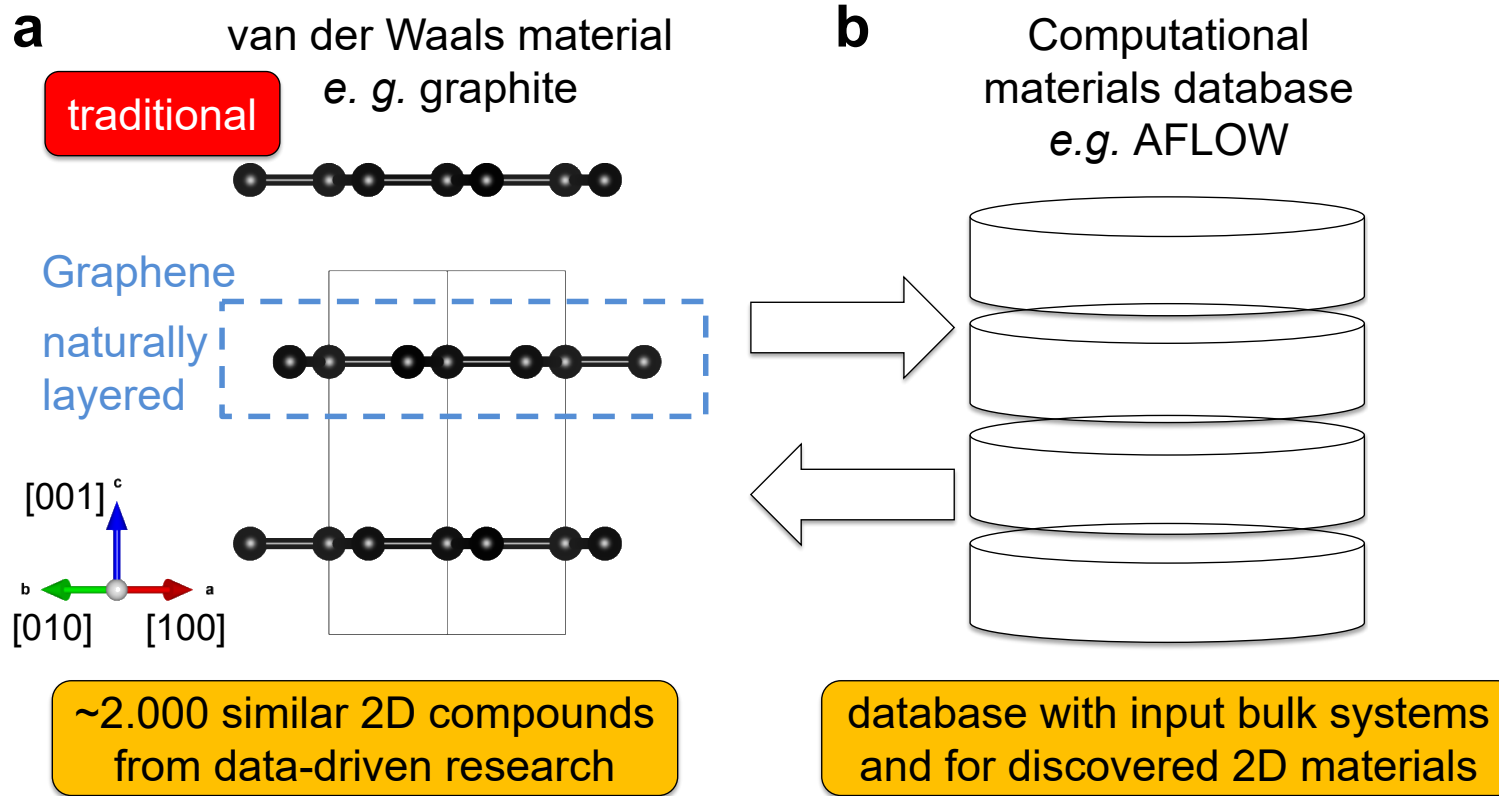
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- Surface Passivation
- Magnetic state switching

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Automatic - FLOW for Materials Discovery



Traditional vs. Data-Driven Materials



- data-driven research predicted several thousands of vdW 2D systems

N. Mounet *et al.*, Nat. Nanotechnol. **13**, 246 (2018)

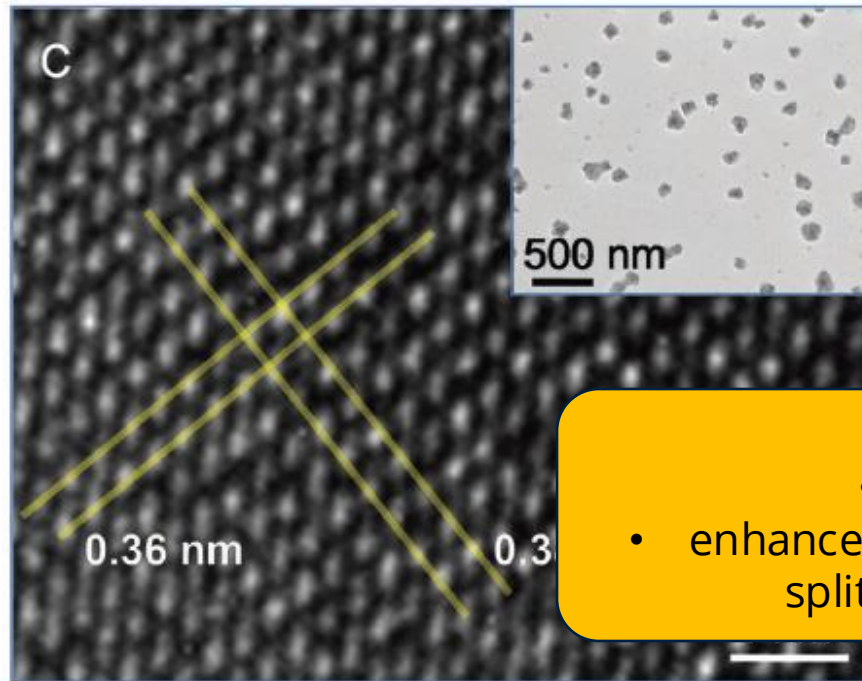
See also: S. Lebegue *et al.*, Phys. Rev. X **3**, 031002 (2013); G. Cheon *et al.*, Nano. Lett. **17**, 1915 (2017)

→ Can we obtain 2D sheets from non-vdW materials?

Electrostatic-Driven Exfoliation and Hybridization of 2D Nanomaterials

Guijian Guan, Jing Xia, Shuhua Liu, Yuan Cheng, Shiqiang Bai, Si Yin Tee, Yong-Wei Zhang,* and Ming-Yong Han*

WO₃ exfoliation



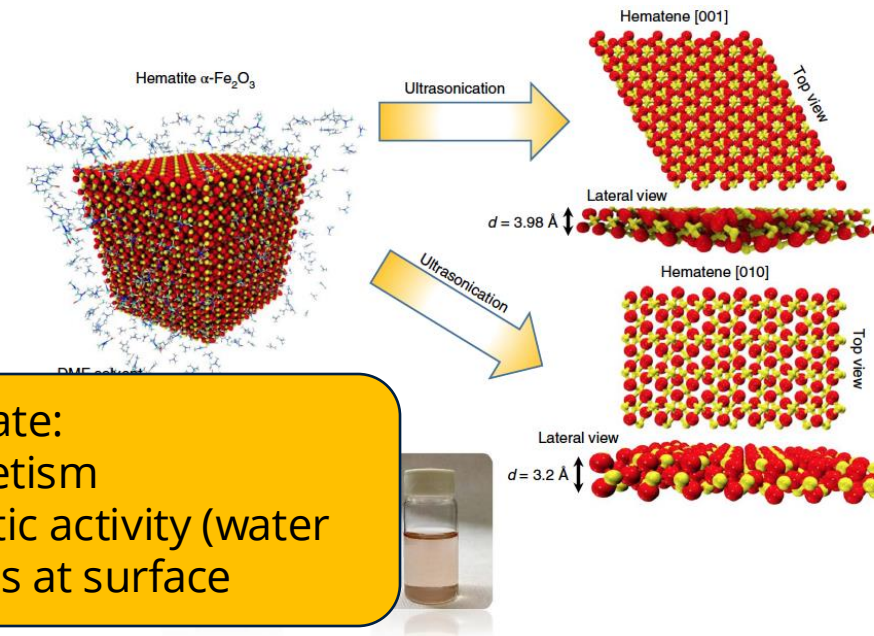
G. Guan *et al.*, *Adv. Mater.* **29**, 1700326 (2017)

results indicate:

