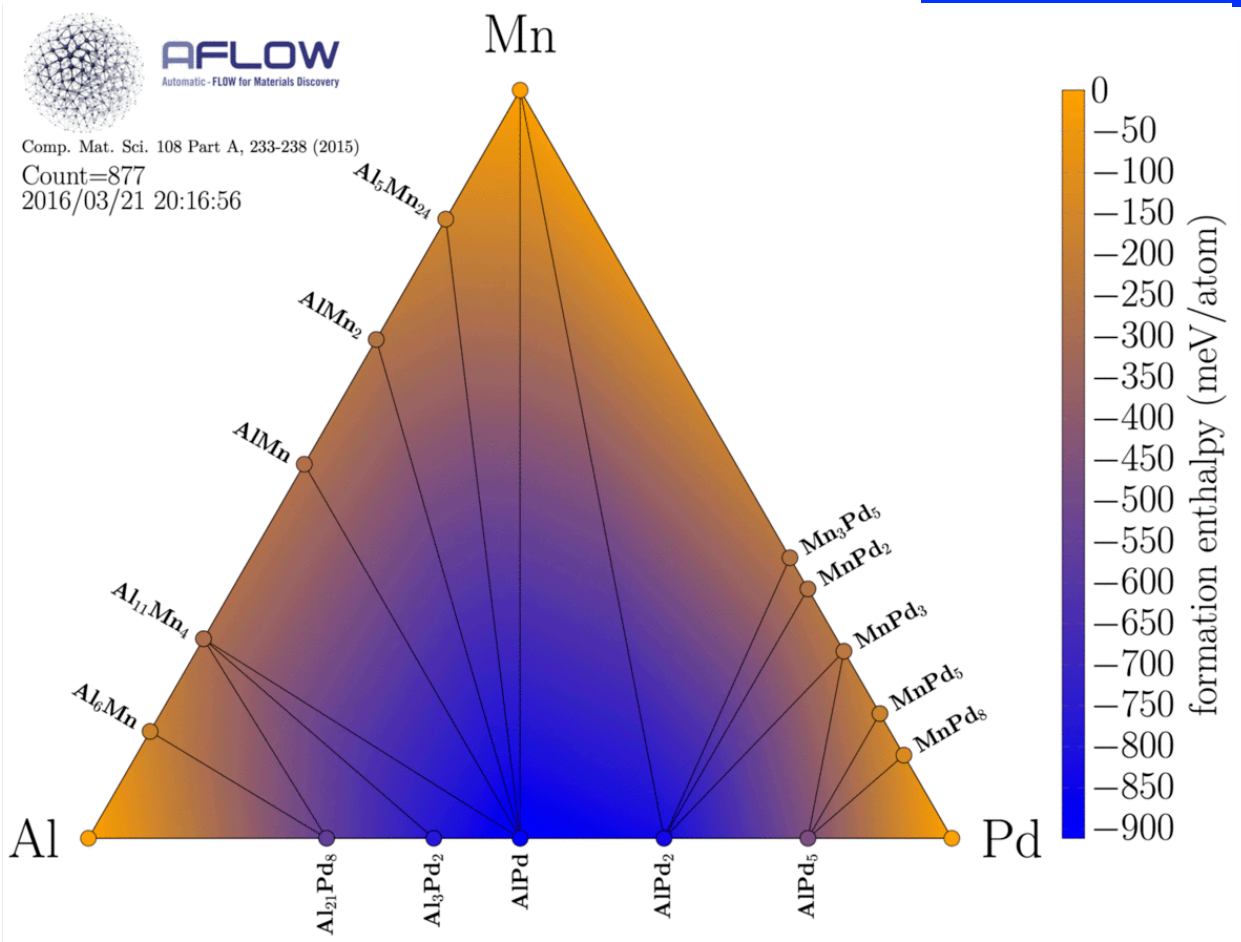
AFLOWLIB Data Repository

CORMAC TOHER
STEFANO CURTAROLO
Materials Science - Duke University
Frisco Rose, Eric Gossett, Harvey Shi, Ichiro Takeuchi, Alexey Kolmogorov, Kesong Yang, Gus Hart, Robert Hanson, Natalio Mingo, Arrigo Calzolari, Amir Natan, Stefano Sanvito, Marco Fornari, Marco Buongiorno Nardelli



