

Accessing training data: materials data APIs

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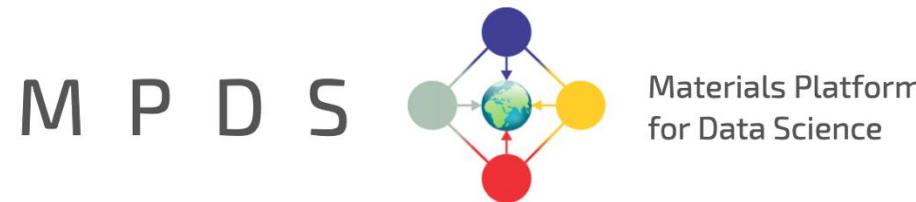
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Accessing online data

- Machine-learning benefits from large quantities of data for training and testing
- Materials data is now available online through websites and programmatically accessible APIs
- Available data includes both experimental (relatively scarce and often requiring license fees) and computational data (relatively plentiful and freely available)
- Experimental materials phase data: Materials Platform for Data Science (commercial):
<https://developer.mpds.io/>



- Experimental materials properties data (e.g. superconductivity): Materials Data Repository:
<https://mdr.nims.go.jp/?locale=en>

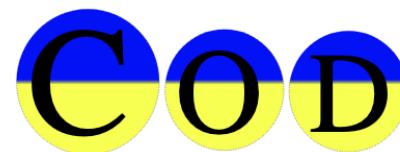


Accessing online data

- Crystallography data:
 - Inorganic Crystal Structure Database (requires purchasing subscription):
<https://icsd.nist.gov/>

NIST Inorganic Crystal Structure Database (ICSD)

- Crystallography Open Database (open-access):
<http://www.crystallography.net/cod/>

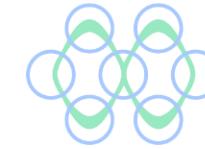


Crystallography Open Database

Accessing online data

- Computational materials data:

