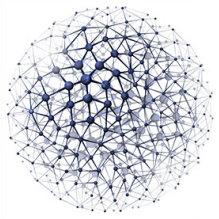
AFLOW Prototype Encyclopedia: Generating crystallographic structures

David Hicks
AFLOW – Technische Universität Dresden – Online

Session 3 (19:00 – 21:00 CET)

Tuesday, September 7th, 2021

Duke UNIVERSITY



AFLOW
Automatic - FLOW for Materials Discovery

NSF

Office of Naval Research
USN ONR
Science & Technology

The search for prototypes

catalogs of structure prototypes



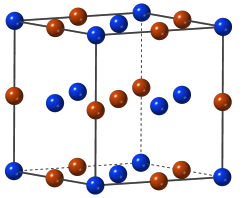
computational hurdles

arbitrary designations

Ex:

compound name: NaCl or MgO

Strukturbericht: B1



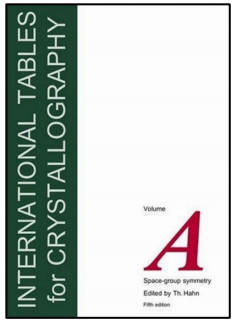
knowledge of crystallography

Ex:

space group #216

Wyckoff position:

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



coordinates

$$\begin{aligned}&\mathrm{Ag}\quad 0,0,0\\&\mathrm{Ag}\quad 0,1/2,1/2\\&\mathrm{Ag}\quad 1/2,0,1/2\\&\mathrm{Ag}\quad 1/2,1/2,0\end{aligned}$$

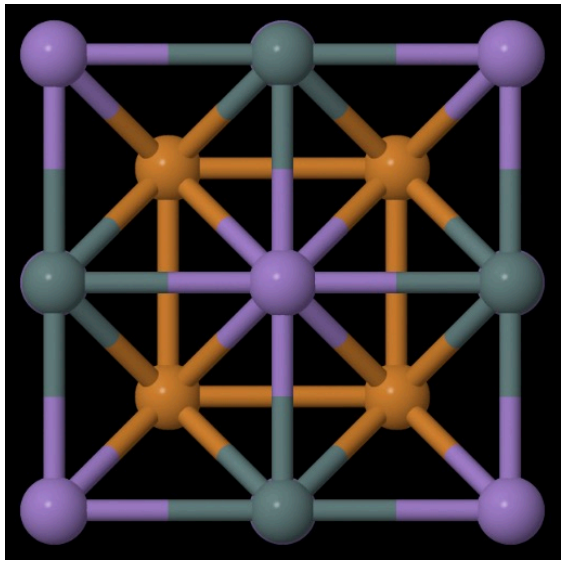
multiplicity — letter designation — representative coordinate

lack methods for materials generation

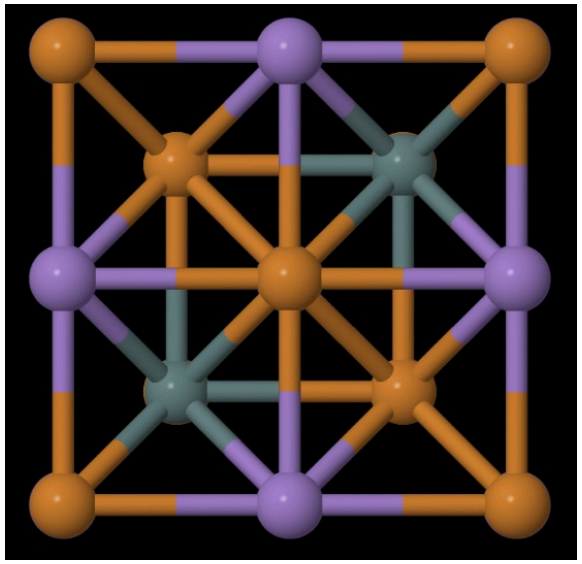
Hahn, Kluwer Academic Publishers (2002)

