Structural analysis and generation of materials: AFLOW-SYM, AFLOW Prototype Encyclopedia, and AFLOW-XtalFinder

Marco Esters, David Hicks

Session 2: 10:00AM – 12:00PM (EST)

Tuesday, February 22nd, 2022

Duke UNIVERSITY

AFLOW
Automatic - FLOW for Materials Discovery

NSF

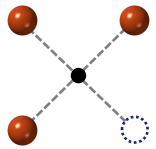
Office of Naval Research
USN ONR
Science & Technology

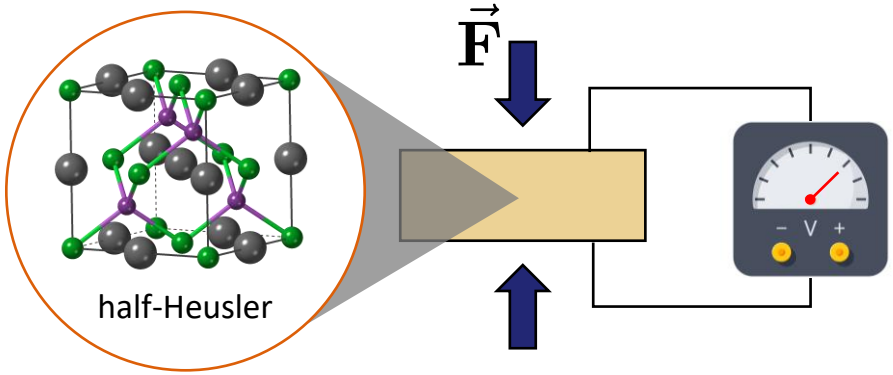
Structure vs properties

understanding structure to guide materials design

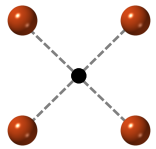
e.g., symmetry and piezoelectricity

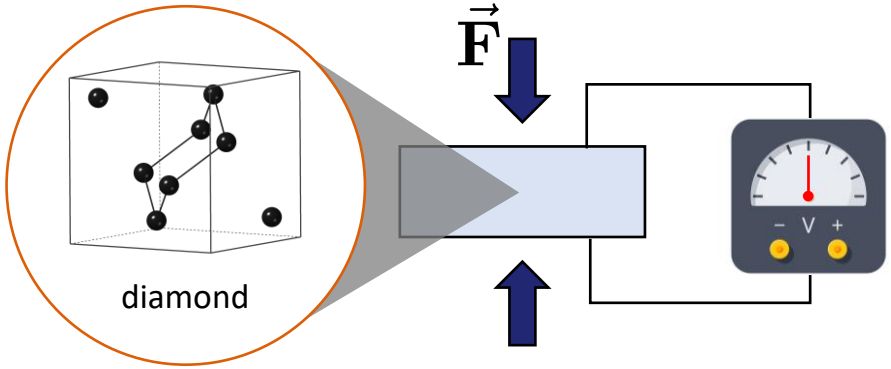
no inversion symmetry



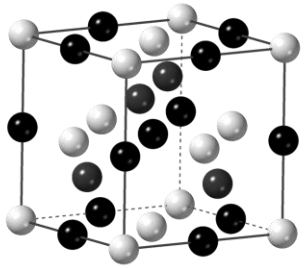


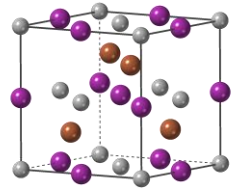
inversion symmetry



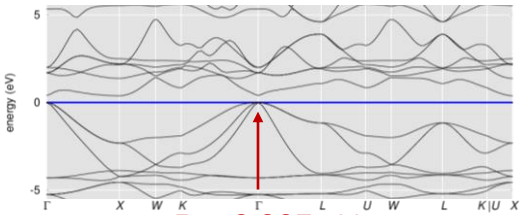


e.g., prototype structures

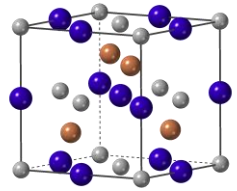




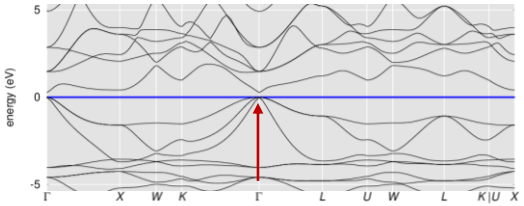
PtSbSc



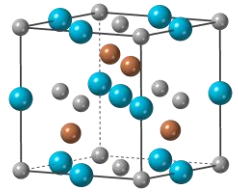
E_g = 0.397 eV



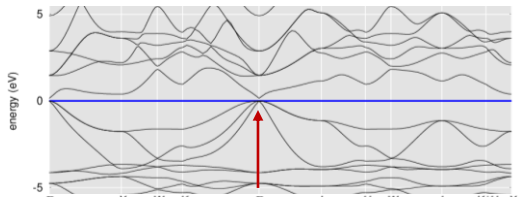
PtSbTb



E_g = 0.276 eV



PtSbHo

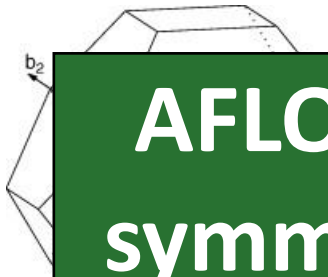


E_g = 0.161 eV

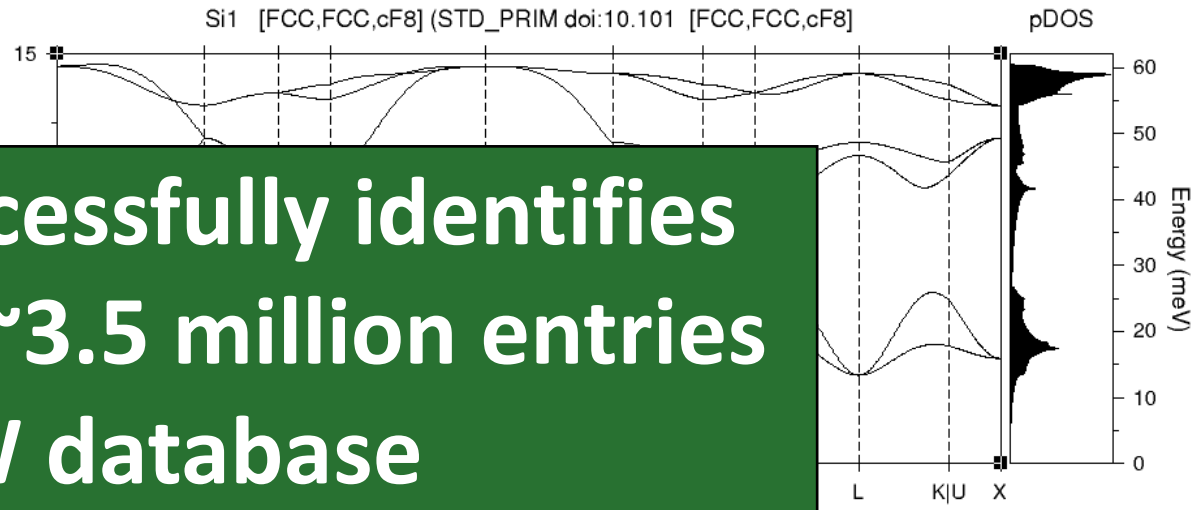
Hahn, Kluwer Academic Publishers (2002); Zou, Tang, and Pan, Proc. Royal Soc. Lond. A **469**, 2012075 (2013)

Symmetry is ubiquitous

Brillouin zones/kpaths/
band structures

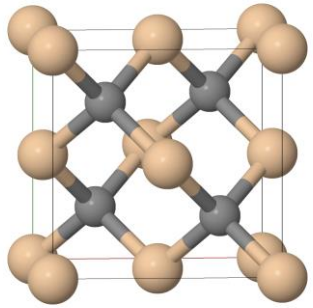


phonon calculations

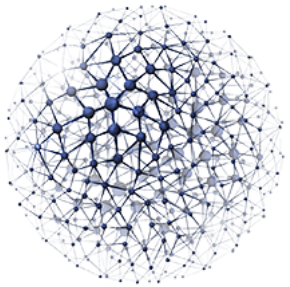


AFLOW-SYM successfully identifies symmetry for all ~3.5 million entries in AFLOW database (no human intervention)

generation/classification



characterization

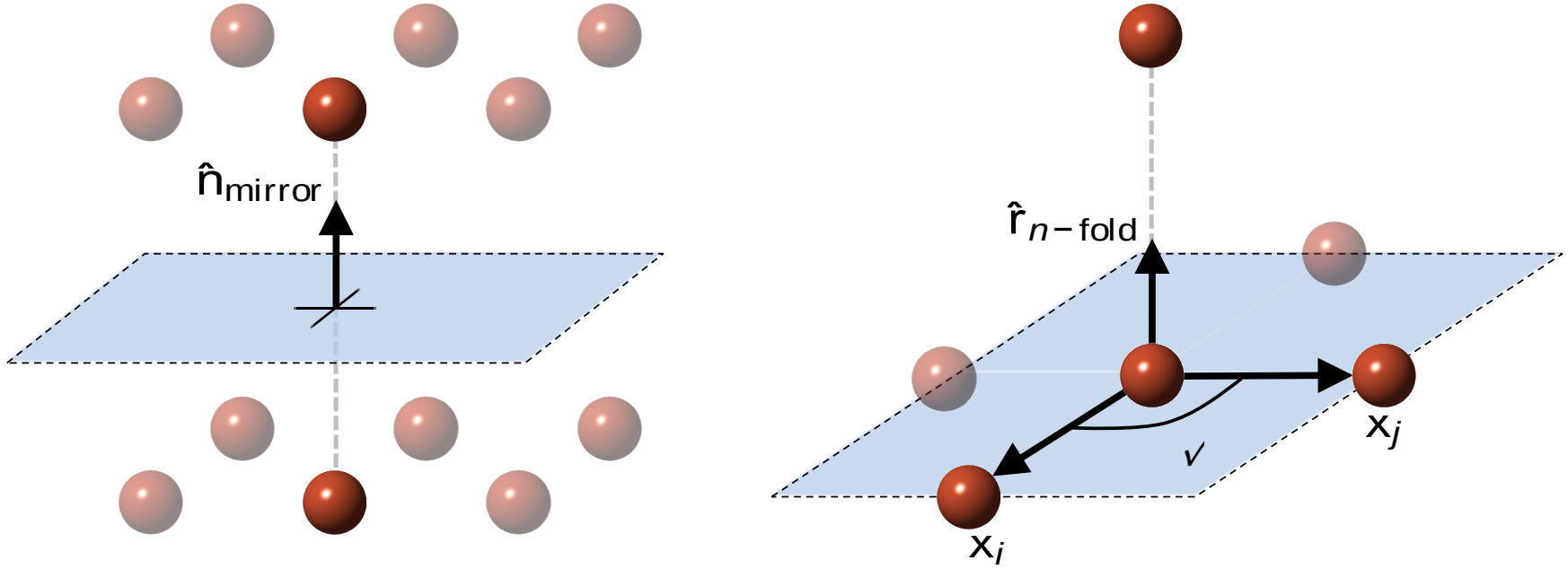


AFLOW
Automatic - FLOW for Materials Discovery

Hicks *et al.*, Acta Cryst. A**74**, 184 (2018), Setyawan and Curtarolo, Comp. Mat. Sci. **49**, 299 (2010)

AFLOW-SYM

AFLOW-SYM tests invariance of crystal under transformations



descriptions:

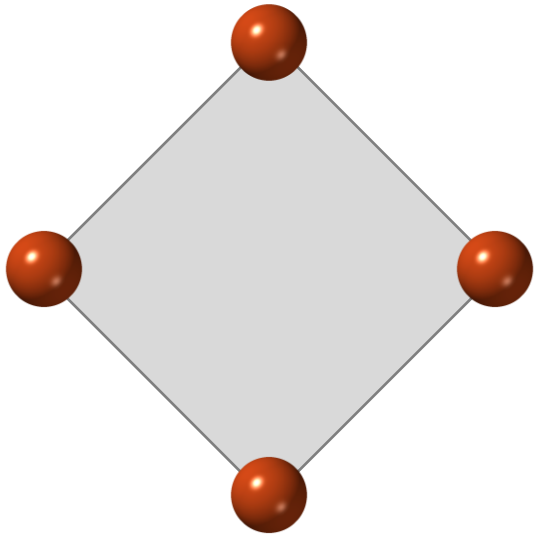
space group	Bravais lattice	conventional cell
Pearson symbol	Wyckoff positions	primitive cell

...