- Materials Project: <https://materialsproject.org/>



- AFLOW: <http://aflow.org/>



- OQMD: <https://oqmd.org/>



- Materials Cloud: <https://www.materialscloud.org/>



- Materials Project Descriptor Database: <http://mpdd.phaseslab.com/>

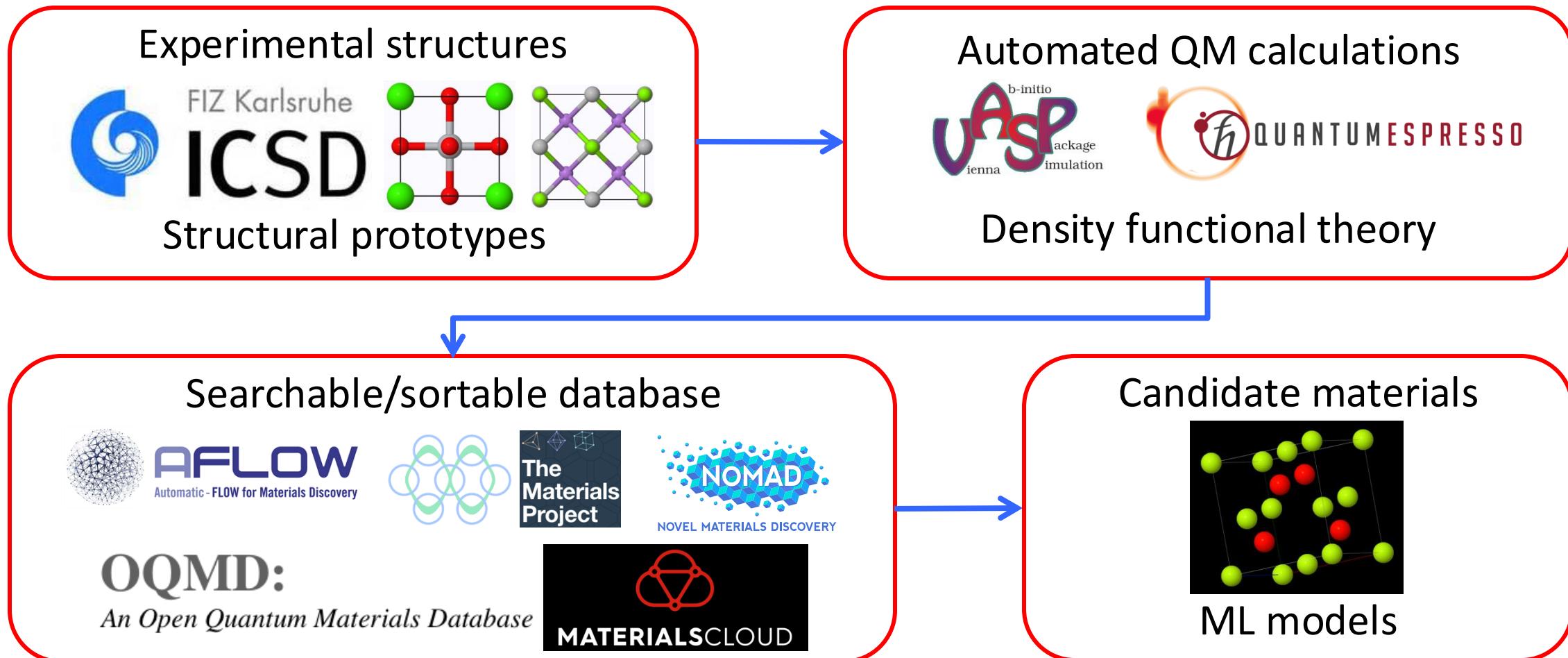
- NOMAD: <https://nomad-lab.eu/>



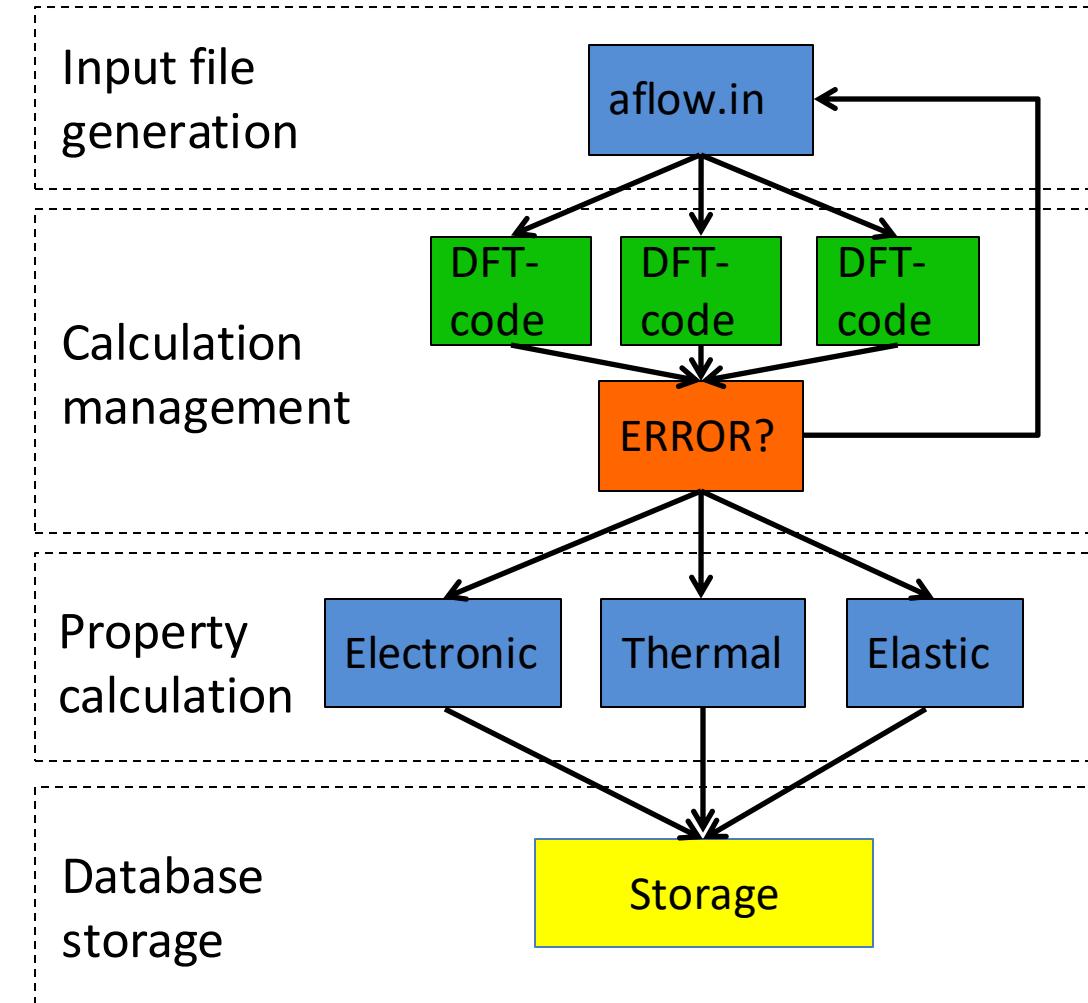
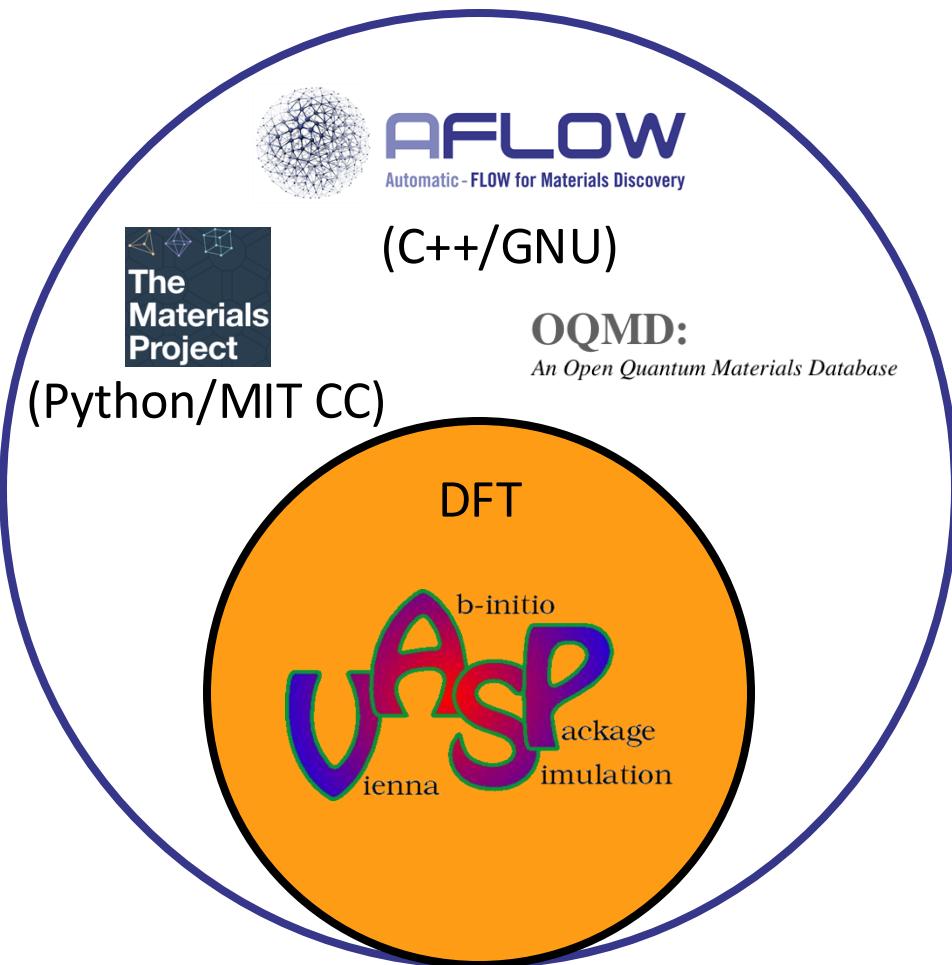
- Common API for materials data: Optimade: <https://www.optimade.org/>