AFLOW: Crystallographic prototypes

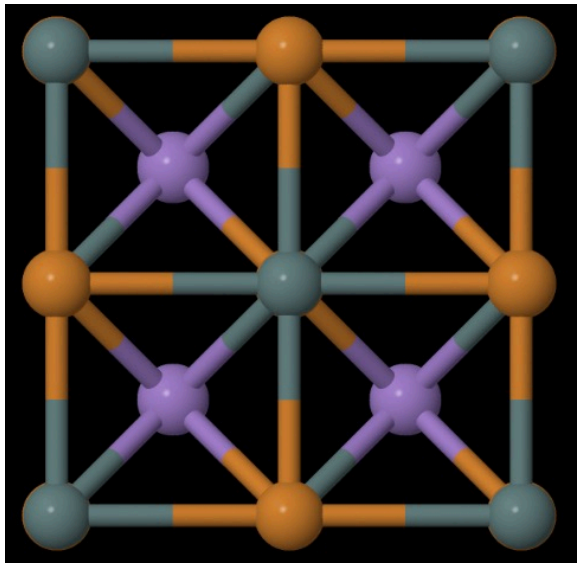
- AFLOW contains built-in structural prototypes:



Prototype T0001:
Heusler structure



Prototype T0002:
Anti-Heusler structure



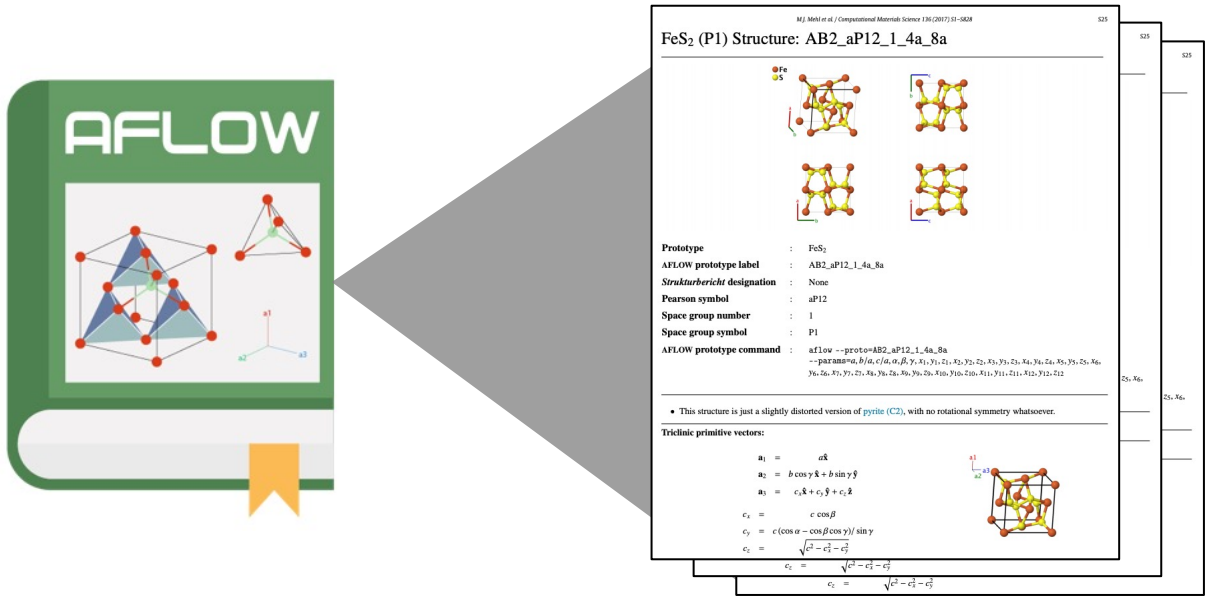
Prototype T0003:
Half-Heusler structure

- Decorating prototypes with different elements allows for automated creation of new hypothetical materials
- ~1,100 prototypes available at 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
- *Strukturbericht*
- historic labels
- similar compounds
- Wyckoff positions
- Pearson symbol
- space group
- explicit coordinates
- lattice vectors
- visualizations

