DFT- code

ERROR?

AFLOW source code now available under GPL 3 materials.duke.edu/AFLOW/

Curtarolo et al., Comput. Mater. Sci. 58, 218 (2012); Calderon et al., Comp. Mat. Sci. 108A, 233 (2015)

**Outline**

**Automated Materials Discovery**

• Ge#ng started with AFLOW:

• Decora8ng crystal prototypes to set up new calcula8ons

• Automated computa8onal materials discovery:

• Symmetry analysis

• Thermodynamic and thermo-mechanical

Experimental structures Automated QM calcula8ons

• Convex hull phase diagrams

• AEL/AGL/APL: Elas8c constants and thermal proper8es

• AFLOW online data repositories

• AFLOW.org online web interface

• AFLOW REST-API

• AFLUX Search-API

Searchable/sortable database

• AFLOW-ML + API

• AFLOW code:

• Installing AFLOW

• Data analysis with AFLOW

• Running AFLOW calcula8ons

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**AFLOW: Integrated infrastructure for computa@onal materials discovery**

AFLOW

DFT-code

**AFLOW: Automa@c FLOW**

Input file generation

DFT- code

aflow.in

Calculation management

calculation Property

Electronic Thermal Elas8c Database storage

Storage

**Outline**

• Ge#ng started with AFLOW:

• Decora8ng crystal prototypes to set up new calcula8ons

• Symmetry analysis

***CORMAC TOHER COREY OSES DAVID HICKS E. Gosse5,***

• Thermodynamic and thermo-mechanical

• Convex hull phase diagrams

• AEL/AGL/APL: Elas8c constants and thermal proper8es

***F. Rose, S. Curtarolo Materials Science***

• AFLOW online data repositories

• AFLOW.org online web interface

• AFLOW REST-API Duke University

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• AFLOW code:

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Density func8onal theory

5

Structural prototypes

ML models

**AFLOW.org: web portal**

**hIp://aflow.org**

**> 1.8 million**

DFT-

**entries**

code

**Advanced Search**

**Crystal Prototypes Machine- learning model**

**Convex AFLOW-online**

**hull (AFLOW-SYM)**

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

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Candidate materials

2

*7/31/18*

*1*

**AFLOW: Crystallographic Prototypes**

**hIp://aflow.org**

**Crystal Prototypes**

Prototype T0003: Half-Heusler structure

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

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**AFLOW: Crystallographic Prototypes**

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

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**AFLOW: Crystallographic Prototypes**

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

**AFLOW: Crystallographic Prototypes**

• AFLOW contains built-in structural prototypes:

• Decora8ng prototypes with different elements allows for automated crea8on of new hypothe8cal materials

• ~600 prototypes available at aflow.org/CrystalDatabase

**AFLOW: Crystallographic Prototypes**

Primitive lattice vectors

Atomic basis vectors

References

Geometry files

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

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Prototype T0001: Heusler structure

Prototype T0002: An8-Heusler structure

Jmol interface

Prototype information

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**AFLOW: Crystallographic Prototypes**

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

Prototype generator

Format options

Structure output

AFLOW command

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**AFLOW: Crystallographic Prototypes**

**AFLOW-SYM**

Exercises:

• Select a prototype from the Library of Crystallographic Prototypes at aflow.org/ CrystalDatabase/. Use the online tool to create a POSCAR for that structure, decorated with elements of your choice.

• 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. Save these structures with appropriate names, as they will be used as part of a later exercise.

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018) D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

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**AFLOW-SYM**

• Mismatch with respect to space group listed in descrip8on of experimental structure in ICSD

D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

**AFLOW-SYM**

minimum in frac8onal ≠ minimum in Cartesian

• AFLOW-SYM consists of robust mapping procedure; takes la#ce skewness into account D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

Cartesian

fractional

θ ˆn

m

cubic orthorhombic triclinic

Cartesian fractional

dmin c

C dmin c

∈

∈

C dmin

f

∈

• AFLOW-SYM tests invariance of crystal under transforma8ons

• Provides informa8on on space group, Pearson symbol, Bravais la#ce, primi8ve and conven8onal cell, etc.

• API keywords:

spacegroup\_relax, Pearson\_symbol\_relax, Bravais\_lattice\_orig, ...

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**a b**

n

mirror

r

n fold

13

**AFLOW-SYM**

• AFLOW-SYM performs self-consistent tolerance scan when transforma8ons are inconsistent with ITC space groups, or when inconsistencies exist between different representa8ons.

D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

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**AFLOW-SYM: AFLOW-Online**

**hIp://aflow.org**

**AFLOW-online (AFLOW-SYM)**

D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

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**a**

**b**

0.1

∈

0

mcl SG: #11

orc SG #59

rhl SG #166

fcc SG #225

0 0.5

1.0 0.3

∈

new

16

x

i

x j θ

*7/31/18*

*3*

**AFLOW-SYM: AFLOW-Online**

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**AFLOW-SYM**

Exercises:

• Use AFLOW-SYM to determine the symmetry proper8es of the structure that you generated using prototype you selected from the Library of Crystallographic Submit here

Prototypes at aflow.org/CrystalDatabase/. What are the space group number and

**Enter**

**when ready**

Pearson symbol for this material?

**POSCAR here**

• Use AFLOW-SYM to determine the symmetry proper8es of the structures that you generated for the prototype A\_hR1\_166\_a. How do the choice of parameters affect the symmetry of the structure?

**Select AFLOW-SYM here**

D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

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**Outline**

**AFLOW-CHULL: Convex Hull Phase Diagram**

• Ge#ng started with AFLOW:

• Decora8ng crystal prototypes to set up new calcula8ons

Convex hull phase diagram: forma8on enthalpy vs. concentra8on

• Symmetry analysis

• Thermodynamic and thermo-mechanical

• Convex hull phase diagrams

• AEL/AGL/APL: Elas8c constants and thermal proper8es

• AFLOW online data repositories

• AFLOW.org online web interface

• AFLOW REST-API

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*\Del B}}) = - (N*

• AFLUX Search-API

• AFLOW-ML + API

• AFLOW code:

• Installing AFLOW

• Data analysis with AFLOW

0 0

0 )

0 0.2 0.4 0.6 0.8 1 Co Ti ∆H(A

x

A

• Running AFLOW calcula8ons

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**AFLOW-CHULL: Convex Hull Phase Diagram**

Ternary convex hull phase diagrams:

23

m o t a / V e m

-100 -100

-200 -200

-10

( y p l a h t

-20

n e n o i t

-300 -300

-30

a m r o f

-400 -400

-40

-500 -500

0

0.2 0.4 0.6 0.8 1 -50

B

x

B

) = H(A

x

A

B

x

B

) - (x

A

H(A) + x

B

H(B))

<latexit sha1\_base64="bWDNN4Q+ifwfLsSm35Kp2ryOAU4="></latexit><latexit sha1\_base64="bWDNN4Q+ifwfLsSm35Kp2ryOAU4="></latexit><latexit sha1\_base64="bWDNN4Q+ifwfLsSm35Kp2ryOAU4="></latexit><latexit sha1\_base64="bWDNN4Q+ifwfLsSm35Kp2ryOAU4="></latexit> API keywords: enthalpy\_formation\_atom, energy\_cell, ... C. Oses et al., submided arXiv:1806.06901 (2018)

