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

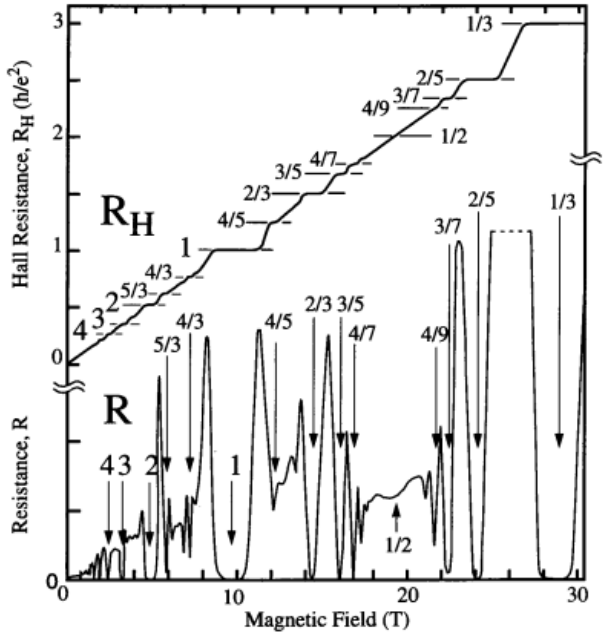
Introduction to 2D materials

- Research interests

Quantum Fractional Hall Effect

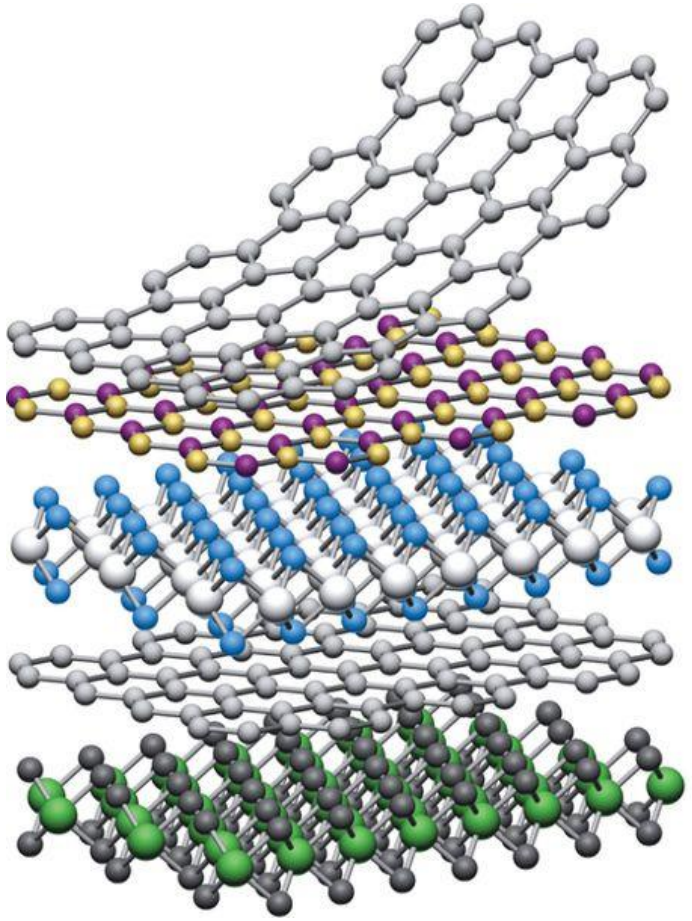
Van der Waals Heterojunction

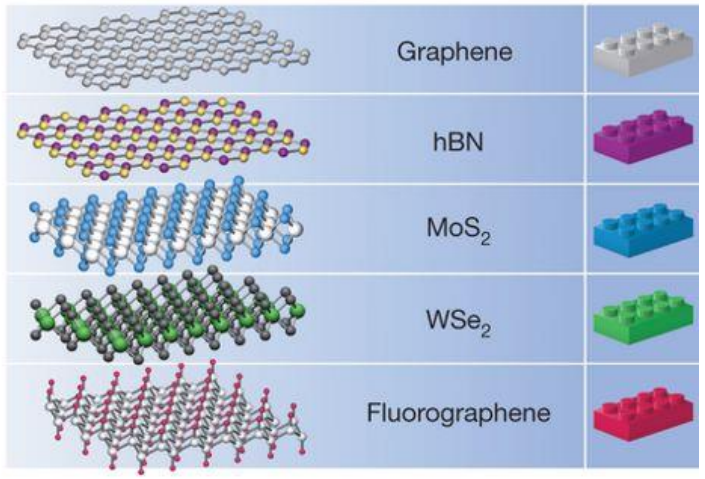
Superconductivity

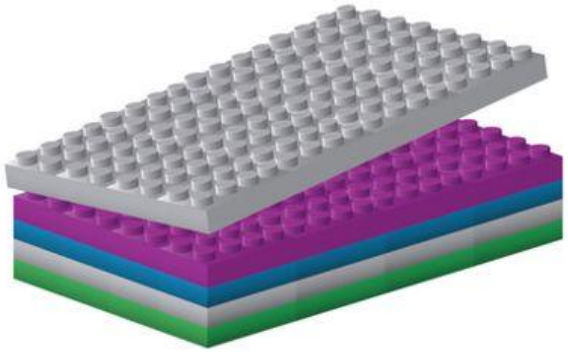


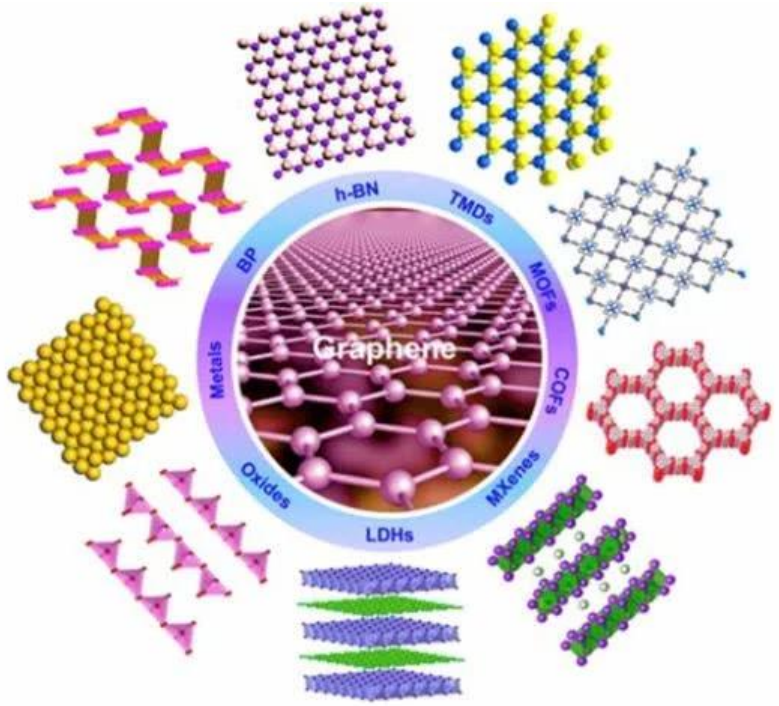
Horst. L. Stormer, Nobel Lecture, 1998

Van der Waals heterostructures









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

2D materials library 2013