prototypes are integrated into AFLOW software = automatic materials generation

part 1
288 prototypes

+

part 2
302 prototypes

+

part 3
510 prototypes

=

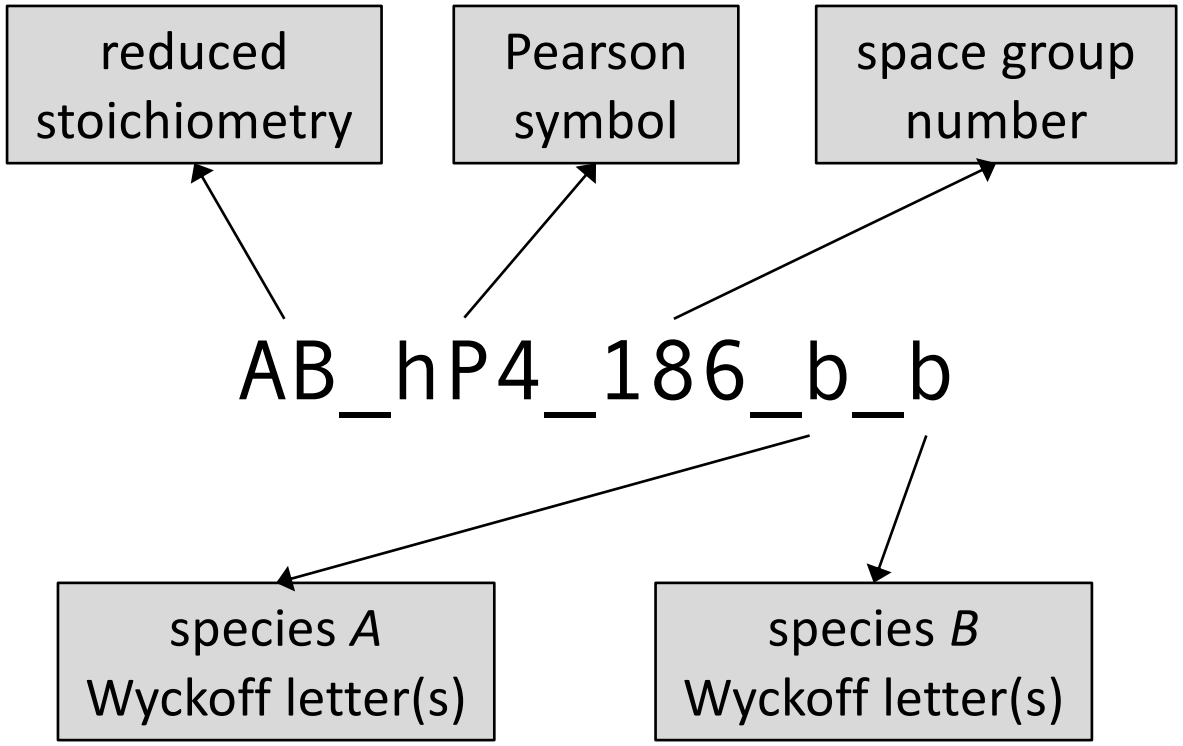
1,100 prototypes

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

