

Data Mining for 2D materials

Group 3

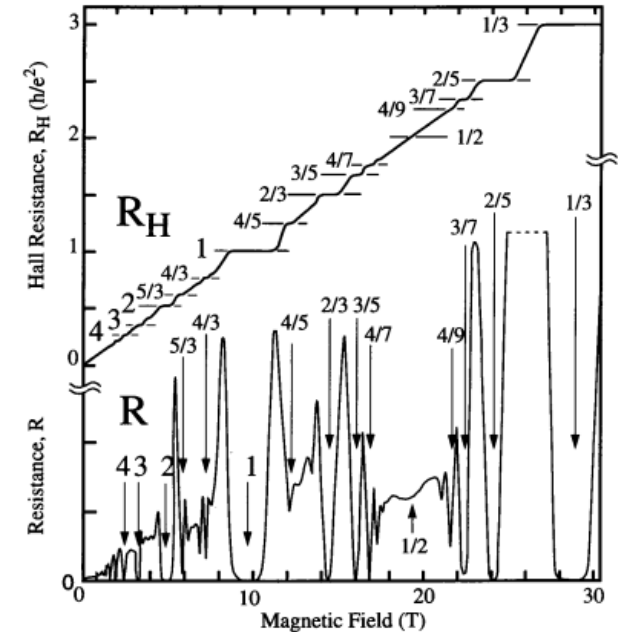
2019/11/12

Outline

- Introduction to 2D materials
- Crystal databases and data mining
- Layered 2D materials searching methods
- Results and further developments

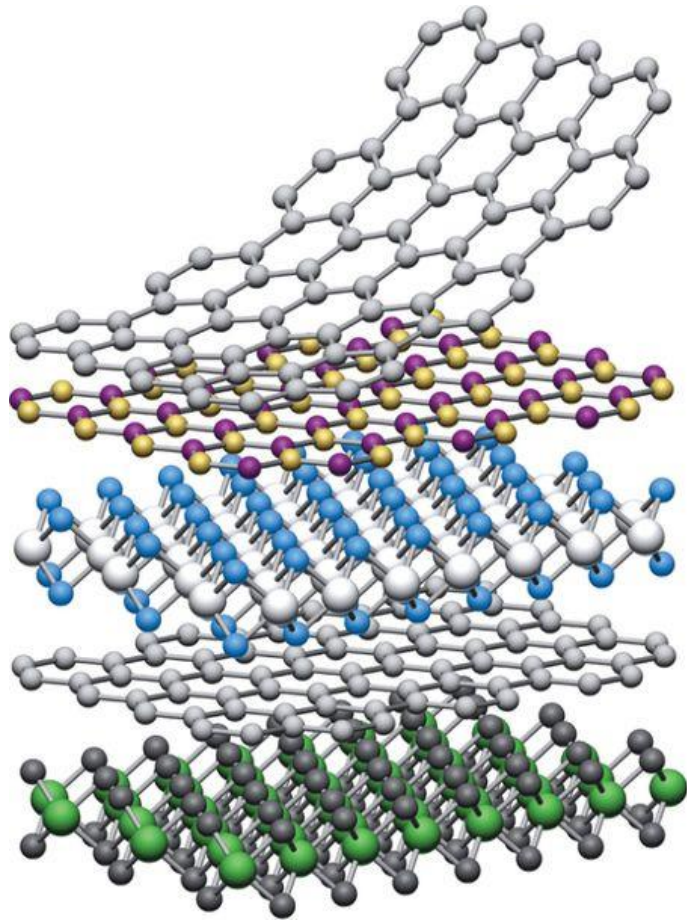
Introduction to 2D materials

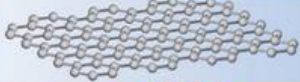

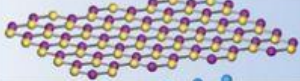

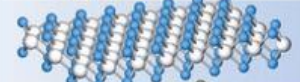

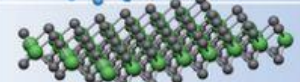
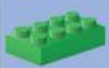
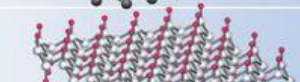

- Research interests
 - Quantum Fractional Hall Effect
 - Van der Waals Heterojunction
 - Superconductivity