<table>
<tr><td>Graphene family</td><td>Graphene</td><td colspan="2">hBN
'white graphene'</td><td>BCN</td><td>Fluorographene</td><td>Graphene oxide</td></tr>
<tr><td rowspan="2">2D chalcogenIdes</td><td colspan="2" rowspan="2">MoS_2, WS_2, $MoSe_2$, WSe_2</td><td colspan="2" rowspan="2">Semiconducting dichalcogenides:
$MoTe_2$, WTe_2,
ZrS_2, $ZrSe_2$ and so on</td><td colspan="2">Metallic dichalcogenides:
$NbSe_2$, NbS_2, TaS_2, TiS_2, $NiSe_2$ and so on</td></tr>
<tr><td colspan="2">Layered semiconductors:
GaSe, GaTe, InSe, Bi_2Se_3 and so on</td></tr>
<tr><td rowspan="2">2D oxides</td><td>Micas,
BSCCO</td><td colspan="2">MoO_3, WO_3</td><td rowspan="2" colspan="2">Perovskite-type:
$LaNb_2O_7$, $(Ca,Sr)_2Nb_3O_{10}$,
$Bi_4Ti_3O_{12}$, $Ca_2Ta_2TiO_{10}$ and so on</td><td>Hydroxides:
$Ni(OH)_2$, $Eu(OH)_2$ and so on</td></tr>
<tr><td>Layered
Cu oxides</td><td>TiO_2, MnO_2, V_2O_5,
TaO_3, RuO_2 and so on</td><td>Others</td></tr>
</table>

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

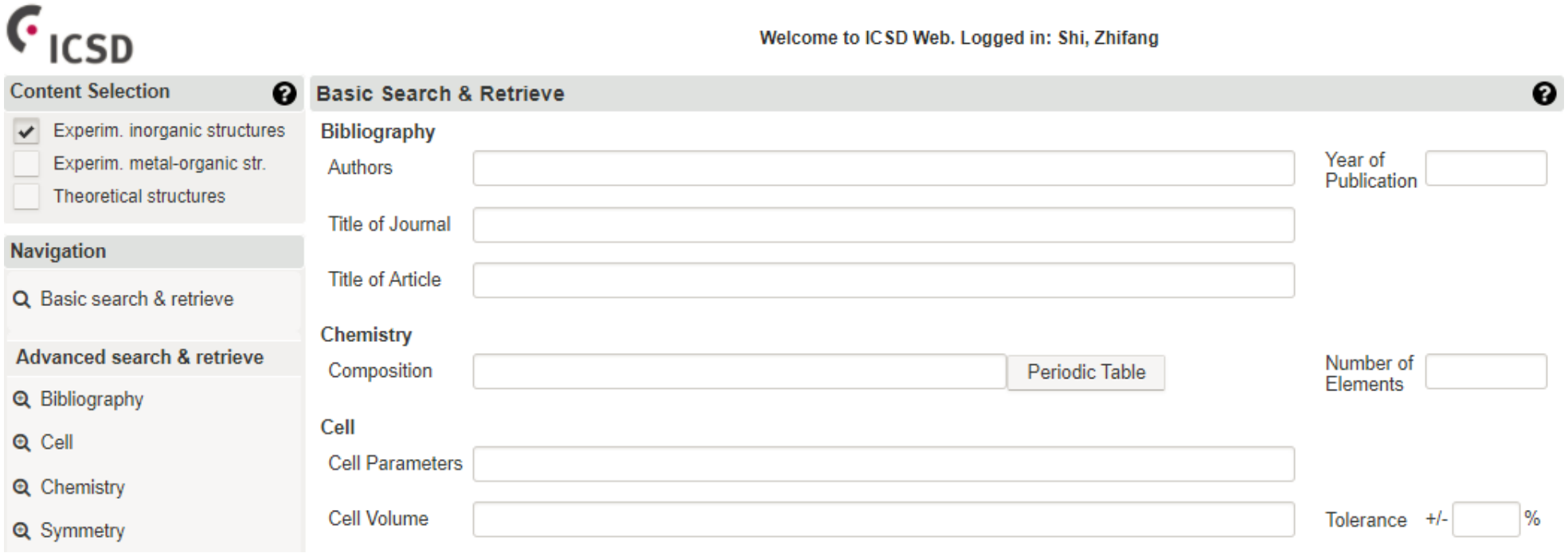
More novel 2D materials?