- ferromagnetism
- enhanced photocatalytic activity (water splitting) → cations at surface

Exfoliation of a non-van der Waals material from iron ore hematite

Aravind Puthirath Balan^{1,2,11}, Sruthi Radhakrishnan^{1,11}, Cristiano F. Woellner³, Shyam K. Sinha⁴, Liangzi Deng⁵, Carlos de los Reyes⁶, Banki Manmadha Rao⁷, Maggie Paulose⁷, Ram Neupane⁷, Amey Apte¹, Vidya Kochat¹, Robert Vajtai¹, Avetik R. Harutyunyan⁸, Ching-Wu Chu^{5,9}, Gelu Costin¹⁰, Douglas S. Galvao³, Angel A. Marti⁶, Peter A. van Aken⁴, Oomman K. Varghese⁷, Chandra Sekhar Tiwary^{1*}, Anantharaman Malie Madom Ramaswamy Iyer^{1,2*} and Pulickel M. Ajayan^{1*}



A. Puthirath Balan *et al.*, *Nat. Nanotechnol.* **13**, 602 (2018)

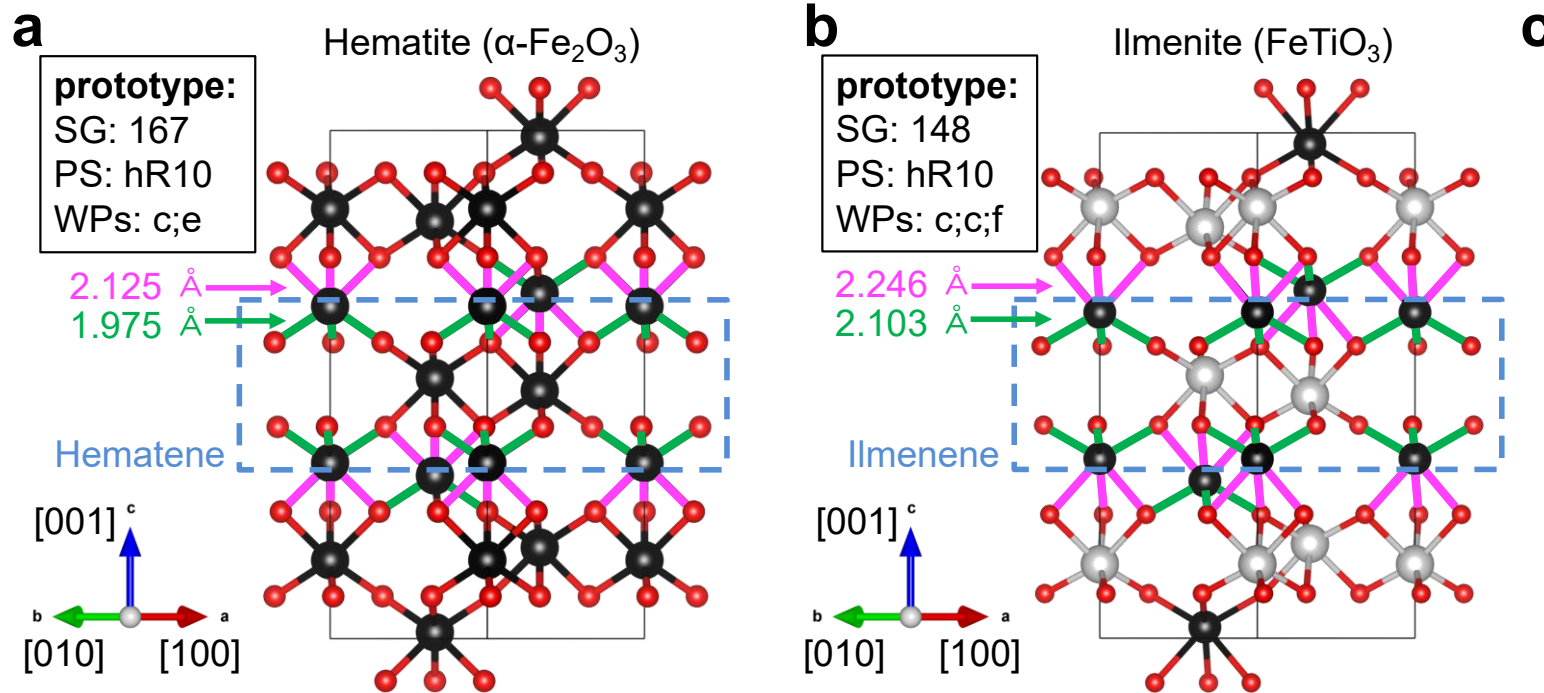
A. Puthirath Balan *et al.*, *Chem. Mater.* **30**, 5923 (2018)

A. Puthirath *et al.*, *J. Phys. Chem. C* **125**, 18927 (2021)

→ Results shatter intuitive understanding of exfoliability (and cleavage)

See also: K. Jiang *et al.*, *Nat. Synth.* **2**, 58 (2023)