Hicks *et al.*, Acta Cryst. A**74**, 184 (2018)

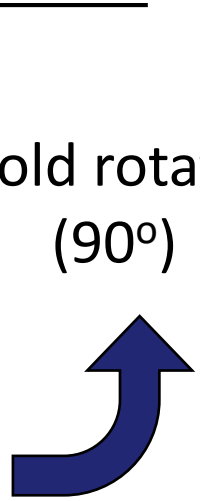
Identifying symmetry elements

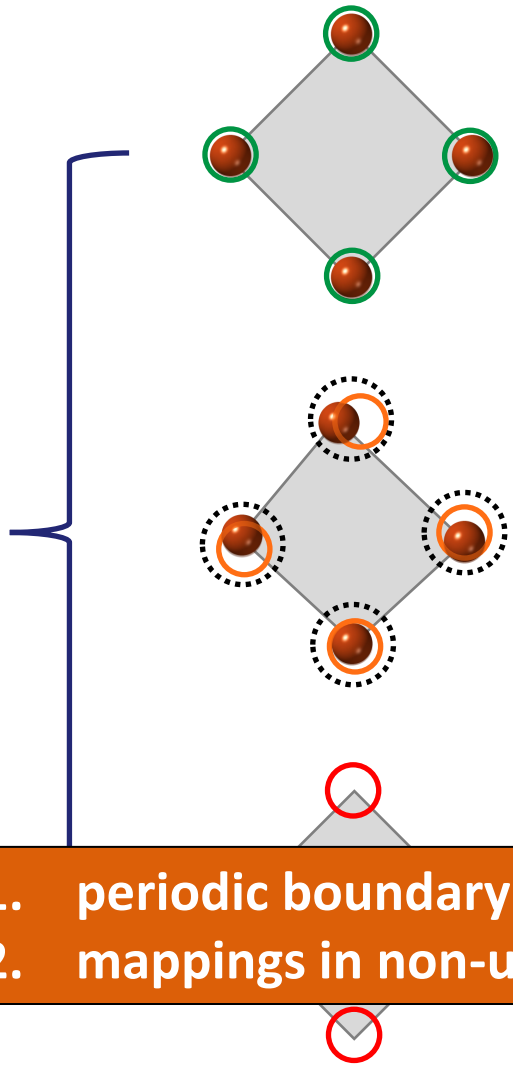
attempt symmetry operation



+

4-fold rotation
(90°)





✓ mapped

✓ mapped

radius ϵ
(threshold for mappings)

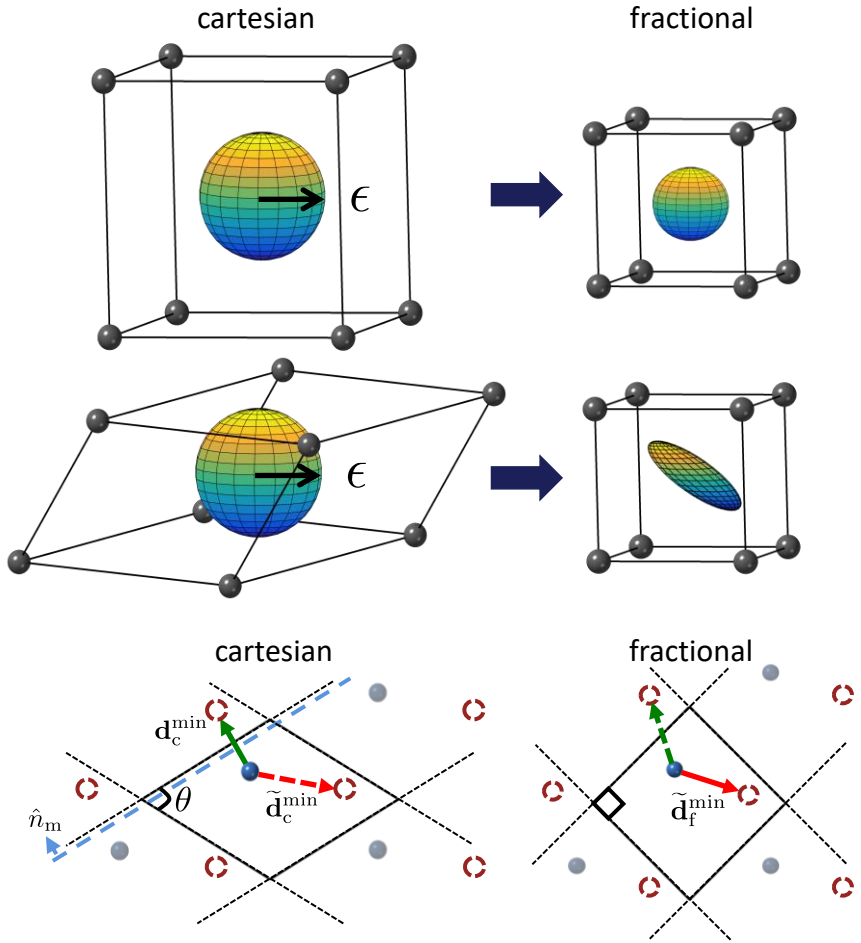
$$||\mathbf{x}_{\text{orig}} - \mathbf{x}_{\text{transformed}}|| \leq \epsilon$$

1. **periodic boundary conditions**
2. **mappings in non-uniform metric spaces**

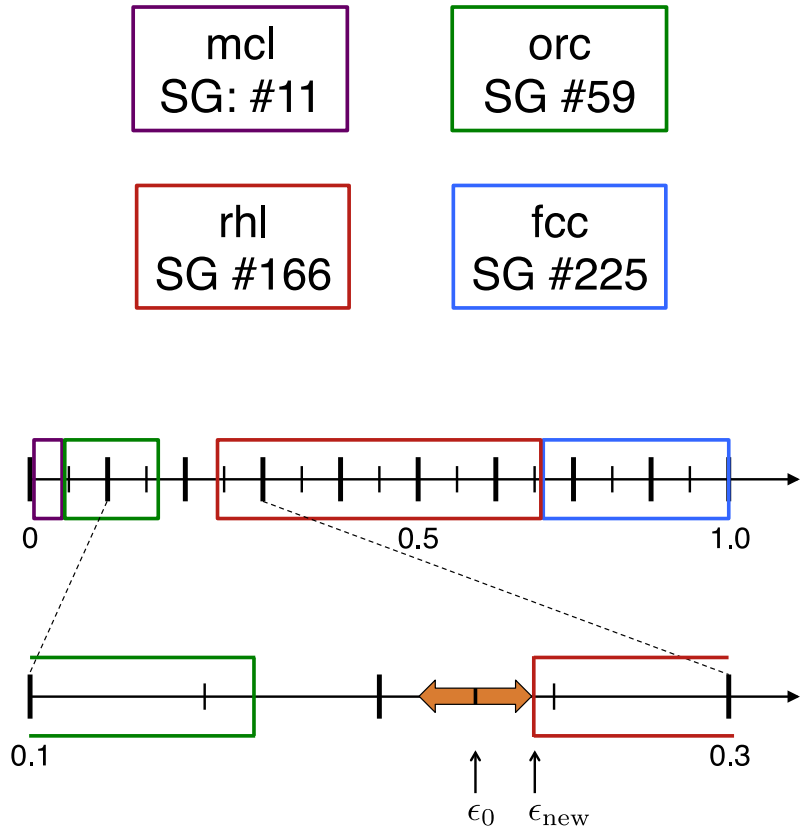
Hicks *et al.*, Acta Cryst. A**74**, 184 (2018)

Algorithm improvements

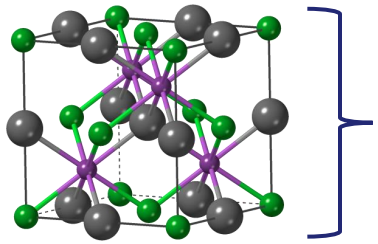
robust mapping procedure
accurate in both direct and reciprocal spaces



adaptive tolerance scheme
ensures self-consistent symmetry



system-specific tolerance
atomic position resolution



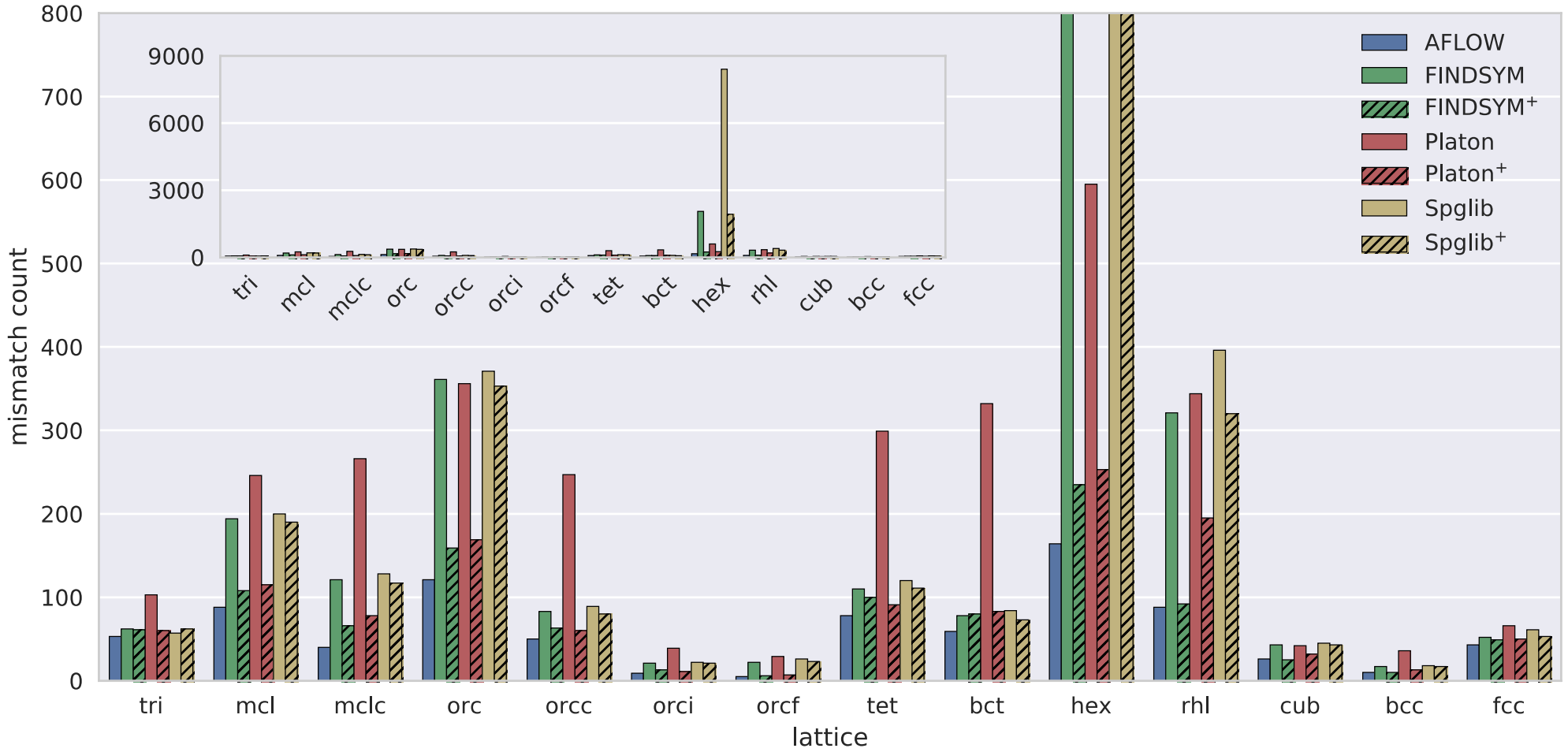
$$\epsilon_{tight} = d_{nn}^{min}/100$$

$$\epsilon_{loose} = d_{nn}^{min}/10$$

single global tolerance

Hicks *et al.*, Acta Cryst. A**74**, 184 (2018)

Benchmark with existing packages

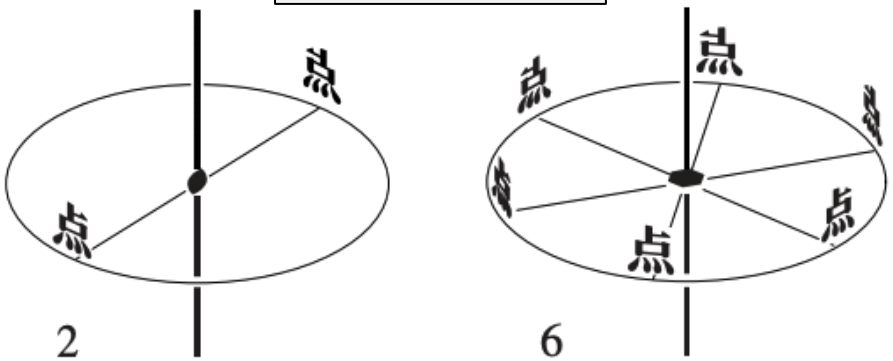


Mismatch with respect to space group listed in description of experimental structure in ICSD