AFLOW
Automatic - FLOW for Materials Discovery

Duke
UNIVERSITY

DEPARTMENT OF THE NAVY
USN
ONR
Science & Technology

CRAY

AFLOWLIB Web Portal

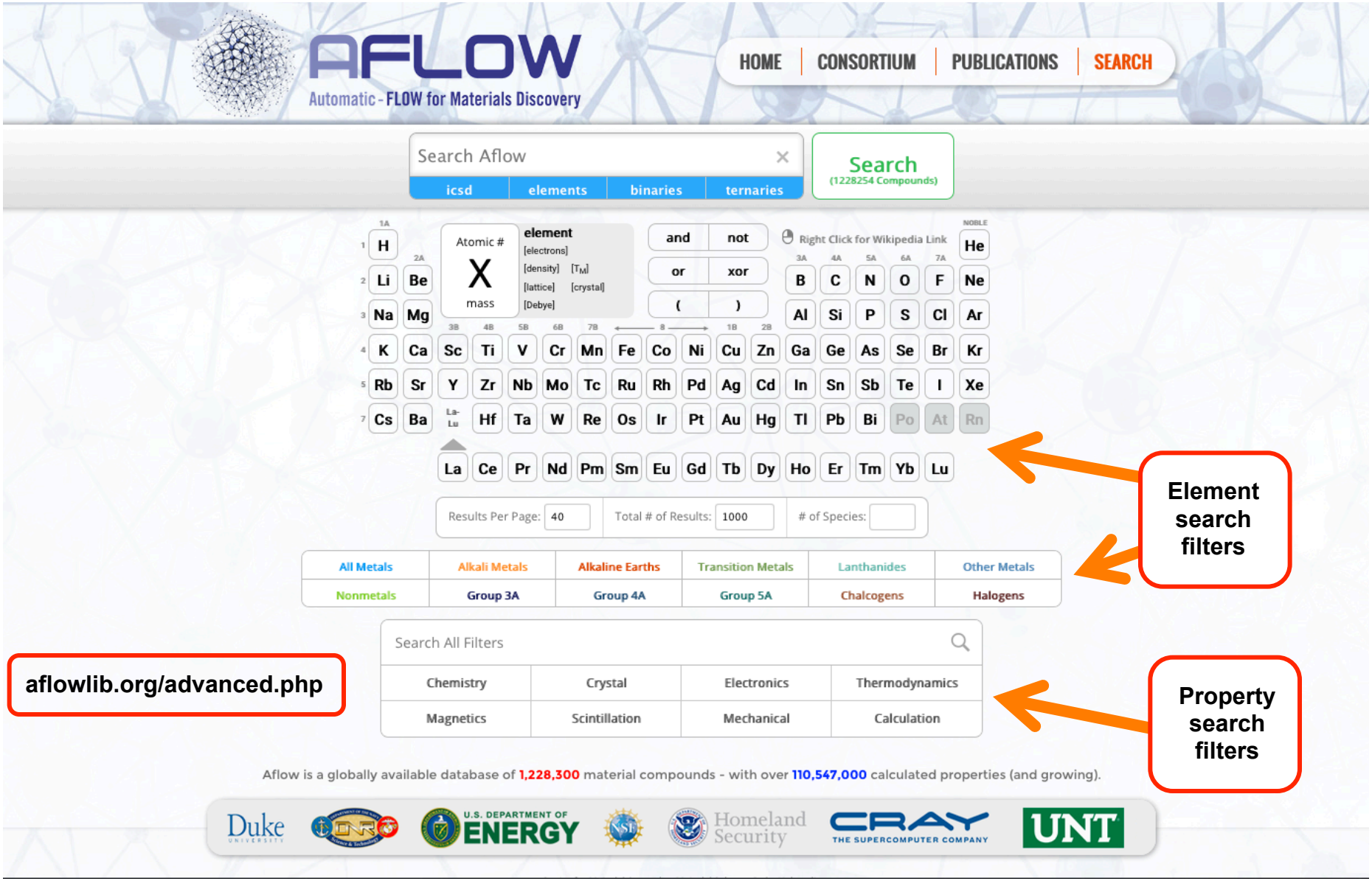
AFLOWLIB.org: web portal

http://aflowlib.org

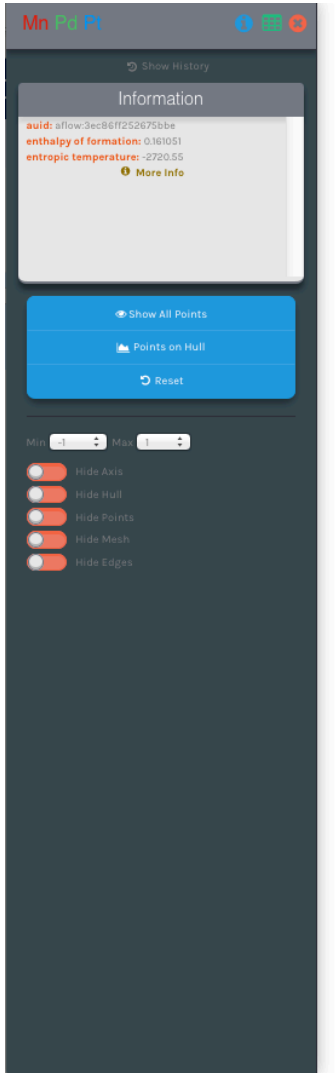
Advanced Search

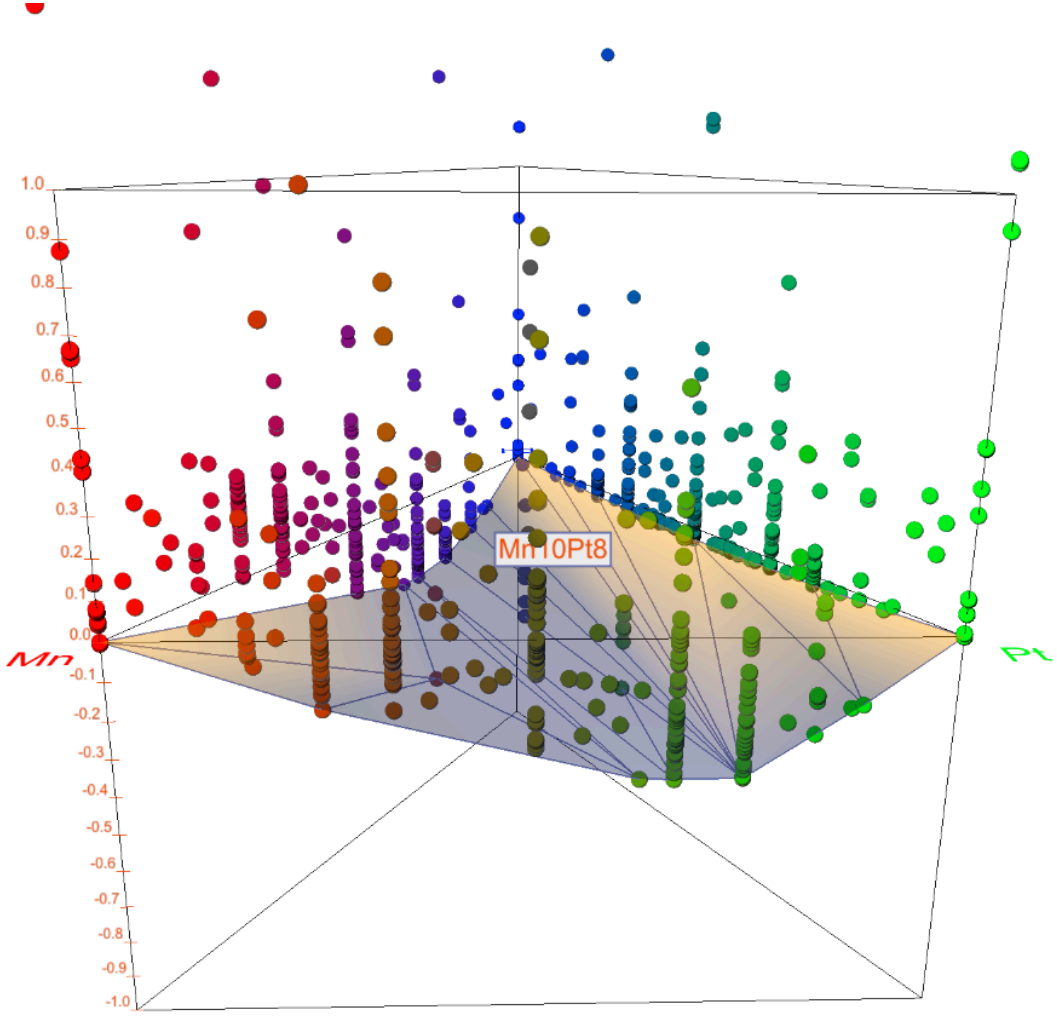
> 1.2 million entries

AFLOWLIB.org: MendeLIB advanced search



AFLOWLIB Online Applications





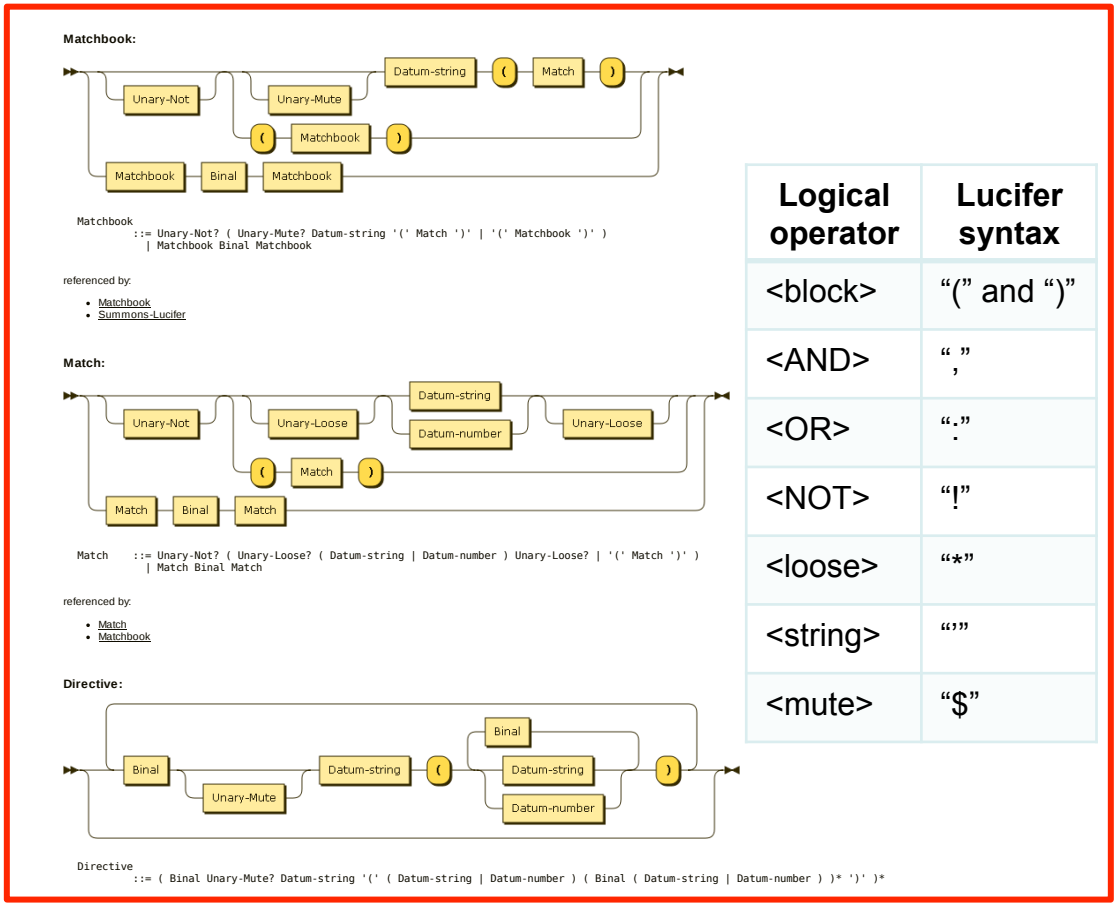
- Interactive online applications for data analysis

AFLOWLIB Search-API

Machine Searchable Materials Data

Comp. Mat. Sci. **93**, 178-192 (2014); DOI=10.1016/j.commatsci.2014.05.014

AFLOWLIB Search-API



Logical operator	Lucifer syntax
<block>	“(” and “)”
<AND>	“ ”
<OR>	“:”
<NOT>	“!”
<loose>	“*”
<string>	“’”
<mute>	“$”