Discovering Non-vdW 2D Materials

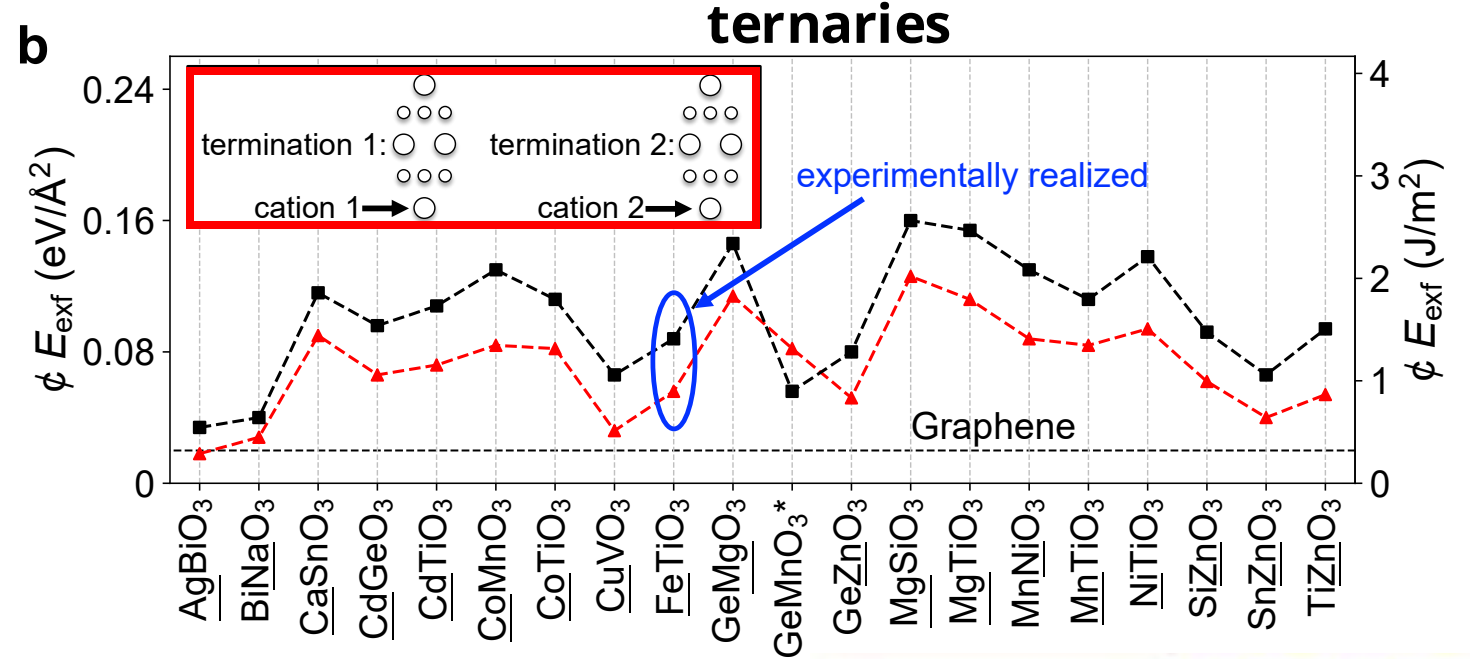
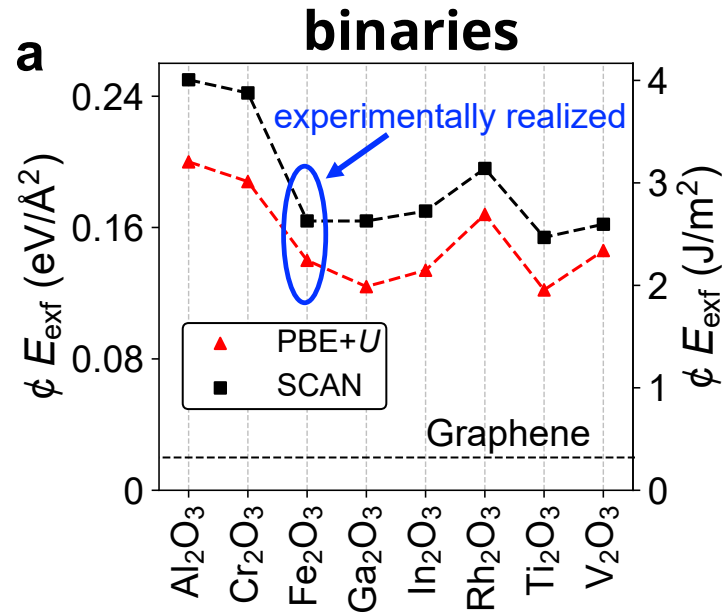


R. Friedrich, M. Ghorbani-Asl, S. Curtarolo and A. V. Krasheninnikov, Nano Lett. **22**, 989 (2022)

T. Barnowsky, A. V. Krasheninnikov, and R. Friedrich, Adv. El. Mats. **9**, 2201112 (2023)

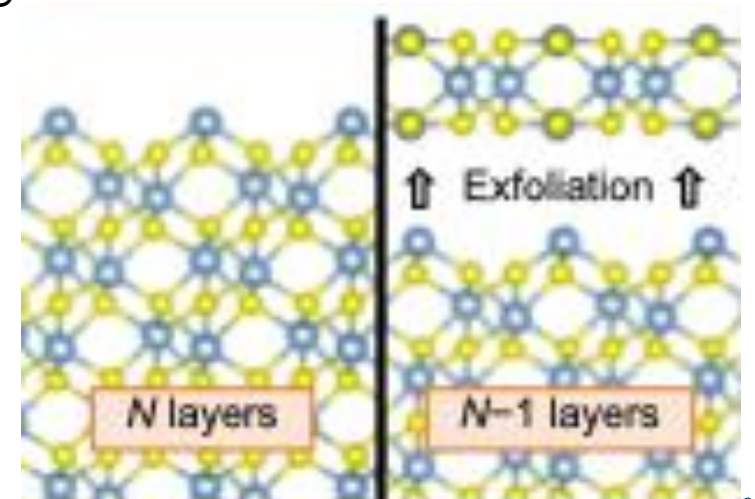
- use structural prototype of first experimentally realized materials to filter AFLOW database
- oxides, sulfides, chlorides