Automated Computational Materials Discovery



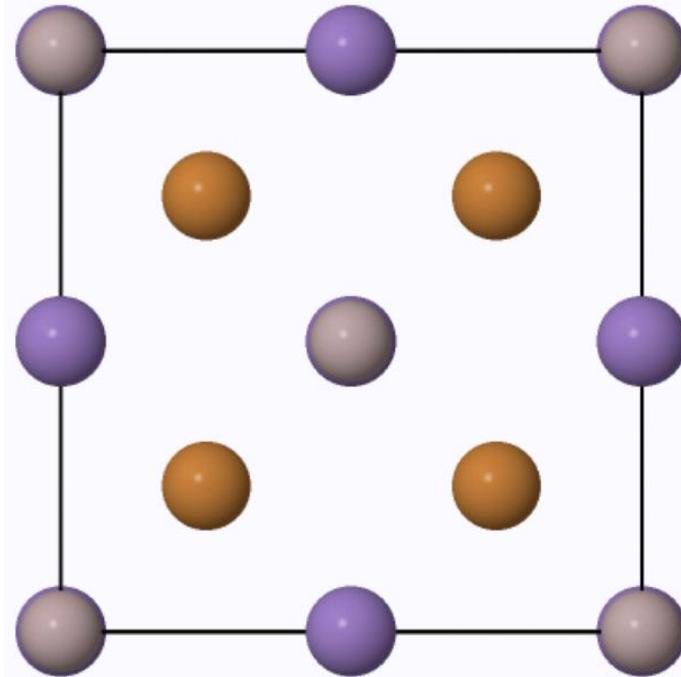
Automated Computational Materials Discovery



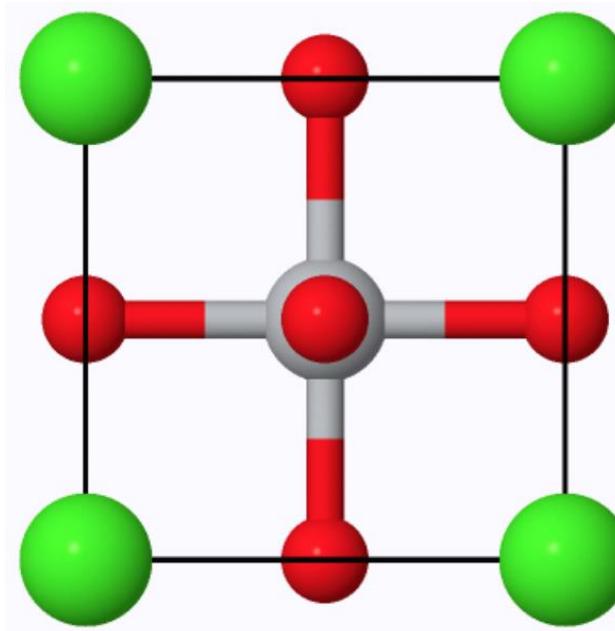
Curtarolo et al., Comput. Mater. Sci. **58**, 218 (2012); Toher et al., “The AFLOW Fleet for Materials Discovery” (2018);
Oses et al., Comput. Mater. Sci. **217**, 111889 (2023)