Hicks *et al.*, Acta Cryst. A**74**, 184 (2018)

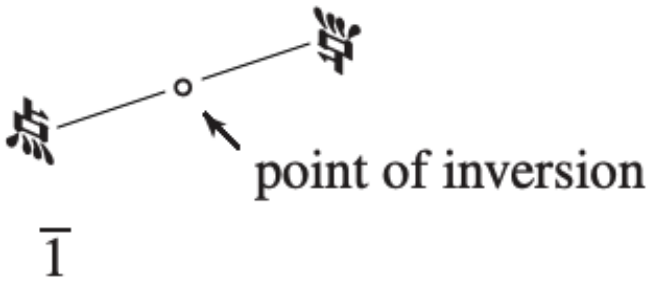
Crystallographic symmetry elements

rotations

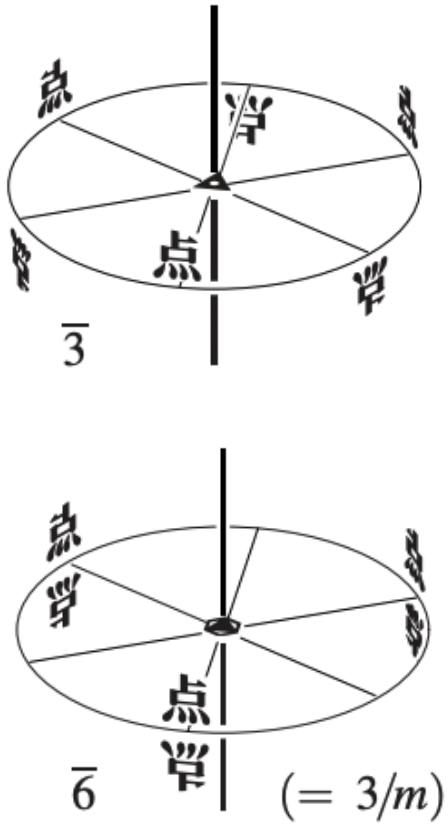


crystallographic restriction theorem: 2-, 3-, 4-, 6-fold

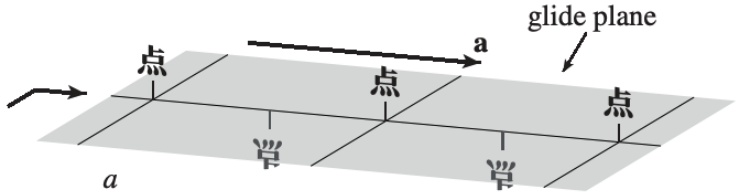
inversion



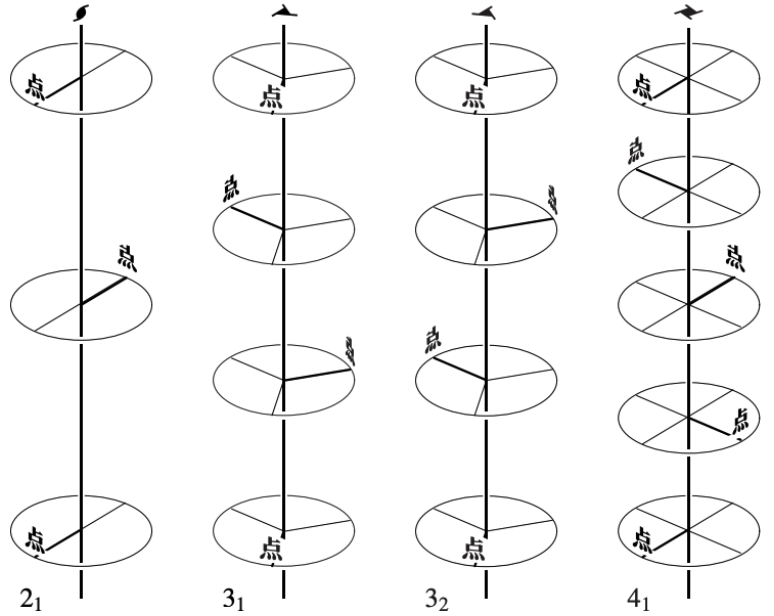
roto-inversions



glides



screws

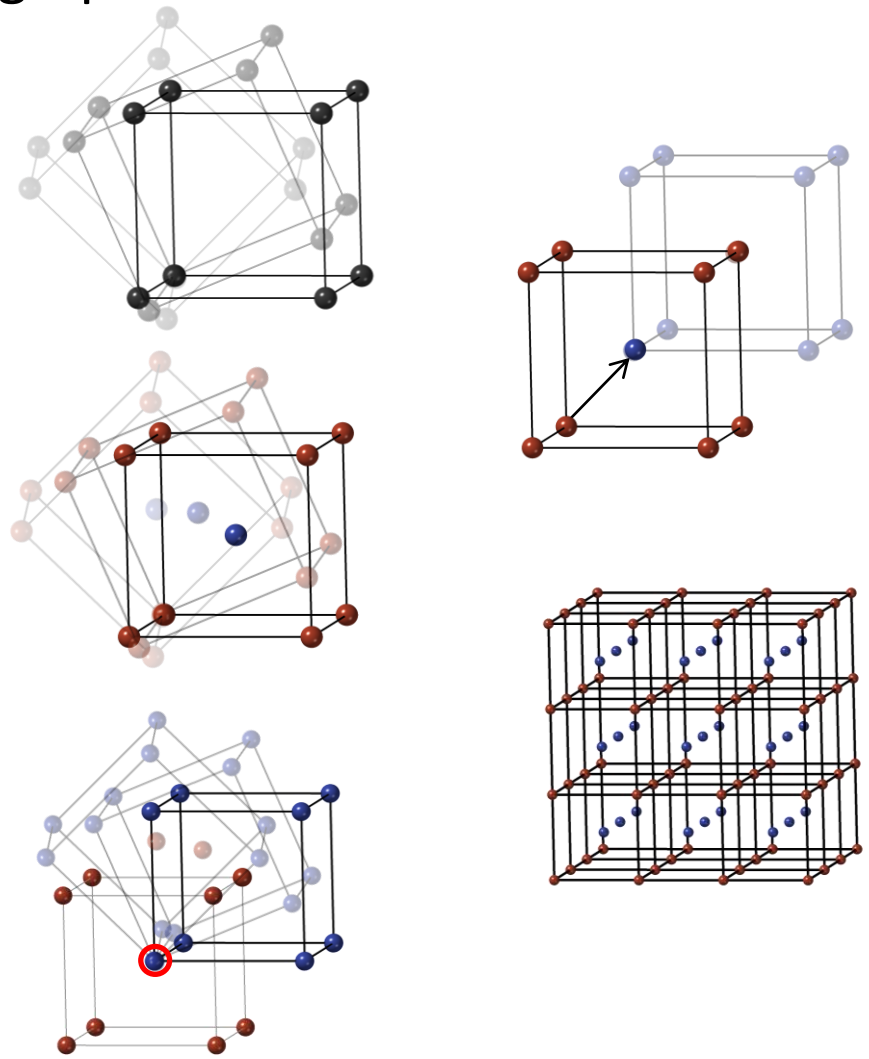


Hicks *et al.*, Acta Cryst. A**74**, 184 (2018), U. Müller, Oxford University Press (2013)

Crystallographic symmetry

Calculates the relevant symmetry groups for crystallographic structures

- lattice point group
- reciprocal lattice point group (BZ symmetry)
- factor group (unit cell symmetry)
- crystallographic point group
- dual of crystallographic point group (IBZ symmetry)
- Patterson symmetry group
- space group
- site point group (atom point symmetry)

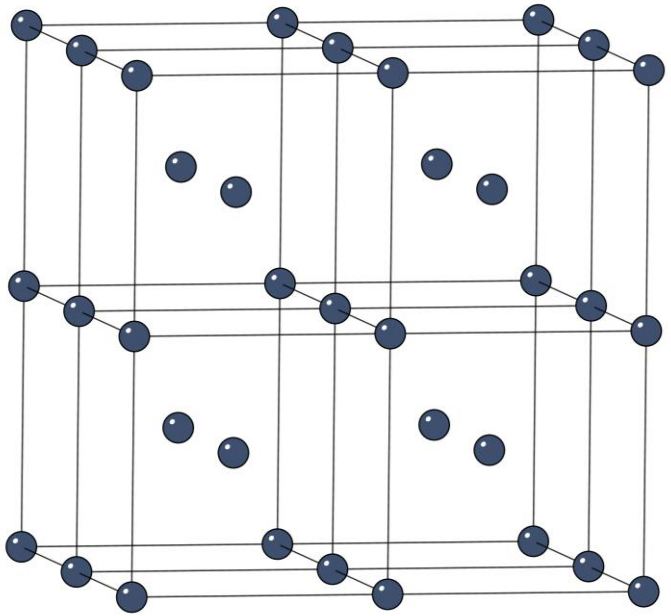


Hicks *et al.*, Acta Cryst. A**74**, 184 (2018)

Crystal-spin symmetry

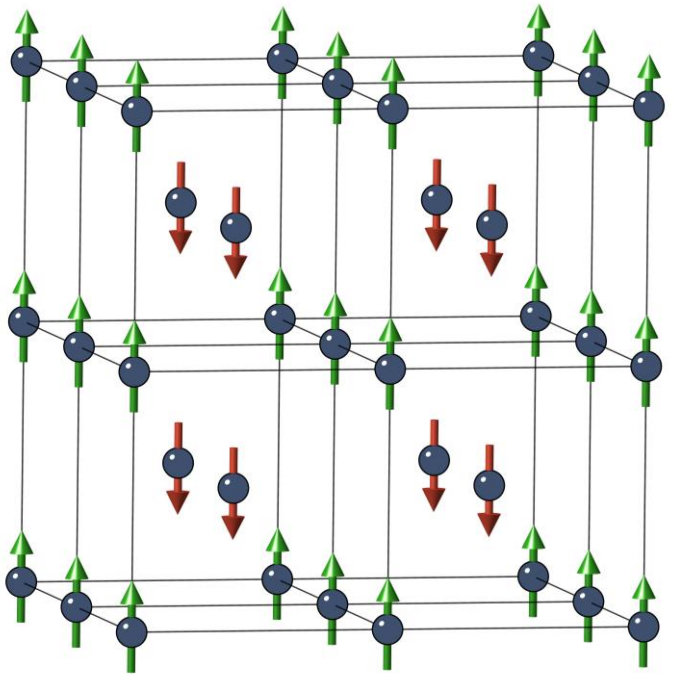
crystal symmetry

$\mathrm{Im\bar{3}m}\ \#\,229$



crystal-spin symmetry

$\mathrm{Pm\bar{3}m}\ \#\,221$



spin – degree of freedom that can break symmetry

crystal symmetry $\geq$ crystal-spin symmetry

Hicks *et al.*, Acta Cryst. A**74**, 184 (2018)

Symmetry descriptions

space group number (1-230)

225

International (Hermann-Mauguin)

$Fm\bar{3}m$

Schoenflies

O_h^5

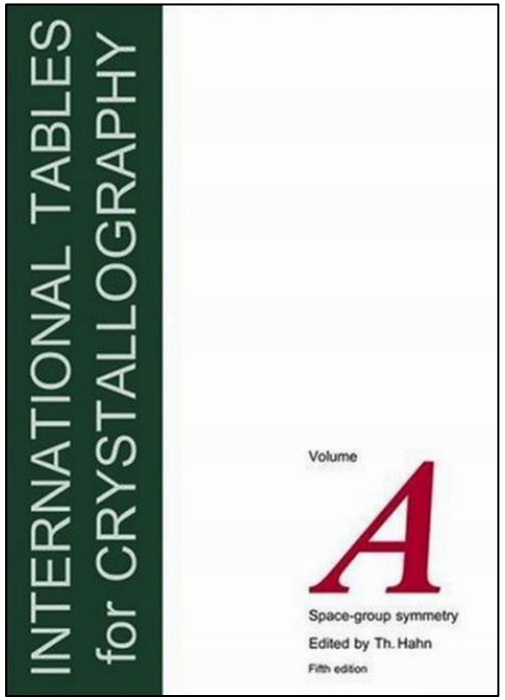
Hall symbol

$F\ 4/m\ {-}3\ 2/m$

Pearson symbol

cF4

consistent with International Tables for Crystallography (ITC)