Exfoliation Energies

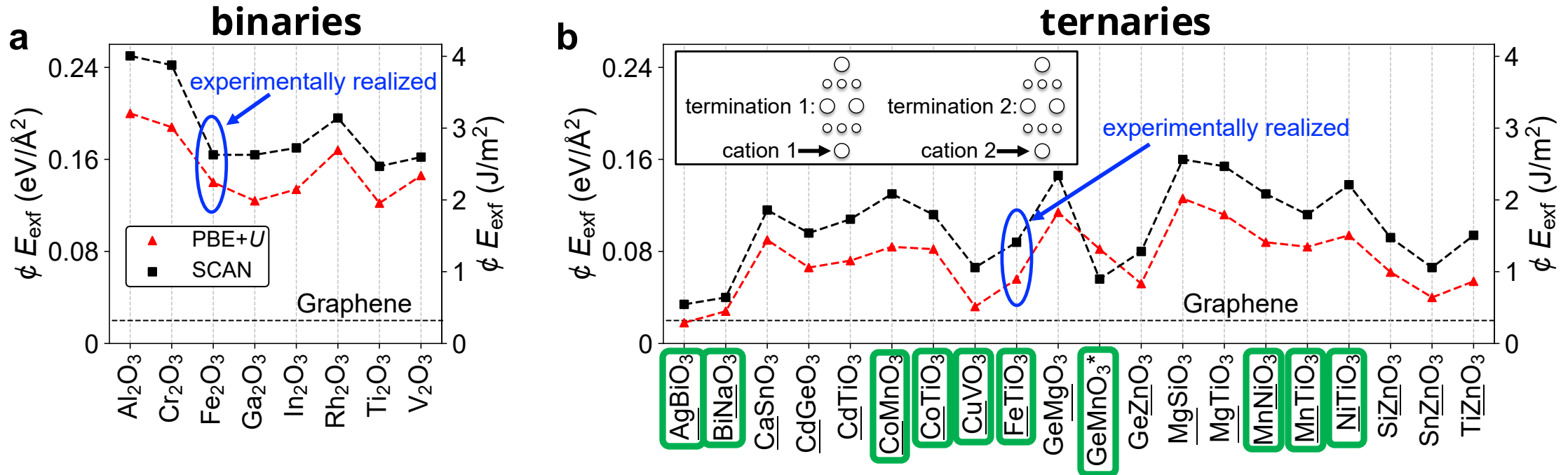


$$\Delta E_{\text{exf}} = \frac{E_{\text{slab}} - E_{\text{bulk}}}{A}$$

J. H. Jung *et al.*, Nano Lett. **18**, 2759 (2018)

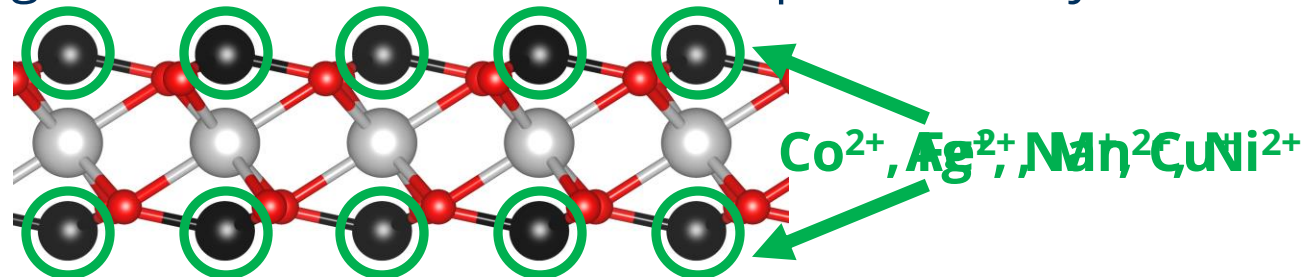


Exfoliation Energies



- all exfoliation energies are close to the ones of exp. realized systems

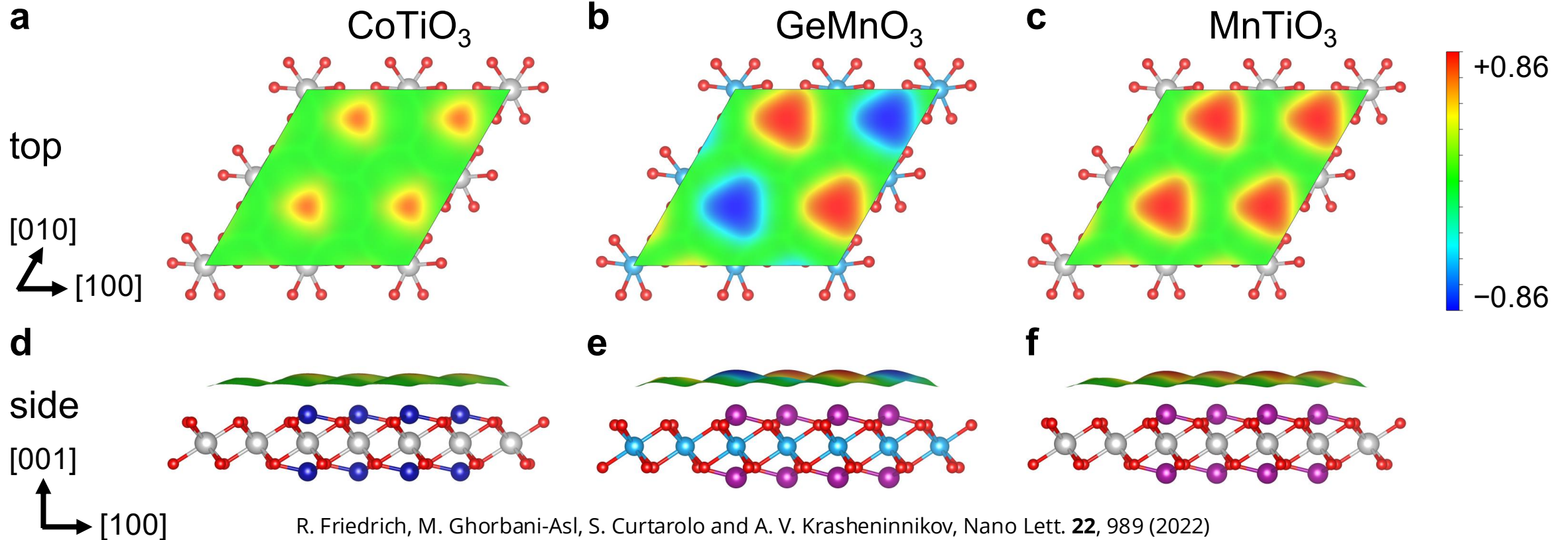
side view



→ easy exfoliation if **cation at surface** is in **low oxidation state**

→ predictive descriptor for future 2D materials discovery

Magnetism



- very diverse surface spin polarization for non-vdW 2D materials

$$P = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}}$$

measurable by spin-polarized scanning tunneling microscopy

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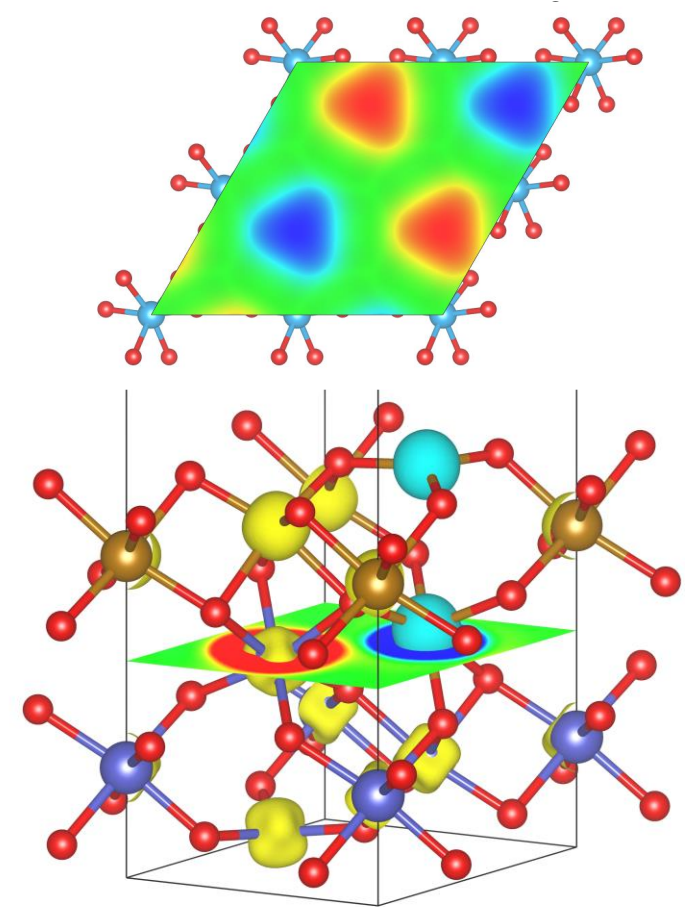
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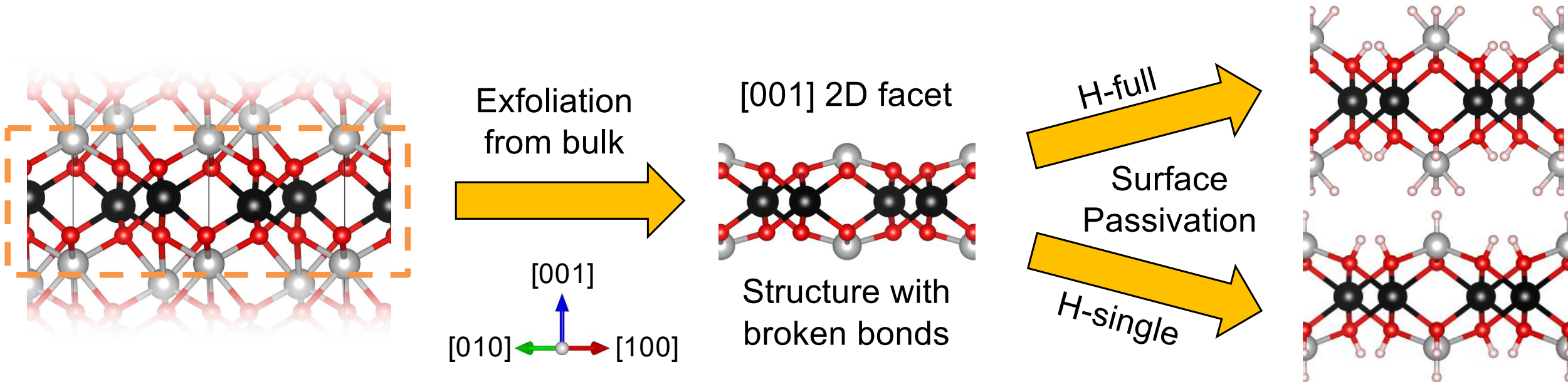
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Surface Passivation of Dangling Bonds