Crystallographic Prototypes

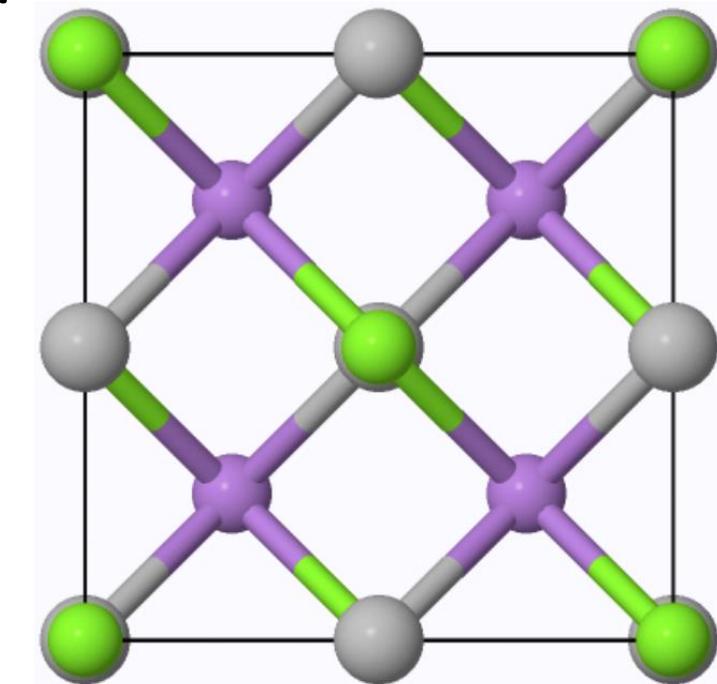
- Search for new materials using structural prototypes:



Heusler structure:
AB₂C_cF16_225_a_c_b



Perovskite structure:
ABC₃_cP5_221_a_b_c



Half-Heusler structure:
ABC_cF12_216_b_c_a

- Decorate prototypes with different elements to generate new hypothetical materials

Mehl et al., Comput. Mater. Sci. **136**, S1-S828 (2017); Hicks et al., Comput. Mater. Sci. **161**, S1-S1011 (2019);
Hicks et al., npj Comput. Mater. **7**, 30 (2021).

AFLOW Web Portal

<https://aflow.org>



HOME | CONSORTIUM | SEMINARS | SCHOOLS | FORUM | SRC

> 700 million properties

AFLOW Schools and Seminars

> 3.5 million entries

breakdown of properties

AFLOW Seminars

AFLOW Schools

Welcome to AFLOW, a globally available database of **3,530,330** material compounds with over **734,308,640** calculated properties, and growing.

3,479,057
form. enthalpies

366,988
band structures

172,488
Bader charges

5,650
elastic properties

5,664
thermal properties

1,738
binary systems

30,289
ternary systems

150,659
quaternary systems

Quick Search

Enter an ICSD Number, [Aflowlib Unique Identifier](#), or advanced search string (e.g. Fe & Si).