- standard space group label
- space group setting
- Wyckoff positions

$$\mathrm{Ag}\quad 4\quad a\quad 0,0,0$$

multiplicity

letter designation

representative coordinate

expand coordinates

$$\mathrm{Ag}\quad 0,0,0 \qquad \mathrm{Ag}\quad 1/2,0,1/2$$
$$\mathrm{Ag}\quad 0,1/2,1/2 \qquad \mathrm{Ag}\quad 1/2,1/2,0$$

Hicks *et al*., Acta Cryst. A**74**, 184 (2018); Hahn, Kluwer Academic Publishers (2002)

AFLOW-SYM: online

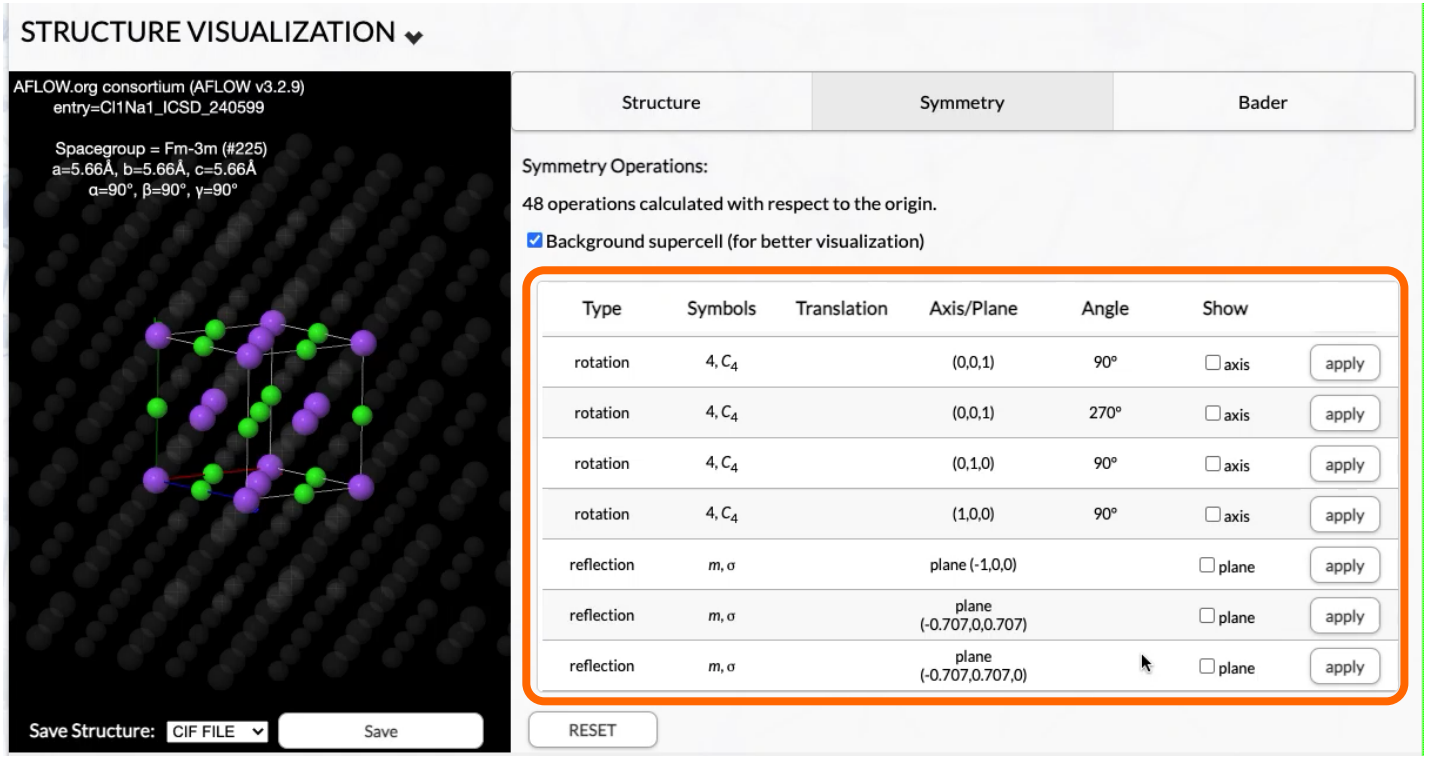
online functionality

https://aflow.org/aflow-online/



visualize symmetry operations

on entry pages of aflow.org



Navigate to AFLOW-Online (aflow.org/aflow-online)

AFLOW Crystal Prototype Encyclopedia

The search for prototypes

catalogs of structure prototypes



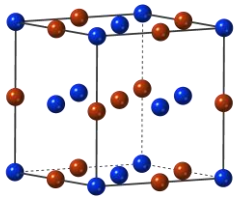
computational hurdles

arbitrary designations

Ex:

compound name: NaCl or MgO

Strukturbericht: B1



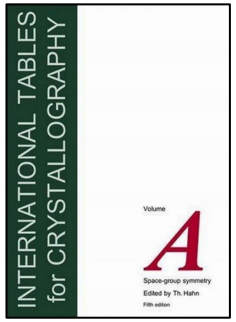
knowledge of crystallography

Ex:

space group #216

Wyckoff position:

$$\mathrm{Ag}\quad 4\quad a\quad 0,0,0$$



coordinates

$$\mathrm{Ag}\quad 0,0,0$$
$$\mathrm{Ag}\quad 0,1/2,1/2$$
$$\mathrm{Ag}\quad 1/2,0,1/2$$
$$\mathrm{Ag}\quad 1/2,1/2,0$$

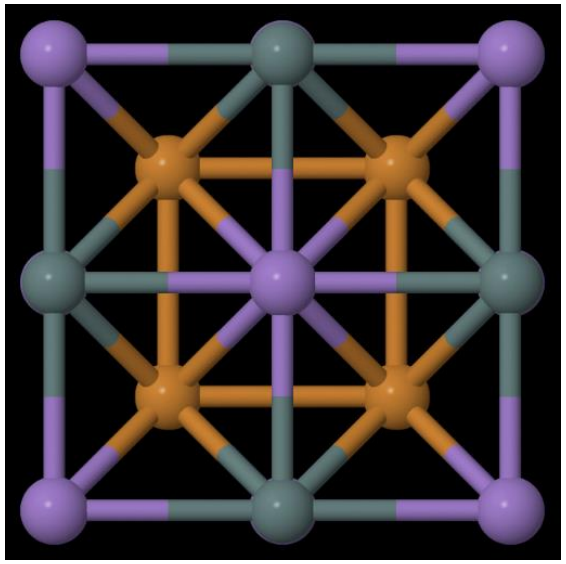
multiplicity — letter designation — representative coordinate

lack methods for materials generation

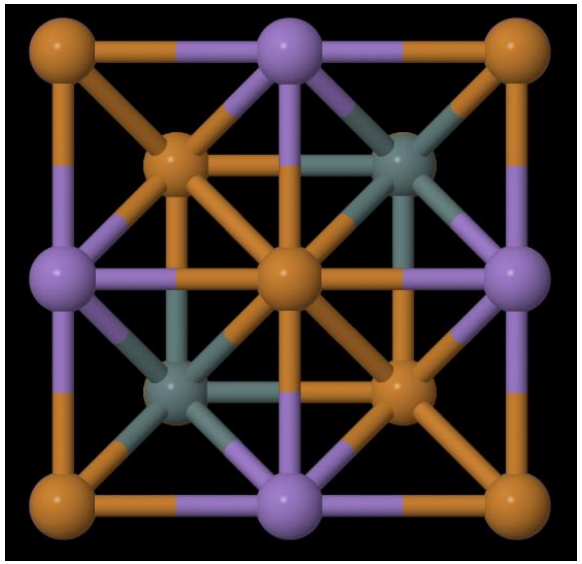
Hahn, Kluwer Academic Publishers (2002)

AFLOW: Crystallographic prototypes

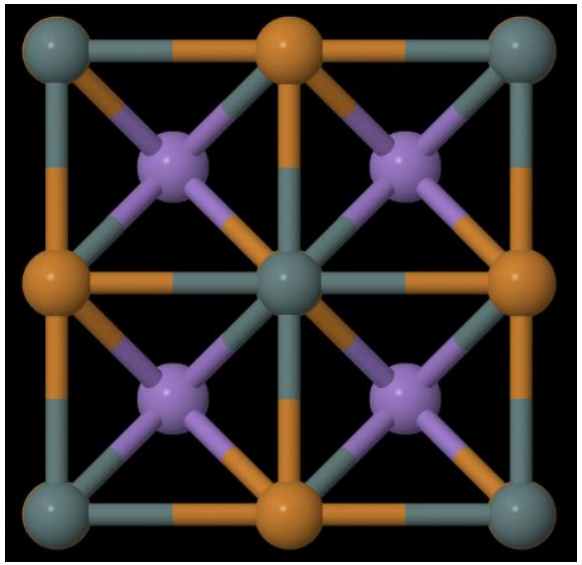
- AFLOW contains built-in structural prototypes:



Prototype T0001:
Heusler structure



Prototype T0002:
Anti-Heusler structure



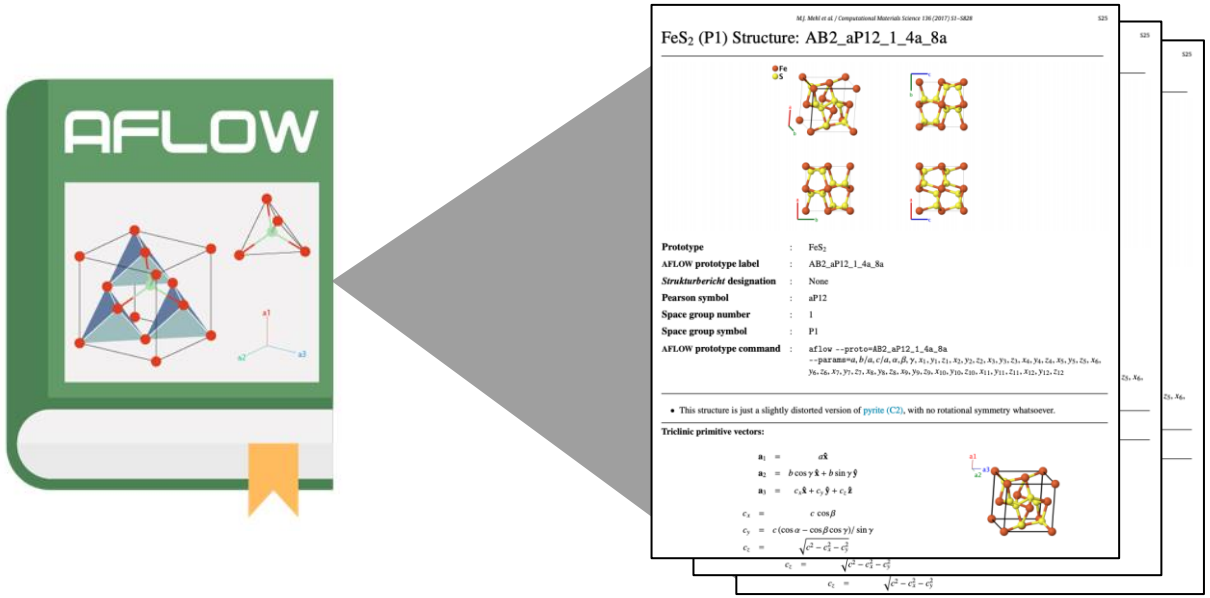
Prototype T0003:
Half-Heusler structure

- Decorating prototypes with different elements allows for automated creation of new hypothetical materials
- ~1,100 prototypes available at https://aflow.org/prototype-encyclopedia/

Mehl *et al.*, Comput. Mater. Sci. **136**, S1 (2017); Hicks *et al.*, Comput. Mater. Sci. **161**, S1 (2019)

Crystal Prototype Encyclopedia

The AFLOW Prototype Encyclopedia



content

- standard label
- historic labels
- Wyckoff positions
- space group
- lattice vectors
- *Strukturbericht*
- similar compounds
- Pearson symbol
- explicit coordinates
- visualizations