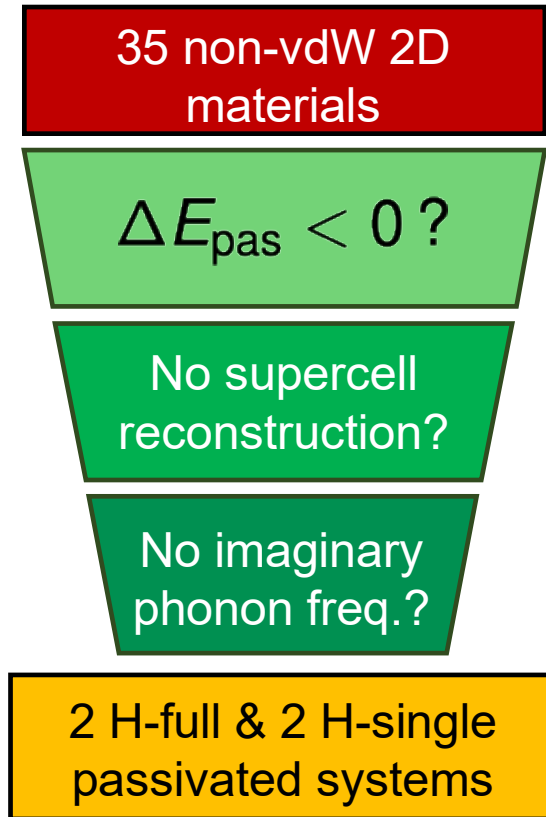
- different surface passivation types mimicking different H chemical potentials



Tom Barnowsky

Filtering Scheme

a

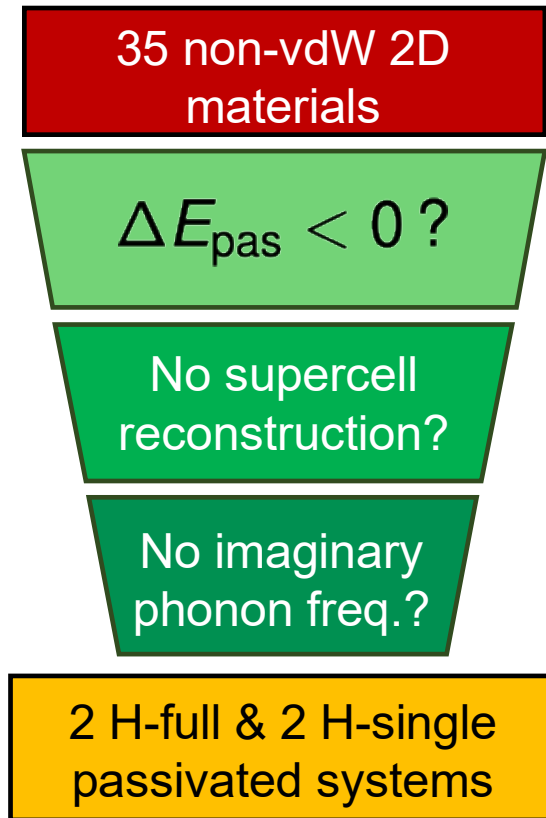


T. Barnowsky, S. Curtarolo, A. V. Krasheninnikov, T. Heine, and R. Friedrich, Nano Letters **24**, 3874 (2024)

- only 4 out of 35 systems pass all stability tests
- special geometry for 2D CdTiO₃:H-single → validated from different starting geometries

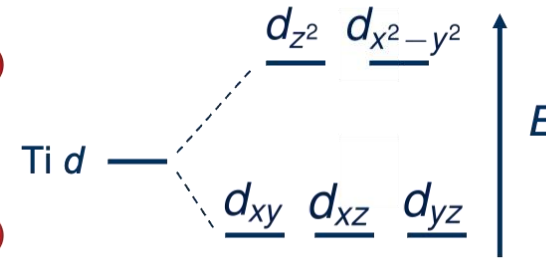
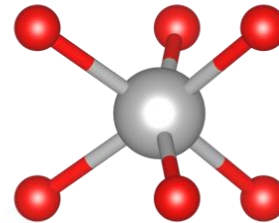
Filtering Scheme

a

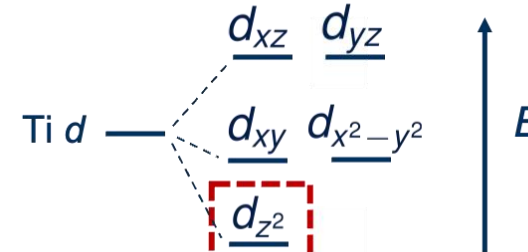
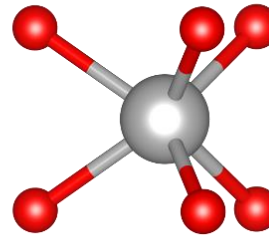


Coordination change during relax.

Octahedral

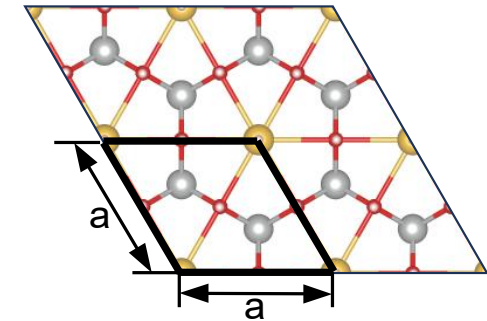
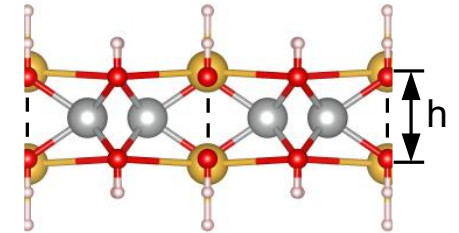


Trigonal-prismatic



e

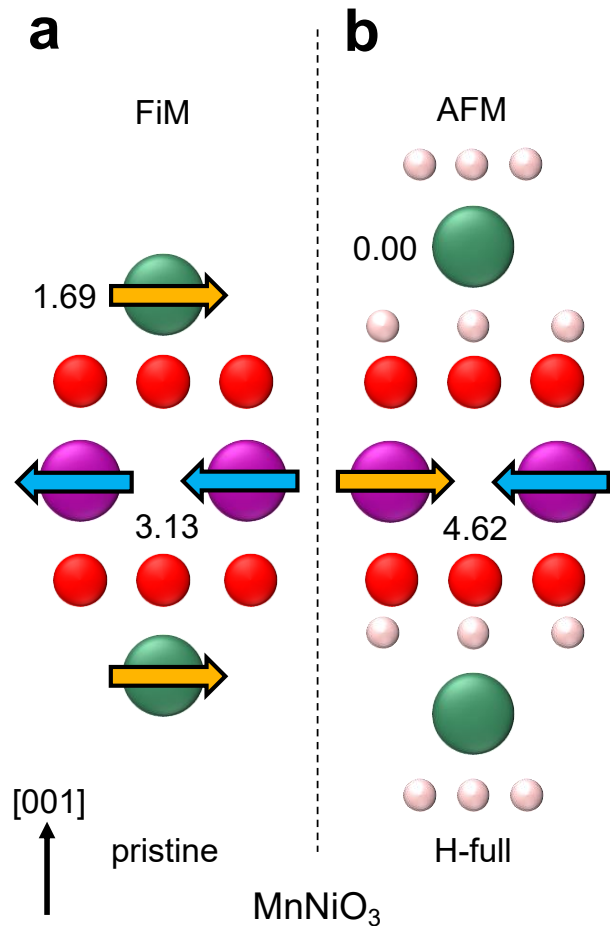
2D $\text{CdTiO}_3\text{:H}$ -single
 $\Delta E_{\text{pas}} = -0.14 \text{ eV/H}_2$