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

- More candidates for Van der Waals heterostructures

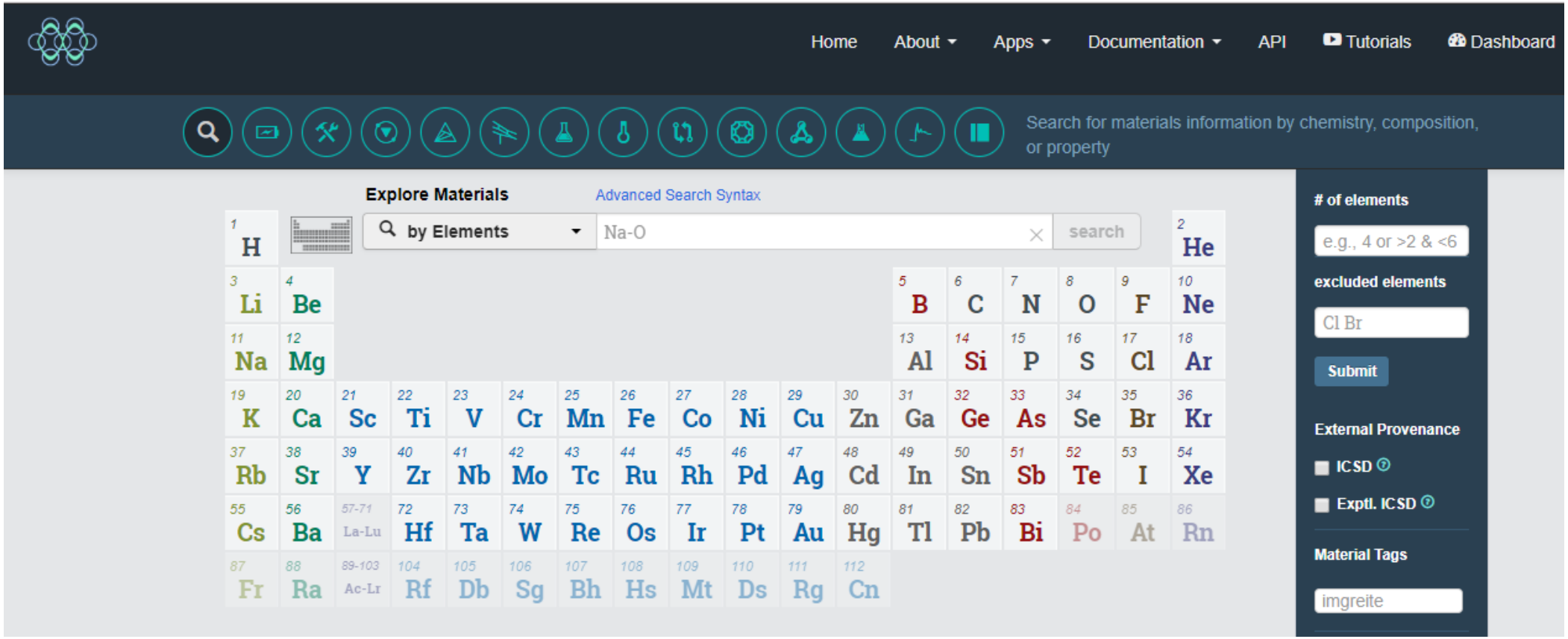
3D crystal databases

- Inorganic Crystal Structure Database (ICSD)



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

Materials Project



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?

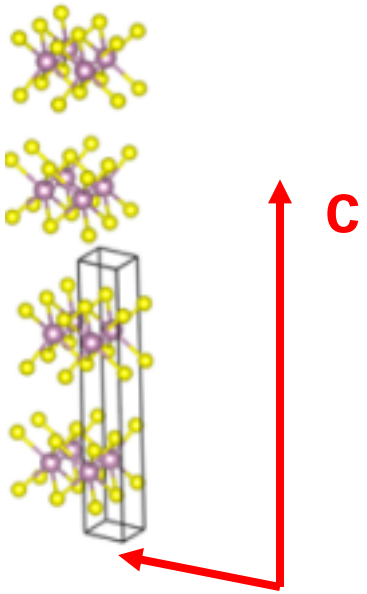
Pioneering attempt to identify layered materials

