

# AFLOWLIB Data Repository

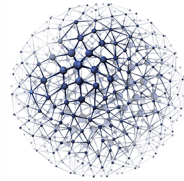
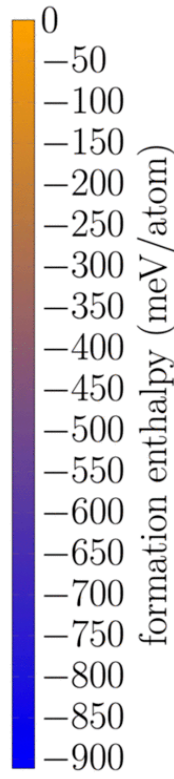
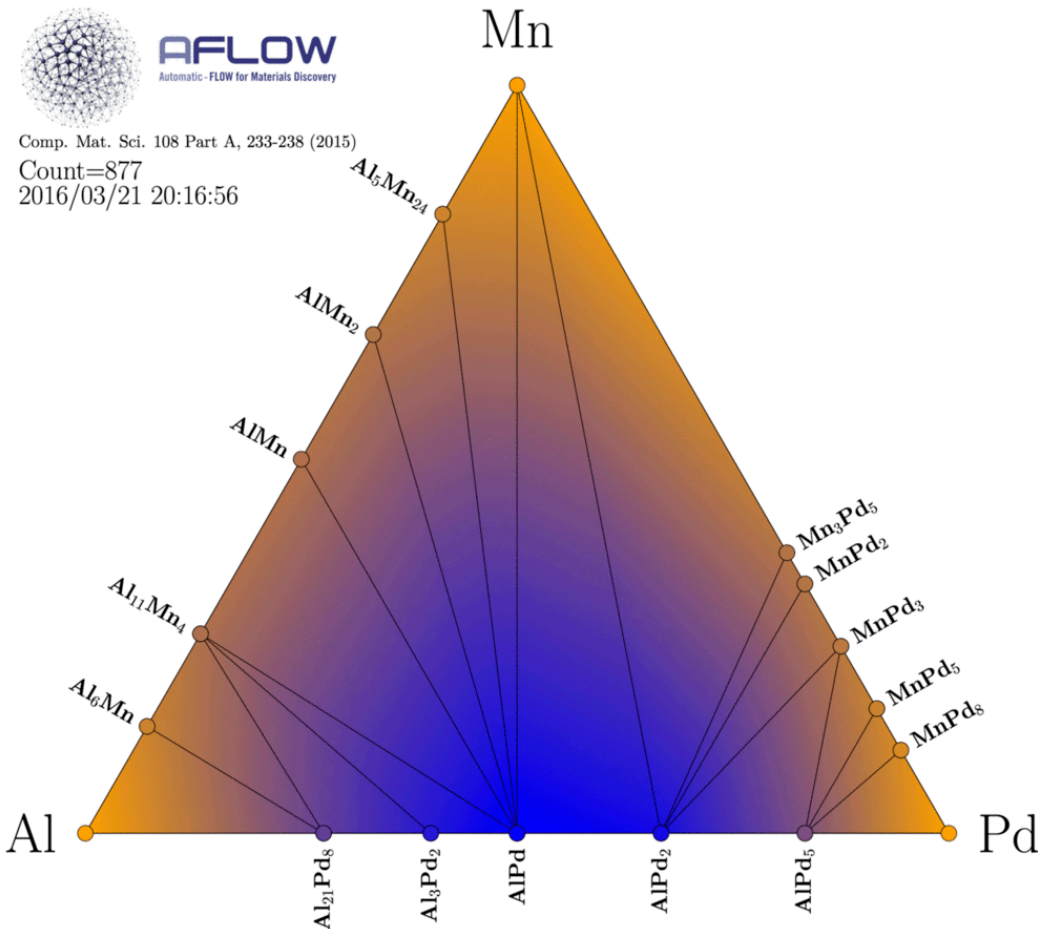
**CORMAC TOHER**  
**STEFANO CURTAROLO**

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



Comp. Mat. Sci. 108 Part A, 233-238 (2015)  
Count=877  
2016/03/21 20:16:56



**AFLOW**  
Automatic - FLOW for Materials Discovery

**Duke**  
UNIVERSITY



**CRAY**

## **AFLOWLIB Web Portal**

# AFLOWLIB.org: web portal

<http://aflowlib.org>

**AFLOW**  
Automatic - FLOW for Materials Discovery

HOME | CONSORTIUM | PUBLICATIONS | SEARCH

Welcome to the AFLOW distributed materials property repository: share with us your passion for innovation and technology.