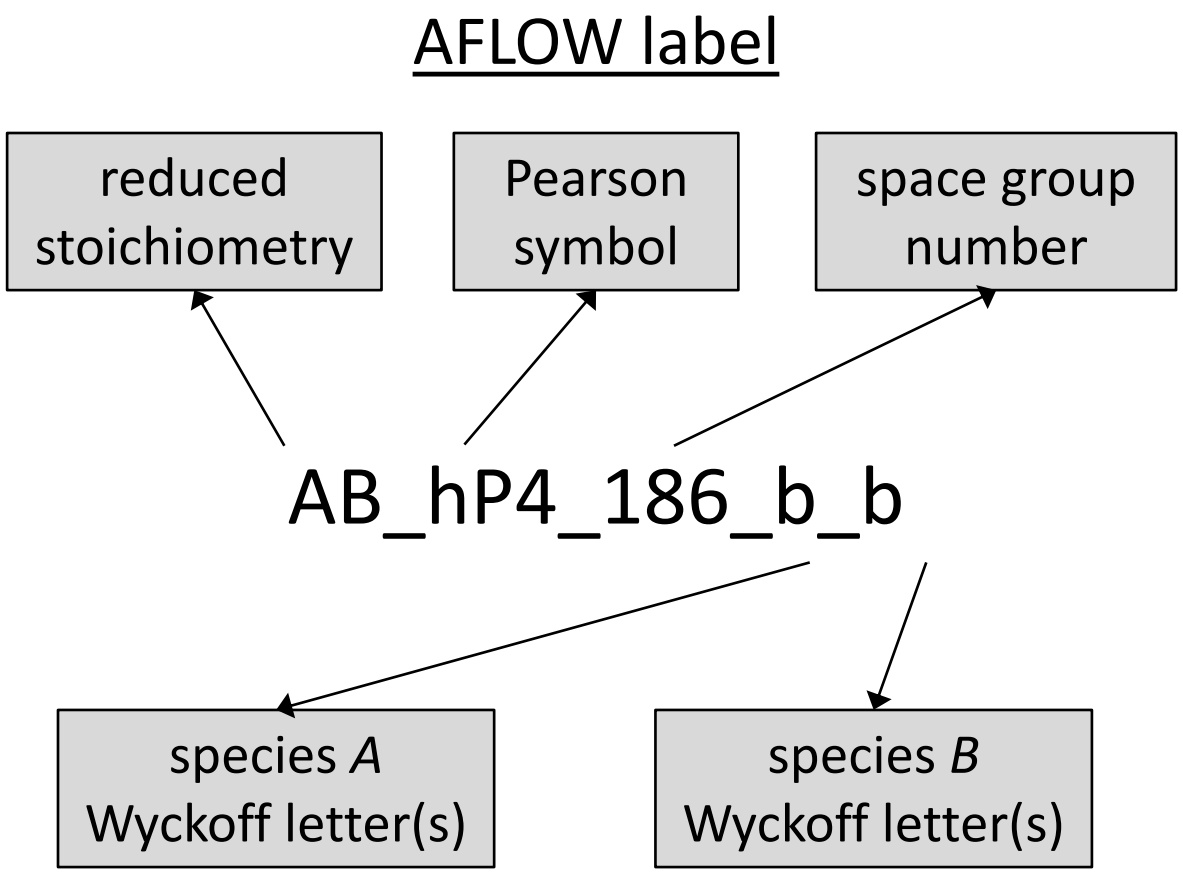
prototypes are integrated into AFLOW software = automatic materials generation

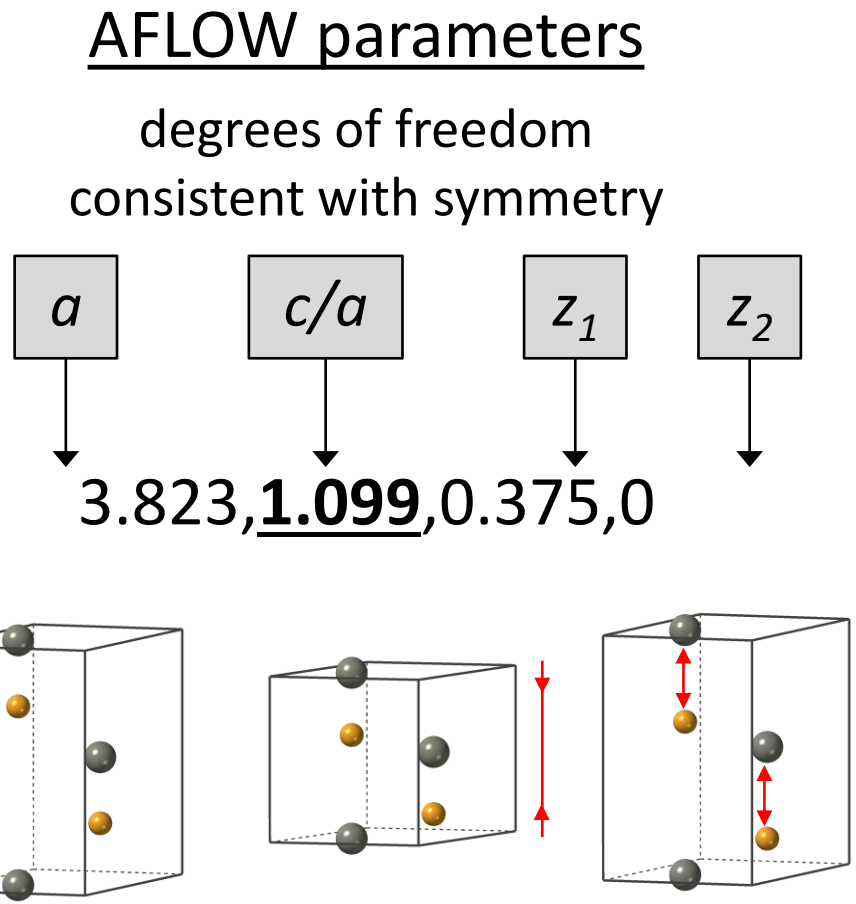
part 1 288 prototypes + **part 2** 302 prototypes + **part 3** 510 prototypes = 1,100 prototypes

Mehl *et al.*, Comput. Mater. Sci. **136**, S1 (2017); Hicks *et al.*, Comput. Mater. Sci. **161**, S1 (2019); Hicks *et al.*, Comput. Mater. Sci. (2021)

Standard designation and generation

Descriptive label and method for generation (*e.g.*, wurtzite)

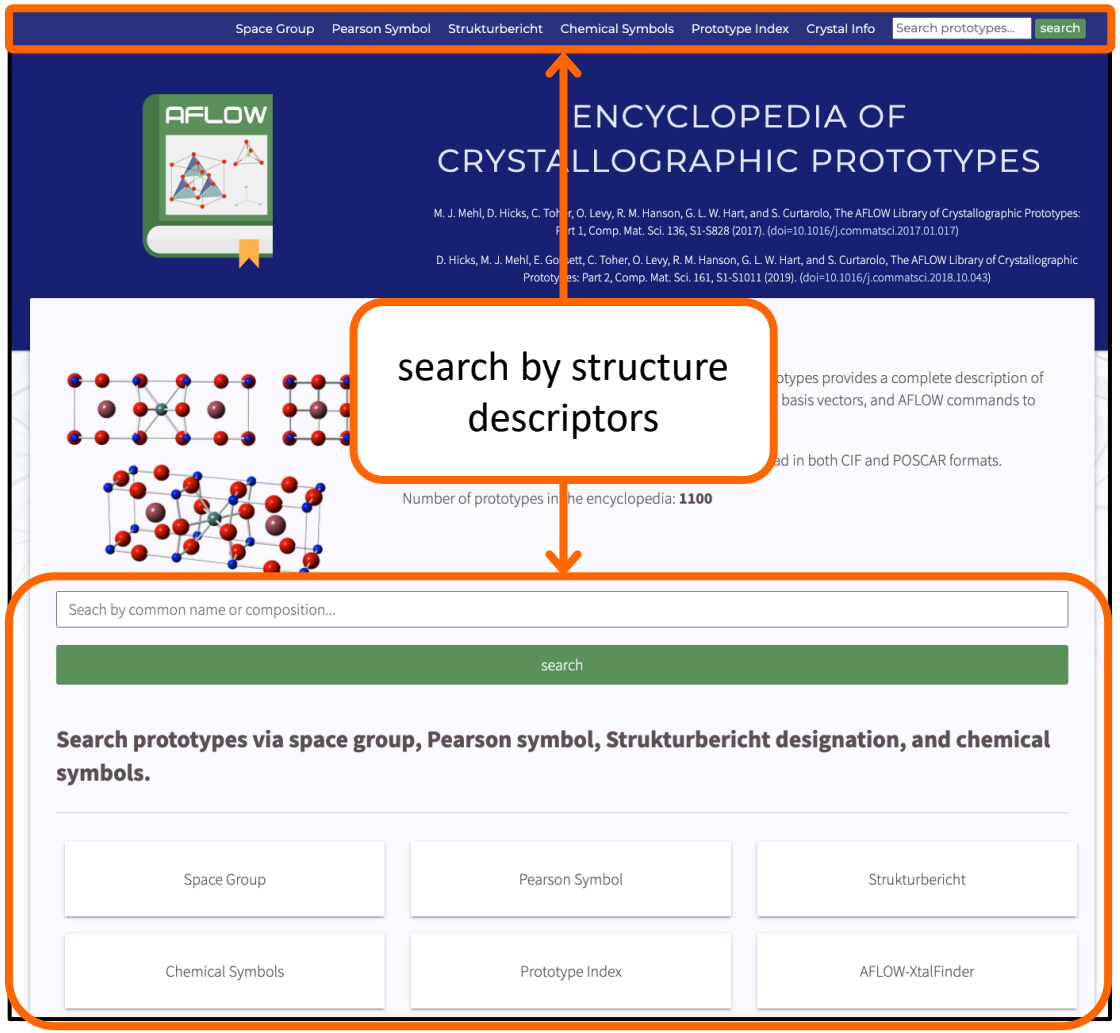


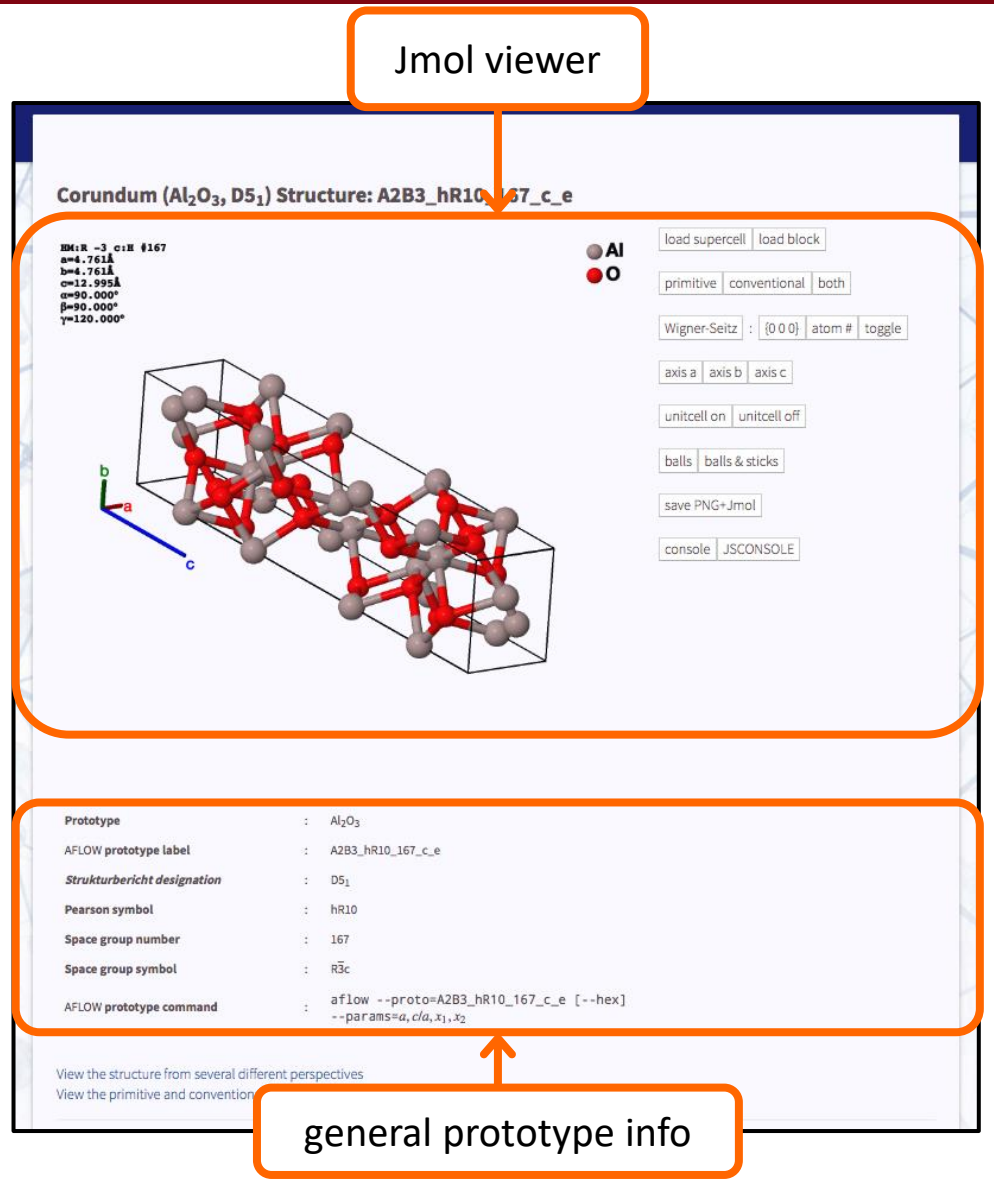


Mehl *et al.*, Comput. Mater. Sci. **136**, S1 (2017); Hicks *et al.*, Comput. Mater. Sci. **161**, S1 (2019); Hicks *et al.*, Comput. Mater. Sci. (2021)