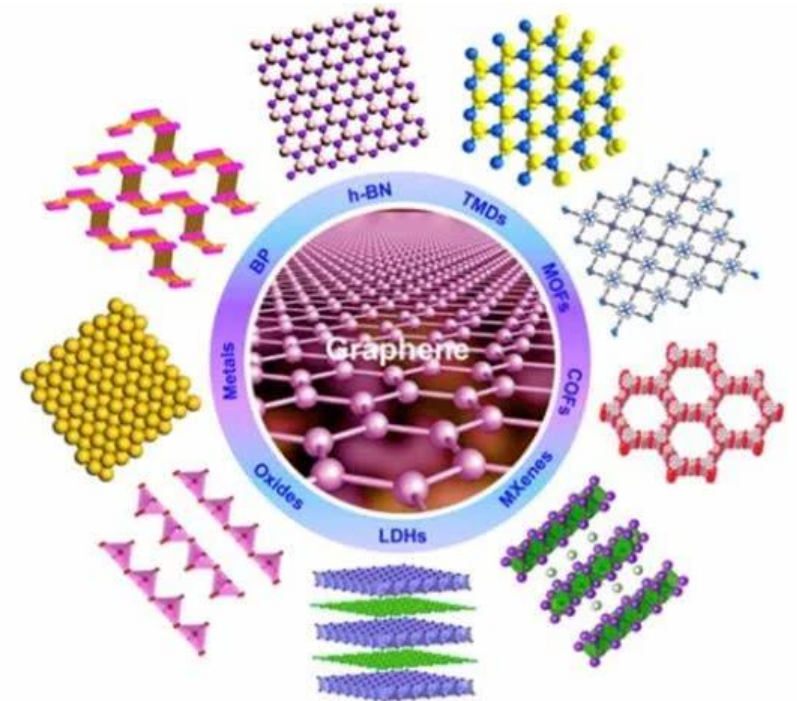
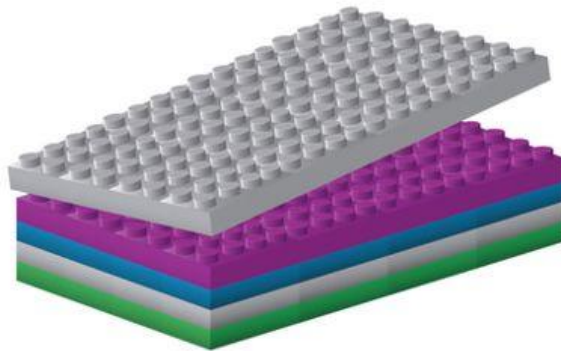


Horst. L. Stormer, Nobel Lecture, 1998

Van der Waals heterostructures



	Graphene	
	hBN	
	MoS ₂	
	WSe ₂	
	Fluorographene	



Geim AK & Grigorieva IV (2013) Van der Waals heterostructures. Nature 499(7459):419-425.

2D materials library 2013

Graphene family	Graphene	hBN 'white graphene'	BCN	Fluorographene	Graphene oxide
2D chalcogenides	MoS ₂ , WS ₂ , MoSe ₂ , WSe ₂		Semiconducting dichalcogenides: MoTe ₂ , WTe ₂ , ZrS ₂ , ZrSe ₂ and so on	Metallic dichalcogenides: NbSe ₂ , NbS ₂ , TaS ₂ , TiS ₂ , NiSe ₂ and so on	
				Layered semiconductors: GaSe, GaTe, InSe, Bi ₂ Se ₃ and so on	
2D oxides	Micas, BSCCO	MoO ₃ , WO ₃	Perovskite-type: LaNb ₂ O ₇ , (Ca,Sr) ₂ Nb ₃ O ₁₀ , Bi ₄ Ti ₃ O ₁₂ , Ca ₂ Ta ₂ TiO ₁₀ and so on		Hydroxides: Ni(OH) ₂ , Eu(OH) ₂ and so on
	Layered Cu oxides	TiO ₂ , MnO ₂ , V ₂ O ₅ , TaO ₃ , RuO ₂ and so on			Others

Geim AK & Grigorieva IV (2013) Van der Waals heterostructures. Nature 499(7459):419-425.