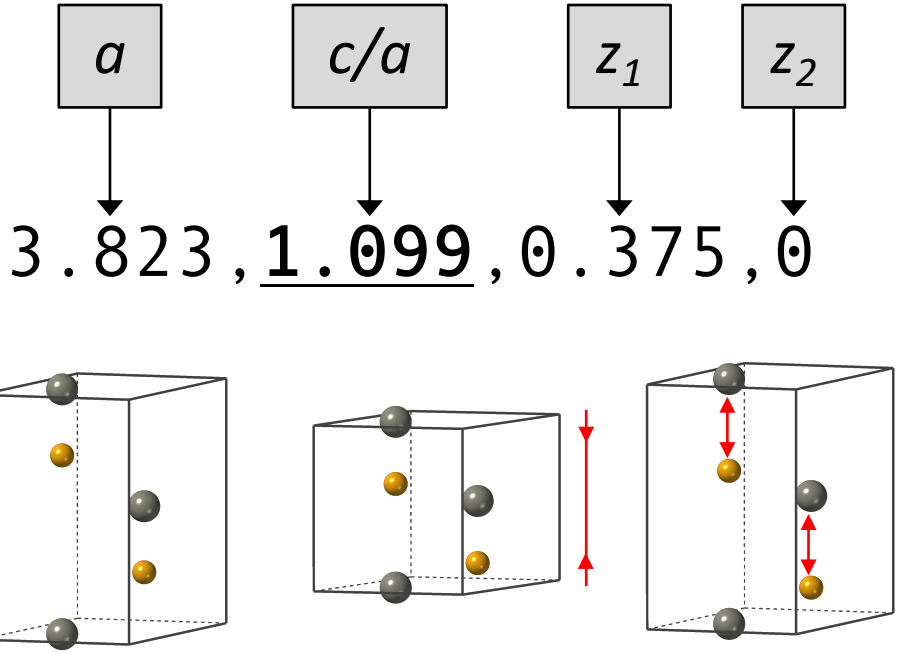
Descriptive label and method for generation (*e.g.*, wurtzite)

AFLOW label



AFLOW parameters

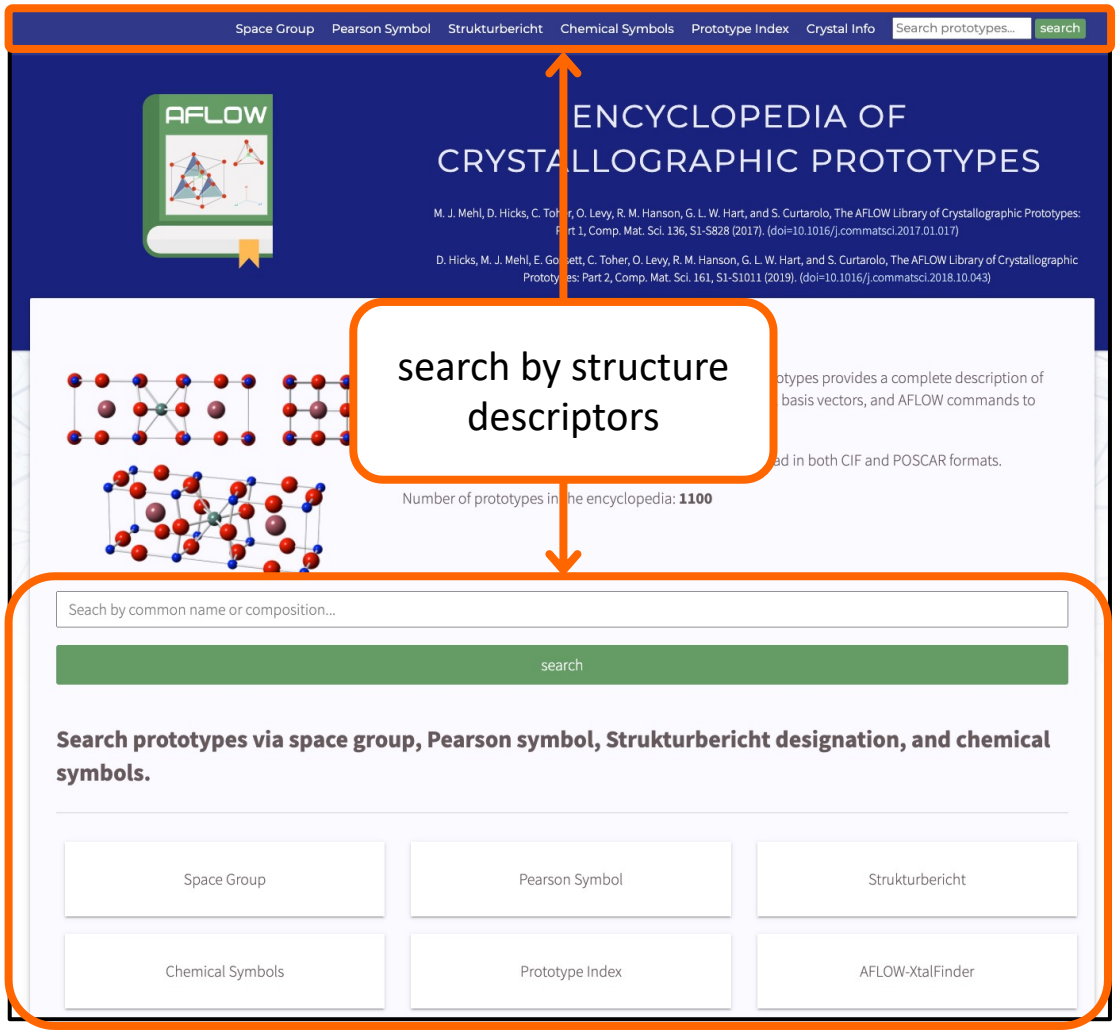
degrees of freedom consistent with symmetry