T. Barnowsky, S. Curtarolo, A. V. Krashennnikov, T. Heine, and R. Friedrich, Nano Letters **24**, 3874 (2024)

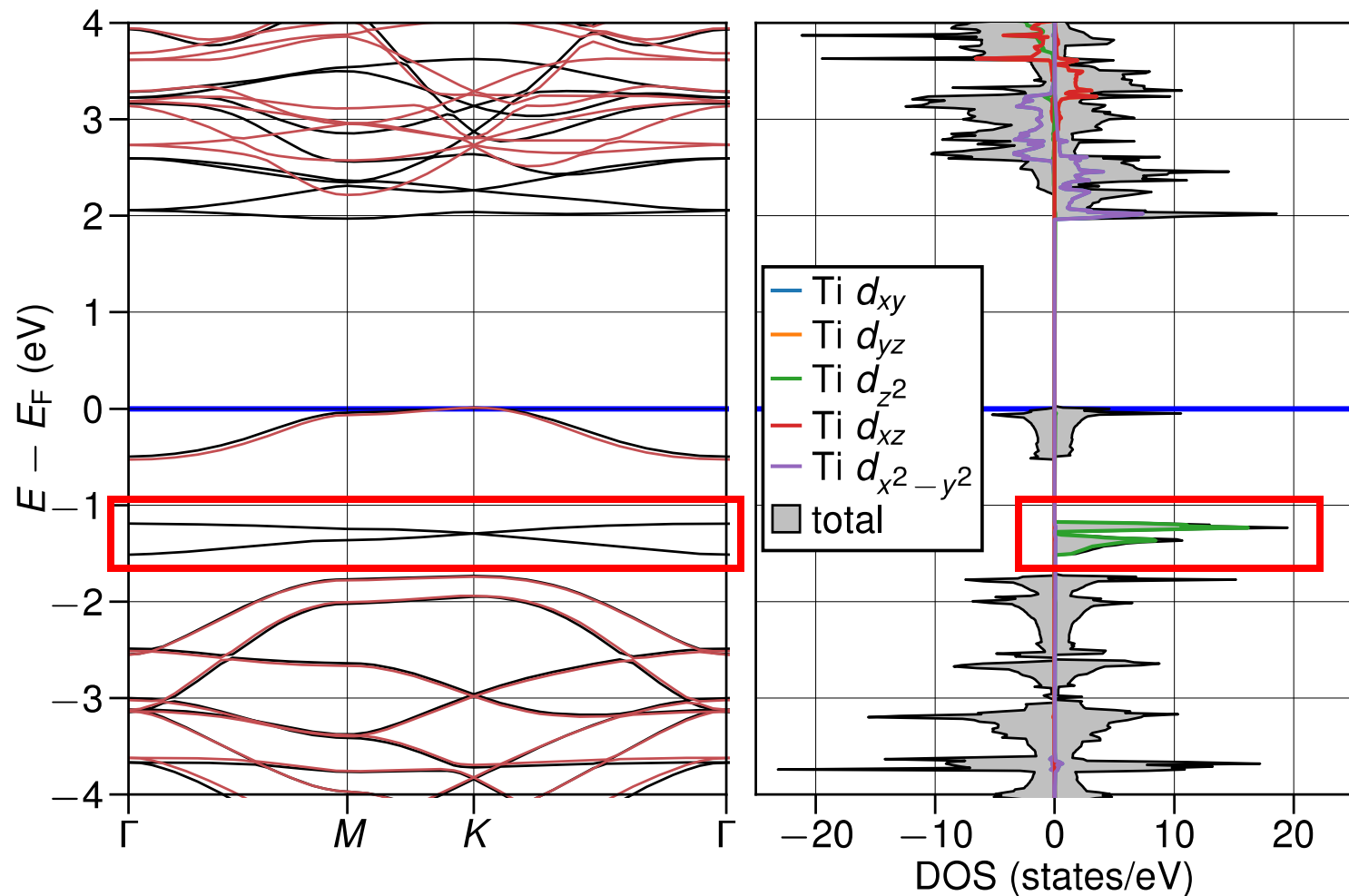
- only 4 out of 35 systems pass all stability tests
- special geometry for 2D $\text{CdTiO}_3\text{:H}$ -single → validated from different starting geometries

Magnetic Configurations



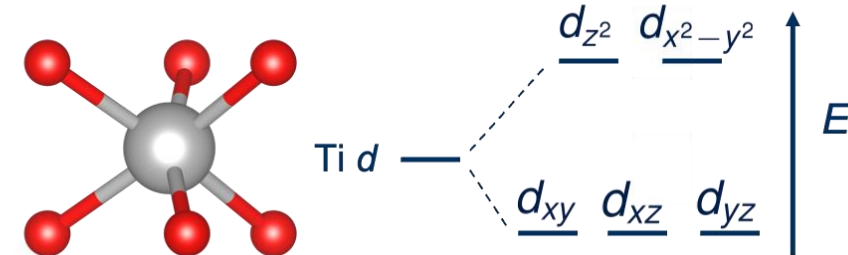
- switching to states with flipped and enhanced moments due to passivation
- onset of ferromagnetism for CdTiO₃:H-single → mean field Curie temperature $T_C^{MF} \sim 10\text{K}$

CdTiO₃:H-single Density of States

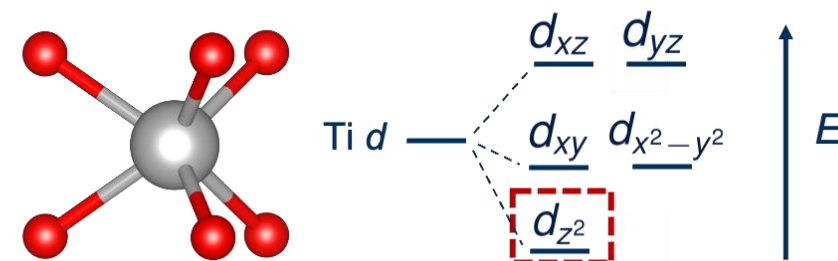


Coordination change during relax.