Interac8ve online applica8on: aflow.org/aflow-chull

C. Oses et al., submided arXiv:1806.06901 (2018)

**AFLOW-CHULL: Data cura@on**

0 0

0

0 0

0

) m o t a / V e m (

-500 -500

-25 -50

-150 -150

-16

y p l a h t n

-1,000 -1,000

-1,500 -1,500

outlier detec8on -75

-100

and -300 -300

removal

-32

e n o i

-125

-450 -450 -150

-48

t a m

-2,000 -2,000

-175

-600 -600 r o f

-200

-64

-225

-750 -750 -2,500 -2,500

0 0 0.2 0.2 0.4 0.4 0.6 0.6 0.8 0.8 1 1 Al Co

0 0 0.2 0.2 0.4 0.4 0.6 0.6 0.8 0.8 1 1 Al

Co 0 0

0 ) m o t a / V e m (

-225 -225

-450 -450

-24

Te3Zr1\_ICSD\_42076 Te3Zr1\_ICSD\_653211

y p l a h t n

-675 -675

structure match

-48

-72

Te3Zr1\_ICSD\_653232 Te3Zr1\_ICSD\_51004 e n o i t a m r o f

-1,125 -1,125 -900 -900

Te3Zr1\_ICSD\_71033

-96

Te3Zr1\_ICSD\_86763 Te3Zr1\_ICSD\_86764 0 0 0.2 0.2 0.4 0.4 0.6 0.6 0.8 0.8 1 1 Te Zr C. Oses et al., submided arXiv:1806.06901 (2018)

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*4*

**AFLOW-CHULL: Thermodynamic analyses**

decomposi8on reac8on stability criterion

0 0

0

0 0

0

*1.5 ~ }\_{3}*

) m o t a / V e m ( y lp a h t n e n o i t

-10 -10

-0.8

-10 -10

-0.8

-1.6

-1.6 -20 -20

-20 -20 -2.4

-2.4

-30 -30

-30 -30 -3.2

-3.2

*eV/atom}*

a m r o f

-40 -40

-4

-40 -40

-4

0 0

0.2 0.2 0.4 0.4 0.6 0.6 0.8 0.8 1 1 0 0 0.2 0.2 0.4 0.4 0.6 0.6 0.8 0.8 1 1 eV/atom}

Pd

Pt

Pd

Pt Pd

2

Pt

3

→ 1.5 PdPt + 0.5 PdPt

3

δ

sc

= 6 meV/atom

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f

= 3 meV/atom

<latexit sha1\_base64="xATScccNm2DbQtv7MOhKNKpmkw4=">AAACE3icbVBNSwMxEM36WetX1aOXYBEEoe6qoB6Eoh56rGCt0JaSTWc1NNldklmhLOt/8OJf8eJBxasXb/4b0w9BrQ8CL+/NMDPPj6Uw6LqfzsTk1PTMbG4uP7+wuLRcWFm9NFGiOdR4JCN95TMDUoRQQ4ESrmINTPkS6n73tO/Xb0EbEYUX2Iuhpdh1KALBGVqpXdhunoFERivttKkY3miVBllGj+ne3fdfweUOw0hl7ULRLbkD0HHijUiRjFBtFz6anYgnCkLkkhnT8NwYWynTKLiELN9MDMSMd9k1NCwNmQLTSgdHZXTTKh0aRNq+EOlA/dmRMmVMT/m2sr+o+ev1xf+8RoLBYSsVYZwghHw4KEgkxYj2E6IdoYGj7FnCuBZ2V8pvmGYcbY55G4L39+RxUtstHZW88/1i+WSURo6skw2yRTxyQMqkQqqkRji5J4/kmbw4D86T8+q8DUsnnFHPGvkF5/0LOcaeiA==</latexit><latexit sha1\_base64="xATScccNm2DbQtv7MOhKNKpmkw4=">AAACE3icbVBNSwMxEM36WetX1aOXYBEEoe6qoB6Eoh56rGCt0JaSTWc1NNldklmhLOt/8OJf8eJBxasXb/4b0w9BrQ8CL+/NMDPPj6Uw6LqfzsTk1PTMbG4uP7+wuLRcWFm9NFGiOdR4JCN95TMDUoRQQ4ESrmINTPkS6n73tO/Xb0EbEYUX2Iuhpdh1KALBGVqpXdhunoFERivttKkY3miVBllGj+ne3fdfweUOw0hl7ULRLbkD0HHijUiRjFBtFz6anYgnCkLkkhnT8NwYWynTKLiELN9MDMSMd9k1NCwNmQLTSgdHZXTTKh0aRNq+EOlA/dmRMmVMT/m2sr+o+ev1xf+8RoLBYSsVYZwghHw4KEgkxYj2E6IdoYGj7FnCuBZ2V8pvmGYcbY55G4L39+RxUtstHZW88/1i+WSURo6skw2yRTxyQMqkQqqkRji5J4/kmbw4D86T8+q8DUsnnFHPGvkF5/0LOcaeiA==</latexit><latexit sha1\_base64="xATScccNm2DbQtv7MOhKNKpmkw4=">AAACE3icbVBNSwMxEM36WetX1aOXYBEEoe6qoB6Eoh56rGCt0JaSTWc1NNldklmhLOt/8OJf8eJBxasXb/4b0w9BrQ8CL+/NMDPPj6Uw6LqfzsTk1PTMbG4uP7+wuLRcWFm9NFGiOdR4JCN95TMDUoRQQ4ESrmINTPkS6n73tO/Xb0EbEYUX2Iuhpdh1KALBGVqpXdhunoFERivttKkY3miVBllGj+ne3fdfweUOw0hl7ULRLbkD0HHijUiRjFBtFz6anYgnCkLkkhnT8NwYWynTKLiELN9MDMSMd9k1NCwNmQLTSgdHZXTTKh0aRNq+EOlA/dmRMmVMT/m2sr+o+ev1xf+8RoLBYSsVYZwghHw4KEgkxYj2E6IdoYGj7FnCuBZ2V8pvmGYcbY55G4L39+RxUtstHZW88/1i+WSURo6skw2yRTxyQMqkQqqkRji5J4/kmbw4D86T8+q8DUsnnFHPGvkF5/0LOcaeiA==</latexit><latexit sha1\_base64="xATScccNm2DbQtv7MOhKNKpmkw4=">AAACE3icbVBNSwMxEM36WetX1aOXYBEEoe6qoB6Eoh56rGCt0JaSTWc1NNldklmhLOt/8OJf8eJBxasXb/4b0w9BrQ8CL+/NMDPPj6Uw6LqfzsTk1PTMbG4uP7+wuLRcWFm9NFGiOdR4JCN95TMDUoRQQ4ESrmINTPkS6n73tO/Xb0EbEYUX2Iuhpdh1KALBGVqpXdhunoFERivttKkY3miVBllGj+ne3fdfweUOw0hl7ULRLbkD0HHijUiRjFBtFz6anYgnCkLkkhnT8NwYWynTKLiELN9MDMSMd9k1NCwNmQLTSgdHZXTTKh0aRNq+EOlA/dmRMmVMT/m2sr+o+ev1xf+8RoLBYSsVYZwghHw4KEgkxYj2E6IdoYGj7FnCuBZ2V8pvmGYcbY55G4L39+RxUtstHZW88/1i+WSURo6skw2yRTxyQMqkQqqkRji5J4/kmbw4D86T8+q8DUsnnFHPGvkF5/0LOcaeiA==</latexit>

C. Oses et al., submided arXiv:1806.06901 (2018)

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C. Oses et al., submided arXiv:1806.06901 (2018)

**AFLOW-CHULL: Convex Hull Phase Diagram**

C. Oses et al., submided arXiv:1806.06901 (2018)

**AFLOW-CHULL: Convex Hull Phase Diagram**

• Click “Download PDF”

**AFLOW-CHULL: Convex Hull Phase Diagram**

Go to aflow.org/aflow-chull and type/select AgAuCd

C. Oses et al., submided arXiv:1806.06901 (2018)

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**AFLOW-CHULL: Convex Hull Phase Diagram**

Click “Highlight Hull Points” and click on one

C. Oses et al., submided arXiv:1806.06901 (2018)

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**AFLOW-CHULL: Convex Hull Phase Diagram**

Click “Highlight Hull Points” and click on one

Exercises:

• What is the distance of Al

17

Co

12

from the hull?