Online application

https://aflow.org/prototype-encyclopedia/





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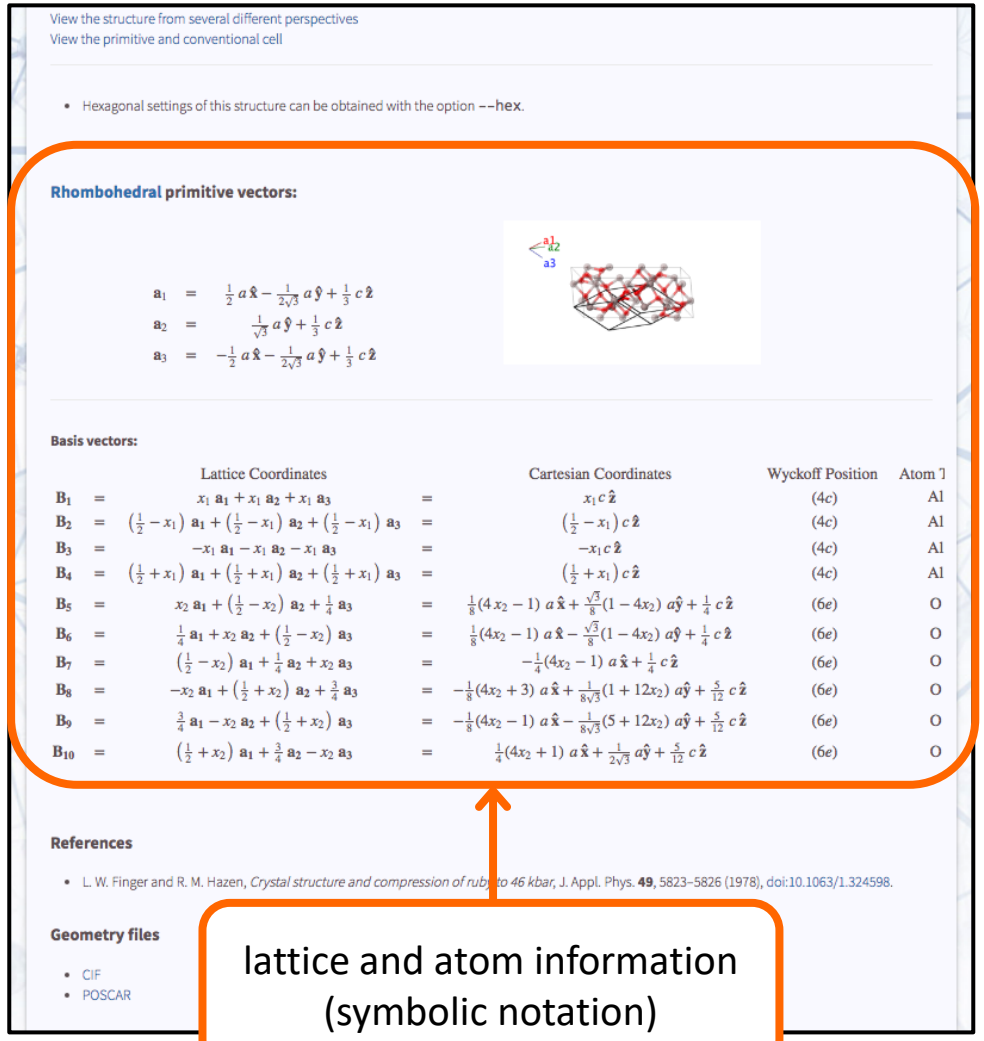
Online application

www.aflow.org/prototype-encyclopedia



lattice and atom information (symbolic notation)

prototype generator



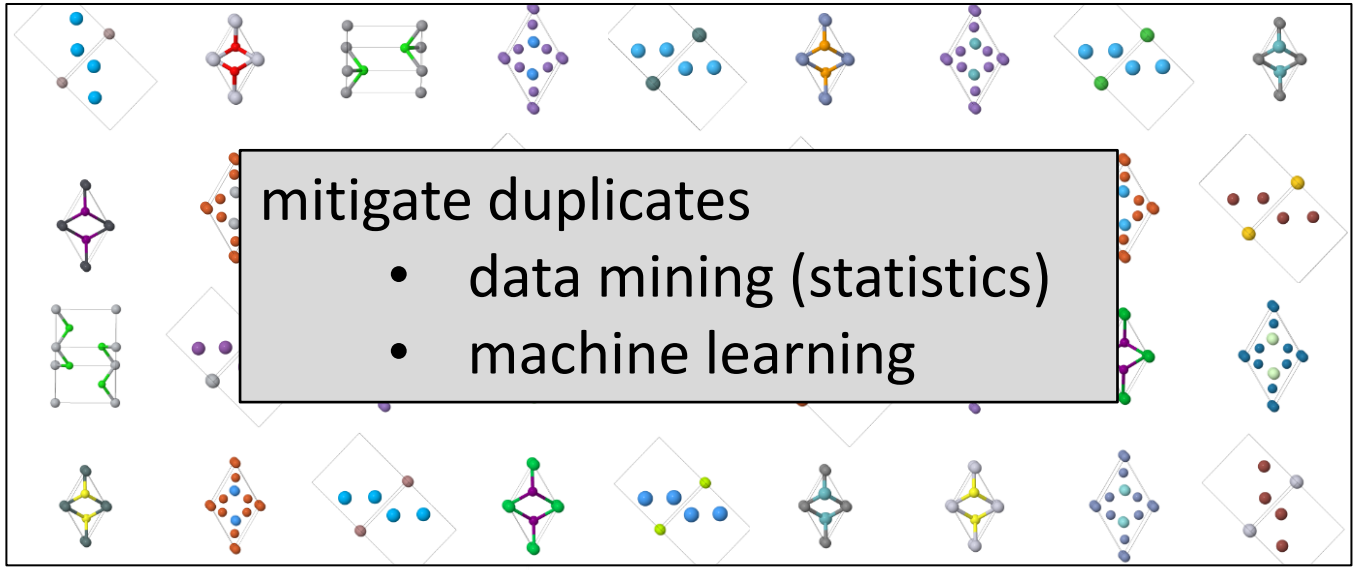
Mehl *et al.*, Comput. Mater. Sci. **136**, S1 (2017); Hicks *et al.*, Comput. Mater. Sci. **161**, S1 (2019); Hicks *et al.*, Comput. Mater. Sci. (2021)

Navigate to Prototype Encyclopedia (aflow.org/prototype-encyclopedia)

AFLOW-XtalFinder

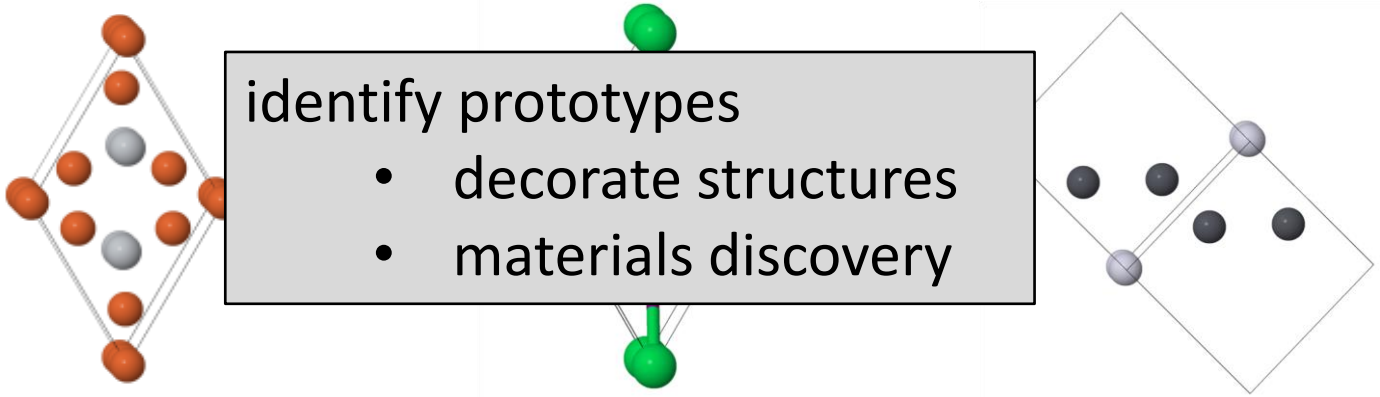
Search for structural diversity

programmatically search for distinct structures in datasets



mitigate duplicates

- data mining (statistics)
- machine learning

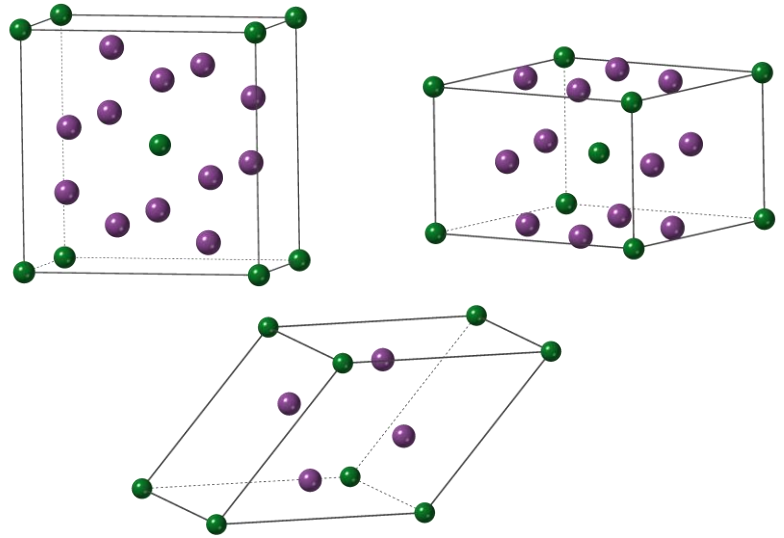


identify prototypes

- decorate structures
- materials discovery

lattice and origin choices obfuscate similarity

Ex:

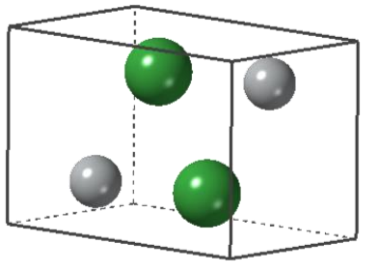


AFLOW-XtalFinder

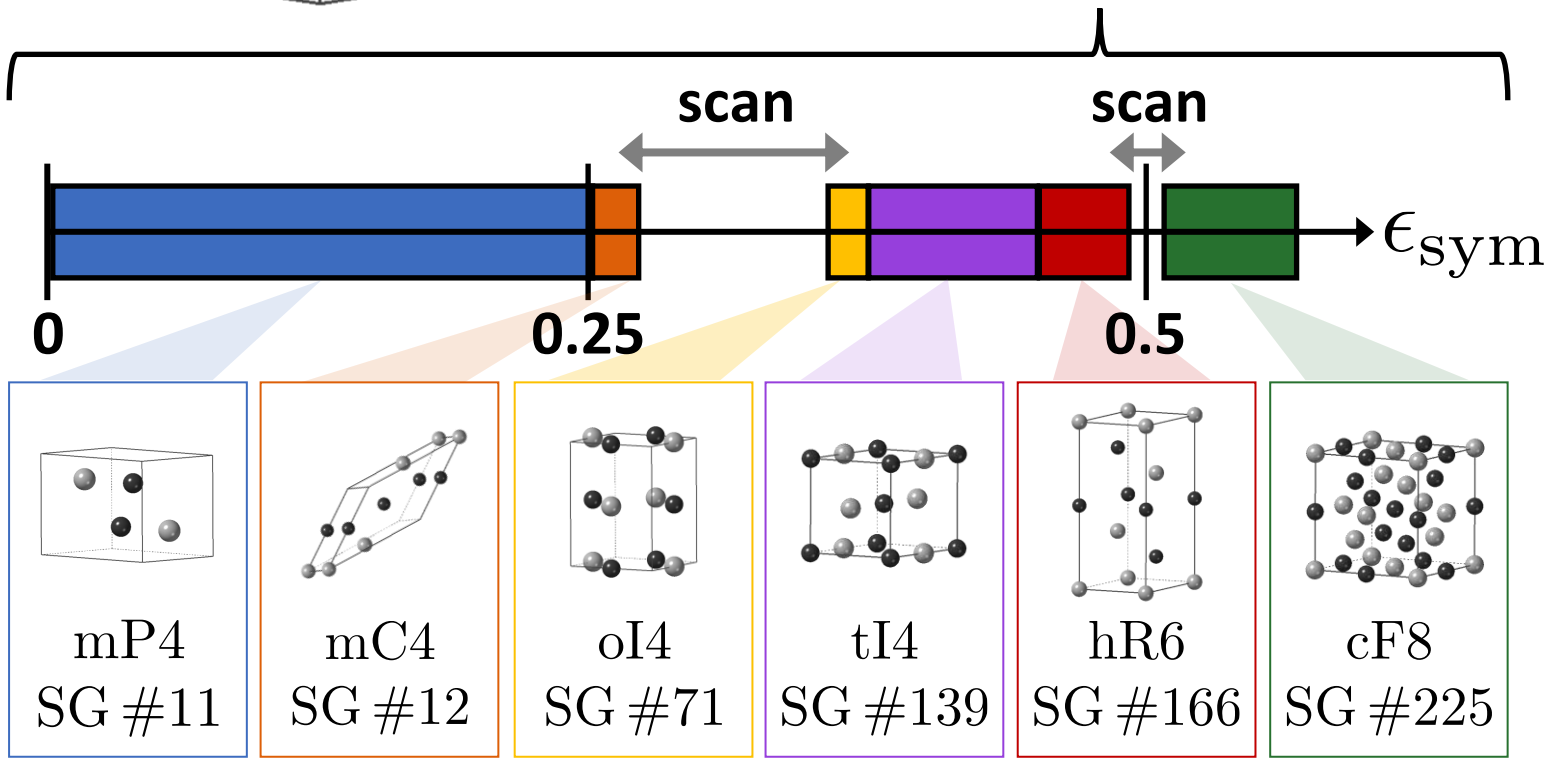
Hicks *et al.*, npj Comput. Mater. **7**, 30 (2021)