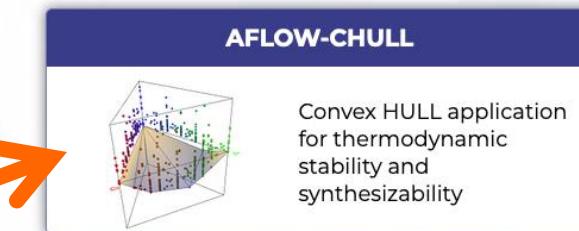
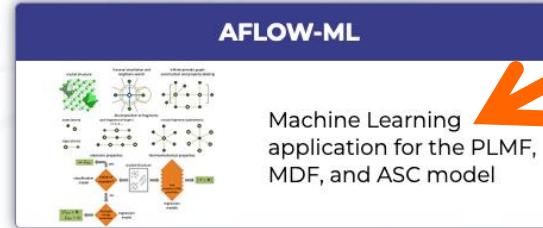
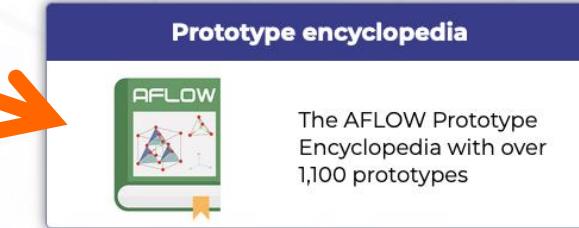
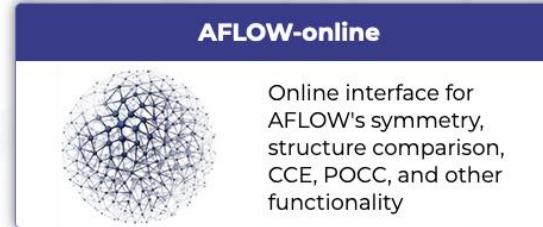
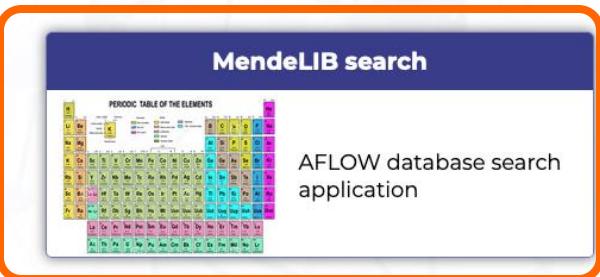
ICSD#, AUID#, search string...

Search

AFLOW Web Portal

Apps and Docs

Crystal
prototype
library



Thermodynamic
stability

ML
application

AFLOW Search Page

The screenshot shows the AFLOW search interface. At the top, there's a navigation bar with links to HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below the navigation is a search bar with options for "ICSD only" and "All AFLOW". A green "Search (60379 entries)" button is on the right, along with a "Display" toggle switch.

The main area features a periodic table with various filters and logic operations overlaid:

- Element group selection:** An orange box labeled "Element group selection" points to the periodic table sections for Metals, Alkali Metals, Alkali Earths, Transition Metals, Lanthanides, Other Metals, Non-Metals, Boron Group, Carbon Group, Pnictogens, Chalcogens, and Halogens.
- Logic operations:** An orange box labeled "Logic operations" points to the logic operators: "and", "not", "or", "xor", and parentheses.
- Number of species:** An orange box labeled "Number of species" points to the "# of species" filter, which includes a dropdown menu set to "=".
- Element selection:** An orange box labeled "Element selection" points to the specific elements As (Arsenic), Sb (Antimony), Te (Tellurium), and Xe (Xenon) highlighted in the periodic table.

At the bottom, logos for Duke University, University at Buffalo, Missouri S&T, NC State University, PennState, NSF, and ONR are displayed, along with the text "Center for Autonomous Materials Design, Materials Science, Duke University".

AFLOW Search Page

The screenshot shows the AFLOW search interface. At the top, there's a navigation bar with links to HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below the navigation bar is a search bar with the placeholder "Search Aflow" and two buttons: "ICSD only" and "All AFLow". To the right of the search bar is a green button labeled "Search (60379 entries)" and a "Display" toggle switch, which is highlighted with a red arrow. The main content area features a large periodic table in the center. Above the periodic table are three sections: "Property Filters" on the left, "Periodic Table" in the middle, and another "Property Filters" section on the right. The "Property Filters" sections contain various filtering options like "and", "not", "or", "xor", and parentheses, along with dropdown menus for "Metals", "Alkali Metals", "Alkali Earths", "Transition Metals", "Lanthanides", "Other Metals", "Non-Metals", "Boron Group", "Carbon Group", "Pnictogens", "Chalcogens", and "Halogens". The "Property Filters" on the right also include a dropdown for "# of species" with options like "2", "He", "Helium", etc. At the bottom of the page, there are logos for Duke University, University at Buffalo, Missouri S&T, NC State University, Penn State, NSF, and ONR.

Slide to Property Filters

Bring property filters onto search page

AFLOW Search Page

The screenshot shows the AFLOW search interface. At the top, there's a navigation bar with links to HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below the navigation is a search bar with dropdowns for "Search Aflow" (set to "ICSD only") and "Display" (set to "All AFLOW"). To the right of the search bar is a green "Search (60379 entries)" button. Below the search area is a "Periodic Table" grid. To the right of the periodic table are several search filters: "and" and "not" operators, a "# of species" dropdown, "or" and "xor" operators, and parentheses. Below these filters is another periodic table grid. At the bottom of the page is a "Property Filters" section with a "Search Properties" input field and a "Clear all" button. This section lists various property categories like Electronic Properties, Magnetic Properties, Mechanical Properties, Thermodynamic Properties, Relaxed Structure, Chemistry, and Calculation Details, each with its own filter options.