- Aim: Programatically expose the same functionality as our web search interface at http://aflowlib.org/advanced.php

AFLOWLIB Search-API: A match is found

- Want to use URL for communication layer, like in our data API: http://aflowlib.duke.edu/AFLOWDATA/ICSD_WEB/ORCC/Ag1As1Na2_ICSD_49007/

- Standard API interfaces in URL's suffer from lack of relationships

- We created a new language called Lucifer to overcome that limitation

- Captures some of the niceties of Structured Query Language without the burden of knowing SQL or the DB schema.

- Fits neatly into the query portion of a URL, but does not interfere with existing ?key=value# nomenclature.

AFLOWLIB Search-API: Lucifer Ignites

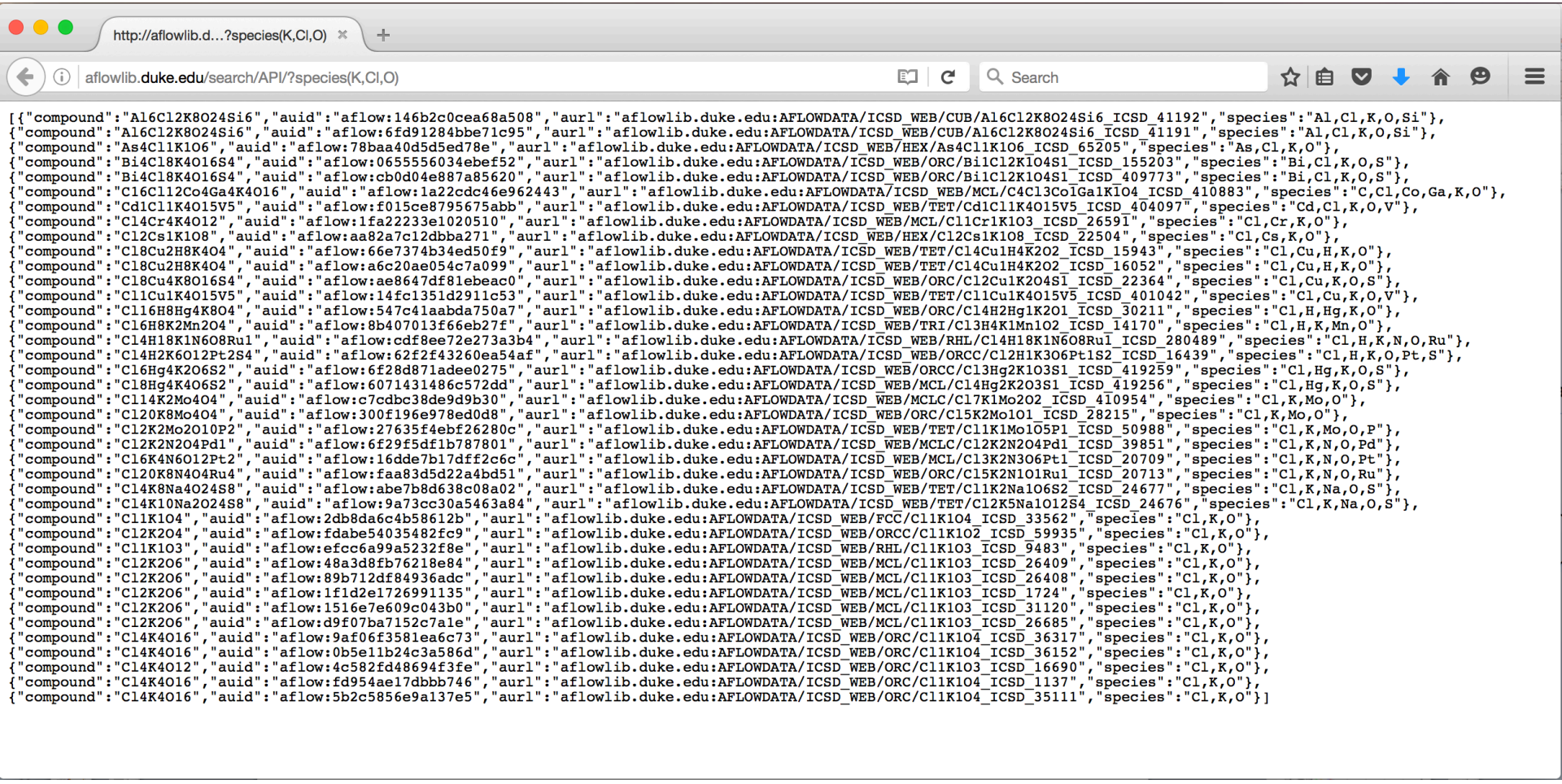
- We have many properties and more are added all the time, so Lucifer is automatic in its property inspection.