Autonomous prototype finder

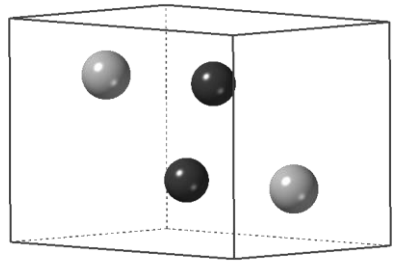
IDENTIFICATION: find prototype of crystalline material



self-consistent crystal prototype finder



ideal prototype designation



$$\begin{array}{llllll} \mathrm{mP4} & A & 2 & e & m \\ P2_1/m\ \#11 & B & 2 & e & m \end{array}$$

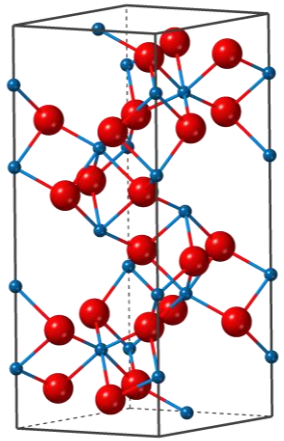
$$\epsilon_{\mathrm{sym}} = d_{\mathrm{nn}}^{\mathrm{min}}/100$$

default, consistent with experiment

Hicks *et al.*, npj Comput. Mater. **7**, 30 (2021)

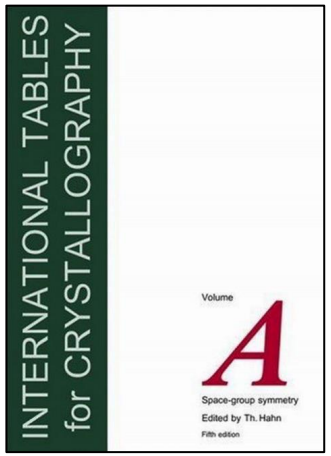
The ideal prototype

CLASSIFICATION: automatically determine standard label and internal degrees of freedom

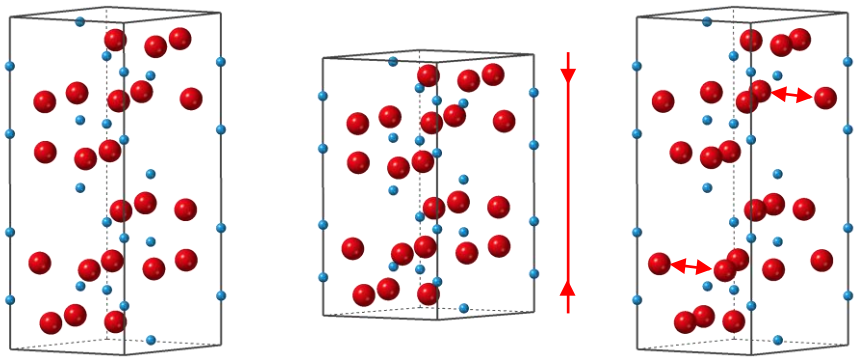


AFLOW label : A2B3_hR10_167_c_e
parameters : $a,c/a,x_1,x_2$
parameter values : 5.22337,2.72958,0.64784,0.9439

consistent with ITC standard



tune-able representation



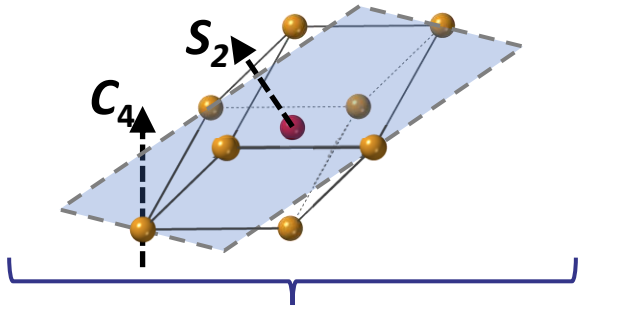
regenerate-able with AFLOW

```
AlO
1.00000
   2.61168  -1.50786   4.75253
   0.00000   3.01571   4.75253
  -2.61168  -1.50786   4.75253
4 6
Direct(10) [A4B6]
   0.35216   0.35216   0.35216  Al
   0.14784   0.14784   0.14784  Al
  -0.35216  -0.35216  -0.35216  Al
   0.85216   0.85216   0.85216  Al
   0.55610  -0.05610   0.25000  O
   0.25000   0.55610  -0.05610  O
  -0.05610   0.25000   0.55610  O
  -0.55610   1.05610   0.75000  O
   0.75000  -0.55610   1.05610  O
   1.05610   0.75000  -0.55610  O
```

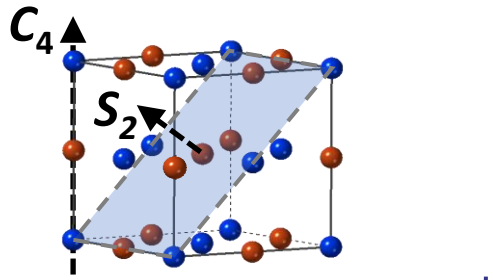
Hicks *et al.*, npj Comput. Mater. **7**, 30 (2021)

Structural uniqueness

symmetry comparison



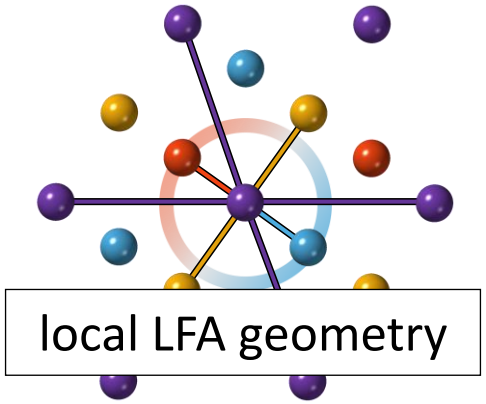
$$C_4 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \ldots \quad S_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



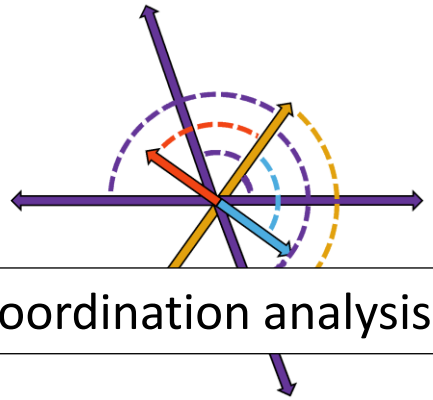
$$C_4 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \ldots \quad S_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

isopointal structures

local geometry comparison



local LFA geometry

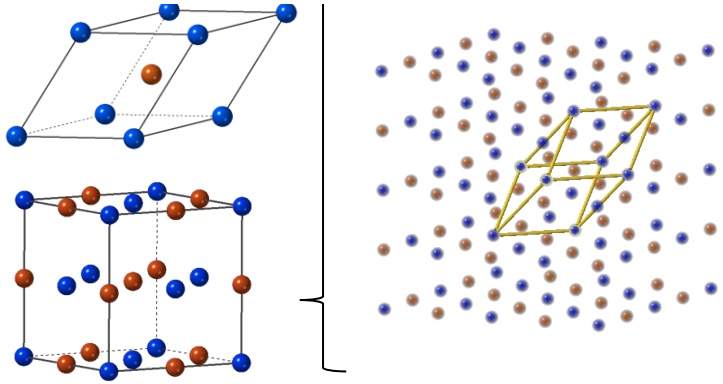


coordination analysis

local snapshots

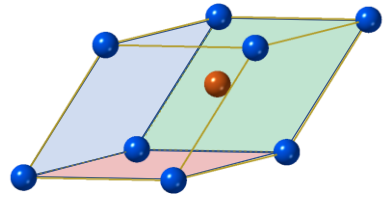
geometric comparison

lattice + origin search

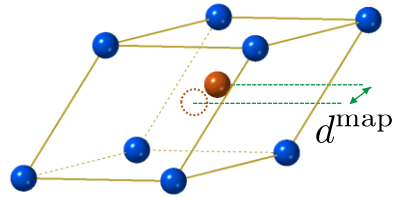


similarity metrics

lattice differences



matched or unmatched atoms



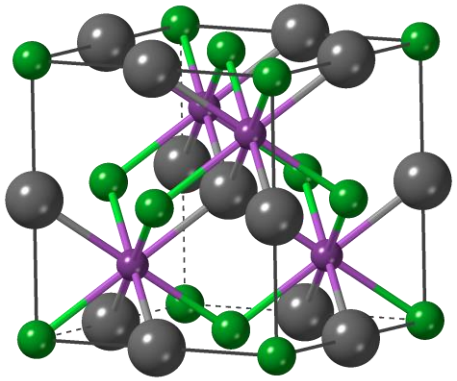
isoconfigurational

Hicks *et al.*, npj Comput. Mater. **7**, 30 (2021)

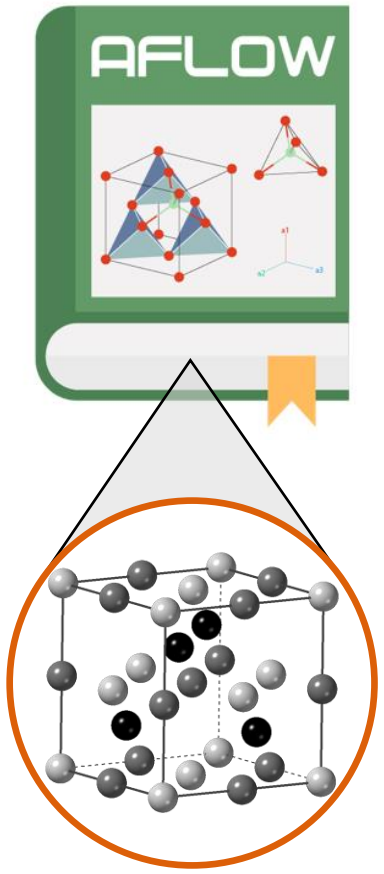
Compare against established prototypes

Compare against structures in AFLOW Prototype Encyclopedia

input structure



?



candidate matches
(similar symmetry, LFA geometry, etc.)

geometric structure mapping

matching entry

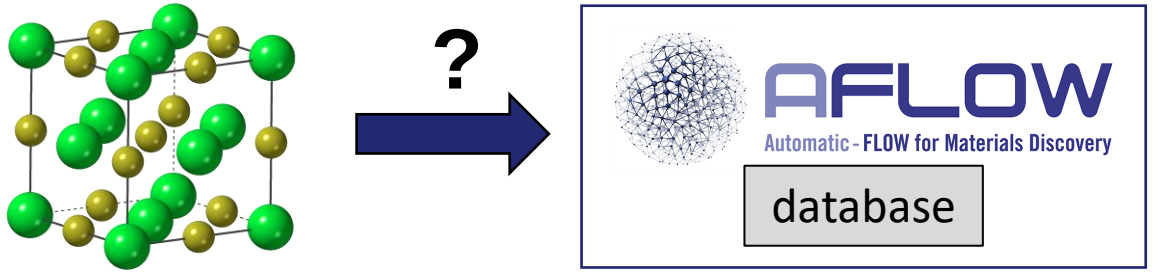
structural mismatch
0.01

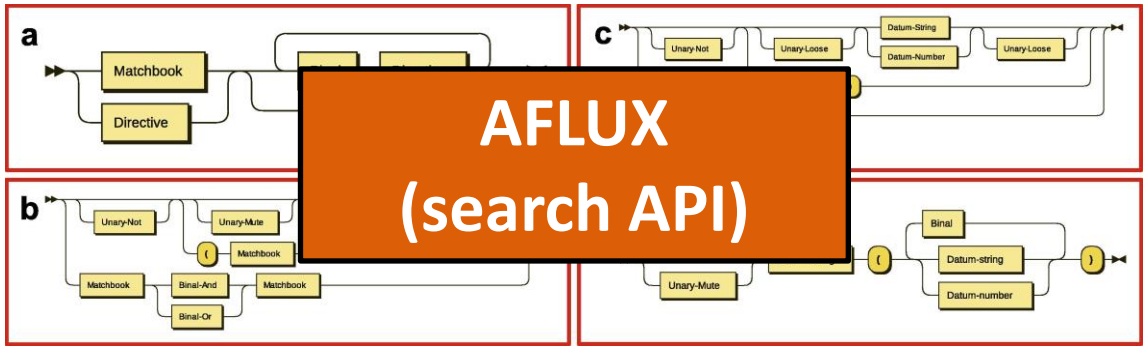
label:
ABC_cF12_216_b_c_a
common name:
half-Heusler
Strukturbericht:
$C1_b$
web:
aflow.org/prototype-encyclopedia/ABC_cF12_216_b_c_a.html
...

