AFLOWLIB Data Repository

AFLOWLIB Web Portal
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).

Quick Search

Advanced search

http://aflowlib.org

> 1.2 million entries

A RESTful API for exchanging Data in AFLOWLIB, Comp. Mat. Sci. 93, 178-192 (2014); DOI=10.1016/j.commatsci.2014.05.014
AFLOWLIB.org: MendeLIB advanced search

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

A RESTful API for exchanging Data in AFLOWLIB, Comp. Mat. Sci. 93, 178-192 (2014); DOI=10.1016/j.commatsci.2014.05.014
AFLOWLIB Online Applications

- Interactive online applications for data analysis
Machine Searchable Materials Data
AFLOWLIB Search-API

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

<table>
<thead>
<tr>
<th>Logical operator</th>
<th>Lucifer syntax</th>
<th>Operator scope</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>&lt;block&gt;</code></td>
<td>“(” and “)”</td>
<td>Intra- and inter-property</td>
</tr>
<tr>
<td><code>&lt;AND&gt;</code></td>
<td>,</td>
<td>Intra- and inter-property</td>
</tr>
<tr>
<td><code>&lt;OR&gt;</code></td>
<td>:</td>
<td>Intra- and inter-property</td>
</tr>
<tr>
<td><code>&lt;NOT&gt;</code></td>
<td>!</td>
<td>Intra-property</td>
</tr>
<tr>
<td><code>&lt;loose&gt;</code></td>
<td>*</td>
<td>Intra-property</td>
</tr>
<tr>
<td><code>&lt;string&gt;</code></td>
<td>””</td>
<td>Inter-property</td>
</tr>
<tr>
<td><code>&lt;mute&gt;</code></td>
<td>”$”</td>
<td>Intra-property</td>
</tr>
</tbody>
</table>
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
• Standalone GUI application for searching AFLOWLIB using search-API
A RESTful API for exchanging Data in AFLOWLIB, Comp. Mat. Sci. 93, 178-192 (2014); DOI=10.1016/j.commatsci.2014.05.014
AFLOWLIB like POSIX: multi-layer system

- SQL database with distributed multilayered structure:

  Server Layer → Project Layer → Set Layer → Entry Layer

- $\text{aurl}=\text{server:AFLOWDATA/project/set/entry/}$

- $\text{aurl}=$aflowlib.duke.edu:AFLOWDATA/LIB2_RAW/AgTi_sv/66/

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

---

A RESTful API for exchanging Data in AFLOWLIB, Comp. Mat. Sci. 93, 178-192 (2014); DOI=10.1016/j.commatsci.2014.05.014
An entry in detail: multi-layer system

aulr=aflowlib.duke.edu:AFLOWDATA/LIB3_RAW/AgCoMn_pv/T0002.A2BC
auid=aflow:AgCoMn_pv/T0002.A2BC:PAW_PBE
aapi=1.0
keywords=aulr,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
density_atom=0
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
AFLOW Standardization
Editor's Choice

The AFLOW standard for high-throughput materials science calculations

Camilo E. Calderon, Jose J. Plata, Cormac Toher, Corey Oses, Ohad Levy, Marco Fornari, Amir Natan, Michael J. Mehl, Gus Hart, Marco Buongiorno Nardelli, Stefano Curtarolo

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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.

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AFLOW Standardization

Default $N_{\text{KPPA}}$ values used in non-BANDS calculations.

<table>
<thead>
<tr>
<th>Database</th>
<th>STATIC</th>
<th>RELAX</th>
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<tbody>
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<td>Heusler</td>
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<td>6000</td>
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<tr>
<td>ICSD</td>
<td>10,000</td>
<td>8000</td>
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Table 4
$U_{\text{eff}}$ Parameters applied to $d$ orbitals.

<table>
<thead>
<tr>
<th>Element</th>
<th>$U_{\text{eff}}$</th>
<th>Refs.</th>
<th>Element</th>
<th>$U_{\text{eff}}$</th>
<th>Refs.</th>
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<tr>
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<td>W</td>
<td>2.2</td>
<td>[39]</td>
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<tr>
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<td>[40]</td>
<td>Tc</td>
<td>2.7</td>
<td>[39]</td>
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<tr>
<td>V</td>
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<td>[41]</td>
<td>Ru</td>
<td>3.0</td>
<td>[39]</td>
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<tr>
<td>Cr</td>
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<td>[42]</td>
<td>Rh</td>
<td>3.3</td>
<td>[39]</td>
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<tr>
<td>Mn</td>
<td>4.0</td>
<td>[42]</td>
<td>Pd</td>
<td>3.6</td>
<td>[39]</td>
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<td>Ag</td>
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<td>[44]</td>
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<tr>
<td>Co</td>
<td>5.0</td>
<td>[41]</td>
<td>Cd</td>
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<td>[45]</td>
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<tr>
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<td>5.1</td>
<td>[41]</td>
<td>In</td>
<td>1.9</td>
<td>[45]</td>
</tr>
<tr>
<td>Cu</td>
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<td>[42]</td>
<td>Sn</td>
<td>3.5</td>
<td>[46]</td>
</tr>
<tr>
<td>Zn</td>
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<td>[39]</td>
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<tr>
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<td>[46]</td>
<td>Au</td>
<td>4.0</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>La</td>
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<td>0.6</td>
<td>[48]</td>
<td>Dy</td>
<td>5.6</td>
<td>0.0</td>
<td>[49]</td>
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<tr>
<td>Ce</td>
<td>7.0</td>
<td>0.7</td>
<td>[50]</td>
<td>Tm</td>
<td>7.0</td>
<td>1.0</td>
<td>[51]</td>
</tr>
<tr>
<td>Pr</td>
<td>6.5</td>
<td>1.0</td>
<td>[52]</td>
<td>Yb</td>
<td>7.0</td>
<td>0.67</td>
<td>[53]</td>
</tr>
<tr>
<td>Nd</td>
<td>7.2</td>
<td>1.0</td>
<td>[18]</td>
<td>Lu</td>
<td>4.8</td>
<td>0.95</td>
<td>[48]</td>
</tr>
<tr>
<td>Sm</td>
<td>7.4</td>
<td>1.0</td>
<td>[18]</td>
<td>Th</td>
<td>5.0</td>
<td>0.0</td>
<td>[54]</td>
</tr>
<tr>
<td>Eu</td>
<td>6.4</td>
<td>1.0</td>
<td>[18]</td>
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<td>4.0</td>
<td>0.0</td>
<td>[55]</td>
</tr>
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<td>0.1</td>
<td>[56]</td>
<td>Dy</td>
<td>5.6</td>
<td>0.0</td>
<td>[49]</td>
</tr>
</tbody>
</table>

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$^a$ 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
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