Octahedral



Trigonal-prismatic



- occupation of $3d_{z^2}$ majority spin bands connected to structural change

Magnetization Density Difference

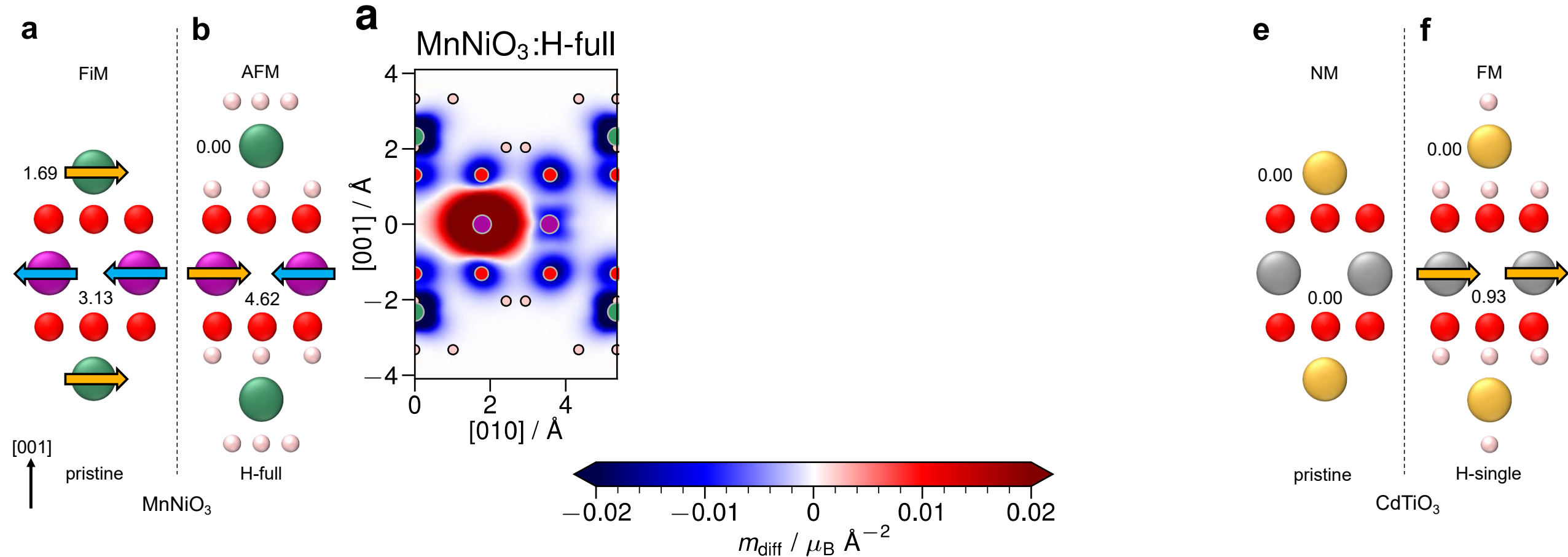
- magnetization density as difference between spin up and spin down electron densities:

$$m(\mathbf{r}) = \mu_B(n_{\uparrow}(\mathbf{r}) - n_{\downarrow}(\mathbf{r}))$$

- magnetization density difference between pristine and passivated systems:

$$m_{\text{diff}}(\mathbf{r}) = m_{\text{passivated}}(\mathbf{r}) - m_{\text{pristine}}^{\text{SCF}}(\mathbf{r})$$

Magnetization Density Difference



T. Barnowsky, S. Curtarolo, A. V. Krashenninnikov, T. Heine, and R. Friedrich, Nano Letters **24**, 3874 (2024)

- local spin symmetry change for MnNiO₃:H-full
- CdTiO₃:H-single: spin transfer to Ti in $3d_{z^2}$ orbital shape

Summary and Conclusions

- data-driven materials design is a powerful tool enabling the discovery of novel compounds
- non-van der Waals 2D materials represent an emerging new class of low-dimensional compounds
- their active cation-terminated surfaces give rise to strong surface spin polarization and magnetic state control through passivation

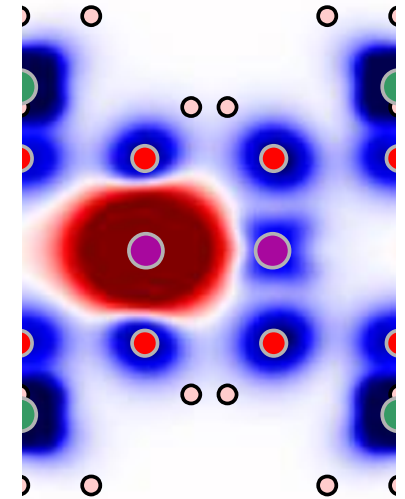
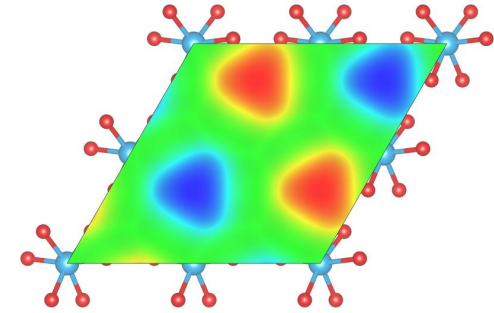
R. Friedrich, M. Ghorbani-Asl, S. Curtarolo and A. V. Krasheninnikov, Nano Lett. **22**, 989 (2022)

T. Barnowsky, A. V. Krasheninnikov, and R. Friedrich, Adv. El. Mats. **9**, 2201112 (2023)

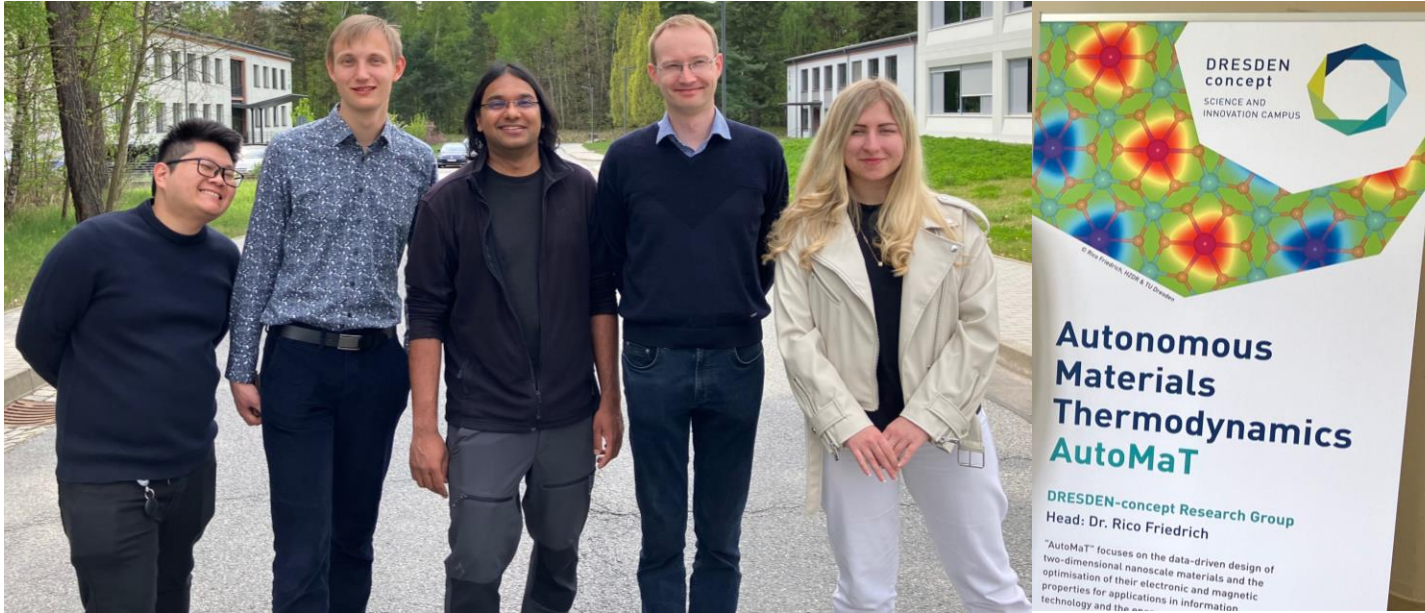
T. Barnowsky, S. Curtarolo, A. V. Krasheninnikov, T. Heine, and R. Friedrich, Nano Letters **24**, 3874 (2024)