• What is the stability criterion of Te

2

Zr?

• What is the energy of the CuZr hull at x = 0.5?

• What is the most stable structure on the MnPdPt hull?

C. Oses et al., submided arXiv:1806.06901 (2018)

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*5*

**AGL: AEL: Elas@c constants**

**Debye-Grüneisen model**

• Apply set of independent normal and shear strains

Different volume cells

E(V) data from DFT

Normal strain Shear strain

*..., , , ,...*

(VASP, QE, etc.)

-7 -7

E E (DFT) (DFT) Polynomial fit -8 -8

*B\_S*

Debye temperature: θ

D

(V)

) V e ( y g r e n E

-10 -10 -9 -9

-11 -11

• Use strain-stress data to calculate elas8c proper8es:

– 6x6 elas8c tensors – Bulk and shear modulus – Poisson ra8o

-12 -12

20 20 30 30 40 40 50 50 60 60 Grüneisen

Heat capacity:

Volume Volume (Å (Å

3 3

) ) parameter: γ

C

V

Fit with polynomial or eqn of state: bulk modulus, B(V) – Combine with AGL (Debye model) to get more accurate

Debye temperature and thermal conduc8vity

La#ce thermal conduc8vity, κ

L

C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017)

C. Toher et al., Phys. Rev. B 90, 174107 (2014); M. A. Blanco et al., Comp. Phys. Commun. 158, 57 (2004)

32

70

70 100 400 1000 2000

Θ

31

**AGL+AEL: Results**

Thermal Conduc8vity (300K)

2000

600

Zincblende/Diamond Rocksalt 1000

Wurzite Equality

Zincblende/Diamond Rocksalt Wurzite 100

Rhombohedral Tetragonal Miscellaneous Equality

0.3

1 2 10 100 1000 5000 κ

l

33

**APL: Phonon calcula@ons**

Debye temperature

AFLOW Phonon Library Interatomic force constants

} }

Φ

↵ ij

=

∂2V ∂r↵

i

∂r

j

400

10

tial

• Correla8on with experimental results is ~0.9

• Using AEL Poisson ra8o improves correla8on by ~5%

Perturb atom, obtain change in force on others

• AGL method suited for rapid screening of thermal proper8es

C. Toher et al., Phys. Rev. B 90, 174107 (2014); C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017) 34

*\om*

100

1

0.3 exp

(K)

Phonon dispersion

exp

(W/(m·K))

∆

F ~

*xp*

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

**AFLOW.org: Thermo-mechanical proper@es**

**Outline**

• AEL-AGL combined workflow has been run for > 5000 materials

• Ge#ng started with AFLOW:

• Decora8ng crystal prototypes to set up new calcula8ons

• Symmetry analysis

• Data is accessible online at aflow.org, via AFLOW REST-API and AFLUX search-API

• Thermodynamic and thermo-mechanical

• Convex hull phase diagrams

• AEL/AGL/APL: Elas8c constants and thermal proper8es

• Elas8c property keywords:

ael\_bulk\_modulus\_vrh, ael\_shear\_modulus\_vrh, ael\_poisson\_ratio, ...

• AFLOW online data repositories

• AFLOW.org online web interface

• AFLOW REST-API

• Thermal proper8es keywords:

agl\_debye, agl\_gruneisen,

• AFLUX Search-API

agl\_heat\_capacity\_Cv\_300K, agl\_thermal\_conductivity\_300K, agl\_thermal\_expansion\_300K, ...

• AFLOW-ML + API

• AFLOW code:

• Installing AFLOW

• Data analysis with AFLOW

• Running AFLOW calcula8ons C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017) 35

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*6*

**AFLOW.org: web portal**

**hIp://aflow.org**

**> 1.8 million entries**

**Advanced Search**

**Crystal Prototypes Machine- learning model**

**Convex AFLOW-online**

**hull (AFLOW-SYM)**

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

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**AFLOW.org: search page**

Exercises:

• Use the advanced search func8onality to find the band gap for SiC in the Selected

zincblende structure (space group number 216).

**Elements**

• Use the advanced search func8onality to find the bulk moduli for materials containing Ti in the AFLOW database. How many results are returned?

• Use the “Restrict Value” budon to limit the search to only entries for which the

**Check box to restrict**

bulk modulus has already been calculated for materials containing Ti. Open the entry page of the material with the highest bulk modulus. What is the la#ce type and space group of this material? Is it a metal or an insulator? search results to specific value range

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

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**AFLOW.org: database organiza@on**

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***aaa"***

**An#entry#in#detail:#mul/0layer#system#**

**AFLOW: REST-API**

**aflow.org**

**c)**

! ! aurl=aflowlib.duke.edu:AFLOWDATA/LIB3\_RAW/AgCoMn\_pv/T0002.A2BC! auid=aflow:AgCoMn\_pv/T0002.A2BC:PAW\_PBE! aapi=1.0!

lattice\_ lattice\_ lattice\_ keywords=aurl,auid,aflow\_api\_version,code,compound,prototype,nspecies,...!

lattice\_ aflowlib\_entry\_date=20140130\_20:34:00\_GMT-5!

**natoms=4 Ins>tute University Laboratory**

aflowlib\_entry\_version=30794! aflow\_version=aflow30293!

nbondxx= nspecies calculation\_cores=1!

Pearson\_ calculation\_memory=539!

Pearson\_ calculation\_time=18347.2!

position

**Project layer**

**ICSD LIB1 LIB2**

corresponding=Stefano\_Sanvito\_sanvitos@tcd.ie!

pp\_type= loop=thermodynamics,bands,magnetic!

pressure node\_CPU\_Cores=12!

prototyp node\_CPU\_MHz=2661!

PV=0! node\_CPU\_Model=Intel(R)\_Xeon(R)\_CPU\_X5650\_@\_2.67GHz!

PV\_atom=

**Set layer**

**CuNb CuV**

node\_RAM\_GB=24!

sg=F-43m code=vasp.4.6.35!

sg2=F-43 composition=2,1,1!

spacegro compound=Ag2Co1Mn1!

spacegro density=8.94193!

species= eentropy=0!

**species\_ entry i entry j**

eentropy\_atom=0!

species\_ Egap=0!

spin=5.1 energy=-20.4051!

spin\_ato energy\_atom=-5.10128!

spinD=0.

**Materials data**

enthalpy=-20.4051!

spinF=0. enthalpy\_atom=-5.10128!

stoichio enthalpy\_formation=1.51248!

type=met enthalpy\_formation\_atom=0.378121!

valence\_ R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

**42 LIB3**

**CuNbV**

**Calculation layer**

**AFLOW.org: search page**

**Number of species=2**

**Added filter for Egap: electronic band bap**

**hIp://aflow.org/advanced.php**

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**AFLOW.org: search page**

**Element group selec@on**

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

**hIp://aflow.org/advanced.php**

**Element selec@on**

**Property**

**Number of Filters**

**species**

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mandatory keywords

optional control keywords

optional materials keywords

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

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*7*

**AFLOW: REST-API**

• Full list of API keywords is available in the online REST-API

• The AFLOW REST-API AFLOW URL (AURL) has the form: documenta8on wiki:

<server>:AFLOWDATA/<project>/<set>/<entry>/?<keyword>

• For example, the AURL for the forma8on enthalpy per atom of the ternary Heusler structure T0001.A2BC with composi8on Cu

2

TiZn is:

aflowlib.duke.edu:AFLOWDATA/LIB3\_RAW/Cu\_pvTi\_svZn/T0001.A2BC/?enthalpy\_formation\_atom

Server Project

Set Layer Entry Keyword Layer

• The URL for the forma8on enthalpy per atom of the ternary Heusler structure T0001.A2BC with composi8on Cu