Property Filters

Search Properties Clear all

| Electronic Properties | | band gap type | Add |
|--------------------------|--|---|--|
| | | Describes if the system is a metal, a semi-metal, or an insulator with direct or indirect band gap. | <input checked="" type="checkbox"/> Display column <input type="checkbox"/> Restrict value from <input type="text" value="1"/> to <input type="text" value="230"/> |
| Magnetic Properties | | electronic band gap | Add |
| | | Electronic band gap. | <input checked="" type="checkbox"/> Display column <input type="checkbox"/> Restrict value equal to <input type="text"/> |
| Mechanical Properties | | | |
| Thermodynamic Properties | | | |
| Relaxed Structure | | | |
| Chemistry | | | |
| Calculation Details | | | |

AFLOW Search Page

The screenshot shows the AFLOW search interface. At the top, the search bar contains "Na, Cl". Below it, under "ICSD only", there are two buttons: "Search (60379 entries)" and "Display". A search result table is shown with columns for element symbols and names. A filter panel on the right allows specifying the number of species (set to 2) and applying logical operators like "and", "not", "or", and "xor". Below the search bar is a periodic table. A "Property Filters" dialog is open, showing categories like Electronic Properties, Magnetic Properties, Mechanical Properties, Thermodynamic Properties, Relaxed Structure, Chemistry, and Calculation Details. Under Electronic Properties, the "band gap type" filter is selected, with an "Add" button highlighted. The "electronic band gap" filter is also shown, with a checkbox checked and a value range of 0 to 17.6792 eV.

Selected Elements

Number of species=2

Added filter for Egap: electronic band gap

Select “Add” to add filter

Check box to restrict search results to specific value range

AFLOW Search Results

Na , Cl

ICSD only All AFLW

Search
(60389 entries)

Display

Structural Information

Requested Properties

Reset Search

Aflux summons:
`https://aflow.org/API/aflux/?species(Na,Cl),$catalog(ICSD),$nspecies(2),Egap(*),$paging(1,1000)`

Results per page

Select page
1 / 2 / 3 / 4 / 5 / 6 / 7 / 8 / 9 / 10 / 11 / 12 / 13 / 14 / 15 / 16 / 17 / 18 / 19 / 20 / 21 / 22 / 23 / 24 / 25 / 26 / 27 / 28 / 29 / 30 / 31 / 32 / 33 / 34 / 35 / 36 / 37 / 38 / 39 / 40 / 41 / 42 / 43 / 44 / 45 / 46 / 47 / 48 / 49 / 50 / 51 / 52 / 53 / 54 / 55 / 56 / 57 / 58 / 59 / 60 / 61 / 62 / 63 / 64 / 65 / 66 / 67 / 68 / 69 / 70 / 71 / 72 / 73 / 74 / 75 / 76 / 77 / 78 / 79 / 80 / 81 / 82 / 83 / 84 / 85 / 86 / 87 / 88 / 89 / 90 / 91 / 92 / 93 / 94 / 95 / 96 / 97 / 98 / 99 / 100

Found 27 entries

ENTRY
CINa [1354bbef4edd80b3]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.06

[API, Out, JSON]

ENTRY
CINa [18ebb85b07a92f89]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.06

[API, Out, JSON]

ENTRY
CINa [182f848dd10cc403]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.06

[API, Out, JSON]

ENTRY
CINa [1cd71114972d46dd]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.04

[API, Out, JSON]

ENTRY
CINa [2f4b5e32510830a0]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.05

[API, Out, JSON]

ENTRY
CINa [39ab5e62afdb5ac0]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.05

[API, Out, JSON]

ENTRY
CINa [4f19021768a3118a]

space group relaxed
Fm $\bar{3}$ *m* (#225)

Pearson symbol relaxed
cF8

electronic band gap (eV)
5.05

[API, Out, JSON]

↑

AFLOW Search Page: Exercises

1. Use the AFLOW Advanced Search Page to find the electronic band gap of SiC with the zincblende structure (space group 216)
2. Use the AFLOW Advanced Search Page to find the electronic band gap of GaN with the wurtzite structure (space group 186)

Materials Project Web Portal



The Materials Project

Apps About ▾ Community ▾ ML API Login



The Materials Project

Harnessing the power of supercomputing and state-of-the-art methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

Login or Register



MP login

- Materials Project database requires registration/login
- Can login using Google/Facebook/Github/Amazon/Microsoft account

Materials Project Web Portal

The Materials Project

Apps About Community ML API

The Materials Project

Harnessing the power of supercomputing and state-of-the-art methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Start Exploring Materials](#) [Search Materials](#) [Browse Apps](#)

MP Materials Explorer

- Select Materials Explorer application to search for materials

Materials Explorer Application

The screenshot shows the Materials Explorer Application interface. On the left, there is a sidebar with various icons representing other explorer applications. The main search bar has placeholder text "e.g. Li-Fe or Li_xFe or Li₃Fe or mp-19017". Below the search bar is a periodic table with three tabs above it: "Only Elements", "At Least Elements", and "Formula". The "At Least Elements" tab is selected. A tooltip box with an orange border contains the text "Enter elements or chemical formula". Another tooltip box on the right contains the text "Filter by only selected elements, at least elements, or chemical formula". A third tooltip box at the bottom right contains the text "Element selection". Orange arrows point from the sidebar icons to the sidebar, from the search bar placeholder to the search bar, and from the "At Least Elements" tab to the element selection grid.