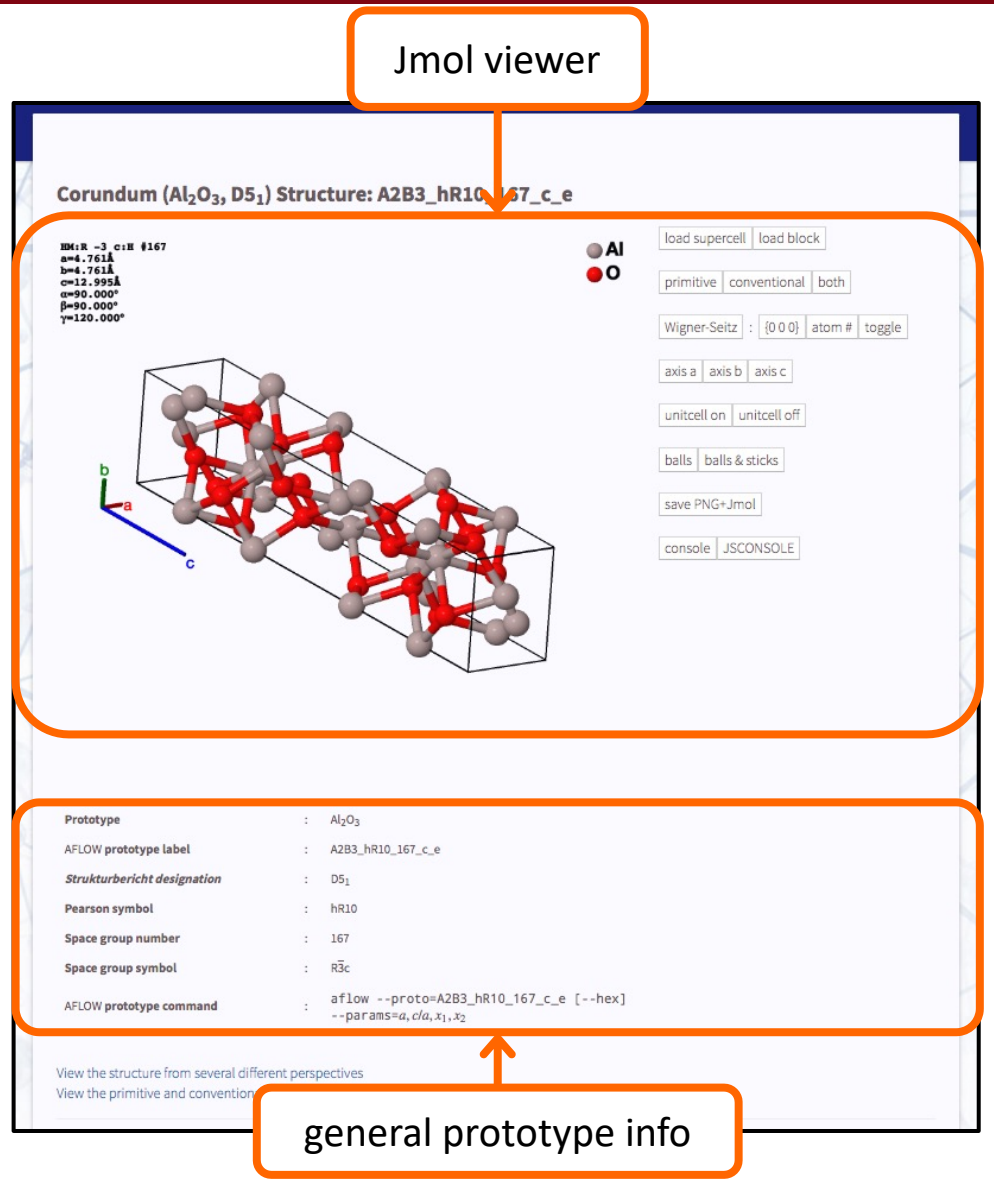


Mehl *et al.*, Comput. Mater. Sci. **136**, S1 (2017); Hicks *et al.*, Comput. Mater. Sci. **161**, S1 (2019); Hicks *et al.*, Comput. Mater. Sci. (2021)