2

TiZn is:

aflowlib.duke.edu/AFLOWDATA/LIB3\_RAW/Cu\_pvTi\_svZn/T0001.A2BC/?enthalpy\_formation\_atom

• The full list of entries in the set Cu-Ti-Zn can be retrieved using:

aflowlib.duke.edu/AFLOWDATA/LIB3\_RAW/Cu\_pvTi\_svZn/?aflowlib\_entries

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014) 44 AFLOW: REST-API

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

**45 AFLOW: REST-API**

• Example python script to access API & download space groups (see

Exercises: AFLOW\_REST\_API\_example.py):

• Use the AFLOW REST-API to download the forma8on enthalpies for all of the

#!/usr/bin/env python

entries in the ternary alloy system AlNiTi (AlNi\_pvTi\_sv). import json, sys, os from urllib import urlopen

• Use the AFLOW REST-API to download the full list of binary alloy systems that are SERVER="http://aflowlib.duke.edu/AFLOWDATA"

available in the LIB2 project. How many alloys systems are available for download? PROJECT="/LIB3\_RAW" SET="/Cu\_pvTi\_svZn" ENTRIES="/?aflowlib\_entries"

• Use the AFLOW REST-API to download the stoichiometries and space groups for all

response=urlopen( SERVER+PROJECT+SET+ENTRIES ).read() response=response.rstrip()

Project: Ternary alloys

Set: CuTiZn alloy system

Keyword: List of entries in this alloy system

of the entries in an alloy system of your choice. How many entries are present in this system?

entry\_list=response.split(",") print(entry\_list)

Download list of entries with urlopen

for i in xrange(len(entry\_list)):

entry=str(entry\_list[i])

Loop through list of entries

URLentry\_sg=SERVER+PROJECT+SET+"/"+entry+"/?spacegroup\_relax" print(URLentry\_sg) response=urlopen( URLentry\_sg ).read() print(response)

Download space group for each entry

R. H. Taylor et al., Comput. Mater. Sci. 93, 178-192 (2014)

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**AFLUX: AFLOW Search-API**

• Aim: Programa8cally expose the same func8onality as our web search interface at hdp://aflow.org/advanced.php

**LUX syntax**

<block> “(” and “)”

<AND> “,” aaa"

<OR> “:”

**An#entry#in#detail:#mul/0layer#system# c)**

! ! aurl=aflowlib.duke.edu:AFLOWDATA/LIB3\_RAW/AgCoMn\_pv/T0002.A2BC!

<NOT> “!”

lattice\_sy auid=aflow:AgCoMn\_pv/T0002.A2BC:PAW\_PBE!

lattice\_sy aapi=1.0!

lattice\_va keywords=aurl,auid,aflow\_api\_version,code,compound,prototype,nspecies,...!

lattice\_va

<loose> “\*” aflowlib\_entry\_date=20140130\_20:34:00\_GMT-5!

natoms=4! aflowlib\_entry\_version=30794!

nbondxx=1. aflow\_version=aflow30293!

nspecies=3 calculation\_cores=1!

Pearson\_sy calculation\_memory=539!

Pearson\_sy calculation\_time=18347.2!

positions=

<string> “’”

corresponding=Stefano\_Sanvito\_sanvitos@tcd.ie!

pp\_type=PA loop=thermodynamics,bands,magnetic!

pressure=0 node\_CPU\_Cores=12!

prototype= node\_CPU\_MHz=2661!

PV=0! node\_CPU\_Model=Intel(R)\_Xeon(R)\_CPU\_X5650\_@\_2.67GHz!

PV\_atom=0!

<mute> “$” node\_RAM\_GB=24!

sg=F-43m#2 code=vasp.4.6.35!

sg2=F-43m# composition=2,1,1!

spacegroup compound=Ag2Co1Mn1!

spacegroup density=8.94193!

species=Ag eentropy=0!

species\_pp eentropy\_atom=0!

species\_pp Egap=0!

spin=5.176 energy=-20.4051!

spin\_atom= energy\_atom=-5.10128!

spinD=0.03 enthalpy=-20.4051!

spinF=0.61 enthalpy\_atom=-5.10128!

stoichiome enthalpy\_formation=1.51248!

type=metal enthalpy\_formation\_atom=0.378121!

valence\_iu entropic\_temperature=-4220.27!

valence\_st

F. Rose et al., Comput. Mater. Sci. 137, 362 (2017).

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**AFLOW.org: web portal**

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mandatory keywords

optional control keywords

optional materials keywords

no references

**Matchbook:**

Matchbook

::= Unary-Not? ( Unary-Mute? Datum-string '(' Match ')' | '(' Matchbook ')' )

| Matchbook Binal Matchbook

referenced by:

Matchbook Summons-­Lucifer

**Match:**

Match ::= Unary-Not? ( Unary-Loose? ( Datum-string | Datum-number ) Unary-Loose? | '(' Match ')' )

| Match Binal Match

referenced by:

Match Matchbook

**Directive:**

**Logical operator**

Directive

::= ( Binal Unary-Mute? Datum-string '(' ( Datum-string | Datum-number ) ( Binal ( Datum-string | Datum-number ) )\* ')' )\*

referenced by:

**Keywords lists**

**AFLUX: AFLOW Search-API**

• AFLUX enables search func8onality through query part of URI

• Supports use of several logical operators

• Operator scope can be inter-property and/or intra-property

Logical operator AFLUX syntax Operator scope <block> “(” and “)” Intra- and inter-property <AND> “,” Intra- and inter-property <OR> “:” Intra- and inter-property <NOT> “!” Intra-property <loose> “\*” Intra-property <string> “’” Inter-property <mute> “$” Intra-property

48 F. Rose et al., Comput. Mater. Sci. 137, 362 (2017).

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**AFLUX: AFLOW Search-API**

49 hdp://aflowlib.duke.edu/search/API/?<matchbook>,<direc8ves>

• Example python script to access AFLUX search-API (see AFLUX\_example.py):

Search API Server Query

#!/usr/bin/env python import json, sys, os from urllib import urlopen

AFLUX Server

• Matchbook:

• Materials keywords with arguments

SERVER="http://aflowlib.duke.edu" API="/search/API/?"

Matchbook: materials keywords

• Example: <server>/?species((Na:K),Cl),nspecies(2),Egap(1\*,\*5),energy\_cell

• Keyword list available from schema direc8ve: <server>/?schema

Directive: return all entries satisfying query

JSON with query results is downloaded

F. Rose et al., Comput. Mater. Sci. 137, 362 (2017).

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MATCHBOOK="species((Na:K),Cl),nspecies(2),Egap(2\*,\*5),energy\_cell" DIRECTIVES="$paging(0)" SUMMONS=MATCHBOOK+","+DIRECTIVES

• Direc8ves:

• Forma#ng instruc8ons with arguments

• “format” takes arguments “json” and “html”

response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8")) for datum in response:

bandgap=[float(x) for x in datum['Egap'].split(",")] energycell=[float(x) for x in datum['energy\_cell'].split(",")]

• “catalog” takes arguments “icsd”, “lib1”, “lib2”, ...

print ("{}, {}, {}".format( datum['auid'], bandgap, energycell))

• “paging” controls number of entries and page displayed, sorted in ascending order of first materials keyword – order can be reversed by using a nega8ve page number in the argument

F. Rose et al., Comput. Mater. Sci. 137, 362 (2017).

**AFLUX: AFLOW Search-API**

**Outline**

Exercises:

• Ge#ng started with AFLOW:

• Decora8ng crystal prototypes to set up new calcula8ons

• Use AFLUX to retrieve the forma8on enthalpies for all of the entries in a ternary

• Symmetry analysis alloy system of your choice.

• Thermodynamic and thermo-mechanical

• Use AFLUX to retrieve the space group numbers of all materials that contain Cu and Ti but not V (the logical NOT operator is denoted by the exclama8on mark “!”).