The Materials Explorer Application interface includes:

- Search Bar:** Enter elements or chemical formula (e.g. Li-Fe or Li_xFe or Li₃Fe or mp-19017)
- Periodic Table Filter:** Select elements to search for materials with **only** these elements. Options include "Only Elements", "At Least Elements", and "Formula".
- Element Selection Grid:** A grid where individual elements can be selected for filtering.
- Sidebar:** Other explorer applications (indicated by icons).

Materials Explorer: Search Results

Filters Reset

- ▶ Composition 1 active
- ▶ Thermodynamics
- ▶ Structural Properties
- ▶ Symmetry
- ▶ Calculated Properties
- ▶ Electronic Structure
- ▶ Magnetism
- ▶ Elasticity
- ▶ Surfaces

Property Filters

13 materials match your search
Showing 1-13

~~×~~ Chemical System: Na-Cl

Columns ▾

| Material ID | Formula | Crystal System | Space Group Symbol | Sites | Energy Above Hull (eV/atom) | Band Gap (eV) |
|-------------|---------------------------------|----------------|----------------------|-------|-----------------------------|---------------|
| ★ mp-22862 | NaCl | Cubic | Fm3m | 2 | 0 | 5.00 |
| mp-1189265 | NaCl ₃ | Orthorhombic | Pnma | 16 | 0 | 2.71 |
| mp-1080771 | NaCl ₇ | Cubic | Pm3 | 8 | 0 | 0.43 |
| mp-1120767 | NaCl | Hexagonal | P6 ₃ /mmc | 12 | 0.06 | 4.38 |
| mp-990084 | Na ₂ Cl | Trigonal | R3m | 3 | 0.10 | 0 |
| mp-1064484 | Na ₃ Cl | Tetragonal | P4/mmm | 4 | 0.14 | 0 |
| mp-1018810 | Na ₂ Cl | Tetragonal | P4/mmm | | 0.14 | 0 |
| ★ mp-22851 | NaCl | Cubic | Pm3m | 2 | 0.15 | 3.97 |
| mp-1069676 | Na ₃ Cl ₂ | Orthorhombic | Cmmm | | | |

Structural Information

NOMAD: Novel Materials Discovery

[NOMAD](#)

[SOLUTIONS](#) ▾ [LEARN](#) ▾ [GET INVOLVED](#) ▾ [ABOUT](#) ▾ [OPEN NOMAD](#)

Search application

NOMAD

Materials science data managed and shared

NOMAD lets you manage and share your materials science data in a way that makes it truly useful to you, your group, and the community. **Free and open source.**

[Open NOMAD →](#)

NOMAD Discord

Join our brand new NOMAD Discord, where you can connect with fellow researchers, share ideas, and get answers.

[Open Discord](#)

USED BY THOUSANDS OF MATERIALS SCIENTISTS

UPLOADED ENTRIES
19,097,756

REPRESENTED MATERIALS
4,335,633

UPLOADED FILES
111.9 TB

 THE UNIVERSITY OF TEXAS AT DALLAS

Erik Jonsson School of Engineering and Computer Science, Department of Materials Science and Engineering 20

NOMAD: Novel Materials Discovery

The screenshot shows the NOMAD software interface. On the left, there is a sidebar with various filters like Material, Elements / Formula, Structure / Symmetry, Method, Precision, DFT, TB, GW, BSE, DMFT, EELS, Workflow, Molecular dynamics, Geometry Optimization, Properties, Electronic, Vibrational, and Mechanical. A red arrow points from the 'Elements / Formula' filter to the periodic table. The periodic table has a green checkmark next to it with the text 'only compositions that exclusively contain these atoms'. A red box labeled 'Element selection' surrounds the periodic table area. In the center, there is a search bar with 'ELEMENTS / FORMULA' and a dropdown set to 'linear'. Below the search bar is a 'Chemical formula hill' section with input fields for 'E.g. H₂O₂, C₂H₅Br' and 'E.g. GaAs, SiC'. To the right, there is a list of entries with columns for 'Upload time' and 'Authors'. A red box labeled 'Search by elements' surrounds the search bar and the periodic table. Another red box labeled 'Return only entries with only these elements' surrounds the green checkmark and the list of entries.