A. Nihei, T. Barnowsky, and R. Friedrich, submitted, arXiv:2503.12209 (2025)

A. P. Balan *et al.*, Materials Today **58**, 164 (2022)



Thank You for Your Attention



Balaram Thakur



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- TU Dresden: Thomas Heine, Alexander Eychmüller, Carsten Timm, Kevin Synnatschke, Michael Ruck, Gianaurelio Cuniberti
- HZDR: Thomas Kühne, Agnieszka Kuc, Mahdi Ghorbani-Asl, Arkady V. Krasheninnikov
- Rice University: Anand B. Puthirath, Aravind Puthirath Balan, Pulickel M. Ajayan
- FZ Jülich: Daniel Wortmann, Gregor Michalick, Gustav Bihlmayer, Stefan Blügel
- IFW Dresden: Axel Lubk, Kornelius Nielsch
- Duke University: Hagen Eckert, Simon Divilov, Stefano Curtarolo
- UT Dallas: Cormac Toher



Paderborn Center for
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Alexander von
HUMBOLDT
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AFLOW.org Search Page

The screenshot shows the AFLOW.org search interface. At the top, there is a navigation bar with links: HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below this is a search bar with a dropdown menu set to 'ICSD only' and a 'Search' button indicating 60379 entries. To the right of the search bar is a 'Display' button. Below the search bar is a 'Periodic Table' section with various filters. Four orange callout boxes with arrows point to specific features: 'Element group selection' points to the 'Filters' section; 'Number of species' points to the '# of species' dropdown; 'Logic operations' points to the 'and', 'or', 'not', and 'xor' buttons; and 'Element selection' points to the periodic table grid.

Element group selection

Number of species

Logic operations

Element selection

AFLOW.org Search Page

The screenshot shows the AFLOW.org Search Page. At the top, there is a navigation bar with links: HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below this is a search bar with the text "Search Aflow" and a dropdown menu currently set to "ICSD only". To the right of the search bar is a green "Search" button with "(60379 entries)" and a "Display" button. Below the search bar is a "Periodic Table" section. On the left of the periodic table is a "Property Filters" section with a list of categories: Metals, Alkali Metals, Alkali Earths, Transition Metals, Lanthanides, Other Metals, Non-Metals, Boron Group, Carbon Group, Pnictogens, Chalcogens, and Halogens. On the right of the periodic table is another "Property Filters" section with a "# of species" dropdown. Two orange arrows point to these sections. The first arrow points to the "Property Filters" on the left, with a callout box that says "Slide to Property Filters". The second arrow points to the "Property Filters" on the right, with a callout box that says "Bring property filters onto search page". At the bottom of the page, there is a footer with logos for Duke University, University at Buffalo, Missouri S&T, NC State University, Penn State, NSF, and ONR. Below the logos is the text "Center for Autonomous Materials Design, Materials Science, Duke University".

AFLOW.org Search Page


AFLOW
 Automatic - FLOW for Materials Discovery

[HOME](#) | [CONSORTIUM](#) | [PUBLICATIONS](#) | [FORUM](#) | [SRC](#) | [SEARCH](#)

Search Aflow
 (60379 entries)

Periodic Table

1 H Hydrogen	2 He Helium
3 Li Lithium	4 Be Beryllium
11 Na Sodium	12 Mg Magnesium
19 K Potassium	20 Ca Calcium
27 Co Cobalt	28 Ni Nickel
35 Br Bromine	36 Kr Krypton
53 I Iodine	54 Xe Xenon
85 At Astatine	86 Rn Radon

Metals Alkali Metals Alkali Earths

Transition Metals Lanthanides Other Metals

Non-Metals Boron Group Carbon Group

Pnictogens Chalcogens Halogens

and not

or xor

()

of species

from 1 to 230

Property Filters

Property Filters

Search Properties

Electronic Properties	band gap type Describes if the system is a metal, a semi-metal, or an insulator with direct or indirect band gap.	Add
Magnetic Properties	electronic band gap Electronic band gap.	Add
Mechanical Properties		
Thermodynamic Properties		
Relaxed Structure		
Chemistry		
Calculation Details		

space group

☒ Display column

☐ Restrict value

from 1 to 230

Pearson symbol

☒ Display column

☐ Restrict value

equal to

AFLOW.org Search Page

The screenshot shows the AFLOW.org search interface. At the top, there's a navigation bar with links: HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below this is a search bar containing "Na, Cl" and a "Search" button (60379 entries). A "Display" button is also present. The "Periodic Table" is shown below the search bar, with elements grouped by categories like Metals, Alkali Metals, Alkali Earths, etc. The "Property Filters" section is at the bottom, showing various filters like Electronic Properties, Mechanical Properties, etc. The "band gap type" filter is highlighted, and the "Add" button is shown. The "electronic band gap" filter is also highlighted, showing a range from 0 to 17.6792 eV. Annotations with orange arrows point to these features:

- Selected Elements:** Points to the search bar containing "Na, Cl".
- Number of species=2:** Points to the "# of species" dropdown menu, which is set to 2.
- Added filter for Egap: electronic band gap:** Points to the "electronic band gap" filter in the Property Filters section.
- Select "Add" to add filter:** Points to the "Add" button in the Property Filters section.
- Check box to restrict search results to specific value range:** Points to the "Restrict value" checkbox for the "electronic band gap" filter.

AFLOW.org Search Page

Live demo examples:

1. Let us use the advanced search functionality to find the band gap for SiC in the zincblende structure (space group number 216).
2. Let us use the advanced search functionality to find the materials containing Sn but not Pb with band gaps between 1 eV and 3 eV in the ICSD catalog of the AFLOW database. How many results are returned?

Alternative server: aflowlib.duke.edu/search/ui/

R. H. Taylor *et al.*, Comput. Mater. Sci. **93**, 178-192 (2014), F. Rose *et al.*, Comput. Mater. Sci. **137**, 362 (2017) ; M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023)

AFLOW.org Search Page

Live demo examples:

1. Let us use the advanced search functionality to find the band gap for SiC in the zincblende structure (space group number 216). → **1.37 eV**
2. Let us use the advanced search functionality to find the materials containing Sn but not Pb with band gaps between 1 eV and 3 eV in the ICSD catalog of the AFLOW database. How many results are returned? → **369 results**

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Entry page for each item of the database

R. H. Taylor *et al.*, Comput. Mater. Sci. **93**, 178-192 (2014), F. Rose *et al.*, Comput. Mater. Sci. **137**, 362 (2017) ; M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023)

AFLOW Software & Apps at aflow.org

AFLOW

Automatic - FLOW for Materials Discovery

S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012)

- written in C++ utilizing VASP as density functional theory program
- AFLOW standard for:
 - *k*-point sets
 - plane wave cutoffs
 - PAW data sets ...

C. E. Calderon *et al.*, Comput. Mater. Sci. **108**, 233 (2015)



G. Kresse and J. Hafner, Phys. Rev. B **49**, 14251 (1994)

G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996)

G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15 (1996)

MendeLIB search



AFLOW database search application

AFLOW-online



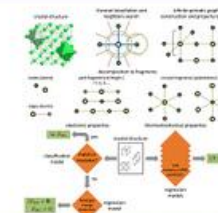
Online interface for AFLOW's symmetry, structure comparison, CCE, POCC, and other functionality

Prototype encyclopedia



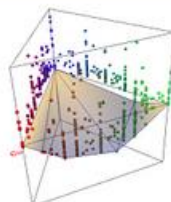
The AFLOW Prototype Encyclopedia with over 1,100 prototypes

AFLOW-ML



Machine Learning application for the PLMF, MDF, and ASC model

AFLOW-CHULL



Convex HULL application for thermodynamic stability and synthesizability

REST-API Docs

AFLOW
REST-API WIKI

Documentation for the AFLOW REST-API

➤ the AFLOW software is structured into purpose dedicated, fully interoperable modules