Aflow is a globally available database of **1,217,595** material compounds - with over **109,583,550** calculated properties (and growing).

Try our Materials Database Search, use our online apps, consult our wiki and publications.

Enter a Compound Name, ICSD Number, [Aflowlib Unique Identifier](#) or advanced search string (ie. Mg & Sn & Cu).

ICSD#, AUID#, element combos...

**Quick Search**

**Advanced search**

**DISCOVER OUR STORY**

Interview

**RECENT PUBLICATIONS**

Entropy Staggered Oxides

Convergence of multi-valley bands as the electronic origin of high thermoelectric performance in CoSb<sub>3</sub> skutterudites

Dysprosium-doped cadmium selenide as a gateway material for mid-infrared plasmonics

Reformulation of DFT+U as a Pseudohybrid Hubbard Density Functional for Accelerated Materials Discovery

**DOCUMENTATION**

[Aflow Rest-API Wiki](#)  
[AFLOW CALCULATE](#)  
[AFLOW ANALYZE](#)

**Apps and Docs**

PERIODIC TABLE OF THE ELEMENTS

MendeLIB Search

Aflow-online

Binary alloy library

**AFLOW REST-API WIKI**

Documentation

Geolocation data

Showcase Material

Duke UNIVERSITY | U.S. DEPARTMENT OF ENERGY | HOMELAND SECURITY | CRAY THE SUPERCOMPUTER COMPANY | UNT

**Advanced Search**

**> 1.2 million entries**

# AFLOWLIB.org: MendeLIB advanced search

**AFLOW**  
Automatic - FLOW for Materials Discovery

HOME | CONSORTIUM | PUBLICATIONS | **SEARCH**

Search Aflow  X

icsd | elements | binaries | ternaries

**Search**  
(1228254 Compounds)

Atomic # **X** element  
[electrons]  
[density] [T<sub>M</sub>]  
[lattice] [crystal]  
[Debye] mass

and not  
or xor  
( )

Right Click for Wikipedia Link

Results Per Page: 40 Total # of Results: 1000 # of Species:

[All Metals](#) [Alkali Metals](#) [Alkaline Earths](#) [Transition Metals](#) [Lanthanides](#) [Other Metals](#)  
[Nonmetals](#) [Group 3A](#) [Group 4A](#) [Group 5A](#) [Chalcogens](#) [Halogens](#)

Search All Filters

Chemistry	Crystal	Electronics	Thermodynamics
Magnetics	Scintillation	Mechanical	Calculation

Aflow is a globally available database of **1,228,300** material compounds - with over **110,547,000** calculated properties (and growing).

Duke UNIVERSITY | ORNL | U.S. DEPARTMENT OF ENERGY | Homeland Security | CRAY THE SUPERCOMPUTER COMPANY | UNT

[aflowlib.org/advanced.php](http://aflowlib.org/advanced.php)