Mehl *et al.*, Comput. Mater. Sci. **136**, S1 (2017); Hicks *et al.*, Comput. Mater. Sci. **161**, S1 (2019); Hicks *et al.*, npj Comput. Mater. **7**, 30 (2021)

Database comparisons

Compare structures to AFLOW database





include API property keywords

e.g., `enthalpy_atom`, `natoms`, `Egap`, `agl_debye`, `kpoints`, `spin_atom`, etc.

Ex: NaCl (AFLOW label: AB_cF8_225_a_b, a=5.64 Å)

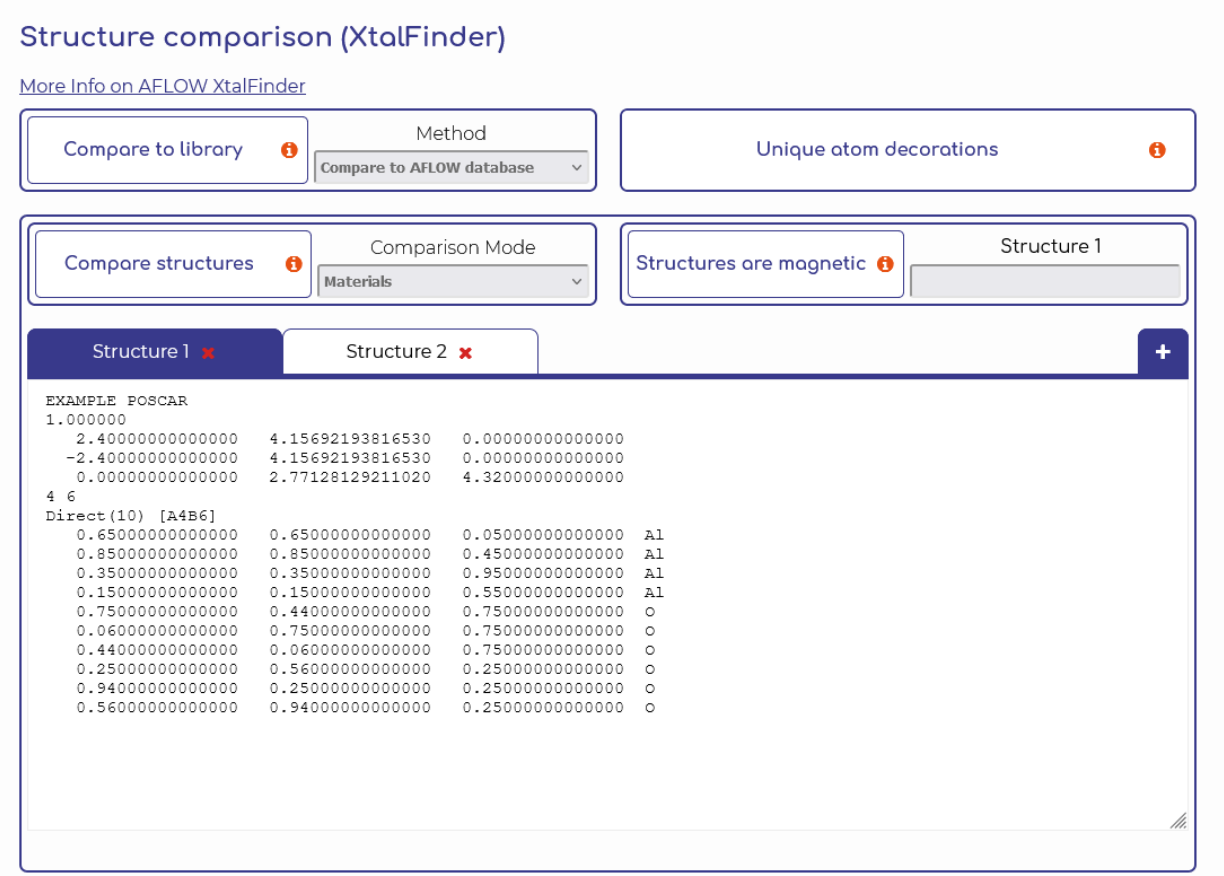
compound	auid	misfit	H_{atom} (eV/atom)	H_{cell} (eV/cell)
Cl1Na1	aflow:ec23029a18d3fec9	0.00384	-3.39049	-6.78098
Cl1Na1	aflow:b2ec4b68e12f3674	0.00415	-3.39056	-6.78112
Cl1Na1	aflow:1354bbef4edd80b3	0.00394	-3.39032	-6.78064
Cl1Na1	aflow:1cd71114972d46dd	0.00525	-3.39078	-6.78157
Cl1Na1	aflow:9017f9c64ead22ab	0.00445	-3.39062	-6.78125
Cl1Na1	aflow:4f19021768a3118a	0.00410	-3.39055	-6.78110
Cl1Na1	aflow:c16c0f1c061f7d3e	0.00435	-3.39061	-6.78121
Cl1Na1	aflow:b5ab343f3a484538	0.00432	-3.39060	-6.78120
Cl1Na1	aflow:182f848dd10cc403	0.00394	-3.39031	-6.78062
Cl1Na1	aflow:a4652bde28e67c3d	0.00350	-3.39041	-6.78082
Cl1Na1	aflow:2f4b5e32510830a0	0.00439	-3.39061	-6.78123
Cl1Na1	aflow:cc41860d69de2888	0.00416	-3.39056	-6.78113
Cl1Na1	aflow:fd711a60dbfba2de	0.00389	-3.39028	-6.78057
Cl1Na1	aflow:e3e31c4914d59e25	0.00390	-3.39029	-6.78059
Cl1Na1	aflow:9a28207fd647e477	0.00390	-3.39029	-6.78059
Cl1Na1	aflow:d996b8d524516c24	0.00391	-3.39030	-6.78059
Cl1Na1	aflow:d241535faf2a4519	0.00525	-3.39101	-6.78202
Cl1Na1	aflow:39ab5e62afdb5ac0	0.00440	-3.39062	-6.78123
Cl1Na1	aflow:9466351a9cbac2c9	0.00390	-3.39030	-6.78059
Cl1Na1	aflow:5699b196418c6044	0.00461	-3.39066	-6.78132
Cl1Na1	aflow:d0c93a9396dc599e	0.00508	-3.39075	-6.78150
Cl1Na1	aflow:55d2cbd0f4018884	0.00416	-3.39013	-6.78026
Cl1Na1	aflow:18ebb85b07a92f89	0.00397	-3.39033	-6.78067
Cl1Na1	aflow:a5755554aaf5d10e	0.00390	-3.39030	-6.78059
Cl1Na1	aflow:82a178672a734c47	0.00548	-3.39082	-6.78165
Cl1Na1	aflow:3bd528dd9f88be7d	0.00406	-3.39233	-6.78466
Cl2Na2	aflow:f4b806d73482566c	0.00361	-3.39121	-13.5648

Rose *et al.*, Comput. Mater. Sci. **137**, 362 (2017); Hicks *et al.*, npj Comput. Mater. **7**, 30 (2021)

AFLOW-XtalFinder: online

online functionality https://aflow.org/aflow-online/

- Compare to library:
  - Find if material exists in the AFLOW database
  - Get isopointal (same symmetry) prototypes
  - Compare to prototype encyclopedia
- Get unique atom decorations
- Compare a set of structures (up to 8)
  - Compare structures taking species into account (Comparison mode: Materials)
  - Compare structures ignoring species (Comparison mode: Structures)



Navigate to AFLOW-Online (aflow.org/aflow-online)

Exercises

1. Navigate to https://aflow.org/prototype-encyclopedia/A2B7C2_tI44_119_i_bdefgh_i. Generate a geometry file with the default parameters and calculate the space group on https://aflow.org/aflow-online? What space group(s) do you find if you change the tolerance from “tight” to “loose”?

2. Navigate to https://aflow.org/prototype-encyclopedia/AB4_cP5_215_a_e and generate a geometry file with the default parameters. Using AFLOW-Online, determine the Wyckoff positions without spin polarization. Now compare the result with a spin polarized material: use the “Magnetic Structure” button to specify spin “up” for some Fe atoms and spin “down” for others (leave C at 0). What is is the new space group and Wyckoff sequence?

3. Navigate to the following AFLOW entry: https://aflow.org/material/?id=aflow:44368cc42c6f60cc. At the bottom of the page, click on the “VASP-CONTCAR” under “Relaxed Structure” and copy the geometry file. On AFLOW-Online, determine the prototype designation via the “AFLOW prototype” button. How many degrees of freedom are there (*i.e.*, # of parameters)? Compare with the data on the entry page.

4. Navigate to the rock salt prototype page. Generate a sodium chloride crystal with the default parameters. On AFLOW-Online, use the “Compare to library” button and “Compare to AFLOW database” method and “Submit”. How many AFLOW entries match to the input? (HINT: Check for “compounds_duplicate=” in the output.)

Python modules

First, download AFLOW source code: https://aflow.org/install-aflow/

Generate Python modules via AFLOW command:

AFLOW-SYM:	`aflow --aflow_sym_python`
AFLOW-XtalFinder:	`aflow --aflow_xtalfinder_python`

Example scripts and functionality at https://aflow.org/aflow-schools

More information

For more functionality, download the AFLOW source code: http://aflow.org/install-aflow/

READMEs:

aflow --readme=symmetry	aflow --readme=prototypes	aflow --readme=xtalfinder

Relevant articles:

AFLOW-SYM:

D. Hicks, C. Oses, R.H. Taylor, E. Gossett, G. Gomez, C. Toher, M.J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: Platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Cryst. A**74**, 184-203 (2018). doi: 10.1107/S2053273318003066

Prototypes:

M.J. Mehl, D. Hicks, C. Toher, O. Levy, R.M. Hanson, G.L.W. Hart, and S. Curtarolo,
The AFLOW Library of Crystallographic Prototypes: Part 1, Comp. Mat. Sci. **136** Supplement, S1–S828 (2017). doi: 10.1016/j.commatsci.2017.01.017

D. Hicks, M.J. Mehl, E. Gossett, C. Toher, O. Levy, R.M. Hanson, G.L.W. Hart, and S. Curtarolo,
The AFLOW Library of Crystallographic Prototypes: Part 2, Comp. Mat. Sci. **161** Supplement, S1-S1011 (2019). doi: 10.1016/j.commatsci.2018.10.043

D. Hicks, M.J. Mehl, M. Esters, C. Oses, O. Levy, G.L.W. Hart, C. Toher, and S. Curtarolo,
The AFLOW Library of Crystallographic Prototypes: Part 3, in press, Comp. Mat. Sci. (2021). arXiv:2012.05961

AFLOW-XtalFinder:

D. Hicks, C. Toher, D.C. Ford, F. Rose, C. De Santo, O. Levy, M.J. Mehl, and S. Curtarolo, *AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes*, npj Comput. Mater. **7**, 30 (2017). doi: 10.1038/s41524-020-00483-4