- 2013 PRX, characterize layered materials by:

Low packing ratio (0.15-0.50)

Large gaps (>2.4 A) between crystallographic planes along the c axis

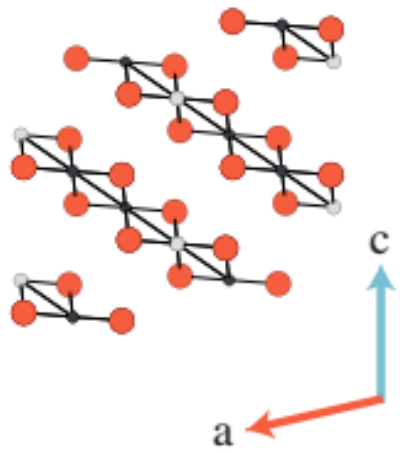
- Discovered almost 100 layered phases!



Leb`egue *et al.* PRX 2013

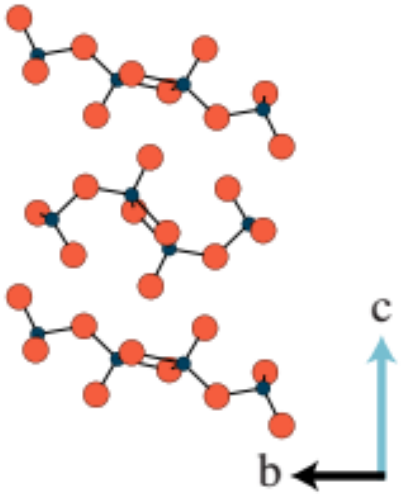
Challenges of layer detection

(a) Co_2NiO_6 (mp-765906)



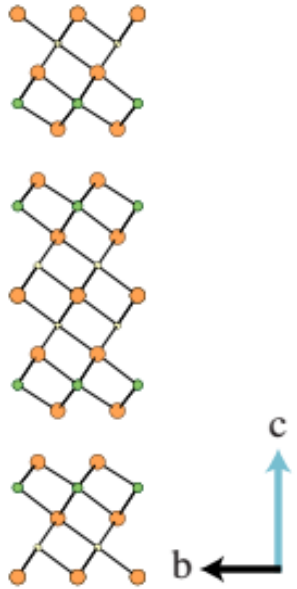
layers not along c axis

(b) V_2O_5 (mp-25643)



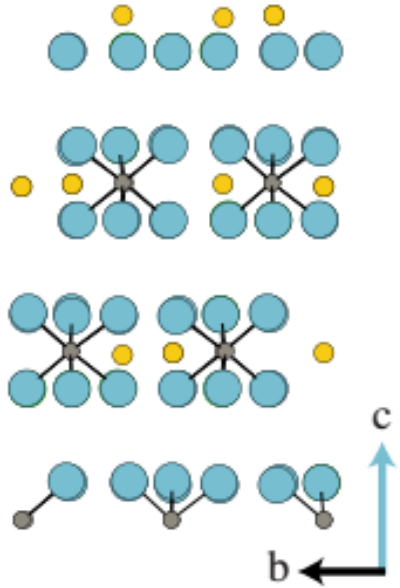
corrugated layers

(c) $Ge_2Te_5As_2$ (mp-14791)



thick layers

(d) Li-WCl_6 (mp-570512)



molecular (nonbonded) layers

Michael Ashton et.al *Phys. Rev. Lett.* 2017

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

Gowoon 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 Marzari[1]

Nature Nanotechnology, 2018

Method

- Step1:

Geometrical screening algorithm for layered materials

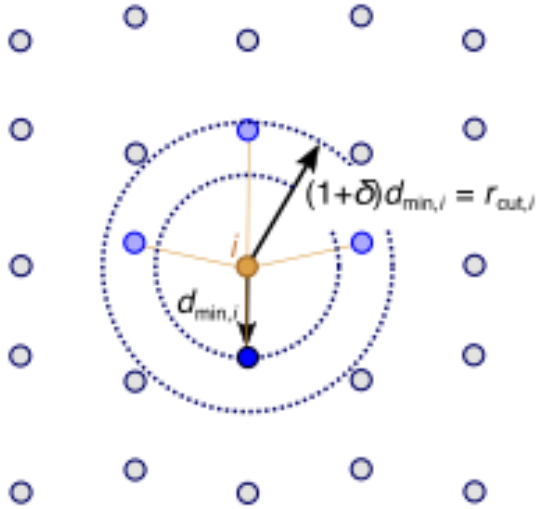
- Step2:

Identify layered materials that easily exfoliable using vdW DFT simulations

Geometrical screening algorithm

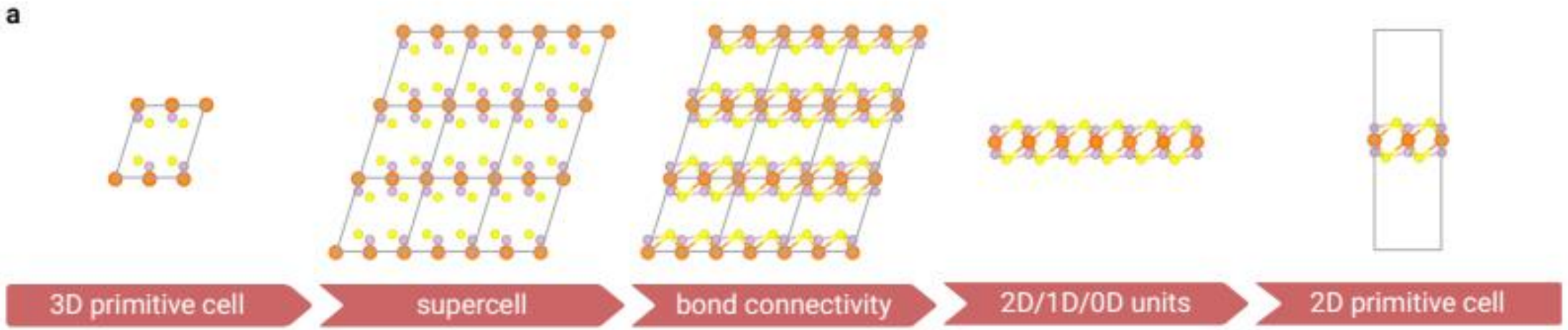
- Find all bonded clusters in the primitive cell, bonds are identified as :