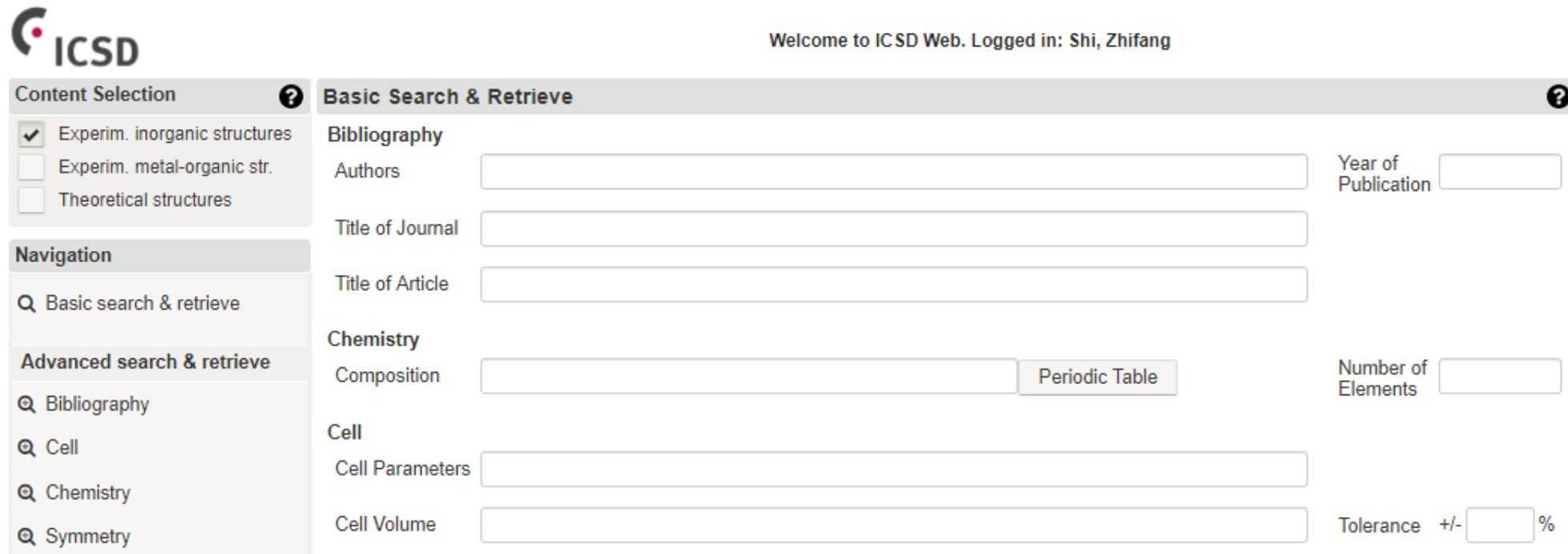
More novel 2D materials?

- Graphene: 0 band gap
- MoS₂: Low electron mobility
- Phosphorene: not stable

- More candidates for Van der Waals heterostructures

3D crystal databases

- Inorganic Crystal Structure Database (ICSD)



The image shows the ICSD (Inorganic Crystal Structure Database) Basic Search & Retrieve interface. The page header includes the ICSD logo and a welcome message: "Welcome to ICSD Web. Logged in: Shi, Zhifang". The interface is divided into several sections:

- Content Selection:** A sidebar with three checkboxes: "Experim. inorganic structures" (checked), "Experim. metal-organic str." (unchecked), and "Theoretical structures" (unchecked).
- Navigation:** A sidebar with search icons for "Basic search & retrieve", "Advanced search & retrieve", "Bibliography", "Cell", "Chemistry", and "Symmetry".
- Basic Search & Retrieve:** The main search area with the following fields:
 - Bibliography:** Authors, Title of Journal, Title of Article, and Year of Publication.
 - Chemistry:** Composition (with a "Periodic Table" button) and Number of Elements.
 - Cell:** Cell Parameters and Cell Volume.
 - Tolerance:** A field for tolerance, labeled "Tolerance +/- %".

<https://icsd.fiz-karlsruhe.de/search/basic.xhtml>

Materials Project

The screenshot displays the Materials Project website interface. At the top, there is a navigation bar with links for Home, About, Apps, Documentation, API, Tutorials, and Dashboard. Below this is a search bar with a magnifying glass icon and a text input field containing "Na-O". To the right of the search bar is a search button labeled "search".