- Simple example search for compounds containing potassium, chlorine and oxygen: http://aflowlib.duke.edu/search/API/?species(K,Cl,O)

- Returns list of compounds in aflowlib.org containing these elements

- Default format is an array of JSON objects, shown 40 at a time; which set is returned is controlled by “paging()” command

AFLOWLIB Search-API: Search Results




```
[{"compound":"Al6Cl2K8O24Si6","auid":"aflow:146b2c0cea68a508","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/CUB/Al6Cl2K8O24Si6_ICSD_41192","species":"Al,Cl,K,O,Si"},
{"compound":"Al6Cl2K8O24Si6","auid":"aflow:6fd91284bbe71c95","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/CUB/Al6Cl2K8O24Si6_ICSD_41191","species":"Al,Cl,K,O,Si"},
{"compound":"As4Cl1K1O6","auid":"aflow:78baa40d5d5ed78e","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/HEX/As4Cl1K1O6_ICSD_65205","species":"As,Cl,K,O"},
{"compound":"Bi4Cl8K4O16S4","auid":"aflow:0655556034ebef52","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Bi1Cl2K1O4S1_ICSD_155203","species":"Bi,Cl,K,O,S"},
{"compound":"Bi4Cl8K4O16S4","auid":"aflow:cb0d04e887a85620","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Bi1Cl2K1O4S1_ICSD_409773","species":"Bi,Cl,K,O,S"},
{"compound":"C16Cl12Co4Ga4K4O16","auid":"aflow:1a22cdc46e962443","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/C4Cl3CoGa1K1O4_ICSD_410883","species":"C,Cl,Co,Ga,K,O"},
{"compound":"Cd1Cl1K4O15V5","auid":"aflow:f015ce8795675abb","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cd1Cl1K4O15V5_ICSD_404097","species":"Cd,Cl,K,O,V"},
{"compound":"Cl4Cr4K4O12","auid":"aflow:1fa22233e1020510","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1Cr1K1O3_ICSD_26591","species":"Cl,Cr,K,O"},
{"compound":"Cl2Cs1K1O8","auid":"aflow:aa82a7c12dbba271","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/HEX/Cl2Cs1K1O8_ICSD_22504","species":"Cl,Cs,K,O"},
{"compound":"Cl8Cu2H8K4O4","auid":"aflow:66e7374b34ed50f9","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl4Cu1H4K2O2_ICSD_15943","species":"Cl,Cu,H,K,O"},
{"compound":"Cl8Cu2H8K4O4","auid":"aflow:a6c20ae054c7a099","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl4Cu1H4K2O2_ICSD_16052","species":"Cl,Cu,H,K,O"},
{"compound":"Cl8Cu4K8O16S4","auid":"aflow:ae8647df81ebeac0","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl2Cu1K2O4S1_ICSD_22364","species":"Cl,Cu,K,O,S"},
{"compound":"Cl1Cu1K4O15V5","auid":"aflow:14fc1351d2911c53","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl1Cu1K4O15V5_ICSD_401042","species":"Cl,Cu,K,O,V"},
{"compound":"Cl16H8Hg4K8O4","auid":"aflow:547c41aabda750a7","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl4H2Hg1K2O1_ICSD_30211","species":"Cl,H,Hg,K,O"},
{"compound":"Cl6H8K2Mn2O4","auid":"aflow:8b407013f66eb27f","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TRI/Cl3H4K1Mn1O2_ICSD_14170","species":"Cl,H,K,Mn,O"},
{"compound":"Cl4H18K1N6O8Ru1","auid":"aflow:cdf8ee72e273a3b4","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/RHL/Cl4H18K1N6O8Ru1_ICSD_280489","species":"Cl,H,K,N,O,Ru"},
{"compound":"Cl4H2K6O12Pt2S4","auid":"aflow:62f2f43260ea54af","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORCC/Cl2H1K3O6Pt1S2_ICSD_16439","species":"Cl,H,K,O,Pt,S"},
{"compound":"Cl6Hg4K2O6S2","auid":"aflow:6f28d871adee0275","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORCC/Cl3Hg2K1O3S1_ICSD_419259","species":"Cl,Hg,K,O,S"},
{"compound":"Cl8Hg4K4O6S2","auid":"aflow:6071431486c572dd","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl4Hg2K2O3S1_ICSD_419256","species":"Cl,Hg,K,O,S"},
{"compound":"Cl14K2Mo4O4","auid":"aflow:c7cdbc38de9d9b30","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCLC/Cl7K1Mo2O2_ICSD_410954","species":"Cl,K,Mo,O"},
{"compound":"Cl20K8Mo4O4","auid":"aflow:300f196e978ed0d8","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl5K2Mo1O1_ICSD_28215","species":"Cl,K,Mo,O"},
{"compound":"Cl2K2Mo2O10P2","auid":"aflow:27635f4ebf26280c","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl1K1Mo1O5P1_ICSD_50988","species":"Cl,K,Mo,O,P"},
{"compound":"Cl2K2N2O4Pd1","auid":"aflow:6f29f5df1b787801","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCLC/Cl2K2N2O4Pd1_ICSD_39851","species":"Cl,K,N,O,Pd"},
{"compound":"Cl6K4N6O12Pt2","auid":"aflow:16dde7b17dff2c6c","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl3K2N3O6Pt1_ICSD_20709","species":"Cl,K,N,O,Pt"},
{"compound":"Cl20K8N4O4Ru4","auid":"aflow:faa83d5d22a4bd51","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl5K2N1O1Ru1_ICSD_20713","species":"Cl,K,N,O,Ru"},
{"compound":"Cl4K8Na4O24S8","auid":"aflow:abe7b8d638c08a02","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl1K2Na1O6S2_ICSD_24677","species":"Cl,K,Na,O,S"},
{"compound":"Cl4K10Na2O24S8","auid":"aflow:9a73cc30a5463a84","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl2K5Na1O12S4_ICSD_24676","species":"Cl,K,Na,O,S"},
{"compound":"Cl1K1O4","auid":"aflow:2db8da6c4b58612b","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/FCC/Cl1K1O4_ICSD_33562","species":"Cl,K,O"},
{"compound":"Cl2K2O4","auid":"aflow:fdabe54035482fc9","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORCC/Cl1K1O2_ICSD_59935","species":"Cl,K,O"},
{"compound":"Cl1K1O3","auid":"aflow:efcc6a99a5232f8e","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/RHL/Cl1K1O3_ICSD_9483","species":"Cl,K,O"},
{"compound":"Cl2K2O6","auid":"aflow:48a3d8fb76218e84","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_26409","species":"Cl,K,O"},
{"compound":"Cl2K2O6","auid":"aflow:89b712df84936adc","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_26408","species":"Cl,K,O"},
{"compound":"Cl2K2O6","auid":"aflow:1f1d2e1726991135","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_1724","species":"Cl,K,O"},
{"compound":"Cl2K2O6","auid":"aflow:1516e7e609c043b0","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_31120","species":"Cl,K,O"},
{"compound":"Cl2K2O6","auid":"aflow:d9f07ba7152c7a1e","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_26685","species":"Cl,K,O"},
{"compound":"Cl4K4O16","auid":"aflow:9af06f3581ea6c73","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_36317","species":"Cl,K,O"},
{"compound":"Cl4K4O16","auid":"aflow:0b5e11b24c3a586d","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_36152","species":"Cl,K,O"},
{"compound":"Cl4K4O12","auid":"aflow:4c582fd48694f3fe","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O3_ICSD_16690","species":"Cl,K,O"},
{"compound":"Cl4K4O16","auid":"aflow:fd954ae17dbbb746","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_1137","species":"Cl,K,O"},
{"compound":"Cl4K4O16","auid":"aflow:5b2c5856e9a137e5","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_35111","species":"Cl,K,O"}]
```