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



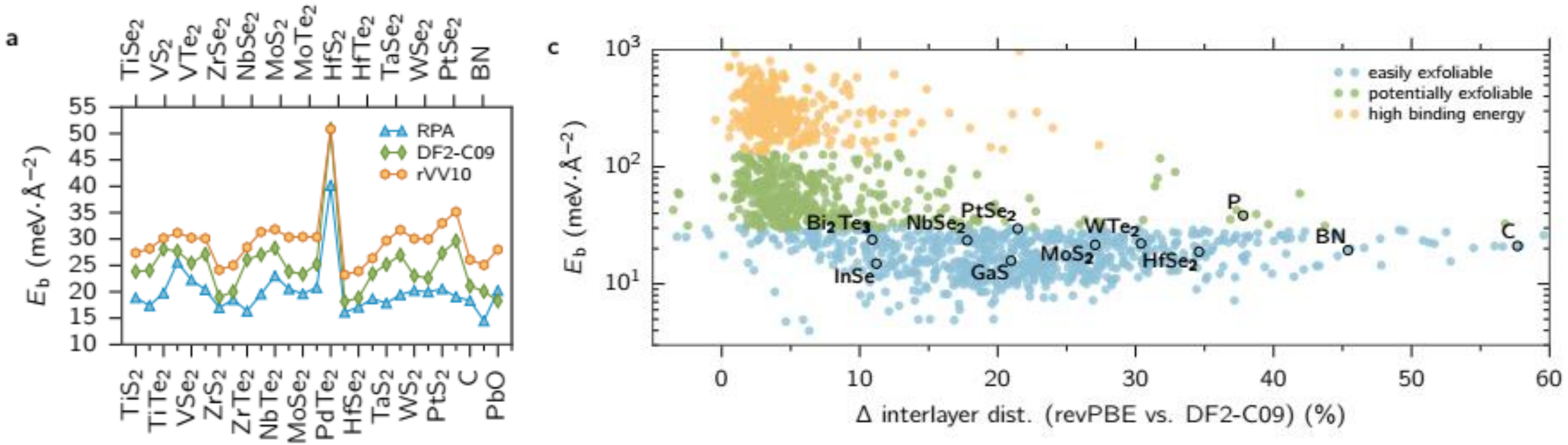
Geometrical screening algorithm

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



Nicolas Mounet ***et.al*** *Arxiv.* 2016

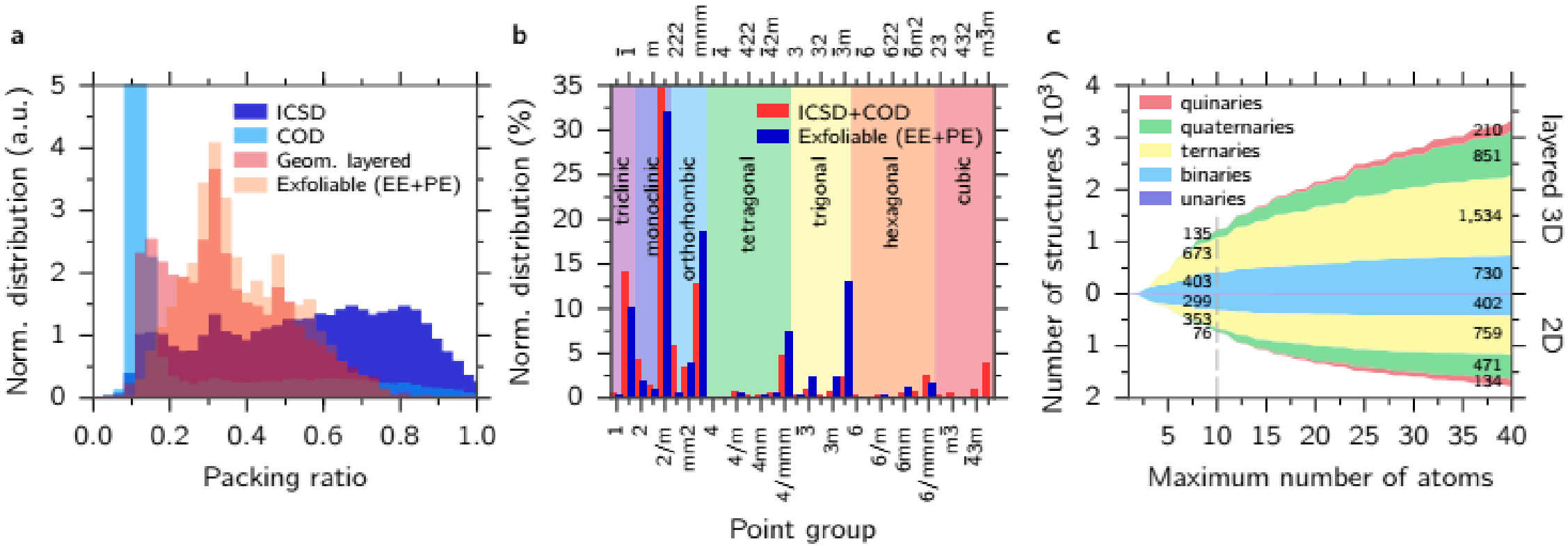
Binding energy



Obtained 1053 easily exfoliable and 791 potentially exfoliable