The main content area features a periodic table of elements. The search results are displayed in a grid format, with elements highlighted in red and blue. The search results for "Na-O" are as follows:

1	2
H	He
Li	Be
Na	Mg
K	Ca
Rb	Sr
Cs	Ba
Fr	Ra
B	C
Al	Si
Ga	Ge
In	Sn
Tl	Pb
N	O
P	S
As	Se
Sb	Te
Bi	Po

On the right side of the interface, there is a sidebar with the following sections:

- # of elements**: A search input field with the example "e.g., 4 or >2 & <6".
- excluded elements**: A search input field with the example "Cl Br".
- Submit**: A blue button.
- External Provenance**: Two checkboxes, "ICSD" and "Exptl. ICSD", both of which are checked.
- Material Tags**: A search input field with the example "imgreite".

<https://www.materialsproject.org>

Quest for novel 2D materials

- By the time of 2016:

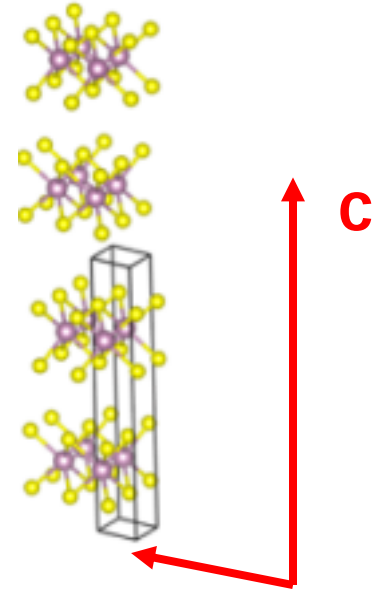
Over 200,000 3D bulk crystals collected in Inorganic Crystal Structure Database (ICSD)

However, only a few dozens of 2D materials have been experimentally synthesised or exfoliated

- Question: How can we find more exfoliable layered materials?

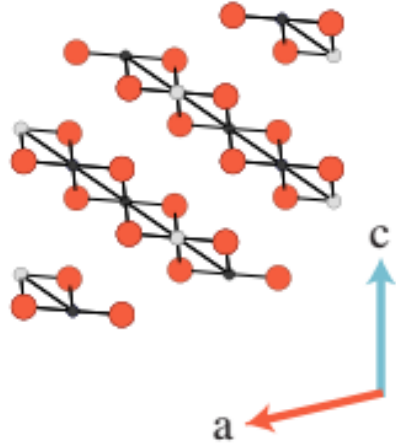
Pioneering attempt to identify layered materials

- 2013 PRX, characterize layered materials by:
Low packing ratio (0.15-0.50)
Large gaps (>2.4 Å) between crystallographic planes along the c axis
- Discovered almost 100 layered phases!



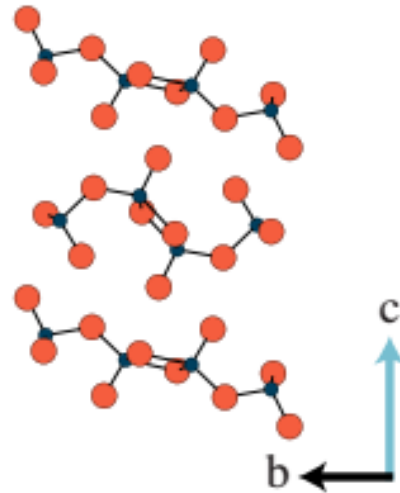
Challenges of layer detection

(a) Co_2NiO_6 (mp-765906)



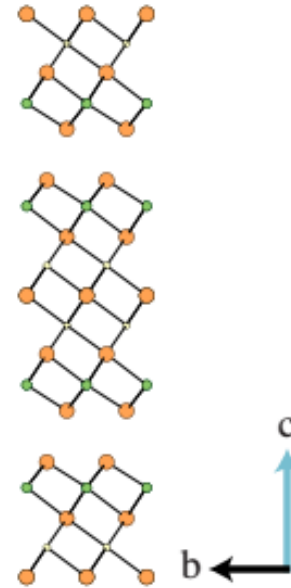
layers not along c axis

(b) V_2O_5 (mp-25643)