- Array of 40 JSON objects returned for search: http://aflowlib.duke.edu/search/API/?species(K,Cl,O)

AFLOWLIB Search-API: Lucifer Operators

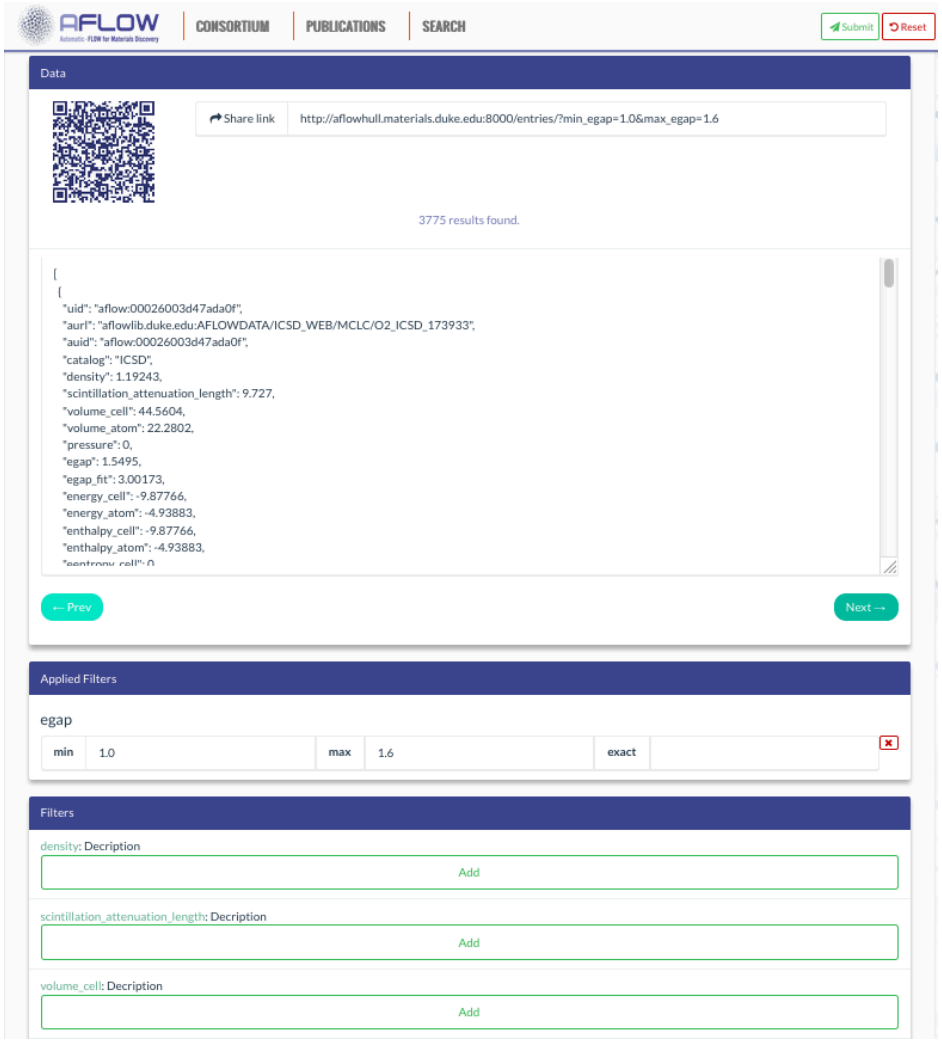
- Lucifer supports use of several logical operators
- Operator scope can be inter-property and/or intra-property