Element search filters

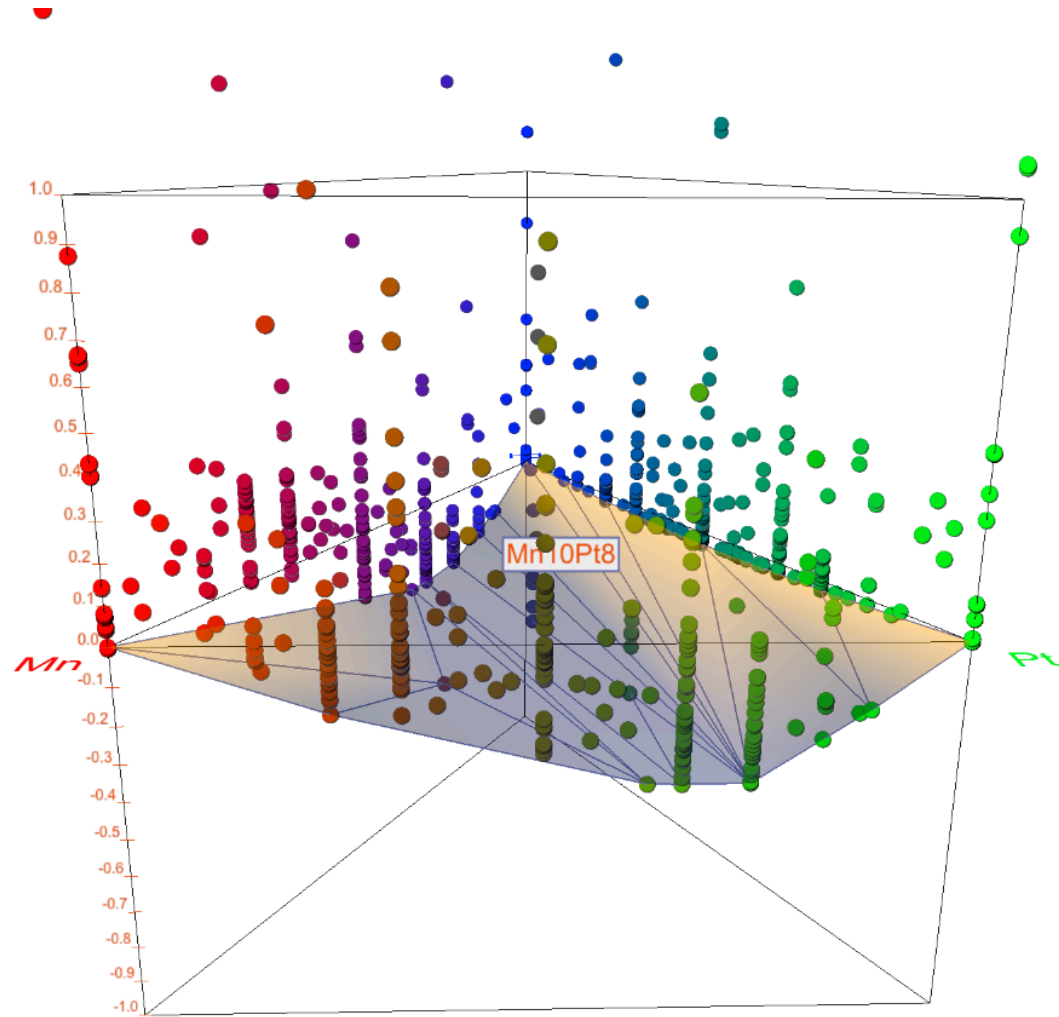
Property search filters



# AFLOWLIB Online Applications

The screenshot shows the AFLOWLIB online application interface. The sidebar on the left contains the following elements:

- Header: Mn Pt Pt
- Show History button
- Information panel with details:
  - aid: aflow:3ec86ff252675bbe
  - enthalpy of formation: 0.161051
  - entropic temperature: -2720.55
  - More Info link
- Show All Points button
- Points on Hull button
- Reset button
- Min and Max sliders (both set to 1)
- Hide Axis, Hide Hull, Hide Points, Hide Mesh, and Hide Edges toggle switches (all currently turned on)