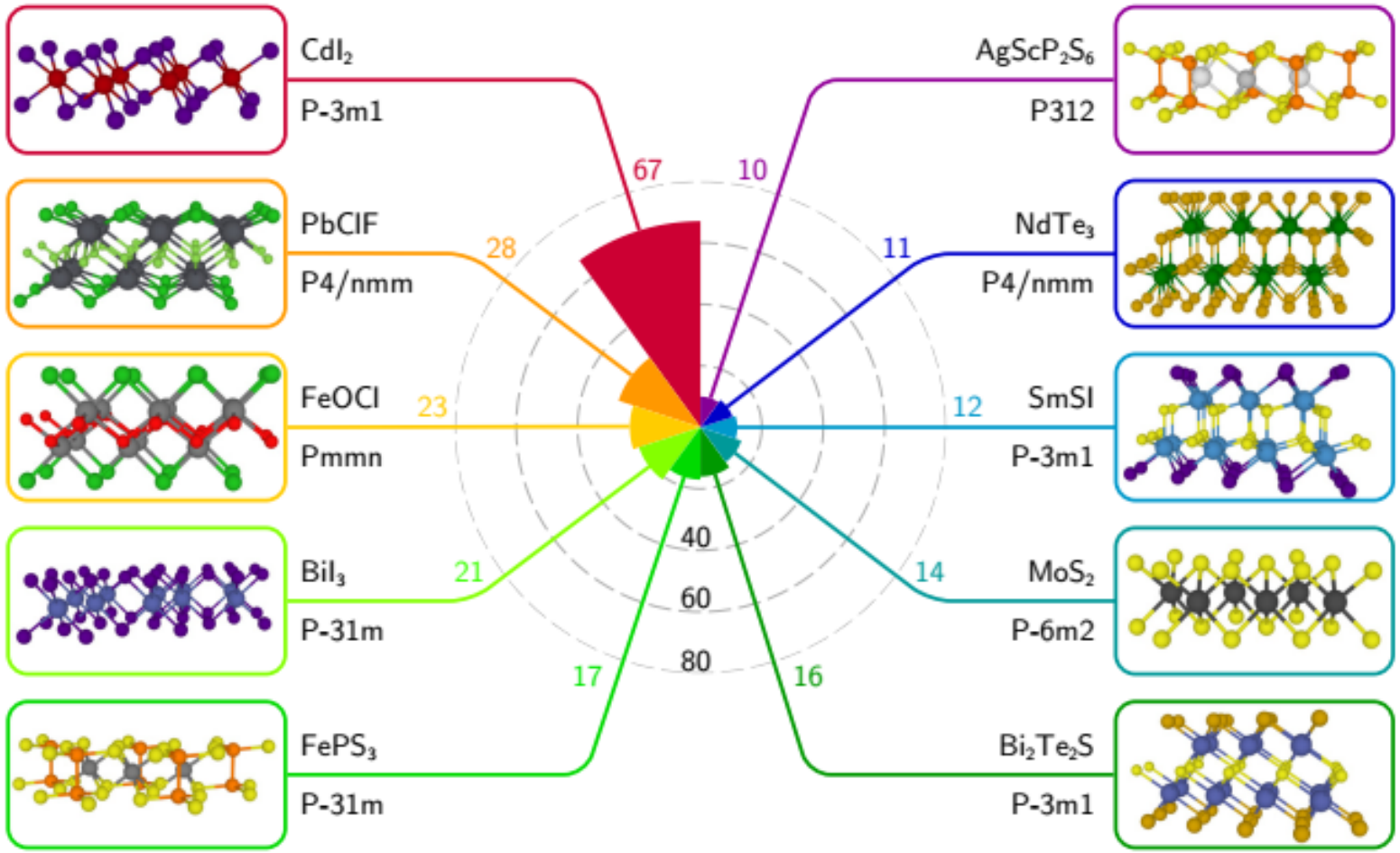
Nicolas Mounet ***et.al*** *Arxiv.* 2016

Statistics of 2D materials



Nicolas Mounet ***et.al*** *Arxiv.* 2016

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 algroithms, started from 2016

- Further developments

2D materials databases, >1000 layered materials

Transition metal dichalcogenides (TMDs)

Questions?