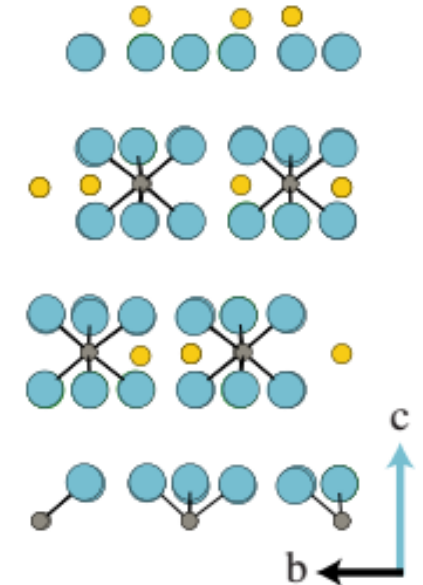
corrugated layers

(c) $\text{Ge}_2\text{Te}_5\text{As}_2$ (mp-14791)



thick layers

(d) Li-WCl_6 (mp-570512)



molecular (nonbonded) layers

Breakthrough

Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials

Michael Ashton,¹ Joshua Paul,¹ Susan B. Sinnott,² and Richard G. Hennig^{1,*}

PRL, 2017

Data Mining for New Two- and One-Dimensional Weakly Bonded Solids and Lattice-Commensurate Heterostructures

Gwoon Cheon,[†] Karel-Alexander N. Duerloo,[‡] Austin D. Sendek,[†] Chase Porter,[§] Yuan Chen,[†]
and Evan J. Reed^{*,‡}

Nano Letters, 2017

Novel two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

Nicolas Mounet,¹ Marco Gibertini,¹ Philippe Schwaller,¹ Andrius Merkys,¹
Ivano E. Castelli,¹ Andrea Cepellotti,¹ Giovanni Pizzi,¹ and Nicola Marzari¹

Nature Nanotechnology, 2018

Method

- Step1:

Geometrical screening algorithm for layered materials

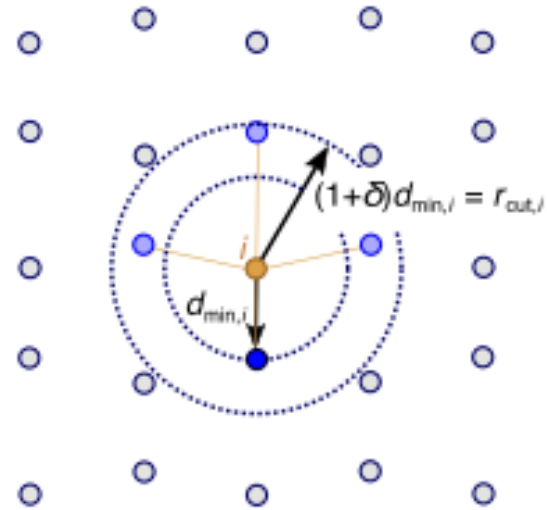
- Step2:

Identify layered materials that easily exfoliable using vdW DFT simulations

Geometrical screening algorithm

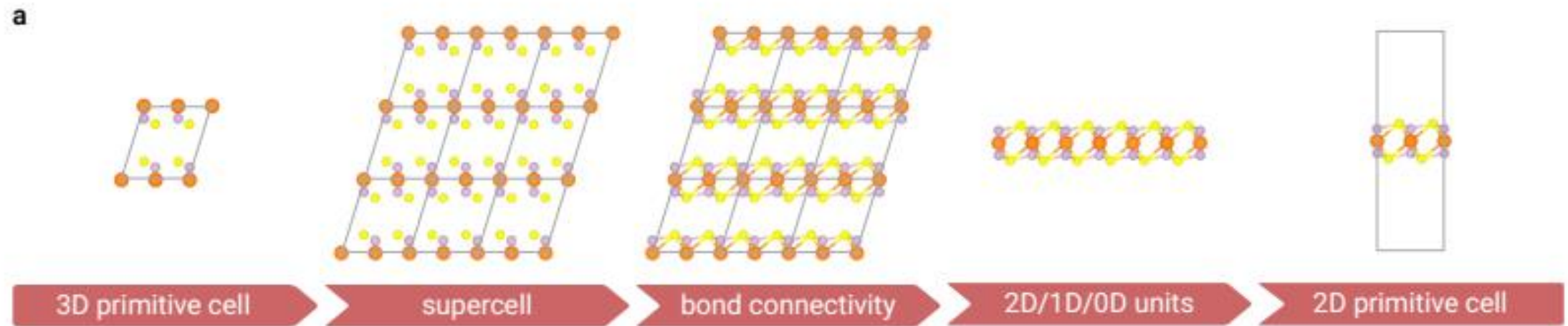
- Find all bonded clusters in the primitive cell, bonds are identified as :