Logical operator	Lucifer 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

AFLOWLIB Search-API: Lucifer Examples

• aflowlib.duke.edu/search/API/?species	Show default DB selection with the species property
• aflowlib.duke.edu/search/API/?species((Na:K),Cl)	Show entries that have NaCl or KCl
• aflowlib.duke.edu/search/API/?species((Na:K),Cl),$nspecies(2)	Show entries that have NaCl or KCl only
• aflowlib.duke.edu/search/API/?species,catalog(icsd:lib2)	Show from both ICSD and Lib2 databases
• aflowlib.duke.edu/search/API/?Egap(1*,*1.6)	Show gaps between 1 and 1.6 eV (inclusive)
• aflowlib.duke.edu/search/API/?Egap(1*),energy_atom	Show entries with gap >= 1 along with energy per atom values
• aflowlib.duke.edu/search/API/?Egap(1*),paging(2)	Show entries with gap >= 1, second set of 40 entries

AFLOWLIB Future Developments

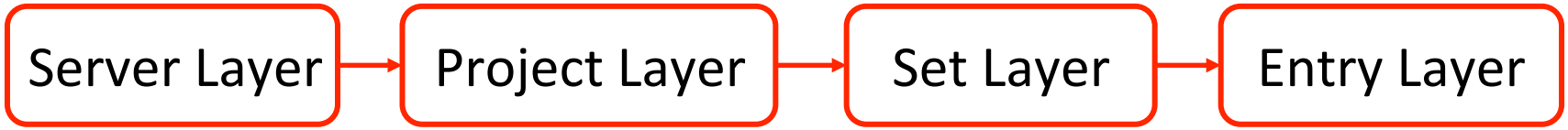


- Standalone GUI application for searching AFLOWLIB using search-API

AFLOWLIB REST-API

AFLOWLIB like POSIX: multi-layer system

- SQL database with distributed multilayered structure:



- $aurl=server:AFLOWDATA/project/set/entry/

- $aurl=aflowlib.duke.edu:AFLOWDATA/LIB2_RAW/AgTi_sv/66/

Server

Project layer

Set layer

Entry

- HTTP access: http://server/AFLOWDATA/project/set/entry
- http://aflowlib.duke.edu/AFLOWDATA/LIB2_RAW/AgTi_sv/66/

An entry in detail: multi-layer system

```
aurl=aflowlib.duke.edu:AFLOWDATA/LIB3_RAW/AgCoMn_pv/T0002.A2BC
auid=aflow:AgCoMn_pv/T0002.A2BC:PAW_PBE
aapi=1.0
keywords=aurl,auid,aflow_api_version,code,compound,prototype,nspecies,...
aflowlib_entry_date=20140130_20:34:00_GMT-5
aflowlib_entry_version=30794
aflow_version=aflow30293
calculation_cores=1
calculation_memory=539
calculation_time=18347.2
corresponding=Stefano_Sanvito_sanvitos@tcd.ie
loop=thermodynamics,bands,magnetic
node_CPU_Cores=12
node_CPU_MHz=2661
node_CPU_Model=Intel(R)_Xeon(R)_CPU_X5650_@_2.67GHz
node_RAM_GB=24
code=vasp.4.6.35
composition=2,1,1
compound=Ag2Co1Mn1
density=8.94193
eentropy=0
eentropy_atom=0
Egap=0
energy=-20.4051
energy_atom=-5.10128
enthalpy=-20.4051
enthalpy_atom=-5.10128
enthalpy_formation=1.51248
```

mandatory **keywords**

optional control **keywords**

optional materials **keywords**

AFLOW Standardization

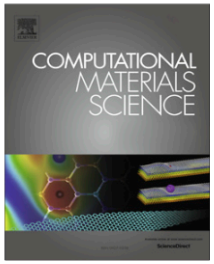
AFLOW Standardization

Computational Materials Science 108 (2015) 233–238

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci



Editor's Choice

The AFLOW standard for high-throughput materials science calculations

Camilo E. Calderon [a], Jose J. Plata [a], Cormac Toher [a], Corey Oses [a], Ohad Levy [a,1], Marco Fornari [b], Amir Natan [c], Michael J. Mehl [d], Gus Hart [e], Marco Buongiorno Nardelli [f], Stefano Curtarolo [g,*]

ARTICLE INFO

Article history:
Received 31 May 2015
Received in revised form 6 July 2015
Accepted 7 July 2015

Keywords:
High-throughput
Materials genomics
AFLOWLIB
VASP

ABSTRACT

The Automatic-Flow (AFLOW) standard for the high-throughput construction of materials science electronic structure databases is described. Electronic structure calculations of solid state materials depend on a large number of parameters which must be understood by researchers, and must be reported by originators to ensure reproducibility and enable collaborative database expansion. We therefore describe standard parameter values for *k*-point grid density, basis set plane wave kinetic energy cut-off, exchange–correlation functionals, pseudopotentials, DFT+U parameters, and convergence criteria used in AFLOW calculations.

AFLOW Standardization

Default N_{KPPRA} values used in non-BANDS calculations.

Database	STATIC	RELAX
Binary Alloy	N.A.	6000
Heusler	10,000	6000
ICSD	10,000	8000

Table 4
U_{eff} parameters applied to *d* orbitals.

Element	U_{eff}	Refs.	Element	U_{eff}	Refs.
Sc	2.9	[38]	W	2.2	[39]
Ti	4.4	[40]	Tc	2.7	[39]
V	2.7	[41]	Ru	3.0	[39]
Cr	3.5	[42]	Rh	3.3	[39]
Mn	4.0	[42]	Pd	3.6	[39]
Fe	4.6	[43]	Ag	5.8	[44]
Co	5.0	[41]	Cd	2.1	[45]
Ni	5.1	[41]	In	1.9	[45]
Cu	4.0	[42]	Sn	3.5	[46]
Zn	7.5	[45]	Ta	2.0	[39]
Ga	3.9	[47]	Re	2.4	[39]
Sn	3.5	[46]	Os	2.6	[39]
Nb	2.1	[39]	Ir	2.8	[39]
Mo	2.4	[39]	Pt	3.0	[39]
Ta	2.0	[46]	Au	4.0	

Table 5
U and *J* parameters applied to selected *f*-block elements.