- Interactive online applications for data analysis

## **Machine Searchable Materials Data**

# AFLOWLIB Search-API



```

aurl=afowlib.duke.edu:afLOWDATA/LTB3_RAW/AgCoMn_pv/T0002.A2BC
auid=aflow:AgCoMn_pv/T0002.A2BC:PAM_PBE
aapi=1.0
keywords=aurl,auid,aflow_api_version,code,compound,prototype,naspecies,...
afowlib_entry_datum=20140130T20:34:00_GHFT-5
afowlib_entry_version=30794
aflow_version=aflow30293
calculation_cores=1
calculation_memory=539
calculation_time=19347.2
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
entropy=0
entropy_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**

**Matchbook:**

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

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

Logical operator	Lucifer syntax
<block>	"(" and ")"
<AND>	" , "
<OR>	"   "
<NOT>	" ! "
<loose>	" * "
<string>	" ' " "
<mute>	" \$ " "

- Aim: Automatically expose the same functionality as our web search interface at <http://afowlib.org/advanced.php>

# AFLOWLIB Search-API: A match is found

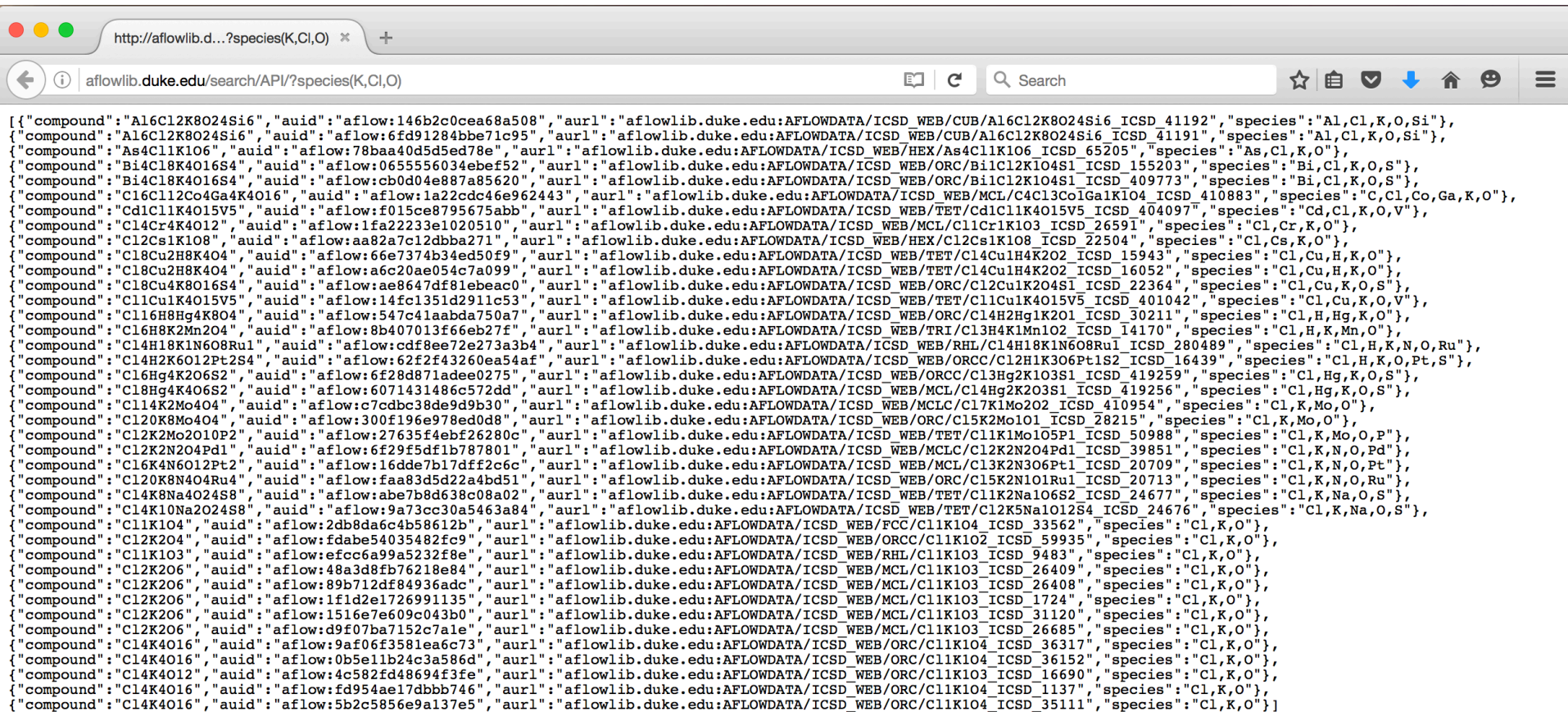
- Want to use URL for communication layer, like in our data API:  
[http://aflowlib.duke.edu/AFLOWDATA/ICSD\\_WEB/ORCC/Ag1As1Na2\\_ICSD\\_49007/](http://aflowlib.duke.edu/AFLOWDATA/ICSD_WEB/ORCC/Ag1As1Na2_ICSD_49007/)
- Standard API interfaces in URL's suffer from lack of relationships
- We created a 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\(K,Cl,O\)](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", "aid": "aflow:146b2c0cea68a508", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/CUB/Al6Cl2K8O24Si6_ICSD_41192", "species": "Al,Cl,K,O,Si"}, {"compound": "Al6Cl2K8O24Si6", "aid": "aflow:6fd91284bbe71c95", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/CUB/Al6Cl2K8O24Si6_ICSD_41191", "species": "Al,Cl,K,O,Si"}, {"compound": "As4Cl1K1O6", "aid": "aflow:78baa40d55ed78e", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/HEX/As4Cl1K1O6_ICSD_65205", "species": "As,Cl,K,O"}, {"compound": "Bi4Cl8K4O16S4", "aid": "aflow:0655556034ebef52", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Bi4Cl8K4O16S4_ICSD_155203", "species": "Bi,Cl,K,O,S"}, {"compound": "Bi4Cl8K4O16S4", "aid": "aflow:cb0d04e887a85620", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Bi4Cl8K4O16S4_ICSD_409773", "species": "Bi,Cl,K,O,S"}, {"compound": "C16Cl12Co4Ga4K4O16", "aid": "aflow:1a22c2c46e962443", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/C4Cl3Co1Ga1K1O4_ICSD_410883", "species": "C,Cl,Co,Ga,K,O"}, {"compound": "Cd1Cl1K4O15V5", "aid": "aflow:f015ce8795675abb", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cd1Cl1K4O15V5_ICSD_404097", "species": "Cd,Cl,K,O,V"}, {"compound": "Cl4Cr4K4O12", "aid": "aflow:1fa22233e1020510", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1Cr1K1O3_ICSD_26591", "species": "Cl,Cr,K,O"}, {"compound": "Cl2Cs1K1O8", "aid": "aflow:aa82a7c12dbba271", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/HEX/Cl2Cs1K1O8_ICSD_22504", "species": "Cl,Cs,K,O"}, {"compound": "Cl8Cu2H8K4O4", "aid": "aflow:66e7374b34ed50f9", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/HEX/Cl8Cu1H4K2O2_ICSD_15943", "species": "Cl,Cu,H,K,O"}, {"compound": "Cl8Cu2H8K4O4", "aid": "aflow:a6c20ae054c7a099", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl4Cu1H4K2O2_ICSD_16052", "species": "Cl,Cu,H,K,O"}, {"compound": "Cl8Cu4K8O16S4", "aid": "aflow:ae8647df81ebeac0", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl2Cu1K2O4S1_ICSD_22364", "species": "Cl,Cu,K,O,S"}, {"compound": "Cl1Cu1K4O15V5", "aid": "aflow:14fc1351d2911c53", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl1Cu1K4O15V5_ICSD_401042", "species": "Cl,Cu,K,O,V"}, {"compound": "Cl16H8Hg4K8O4", "aid": "aflow:547c41aabda750a7", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl14H2Hg1K2O1_ICSD_30211", "species": "Cl,H,Hg,K,O"}, {"compound": "Cl6H8K2Mn2O4", "aid": "aflow:8b407013f66eb27f", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TRI/Cl3H4K1Mn1O2_ICSD_14170", "species": "Cl,H,K,Mn,O"}, {"compound": "Cl4H18K1N6O8Ru1", "aid": "aflow:cdf8ee72e273a3b4", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/RHL/Cl4H18K1N6O8Ru1_ICSD_280489", "species": "Cl,H,K,N,O,Ru"}, {"compound": "Cl4H2K6O12Pt2S4", "aid": "aflow:62f2f43260ea54af", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORCC/Cl2H1K3O6Pt1S2_ICSD_16439", "species": "Cl,H,K,O,Pt,S"}, {"compound": "Cl6Hg4K2O6S2", "aid": "aflow:6f28d871adee0275", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORCC/Cl3Hg2K1O3S1_ICSD_419259", "species": "Cl,Hg,K,O,S"}, {"compound": "Cl8Hg4K4O6S2", "aid": "aflow:6071431486c572dd", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl4Hg2K2O3S1_ICSD_419256", "species": "Cl,Hg,K,O,S"}, {"compound": "Cl14K2Mo4O4", "aid": "aflow:c7cdbc38de9d9b30", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl17K1Mo2O2_ICSD_410954", "species": "Cl,K,Mo,O"}, {"compound": "Cl20K8Mo4O4", "aid": "aflow:300f196e978ed0d8", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl5K2Mo1O1_ICSD_28215", "species": "Cl,K,Mo,O"}, {"compound": "Cl2K2Mo2O10P2", "aid": "aflow:27635f4ebf26280c", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl1K1Mo1O5P1_ICSD_50988", "species": "Cl,K,Mo,O,P"}, {"compound": "Cl2K2N2O4Pd1", "aid": "aflow:6f29f5df1b787801", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl2K2N2O4Pd1_ICSD_39851", "species": "Cl,K,N,O,Pd"}, {"compound": "Cl6K4N6O12Pt2", "aid": "aflow:16dde7b17dff2c6c", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl3K2N3O6Pt1_ICSD_20709", "species": "Cl,K,N,O,Pt"}, {"compound": "Cl20K8N4O4Ru4", "aid": "aflow:faa83d5d22a4bd51", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl5K2N1O1Ru1_ICSD_20713", "species": "Cl,K,N,O,Ru"}, {"compound": "Cl4K8Na4O24S8", "aid": "aflow:abe7b8d638c08a02", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl1K2Na1O6S2_ICSD_24677", "species": "Cl,K,Na,O,S"}, {"compound": "Cl4K10Na2O24S8", "aid": "aflow:9a73cc30a5463a84", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/Cl2K5Na1O12S4_ICSD_24676", "species": "Cl,K,Na,O,S"}, {"compound": "Cl1K1O4", "aid": "aflow:2db8da6c4b58612b", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/FCC/Cl1K1O4_ICSD_33562", "species": "Cl,K,O"}, {"compound": "Cl2K2O4", "aid": "aflow:fdabe54035482fc9", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORCC/Cl1K1O2_ICSD_59935", "species": "Cl,K,O"}, {"compound": "Cl1K1O3", "aid": "aflow:efcc6a99a5232f8e", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/RHL/Cl1K1O3_ICSD_9483", "species": "Cl,K,O"}, {"compound": "Cl2K2O6", "aid": "aflow:48a3d8fb76218e84", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_26409", "species": "Cl,K,O"}, {"compound": "Cl2K2O6", "aid": "aflow:89b712df84936adc", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_26408", "species": "Cl,K,O"}, {"compound": "Cl2K2O6", "aid": "aflow:1f1d2e1726991135", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_1724", "species": "Cl,K,O"}, {"compound": "Cl2K2O6", "aid": "aflow:1516e7e609c043b0", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_31120", "species": "Cl,K,O"}, {"compound": "Cl2K2O6", "aid": "aflow:d9f07ba7152c7ale", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCL/Cl1K1O3_ICSD_26685", "species": "Cl,K,O"}, {"compound": "Cl4K4O16", "aid": "aflow:9af06f3581ea6c73", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_36317", "species": "Cl,K,O"}, {"compound": "Cl4K4O16", "aid": "aflow:0b5e11b24c3a586d", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_36152", "species": "Cl,K,O"}, {"compound": "Cl4K4O12", "aid": "aflow:4c582fd48694f3fe", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O3_ICSD_16690", "species": "Cl,K,O"}, {"compound": "Cl4K4O16", "aid": "aflow:fd954ae17dbbb746", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/Cl1K1O4_ICSD_1137", "species": "Cl,K,O"}, {"compound": "Cl4K4O16", "aid": "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\(K,Cl,O\)](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

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



# AFLOWLIB Future Developments

The screenshot displays the AFLOWLIB search interface. At the top, there is a navigation bar with the AFLOW logo (AFLOW Consortium: FLM for Materials Society), links for CONSORTIUM, PUBLICATIONS, and SEARCH, and buttons for Submit and Reset. The main content area is titled "Data" and features a QR code, a "Share link" button, and a URL: [http://aflowlib.materials.duke.edu:8000/entries/?min\\_egap=1.0&max\\_egap=1.6](http://aflowlib.materials.duke.edu:8000/entries/?min_egap=1.0&max_egap=1.6). Below this, it indicates "3775 results found." and displays a JSON object representing a search result:

```
{
  "uid": "aflow:00026003d47ada0f",
  "auri": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/MCLC/O2_ICSD_173933",
  "auid": "aflow:00026003d47ada0f",
  "catalog": "ICSD",
  "density": 1.19243,
  "scintillation_attenuation_length": 9.727,
  "volume_cell": 44.5604,
  "volume_atom": 22.2802,
  "pressure": 0,
  "egap": 1.5495,
  "egap_fit": 3.00173,
  "energy_cell": -9.87766,
  "energy_atom": -4.93883,
  "enthalpy_cell": -9.87766,
  "enthalpy_atom": -4.93883,
  "entropy_cell": 0
}
```

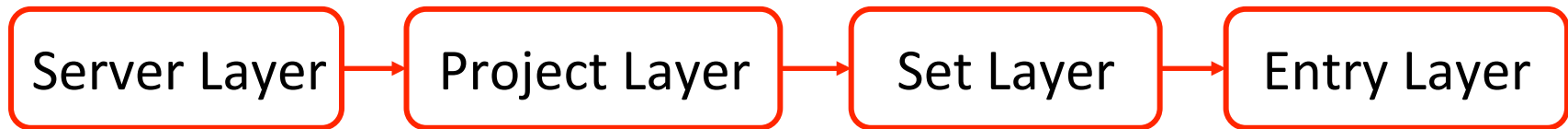
Navigation buttons for "Prev" and "Next" are visible. Below the data section, the "Applied Filters" section shows the filter "egap" with a range from "min 1.0" to "max 1.6" and an "exact" option. The "Filters" section lists three filters: "density: Description", "scintillation\_attenuation\_length: Description", and "volume\_cell: Description", each with an "Add" button.

- Standalone GUI application for searching AFLOWLIB using search-API

## **AFLOWLIB REST-API**

# AFLOWLIB like POSIX: multi-layer system

- SQL database with distributed multilayered structure:



- `$curl=server:AFLOWDATA/project/set/entry/`
- `$curl=afowlib.duke.edu:AFLOWDATA/LIB2_RAW/AgTi_sv/66/`  

The diagram shows the URL `$curl=afowlib.duke.edu:AFLOWDATA/LIB2_RAW/AgTi_sv/66/` with red brackets underneath. The first bracket under `afowlib.duke.edu` is labeled 'Server'. The second bracket under `AFLOWDATA/LIB2_RAW` is labeled 'Project layer'. The third bracket under `AgTi_sv` is labeled 'Set layer'. The fourth bracket under `66/` is labeled 'Entry layer'.
- HTTP access: <http://server/AFLOWDATA/project/set/entry>
- `http://afowlib.duke.edu/AFLOWDATA/LIB2_RAW/AgTi_sv/66/`

# An entry in detail: multi-layer system