Online application

www.aflow.org/prototype-encyclopedia





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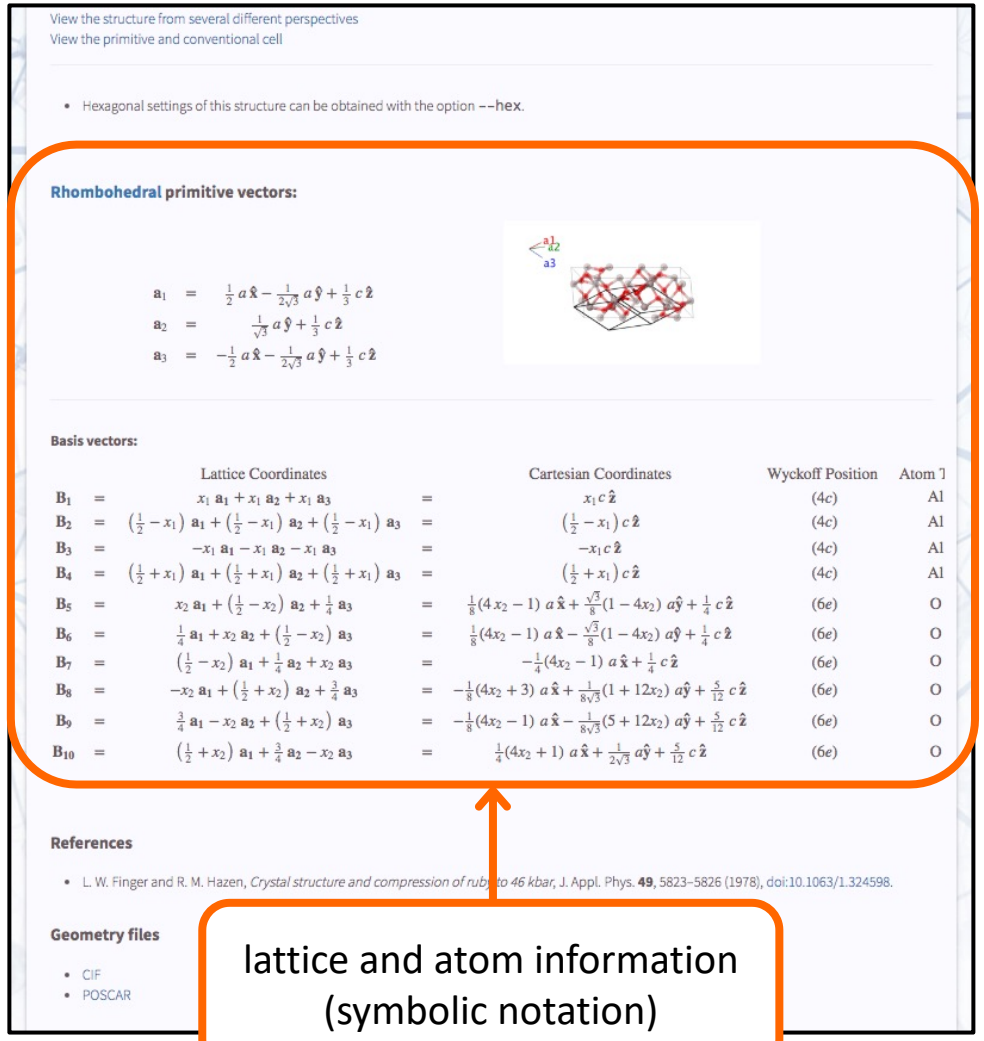