Element	*U*	*J*	Refs.	Element	*U*	*J*	Refs.
La	8.1	0.6	[48]	Dy	5.6	0.0	[49]
Ce	7.0	0.7	[50]	Tm	7.0	1.0	[51]
Pr	6.5	1.0	[52]	Yb	7.0	0.67	[53]
Nd	7.2	1.0	[18]	Lu	4.8	0.95	[48]
Sm	7.4	1.0	[18]	Th	5.0	0.0	[54]
Eu	6.4	1.0	[18]	U	4.0	0.0	[55]
Gd	6.7	0.1	[56]				

Projector-Augmented Wavefunction (PAW) potentials, parameterized for the LDA, PW91, and PBE functionals, included in the AFLOW standard. The PAW-PBE combination is used as the default for ICSD, Binary Alloy and Heusler databases.

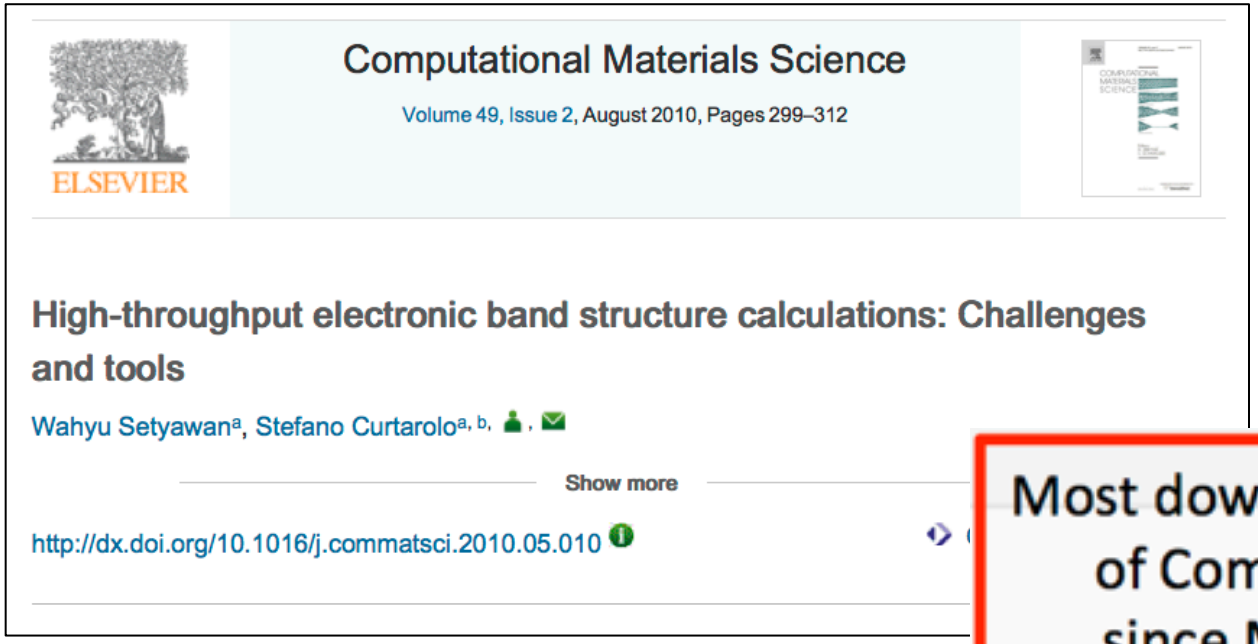
Element	Label	Element	Label	Element	Label
H	H	Se	Se	Gd[b]	Gd_3
He	He	Br	Br	Tb	Tb_3
Li	Li_sv	Kr	Kr	Dy	Dy_3
Be	Be_sv	Rb	Rb_sv	Ho	Ho_3
B	B_h	Sr	Sr_sv	Er	Er_3
C	C	Y	Y_sv	Tm	Tm
N	N	Zr	Zr_sv	Yb	Yb
O	O	Nb	Nb_sv	Lu	Lu
F	F	Mo	Mo_pv	Hf	Hf
Ne	Ne	Tc	Tc_pv	Ta	Ta_pv
Na	Na_pv	Ru	Ru_pv	W	W_pv
Mg	Mg_pv	Rh	Rh_pv	Re	Re_pv
Al	Al	Pd	Pd_pv	Os	Os_pv
Si	Si	Ag	Ag	Ir	Ir
P	P	Cd	Cd	Pt	Pt
S	S	In	In_d	Au	Au
Cl	Cl	Sn	Sn	Hg	Hg
Ar	Ar	Sb	Sb	Tl	Tl_d
K	K_sv	Te	Te	Pb	Pb_d
Ca	Ca_sv	I	I	Bi	Bi_d
Sc	Sc_sv	Xe	Xe	Po	Po
Ti	Ti_sv	Cs	Cs_sv	At	At
V	V_sv	Ba	Ba_sv	Rn	Rn
Cr	Cr_pv	La	La	Fr	Fr
Mn	Mn_pv	Ce	Ce	Ra	Ra
Fe	Fe_pv	Pr	Pr	Ac	Ac
Co	Co	Nd	Nd	Th	Th_s
Ni	Ni_pv	Pm	Pm	Pa	Pa
Cu	Cu_pv	Sm[a]	Sm	U	U
Zn	Zn	Sm[b]	Sm_3	Np	Np_s
Ga	Ga_h	Eu	Eu	Pu	Pu_s
As	As	Gd[a]	Gd		

[a] PBE potentials only.
[b] LDA and PW91 potentials only.

AFLOWLIB Band Structure Standard

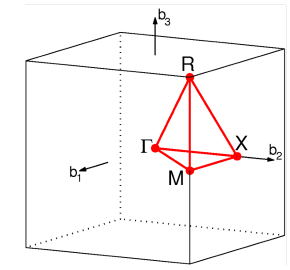
an apparently simple problem requiring a complex solution

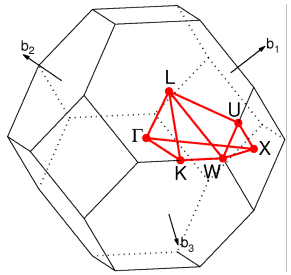
1. *Work out all the prototype definitions/symmetries:*
2. *Define standards in reciprocal space (on-line):*
3. *Standard needs to be quick.*

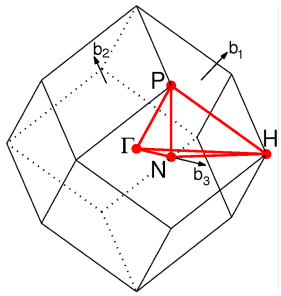


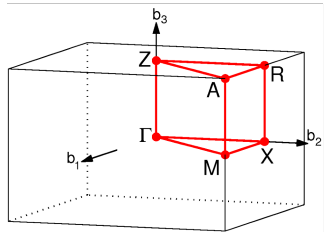
Most downloaded article of Comp. Mat. Sci. since March 2013