```
aurllib.duke.edu:AFLOWDATA/LIB3_RAW/AgCoMn_pv/T0002.A2BC
auid=aflow:AgCoMn_pv/T0002.A2BC:PAW_PBE
aapi=1.0
keywords=aurllib.duke.edu:AFLOWDATA/LIB3_RAW/AgCoMn_pv/T0002.A2BC,aflow:AgCoMn_pv/T0002.A2BC:PAW_PBE,aflow_api_version,code,compound,prototype,nspecies,...
```

mandatory  
keywords

```
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
```

optional  
control  
keywords

```
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
```

optional  
materials  
keywords



## **AFLOW Standardization**

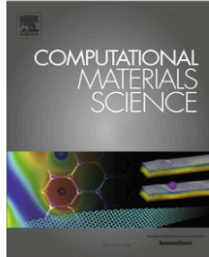
# AFLOW Standardization

Computational Materials Science 108 (2015) 233–238

Contents lists available at [ScienceDirect](#)

## Computational Materials Science

journal homepage: [www.elsevier.com/locate/commatsci](http://www.elsevier.com/locate/commatsci)



Editor's Choice

### The AFLOW standard for high-throughput materials science calculations



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

#### 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.

© 2015 Elsevier B.V. All rights reserved.

# 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**

$U_{\text{eff}}$  parameters applied to  $d$  orbitals.

Element	$U_{\text{eff}}$	Refs.	Element	$U_{\text{eff}}$	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 <sup>b</sup>	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 <sup>a</sup>	Sm	U	U
Zn	Zn	Sm <sup>b</sup>	Sm_3	Np	Np_s
Ga	Ga_h	Eu	Eu	Pu	Pu_s
As	As	Gd <sup>a</sup>	Gd		

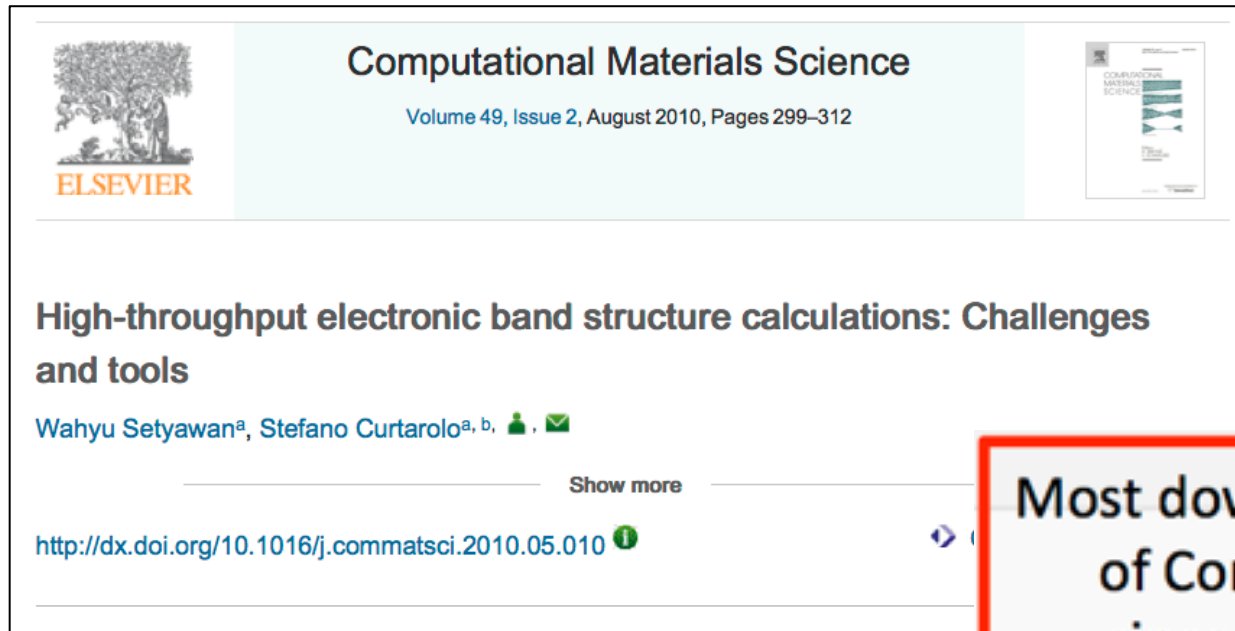
<sup>a</sup> PBE potentials only.

<sup>b</sup> 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.*



The screenshot shows the top portion of a journal article page. On the left is the Elsevier logo, which features a tree and the word 'ELSEVIER'. To the right of the logo, the journal title 'Computational Materials Science' is displayed in a large, bold font. Below the title, the volume and issue information 'Volume 49, Issue 2, August 2010, Pages 299–312' is shown in a smaller font. On the far right, there is a small thumbnail image of the journal cover. Below the journal information, the article title 'High-throughput electronic band structure calculations: Challenges and tools' is prominently displayed in a bold font. Underneath the title, the authors 'Wahyu Setyawan<sup>a</sup>, Stefano Curtarolo<sup>a, b</sup>' are listed, followed by small icons for a person and an envelope. A 'Show more' link is visible below the authors. At the bottom of the article information, the DOI link 'http://dx.doi.org/10.1016/j.commatsci.2010.05.010' is provided with a small circular icon next to it.

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





# Acknowledgements

- Prof. Stefano Curtarolo, Director, Center for Materials Genomics
- Dr. Frisco Rose, Harvey Shi, Eric Gossett: online database implementation