• Convex hull phase diagrams

• AEL/AGL/APL: Elas8c constants and thermal proper8es

• Use AFLUX to retrieve the band gaps of all of the materials that have a calculated bulk modulus between 200GPa and 300GPa.

• AFLOW online data repositories

• AFLOW.org online web interface

• AFLOW REST-API

• AFLUX Search-API

• Use AFLUX to retrieve the materials in the ICSD catalog that contain the element Sn but not Pb, and that have a band gap between 1 and 3eV. How many such

• AFLOW-ML + API materials are available?

• AFLOW code:

• Installing AFLOW

• Data analysis with AFLOW

• Running AFLOW calcula8ons F. Rose et al., Comput. Mater. Sci. 137, 362 (2017). 52

**AFLOW Machine Learning**

**AFLOW Machine Learning**

• AFLOW data for > 26,674 materials on AFLOW.org used to train gradient boos8ng decision trees machine-learning model

• Connected atoms form structure fragments descriptors

• Predic8ons proper8es

b Voronoi based neighbors tessella/on on search

structural and

morphology c

infinite periodic and graph

elemental construc/on and property labeling

**d**

decomposi/on to fragments

O. Isayev et al., Nat. Commun. 8, 15679 (2017).

53

**d**

re

• Atomic nodes in structure fragments are decorated with elemental proper8es to form Property-Labeled Materials Fragments (PLMF)

• Voronoi tessella8on used to determine atomic connec8vity

• Proper8es used include number of valence electrons, ioniza8on

• Atoms which share a Voronoi cell face are connected to form a graph

poten8al, electron affinity, electronega8vity, covalent radii, etc.

O. Isayev et al., Nat. Commun. 8, 15679 (2017).

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decomposi/on to fragments

edges (bonds) nodes (atoms)

path fragments of length l, l = 2, 3, ...

**AFLUX: AFLOW Search-API**

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circular fragments (polyhedrons)

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*9*

**AFLOW.org: web portal**

**hIp://aflow.org**

**Machine- learning model**

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

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**AFLOW Machine Learning**

• Model predicts electronic and thermo-mechanical proper8es

4

regression models

FIG. 2. Outline of the modeling work-flow. ML models are represented by orange diamonds. Target properties predicted

• Model predicts electronic band gap for non-metals

O. Isayev et al., Nat. Commun. 8, 15679 (2017).

**AFLOW AFLOW Machine Learning**

**Machine Learning**

• Par8al dependence on elemental proper8es can be used to

• Par8al dependence of proper8es on descriptors: formulate design rules for new materials

• Good agreement of predic8ons with both DFT and experiment

**a b c**

Par8al dependence: metal vs. insulator

B,G : r2 = 0.99;θ

D Par8al dependence: Band gap vs. ioniza8on poten8al

: r2 = 0.97 O. Isayev et al., Nat. Commun. 8, 15679 (2017). O. Isayev et al., Nat. Commun. 8, 15679 (2017).

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**Electronic Proper1es Thermo-Mechanical Proper1es**

no E

BG

metal or insulator?

1E

BG

classifica4on model

∈ R :

regression E

BG

> 0l

model

band gap energy predic4on

yes

no

**crystal structure**

bulk modulus (VRH) predic4on

1X ∈ Rl

**AFLOW Machine Learning**

• ML model trained on 26674 unique GGA+U band structures from AFLOW.org to predict metal vs. insulator and electronic band gap

ML predic8on vs. DFT+U calcula8on

Sta8s8cs for 5-fold cross- valida8on for electronic band gap:

• RMSE: 0.51eV

• MAE: 0.35eV

• r2: 0.90

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O. Isayev et al., Nat. Commun. 8, 15679 (2017).

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**AFLOW-ML Online**

• Models are available online at aflow.org/aflow-ml

O. Isayev et al., Nat. Commun. 8, 15679 (2017), E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

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**AFLOW-ML API**

• Models are now programma8cally accessible via AFLOW-ML API

E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

**AFLOW-ML API**

• Post POSCAR (for VASP version 5) to API using e.g. cURL:

Mg1O1 [FCC,FCC,cF8] (STD\_PRIM doi:10.1016/j.commatsci.2010.05.010)

POST

Endpoint <model>/prediction POSCAR

**Response**

1.224745

0.00000000000000 1.73622980869126 1.73622980869126 task object (which includes {id})

1.73622980869126 0.00000000000000 1.73622980869126 1.73622980869126 1.73622980869126 0.00000000000000 Mg O 1 1 T E G

Direct(2) [A1B1]

0.00000000000000 0.00000000000000 0.00000000000000 Mg 0.50000000000000 0.50000000000000 0.50000000000000 O

Prediction

**yes**

status =

Endpoint /prediction/result/{id}

> curl http://aflow.org/API/aflow-ml/v1.0/plmf/prediction

"SUCCESS"

**Response**

status or prediction object

--data-urlencode file@POSCAR

• Receive JSON file with task ID:

{

"id": "531c2817-ee51-4a23-be61-6e8ca6f31aec", no

"model": "plmf", "results\_endpoint": "/prediction/result/531c2817-ee51-4a23-be61-6e8ca6f31aec" }

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E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

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**AFLOW-ML API**

• Use task ID to query endpoint to retrieve results:

E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

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**AFLOW-ML API**

• Example python script to access AFLOW-ML API (part 1 of AFLOW-

> curl http://aflow.org/API/aflow-ml/v1.0/prediction/result/531c2817-ee51-4a23-be61-6e8ca6f31aec

ML\_example.py): #!/usr/bin/env python

• Receive JSON file with results:

import json, sys, os from urllib import urlopen

{

"citation": "10.1038/ncomms15679",

from urllib import urlencode import urllib2 "description": "The job has completed.",

from time import sleep "ml\_ael\_bulk\_modulus\_vrh": 144.522, "ml\_ael\_shear\_modulus\_vrh": 104.453, "ml\_agl\_debye": 777.163, "ml\_agl\_heat\_capacity\_Cp\_300K": 4.33, "ml\_agl\_heat\_capacity\_Cp\_300K\_per\_atom": 2.194,

SERVER="http://aflow.org" API="/API/aflow-ml/v1.0" MODEL="plmf"

"ml\_agl\_heat\_capacity\_Cv\_300K": 4.178, "ml\_agl\_heat\_capacity\_Cv\_300K\_per\_atom": 2.139,

poscar=open('POSCAR', 'r').read() "ml\_agl\_thermal\_conductivity\_300K": 3.509,

encoded\_data = urlencode({'file': poscar,}) "ml\_agl\_thermal\_expansion\_300K": 6.18e-05, "ml\_egap": 3.375, "ml\_egap\_type": "Insulator", "ml\_energy\_per\_atom": -5.742, "model": "plmf", "status": "SUCCESS" }

AFLOW-ML API server

PLMF model

Read and encode POSCAR structure file

url = SERVER + API + "/" + MODEL + "/prediction" request\_task = urllib2.Request(url, encoded\_data)

Post POSCAR to ML API server

task = urllib2.urlopen(request\_task).read() task\_json = json.loads(task)

Extract results results\_endpoint = task\_json["results\_endpoint"]

endpoint from results\_url = SERVER + API + results\_endpoint

returned task

E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

object

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**AFLOW-ML API**

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**AFLOW-ML API**

• Example python script to access AFLOW-ML API (part 2 of AFLOW- ML\_example.py):

incomplete = True while incomplete:

request\_results = urllib2.Request(results\_url) results = urllib2.urlopen(request\_results).read()

Query results endpoint until results are retrieved

• AFLOW-ML API Python client can be downloaded from:

hdp://aflow.org/src/aflow-ml/

results\_json = json.loads(results) if results\_json["status"] == 'PENDING':

sleep(10) continue elif results\_json["status"] == ’STARTED':

sleep(10)