lattice and atom information (symbolic notation)

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)

Prototype commands

- AFLOW Crystallographic Prototype Encyclopedia (approx. 1,100)

```
aflow --proto=AB_hP4_186_b_b --params=3.823,1.638,0.375,0.0
```

label parameters

- AFLOW Standard Prototypes (approx. 700)

```
aflow --proto=T0001.A2BC
```

  - generally numbered labels
  - hard-coded prototypes; no degrees of freedom

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)

Create geometry files

- Decorate rock-salt prototype AB_cF8_225_a_b with MgO:

```
aflow --proto=AB_cF8_225_a_b:Mg:O --params=3.5
```

```
MgO/AB_cF8_225_a_b params=3.5 SG#=225
1.000000
   0.0000000000000   1.7500000000000   1.7500000000000
   1.7500000000000   0.0000000000000   1.7500000000000
   1.7500000000000   1.7500000000000   0.0000000000000
1 1
Direct(2) [A1B1]
   0.0000000000000   0.0000000000000   0.0000000000000  Mg
   0.5000000000000   0.5000000000000   0.5000000000000  O
```

- Variety of possible geometry file formats by adding options:

VASP	CIF	FHI-AIMS	Quantum Espresso	ABINIT	ELK
`--vasp`	`--cif`	`--aims`	`--qe`	`--abinit`	`--elk`

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)

Create geometry files

- Control atomic site decoration:

```
aflow --proto=AB_cF8_225_a_b.BA:Mg:O --params=3.5
```

```
MgO/AB_cF8_225_a_b.BA params=3.5 SG=225
1.000000
   0.0000000000000   1.7500000000000   1.7500000000000
   1.7500000000000   0.0000000000000   1.7500000000000
   1.7500000000000   1.7500000000000   0.0000000000000
1 1
Direct(2) [A1B1]
   0.5000000000000   0.5000000000000   0.5000000000000  Mg
   0.0000000000000   0.0000000000000   0.0000000000000  O
```

- Automatic volume scaling based on atomic elements:

```
aflow --proto=AB_cF8_225_a_b.AB:Mg:O --params=-1
```

```
MgO/AB_cF8_225_a_b.AB params=-1 SG=225
-30.600100
   0.0000000000000   0.5000000000000   0.5000000000000
   0.5000000000000   0.0000000000000   0.5000000000000
   0.5000000000000   0.5000000000000   0.0000000000000
```

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)