$$d_{i,j} < r_i^{vdW} + r_j^{vdW} - \Delta$$

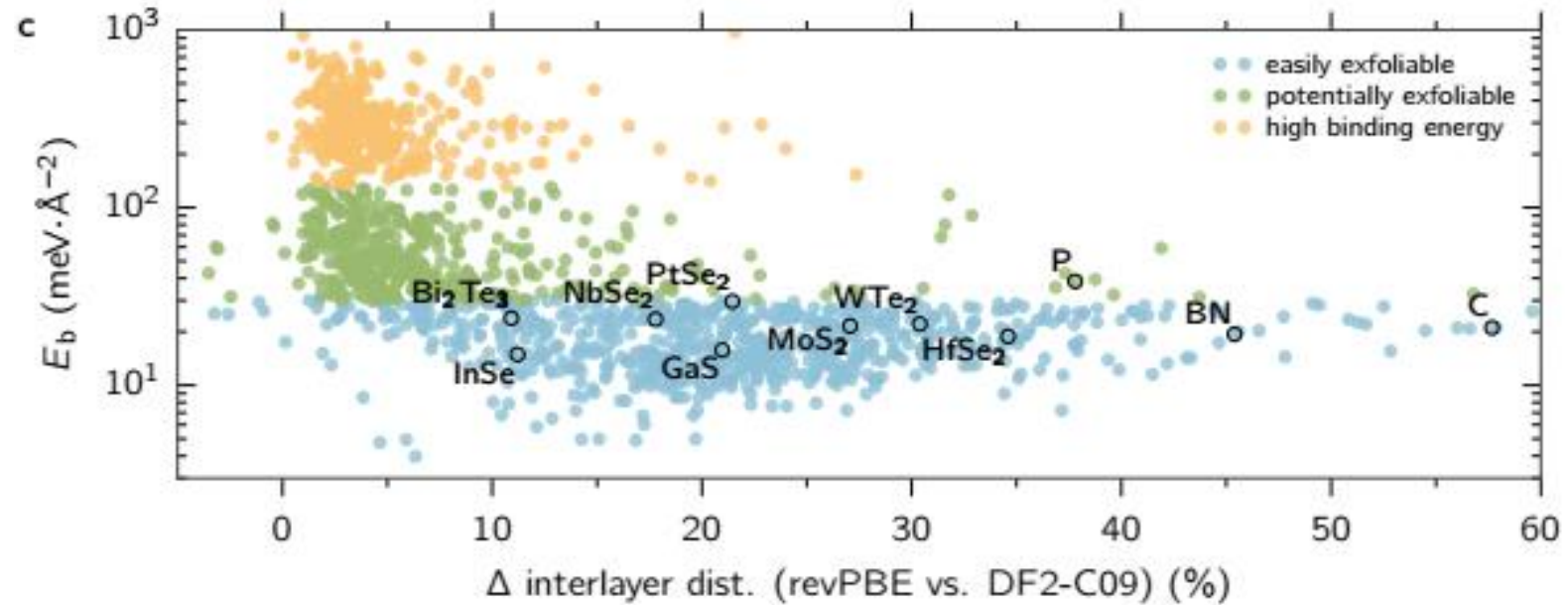
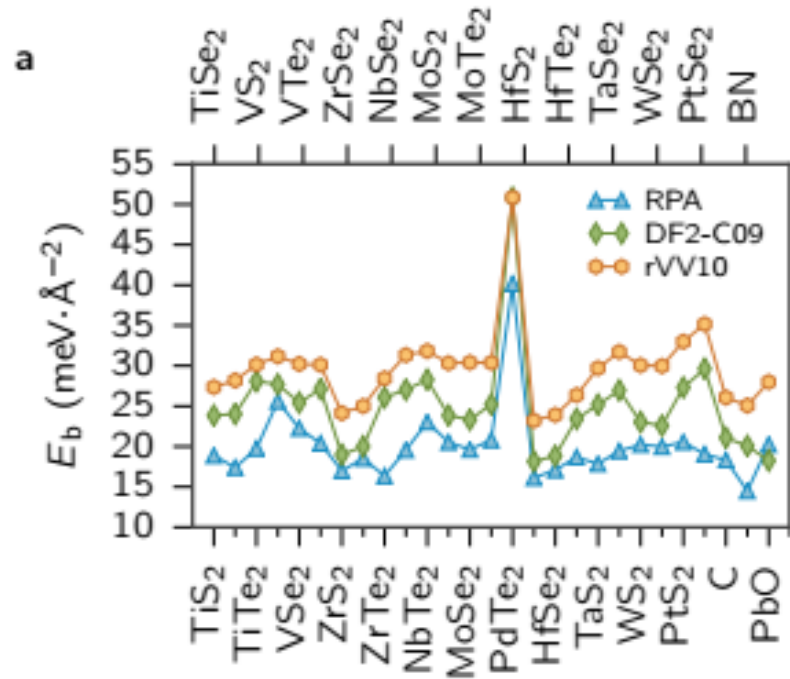