If prediction is incomplete, wait and requery endpoint

continue elif results\_json["status"] == 'FAILURE':

print("Error: prediction failure") incomplete = False elif results\_json["status"] == 'SUCCESS':

Print error message for prediction failure

print("Successful prediction") print(results\_json)

Print results for incomplete = False

successful prediction

E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

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E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

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**AFLOW: Installa@on**

• Install AFLOW (perform with every new version)

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

**AFLOW-ML API**

• AFLOW-ML API Python client can be installed using “setup.py” script

Exercises: included in client

• Convert the POSCAR files, generated previously using the AFLOW prototype

python setup.py install

modules, to the format used by version 5 of VASP by adding the addi8onal line with the element symbols. Upload the POSCARs to the aflow.org/aflow-ml page, and generate predic8ons. Are these materials predicted to be metals or

• AFLOW-ML API Python client can be run using a script of this form:

insulators?

from AFLOWml.client import AFLOWmlAPI

• Use the AFLOW-ML API to obtain predic8ons for both the plmf and mfd models for from pprint import pprint

these structures, and retrieve the results in JSON format. For the structures generated using the prototype A\_hR1\_166\_a, how does the value of c/a affect the

with open('test.poscar', 'r') as input\_file:

ml = AFLOWmlAPI()

elas8c moduli and electronic band gap? What proper8es can you obtain using the mfd model? data = ml.get\_prediction(input\_file.read(), 'plmf') pprint(data)

E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018). E. Gossed et al., Comput. Mater. Sci. 152, 134-145 (2018).

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**Outline**

**AFLOW: Installa@on**

• Ge#ng started with AFLOW:

• Decora8ng crystal prototypes to set up new calcula8ons

• AFLOW can be installed using the xaflow script.

• Symmetry analysis

• Install xaflow (perform once)

• Thermodynamic and thermo-mechanical

• Convex hull phase diagrams

• AEL/AGL/APL: Elas8c constants and thermal proper8es

• AFLOW online data repositories

• AFLOW.org online web interface

• AFLOW REST-API

• AFLUX Search-API

• AFLOW-ML + API

• AFLOW code:

• Installing AFLOW

• Data analysis with AFLOW

• Running AFLOW calcula8ons

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

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**AFLOW: Configura@on**

• AFLOW can be configured with the .aflow.rc file

1. Run xaflow

xaflow - xaflow compiles AFLOW in ~/src/AFLOW by default - To change the compila8on directory, run

xaflow AWD=/home/src/AFLOW 2. Install the newly compiled executable to your path

xaflow install

- xaflow installs AFLOW to ~/bin by default - To change the compila8on directory, run

xaflow install ULB=/usr/local/bin 3. Run aflow

aflow

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

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**AFLOW-ML API**

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1. Download xaflow

wget materials.duke.edu/AFLOW/xaflow

2. Move/copy xaflow somewhere in your path

mkdir ~/bin export PATH=~/bin:$PATH mv xaflow ~/bin/xaflow

3. Ensure the file can be executed

chmod 555 ~/bin/xaflow

4. Check that xaflow is in your path

which xaflow

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• Machine se#ngs

– MPI op8ons 1. Dow

wge 2. Mov

– Binary paths – Database paths

mv 3. Ensu chm 4. Chec whi - A ret 5. Run

xafl - xaflo

• AFLOW se#ngs $(HO

– Output file names - The c

xafl

– Graphic se#ngs (Gnuplot, LaTeX)

6. Insta

xafl - By de - The i xafl

• VASP specific se#ngs

– POTCAR paths (pseudo poten8als files) – Precision defaults (k-points scheme, minimiza8on algorithm, energy cutoff, etc.) – Run se#ng defaults (spin-polarized calcula8on, symmetry determina8on, etc.)

aflow --readme=aflowrc

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1. Dow

wge 2. Mov

mv 3. Ensu chm 4. Chec whi - A ret 5. Run

xafl - xaflo $(HO - The c

xafl 6. Insta xafl - By de - The i xafl

1. Dow

wge 2. Mov

mv 3. Ensu chm 4. Chec whi - A ret 5. Run

xafl - xaflo $(HO - The c

xafl 6. Insta xafl - By de - The i xafl

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**AFLOW: Crystallographic Prototypes**

• Decorate rock-salt prototype AB\_cF8\_225\_a\_b with MgO:

aflow --proto=AB\_cF8\_225\_a\_b:Mg:O --params=3.5

AB\_cF8\_225\_a\_b params=3.5 SG#=225 [ANRL doi: arXiv:1607.02532] 1.000000

0.00000000000000 1.75000000000000 1.75000000000000 1.75000000000000 0.00000000000000 1.75000000000000 1.75000000000000 1.75000000000000 0.00000000000000 1 1 Direct(2) [A1B1]

0.00000000000000 0.00000000000000 0.00000000000000 Mg 0.50000000000000 0.50000000000000 0.50000000000000 O

• Use Heusler prototype T0001.A2BC to create aflow.in file for Cu

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**AFLOW: High throughput aflow.in’s**

• 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

• Pre-defined sets

aflow --aflow\_proto=T0001.A2BC:LIB3:LIB3:LIB3

TiZn:

• Full prototype lis8ngs

aflow --aflow\_proto=T0001.A2BC:Cu:Ti:Zn

AFLOW Standard

AFLOW Crystallographic Library

aflow --protos

http://aflow.org/CrystalDatabase

• Variety of possible ab-inifio formats by adding op8ons:

VASP

FHI-AIMS

Quantum Espresso

ABINIT

Have fun! --vasp

--aims

--qe

--abinit

M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018)

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

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**AFLOW: Crystallographic Prototypes**

**AFLOW-SYM**

Exercises:

• Point, factor, site-symmetry, and space group opera8ons are calculated via:

• Use the aflow --proto command with the appropriate op8ons as described on the

aflow --aflowSYM < POSCAR online prototype page to generate a POSCAR for the same structure used in the previous exercise, decorated with elements of your choice.

• Tolerance values and output format can be set using the op8ons:

aflow --aflowSYM=0.0001 --print=json < POSCAR

• Generate structures for the prototype A\_hR1\_166\_a using an element and value of

• Space-group symmetry informa8on (number/symbol, Wyckoff posi8ons, cell a of your choice, with c/a values of 0.5, 0.612, 1.0, 1.225, 1.5, 2.45, and 3.0. Save

se#ng, etc.) consistent with ITC conven8ons: these structures with appropriate names, as they will be used as part of a later

aflow --sgdata=0.0001 --print=json < POSCAR exercise.