Create geometry files

- Enumerated parameter sets:

```
aflow --proto=AB2C_oP16_62_c_2c_c.ABC:Cu:S:Sb
--params=-1,0.630741110003,2.4086075108,0.2522,0.8276,0.6221,0.095,0.8706,0.8244,0.226,0.06333
```

vs

```
aflow --proto=AB2C_oP16_62_c_2c_c-001.ABC:Cu:S:Sb
```

- Don't know what parameter sets are available?

```
aflow --proto=AB2_oP6_58_a_g
```

```
anrl::getANRLParameters(): ERROR - AB2_oP6_58_a_g has 3 preset parameter set(s):
 AB2_oP6_58_a_g-001 : -1,1.03044871795,0.673076923077,0.275,0.325
 AB2_oP6_58_a_g-002 : -1,0.917942176871,0.601615646259,0.66667,0.25
 AB2_oP6_58_a_g-003 : -1,1.22049228277,0.761913333033,0.2004,0.3787
 AB2_oP6_58_a_g-004 : -1,1.1965466,0.67115528,0.8682,0.5945
 AB2_oP6_58_a_g-005 : -1,1.2288051,0.58567724,0.414,0.068
```

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)

Generate aflow.in files

- Use Heusler prototype T0001.A2BC to create aflow.in file for Cu_2TiZn:

```
aflow --aflow_proto=T0001.A2BC:Cu:Ti:Zn
```

- Comma separated prototypes:

```
aflow --aflow_proto=T0001.A2BC,TFCC001.ABC:Ag,Au,Cu,Fe:Mn,Ti:Zn
```

- Comma separated species:

```
aflow --aflow_proto=T0001.A2BC:Ag,Au,Cu,Fe:Mn,Ti:Zn
```

- Include degrees of freedom for relevant prototypes:

```
aflow --aflow_proto=AB_cF8_225_a_b.AB:Mg:O --params=-1
```

- NOTE: Since we are not using VASP, add the following option when using --aflow_proto:

```
--generate_aflowin_only
```

Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012); Curtarolo *et al.*, Comput. Mater. Sci. **58**, 227 (2012)

Available prototypes

- List of prototypes:

```
aflow --protos
```

OR

AFLOW Prototype Encyclopedia

```
http://aflow.org/prototype-encyclopedia
```

- Search for specific prototypes:

```
aflow --prototype_labels --nspecies=2 --stoichiometry=1,2 --sg=225
```

583,584,691.AB,691.BA,1027.AB,1027.BA,1218.AB,1218.BA,AB2_cF12_225_a_c

- Additional information is available in README:

```
aflow --readme=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)

Exercises

1. [ONLINE EXERCISE] Generate POSCARs for the following structures via the AFLOW online generator: 1) diamond, 2) caswellsilverite, 3) spinel (ternary), 4) calaverite (Struk. *C34*), 5) brookite, 6) sulvanite. What are the AFLOW labels of these structures?

2. Generate structures for the prototype A_hR1_166_a using an element and value of *a* of your choice, with *c*/*a* values of 0.5, 0.612, 1.0, 1.225, 1.5, 2.45, and 3.0. Calculate the space group (--aflowSG) of each of the structures.

3. Generate two quaternary Heusler structures (ABCD_cF16_216_c_d_b_a) with the –params=-1 and decorate it with the following elements: Ag, Cu, Fe, Mn. For the first structure, Put Ag, Cu, Fe, and Mn on Wyckoff sites b, a, c, and d, respectively for the first structure. For the second structure, put Ag, Cu, Fe, Mn on Wyckoff sites d, b, c, and a, respectively. Keep the species in ALPHABETICAL order and use the decoration functionality. Note: Wyckoff a is (0,0,0), b is (1/2,1/2,1/2), c is (1/4,1/4,1/4), and d is (3/4,3/4,/3/4).

4. Generate the Heusler structure (T0001.A2BC) and decorate with elements of your choice. Determine the space group, Wyckoff positions, and Pearson symbol of this prototype. What would the corresponding AFLOW prototype label be?

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)

More information

AFLOW Prototypes README:

```
aflow --readme=prototypes
```

AFLOW Prototype articles:

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