Geometrical screening algorithm

- Consider a bonded manifold as layer, if periodic in two independent directions

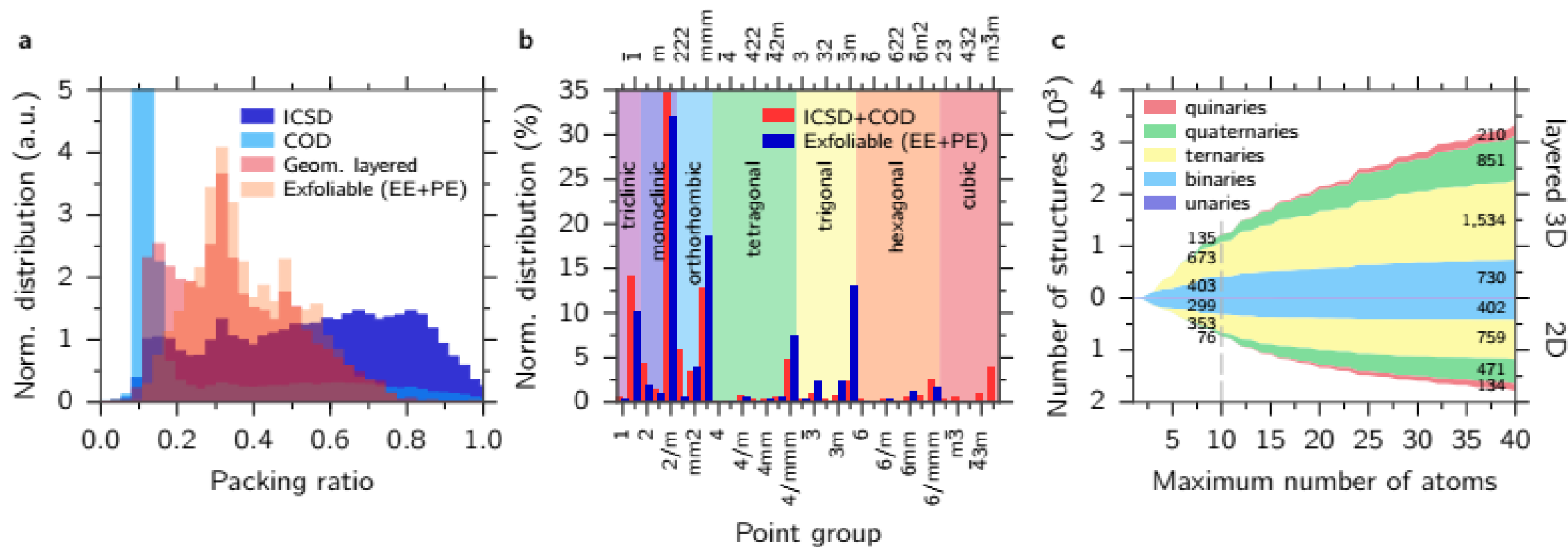


Binding energy

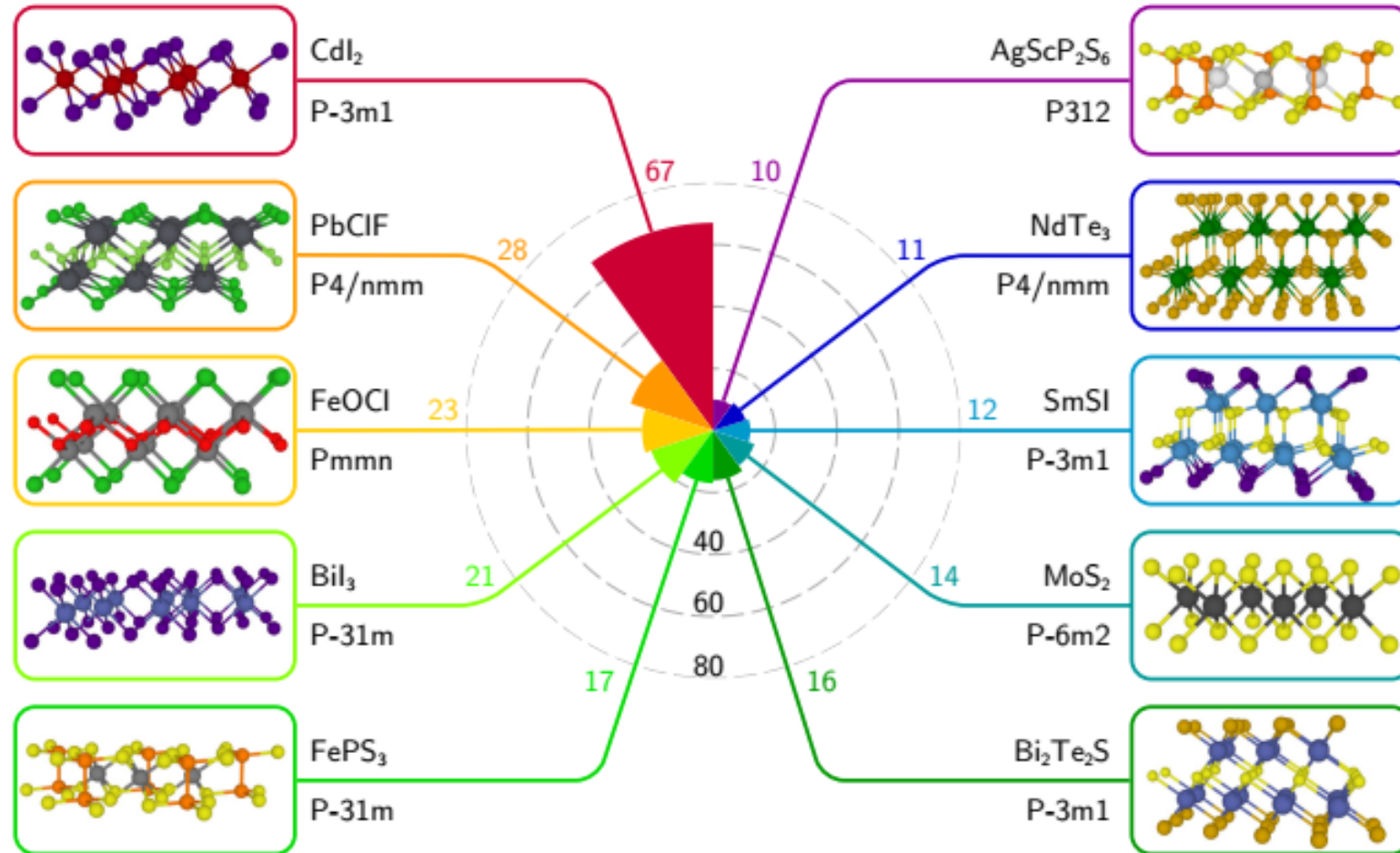


Obtained 1053 easily exfoliable and 791 potentially exfoliable

Statistics of 2D materials



2D materials prototypes



Further developments

- Contributed to:

Magnetic 2D materials and heterostructures

Ultrathin layers of transition metal dichalcogenides (TMDs)

Summary

- Data mining of layered materials

100 layered phases discovered by intuitive criteria , 2013

>1000 unique layered materials discovered by optimized algorithms, started from 2016

- Further developments

2D materials databases, >1000 layered materials

Transition metal dichalcogenides (TMDs)

Questions?