• Extended crystallographic data (crystal, la#ce, superla#ce, symmetry descrip8ons) can be extracted using:

aflow --edata=0.0001 --print=json < POSCAR

• Other standalone symmetry commands: Space-group number/symbol

Pearson symbol aflow --aflowSG < POSCAR

aflow --pearson < POSCAR

Wyckoff positions (POSCAR format)

Standard primitive cell aflow --wyccar < POSCAR

aflow --sprim < POSCAR M. J. Mehl et al., Comput. Mater. Sci. 136, S1-S828 (2017); D. Hicks et al., submided (2018) 75

D. Hicks et al., Acta Cryst. A74, 184-203 (2018)

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**AFLOW-CHULL: Convex Hull Phase Diagram**

• Output format can be specified as usual

• Directly query a structure’s stability criterion

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**AFLOW: aflow.in file**

• The aflow.in file:

aflow --chull --alloy=MnPd --print=json,txt,pdf

[AFLOW] [AFLOW]SYSTEM=Cu\_pvTi\_svZn.T0001.A2BC

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

System name

• Directly query a structure’s distance from the hull

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [AFLOW] input file for aflow [AFLOW\_MODE=VASP] [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* aflow --chull --alloy=MnPd --d2h=aflow:9001c322296fc162

[AFLOW\_MODE\_ZIP=xz] [AFLOW\_MODE\_BINARY=vasp46s] [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* #[AFLOW\_MODE\_MPI] [AFLOW\_MODE\_MPI\_MODE]NCPUS=MAX

aflow --chull --alloy=MnPd --sc=aflow:4fc97e549ca17d4e

[AFLOW\_MODE\_MPI\_MODE]COMMAND ="mpirun -np" [AFLOW\_MODE\_MPI\_MODE]AUTOTUNE [AFLOW\_MODE\_MPI\_MODE]BINARY="mpivasp46s"

• Directly query the energy of the hull at a par8cular stoichiometry

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [AFLOW\_SYMMETRY]CALC #[AFLOW\_SYMMETRY]SGROUP\_WRITE #[AFLOW\_SYMMETRY]SGROUP\_RADIUS=7.77 aflow --chull --alloy=MnPd --hull\_energy=0.25

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* #[AFLOW\_NEIGHBOURS]CALC [AFLOW\_NEIGHBOURS]RADIUS=7.7

• High throughput inputs

[AFLOW\_NEIGHBOURS]DRADIUS=0.1 [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* #[AFLOW\_APL]CALC // README\_AFLOW\_APL.TXT aflow --chull --alloy=MnPt,PdPt

[AFLOW\_APL]ENGINE=DM // README\_AFLOW\_APL.TXT [AFLOW\_APL]DMAG=0.015 // README\_AFLOW\_APL.TXT [AFLOW\_APL]MINATOMS=100 // README\_AFLOW\_APL.TXT aflow --chull --alloy=Mn,Pd:Pt

#[AFLOW\_APL]SUPERCELL=3x3x3 // README\_AFLOW\_APL.TXT [AFLOW\_APL]DC=y // README\_AFLOW\_APL.TXT [AFLOW\_APL]DPM=y // README\_AFLOW\_APL.TXT aflow --chull --alloy=LIB2:LIB2

[AFLOW\_APL]ZEROSTATE=y // README\_AFLOW\_APL.TXT [AFLOW\_APL]DOS=y // README\_AFLOW\_APL.TXT [AFLOW\_APL]TP=y // README\_AFLOW\_APL.TXT C. Oses et al., submided arXiv:1806.06901 (2018)

[AFLOW\_APL]TPT=0:2000:10 // README\_AFLOW\_APL.TXT README for more op8ons/help

aflow --readme=chull

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**AFLOW: aflow.in file**

• The aflow.in file:

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [VASP\_RUN]RELAX\_STATIC\_BANDS=2 // GENERATE | STATIC | RELAX=N | RELAX\_STATIC=N | STATIC\_BANDS | RELAX\_STATIC\_BANDS=N | REPEAT\_BANDS [,DS[,DD[,DSCF]]] [VASP\_FORCE\_OPTION]NEGLECT\_NOMIX #[VASP\_FORCE\_OPTION]KPOINTS=keyword[,keyword] // EVEN | ODD | KSHIFT\_GAMMA\_EVEN | KSHIFT\_GAMMA\_ODD | KSCHEME\_MONKHORST\_PACK | KSCHEME\_GAMMA | GAMMA | KEEPK | IBZKPT [VASP\_FORCE\_OPTION]SYM=ON // ON | OFF (default ON) [VASP\_FORCE\_OPTION]AUTO\_PSEUDOPOTENTIALS=potpaw\_PBE // pot\_LDA | pot\_GGA | potpaw\_LDA | potpaw\_GGA | potpaw\_PBE | potpaw\_LDA\_KIN | potpaw\_PBE\_KIN [VASP\_FORCE\_OPTION]NBANDS // Estimate Bands (better than VASP) #[VASP\_FORCE\_OPTION]PSTRESS=0.0 // Pressure in kBar (1kB=0.1GPa) #[VASP\_FORCE\_OPTION]EDIFFG=-0.001 // EDIFFG for relaxed forces #[VASP\_FORCE\_OPTION]ENMAX\_MULTIPLY=1.4 // Multiplication of the max(pseudopotential\_cutoffs) #[VASP\_FORCE\_OPTION]POTIM=0.5 // ionic time-step [VASP\_FORCE\_OPTION]SPIN=ON // (ON | OFF (default ON)), REMOVE\_RELAX\_1 | \_2 #[VASP\_FORCE\_OPTION]AUTO\_MAGMOM=ON // ON | OFF (default OFF) [VASP\_FORCE\_OPTION]RELAX\_MODE=ENERGY // (ENERGY | FORCES | ENERGY\_FORCES | FORCES\_ENERGY) (default: DEFAULT\_VASP\_FORCE\_OPTION\_RELAX\_MODE\_SCHEME in .aflow.rc) [VASP\_FORCE\_OPTION]PREC=ACCURATE // (LOW | MEDIUM | NORMAL | HIGH | ACCURATE), PRESERVED (default: DEFAULT\_VASP\_FORCE\_OPTION\_PREC\_SCHEME in .aflow.rc) [VASP\_FORCE\_OPTION]ALGO=FAST // (NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED (default: DEFAULT\_VASP\_FORCE\_OPTION\_ALGO\_SCHEME in .aflow.rc) #[VASP\_FORCE\_OPTION]METAGGA=NONE // (TPSS | RTPSS | M06L | MBJL | SCAN | MS0 | MS1 | MS2 | NONE) (default: DEFAULT\_VASP\_FORCE\_OPTION\_METAGGA\_SCHEME in .aflow.rc) #[VASP\_FORCE\_OPTION]IVDW=0 // (number\_for\_VASP\_see\_manual\_for\_IVDW | 0) (default: DEFAULT\_VASP\_FORCE\_OPTION\_IVDW\_SCHEME in .aflow.rc) [VASP\_FORCE\_OPTION]RELAX\_ALL #[VASP\_FORCE\_OPTION]NOTUNE [VASP\_FORCE\_OPTION]TYPE=DEFAULT // (METAL | INSULATOR | SEMICONDUCTOR | DEFAULT) (default DEFAULT) [VASP\_FORCE\_OPTION]CONVERT\_UNIT\_CELL=SPRIM,MINK // (SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART, FRAC, PRES) #[VASP\_FORCE\_OPTION]VOLUME+=10.0 [VASP\_FORCE\_OPTION]VOLUME\*=1.05 [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

**AFLOW: aflow.in file**

• The aflow.in file:

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [VASP\_INCAR\_MODE\_EXPLICIT]START

Calculation type

SYSTEM=Cu\_pvTi\_svZn.T0001.A2BC #PSTRESS=000 # Pressure in kBar (1kB=0.1GPa) # for hand modification #EDIFFG=-0.001 # For relaxed forces # for hand modification #POTIM=-0.001 # default # for hand modification

Explicit INCAR #NBANDS=XX #IALGO=48 # for hand modification # for hand modification

additions

[VASP\_INCAR\_MODE\_EXPLICIT]STOP

Exchange- correlation functional

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [VASP\_KPOINTS\_MODE\_IMPLICIT] [VASP\_KPOINTS\_FILE]KSCHEME=M [VASP\_KPOINTS\_FILE]KPPRA=6000 [VASP\_KPOINTS\_FILE]STATIC\_KSCHEME=M [VASP\_KPOINTS\_FILE]STATIC\_KPPRA=10000

k-point grid settings [VASP\_KPOINTS\_FILE]BANDS\_LATTICE=AUTO Relaxation mode

[VASP\_KPOINTS\_FILE]BANDS\_GRID=20 [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Basis cut-off

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**AFLOW: aflow.in file**

• The aflow.in file:

[AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [VASP\_POSCAR\_MODE\_EXPLICIT]START Cu\_pvTi\_svZn/T0001.A2BC - (T0001.A2BC) - AlCu2Mn [A2BC] (T0001.A2BC) & Fm(-3)m & #225 & cF16 & Navy HTQC Project (use of T0001.proto) -56.218000

0.00000000000000 1.00000000000000 1.00000000000000 1.00000000000000 0.00000000000000 1.00000000000000 1.00000000000000 1.00000000000000 0.00000000000000 2 1 1 Direct(4) [A2B1C1]

0.75000000000000 0.75000000000000 0.75000000000000 Cu\_pv 0.25000000000000 0.25000000000000 0.25000000000000 Cu\_pv 0.00000000000000 0.00000000000000 0.00000000000000 Ti\_sv 0.50000000000000 0.50000000000000 0.50000000000000 Zn [VASP\_POSCAR\_MODE\_EXPLICIT]STOP [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* [VASP\_POTCAR\_MODE\_IMPLICIT] [VASP\_POTCAR\_FILE]Cu [VASP\_POTCAR\_FILE]Ti [VASP\_POTCAR\_FILE]Zn [AFLOW] potpaw\_PBE: Cu\_pv Ti\_sv Zn [AFLOW] COMPOSITION\_PP=|Cu\_pv2|Ti\_sv1|Zn1| [AFLOW] COMPOSITION=|Cu2|Ti1|Zn1| [AFLOW] VOLUME(A^3)=|12.0159|17.1035|15.0827| [AFLOW] MASS(amu)=|63.546|47.9|65.38| [AFLOW] \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

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**Running AFLOW**

• VASP calcula8ons can be run through AFLOW using commands of this form:

• The AFLOW monitor op8on can be used to monitor jobs to prevent them consuming excessive resources and crashing the computer:

• A typical job submission script should contain something like the following:

aflow --run --force --D <run directory path>

POSCAR: VASP geometry

aflow --monitor input file

touch log.$PBS\_JOBID aflow --monitor >> log.$PBS\_JOBID &

POTCAR: VASP

aflow --run --force --D ./ >> log.$PBS\_JOBID pseudopotential • AFLOW creates a “LOCK” file in directories when it starts to run VASP,

preven8ng future AFLOW runs in that directory. To run, e.g., an APL (phonon) calcula8on in the same directory, change the name used for the LOCK file as follows:

aflow --use\_LOCK=apl.LOCK --multi --D <run directory path>

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**AEL: Elas@c constants**

**AEL: Elas@c constants**

• AFLOW-AEL is run by including the following line in the aflow.in:

Exercises:

[AFLOW\_AEL]CALC

• Add the appropriate line to run an AEL calcula8on to the aflow.in file created using

• The number and size of the normal and shear strains can be set using

the Heusler prototype in the previous exercise.

the following lines:

• Use the command aflow --run --generate\_aflowin\_only to create the subdirectories [AFLOW\_AEL]NNORMALSTRAINS=<number> [AFLOW\_AEL]NSHEARSTRAINS=<number> [AFLOW\_AEL]NORMALSTRAINSTEP=<number> [AFLOW\_AEL]SHEARSTRAINSTEP=<number>

aflow --multi --D <directory path>

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for this AEL calcula8on. (Note: this will not perform any DFT calcula8ons, which would require VASP to be installed on your computer and can be computa8onally expensive. To run DFT calcula8ons, leave out the op8on --generate\_aflowin\_only.

• Symmetry can be used to reduce the number of independent

Use the command aflow --mul8 --D ./ to run all subdirectories). How many subdirectories are created? direc8ons by including the following lines:

[AFLOW\_AEL]STRAINSYMMETRY=ON

• DFT calcula8ons can be run for the strained structures in all of the subdirectories using the following command:

• Copy the aflow.in file to a new directory, and add the op8on to switch on the use of symmetry to determine number of independent direc8ons. Re-run the command to generate the subdirectories. How many subdirectories are created now?

C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017) C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017)

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**AGL: Debye-Grüneisen model**

• AFLOW-AGL is run by including the following line in the aflow.in:

[AFLOW\_AGL]CALC

• The number and size of the isotropic strains applied to the structures can be set using the following lines:

[AFLOW\_AGL]NSTRUCTURES=<number> [AFLOW\_AGL]STRAINSTEP=<number>

• The value of the Poisson ra8o used to calculate the Debye temperature can be set using the following line:

[AFLOW\_AGL]POISSON=<number>

• DFT calcula8ons can be run for the strained structures using the following command:

C. Toher et al., Phys. Rev. B 90, 174107 (2014); C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017)

**AGL: Debye-Grüneisen model**

Exercises:

• Add the appropriate line to run an AGL calcula8on to the aflow.in file created using the Heusler prototype in the previous exercise.

• Use the command aflow --run --generate\_aflowin\_only to create the subdirectories for this calcula8on. (Note: this will not perform any DFT calcula8ons, which would require VASP to be installed on your computer and can be computa8onally expensive. To run DFT calcula8ons, leave out the op8on --generate\_aflowin\_only. Use the command aflow --mul8 --D ./ to run all subdirectories). How many subdirectories are created?

• AEL can be called to calculate the Poisson ra8o using the following line:

[AFLOW\_AGL]AELPOISSONRATIO=ON

• Copy the aflow.in file to a new directory, and add the op8on to use AEL to calculate the Poisson ra8o. Re-run the command to generate the subdirectories. What structures are created?

aflow --multi --D <directory path>

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C. Toher et al., Phys. Rev. B 90, 174107 (2014); C. Toher et al., Phys. Rev. Mater. 1, 015401 (2017)

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**APL: Phonon calcula@ons**

• AFLOW-APL is run by uncommen8ng the following line in the aflow.in:

[AFLOW\_APL]CALC

• Addi8onal parameters:

[AFLOW\_APL]ENGINE=DM [AFLOW\_APL]DMAG=0.015 [AFLOW\_APL]MINATOMS=100 #[AFLOW\_APL]SUPERCELL=3x3x3 [AFLOW\_APL]DC=y [AFLOW\_APL]DCUSERPATH=G-X|X-U|K-G|G-L [AFLOW\_APL]DPM=y [AFLOW\_APL]ZEROSTATE=y [AFLOW\_APL]POLAR=y [AFLOW\_APL]DOS=y [AFLOW\_APL]TP=y [AFLOW\_APL]TPT=0:2000:10 [AFLOW\_APL]KPPRA=2000

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**APL: Phonon calcula@ons**

• Followed by the usual run command

• Alterna8vely, a fresh aflow.in can be created with the line already uncommented aflow --run --LOCK=apl.LOCK

aflow --aflow\_proto=T0001.A2BC:Cu:Ti:Zn --module=apl

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• DFT calcula8ons can be run for the strained structures using the following command:

aflow --multi --D <directory path>

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

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**APL: Phonon calcula@ons**

**Conclusions**

Exercises:

• Add/uncomment the appropriate line to run an APL calcula8on to the aflow.in file created using the Heusler prototype in the previous exercise.

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• Automa8c materials design frameworks can generate large quan88es of materials data and combine mul8ple DFT calcula8ons to predict thermodynamic stability and thermo-mechanical proper8es

• Use the command aflow --run --generate\_aflowin\_only to create the subdirectories for this calcula8on. (Note: this will not perform any DFT calcula8ons, which would

• AFLOW data is accessible via aflow.org web portal, AFLOW REST-API, and AFLUX Search-API require VASP to be installed on your computer and can be computa8onally expensive. To run DFT calcula8ons, leave out the op8on --generate\_aflowin\_only. Use the command aflow --mul8 --D ./ to run all subdirectories). How many subdirectories are created? How many atoms do the supercells contain?

• Calculated AFLOW data for electronic and thermo-mechanical proper8es is being used to train machine-learning models to predict these quan88es, which are accessible by AFLOW-ML API

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