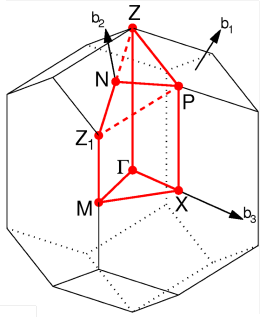
STANDARD in Real Space and Reciprocal Space

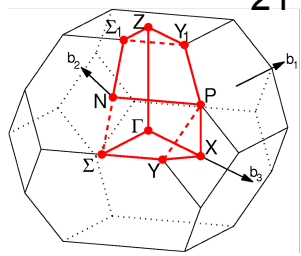


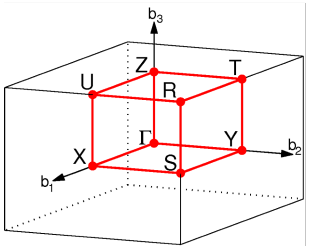


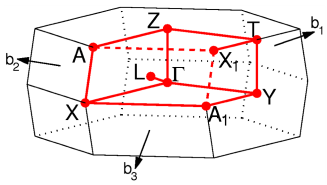


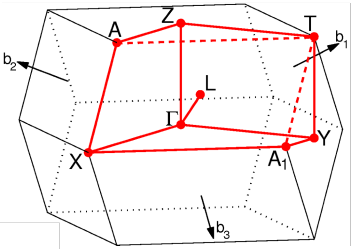


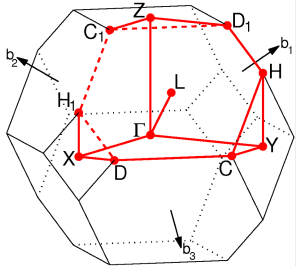


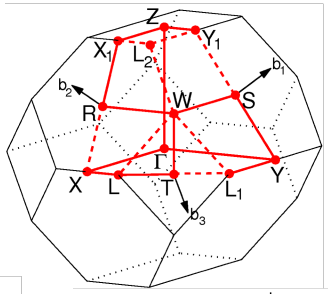


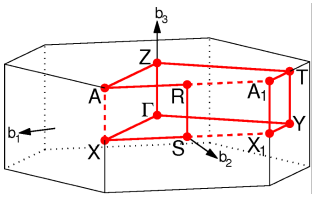


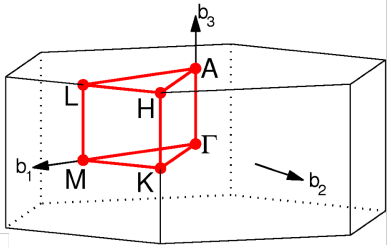


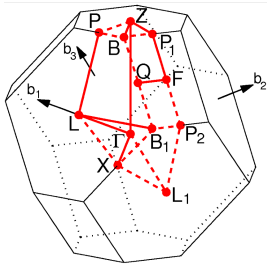


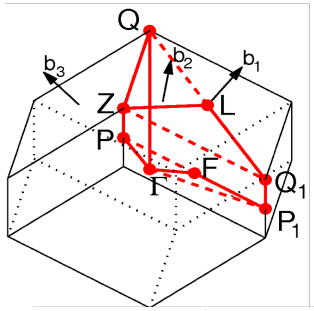


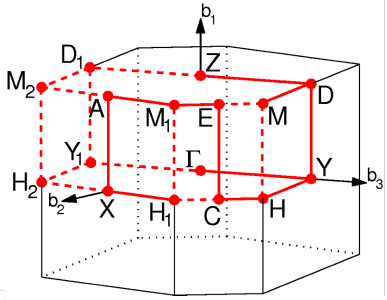


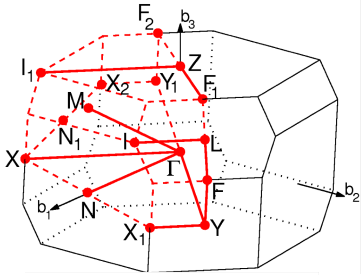


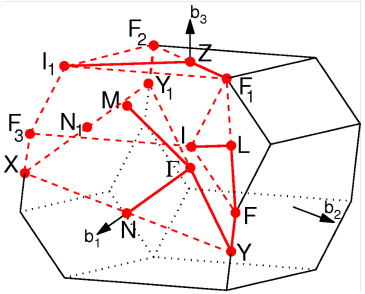


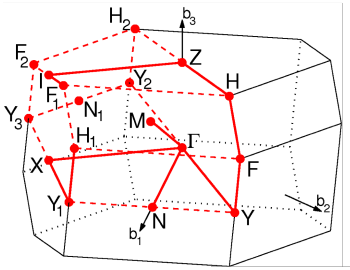


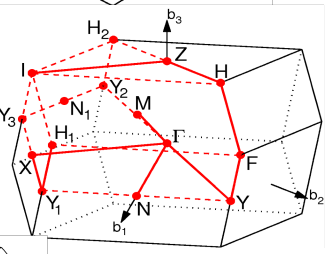


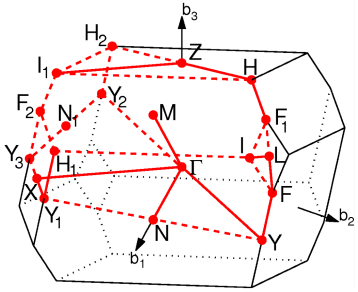


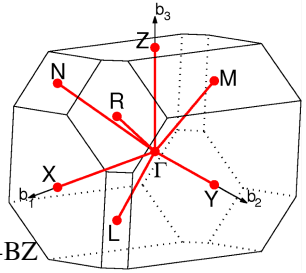


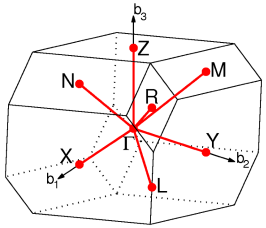


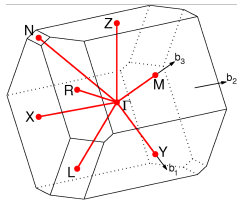


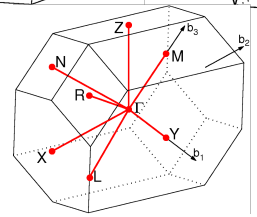












ht-BZ

Acknowledgements

- Prof. Stefano Curtarolo, Director, Center for Materials Genomics

- Dr. Frisco Rose, Harvey Shi, Eric Gossett: online database implementation