PUBLISH EXPLORE ANALYZE ABOUT

Entries

FILTERS

Material

Elements / Formula

Structure / Symmetry

Method

Precision

DFT

TB

GW

BSE

DMFT

EELS

Workflow

Molecular dynamics

Geometry Optimization

Properties

Electronic

Vibrational

Mechanical

7.5k

ELEMENTS / FORMULA

Elements

linear

only compositions that exclusively contain these atoms

Chemical formula hill

linear

Chemical formula IUPAC

linear

Chemical formula reduced

linear

Chemical formula anonymous

linear

Upload time ↓

Authors

1/2/2025, 4:55:20 AM Cecilia Vona

12/19/2024, 6:12:36 AM Miguel Marques

Element selection

Search by elements

Return only entries with only these elements

NOMAD: Novel Materials Discovery

The screenshot shows the NOMAD interface. On the left is a sidebar with various filters like Material, Elements / Formula, and Method. The main area has a search bar at the top with the placeholder "Type your query or keyword here". Below it is a search interface with buttons for "Exclusive" and "Elements", and a search term "Na AND Cl" with a delete button. There are also buttons for "+ TERMS", "+ HISTOGRAM", "+ SCATTER PLOT", and "+ PERIODIC TABLE". A large orange arrow points from a callout box labeled "Search query" to the search bar. Another orange arrow points from a callout box labeled "Search results" to the list of search results. The results table has columns for Name, Formula, Entry type, Upload time, and Authors. Most entries are for NaCl simulations, while one is for NaCl3.

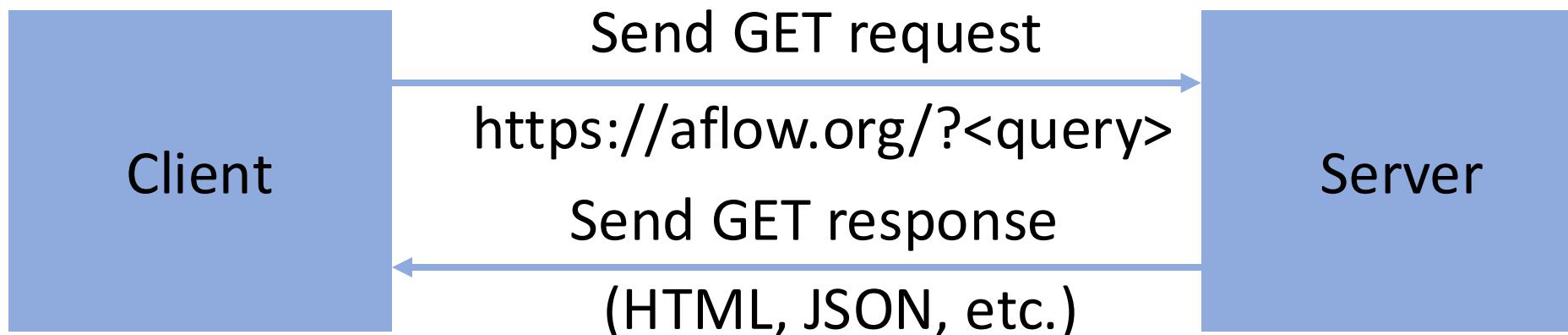
| Name | Formula | Entry type | Upload time | Authors |
|--|---------|---------------------------|------------------------|----------------|
| NaCl exciting DFT SinglePoint simulation | CINa | exciting DFT SinglePoint | 1/2/2025, 4:55:20 AM | Cecilia Vona |
| NaCl exciting DFT SinglePoint simulation | CINa | exciting DFT SinglePoint | 1/2/2025, 4:55:20 AM | Cecilia Vona |
| NaCl exciting DFT SinglePoint simulation | CINa | exciting DFT SinglePoint | 1/2/2025, 4:55:20 AM | Cecilia Vona |
| NaCl exciting DFT SinglePoint simulation | CINa | exciting DFT SinglePoint | 1/2/2025, 4:55:20 AM | Cecilia Vona |
| NaCl exciting DFT SinglePoint simulation | CINa | exciting DFT SinglePoint | 1/2/2025, 4:55:20 AM | Cecilia Vona |
| NaCl exciting DFT SinglePoint simulation | CINa | exciting DFT SinglePoint | 1/2/2025, 4:55:20 AM | Cecilia Vona |
| NaCl3 VASP GeometryOptimization simulation | Cl6Na2 | VASP GeometryOptimization | 12/19/2024, 6:12:36 AM | Miguel Marques |
| NaCl3 VASP GeometryOptimization simulation | Cl6Na2 | VASP GeometryOptimization | 12/19/2024, 6:12:36 AM | Miguel Marques |
| NaCl3 VASP DFT SinglePoint simulation | Cl6Na2 | VASP DFT SinglePoint | 12/19/2024, 6:12:36 AM | Miguel Marques |
| | Cl6Na2 | VASP GeometryOptimization | 12/19/2024, 6:12:36 AM | Miguel Marques |

Accessing online data

- Specific materials or molecules can be searched for directly using web portals
- However, machine-learning models often require large data sets for training on
- Therefore, it is useful to be able to search for and download data programmatically
- This is performed through an Application Programming Interface (API)
- Examples: Materials Project API (for Materials Project API); AFLUX (for AFLOW database: aflow.org); AiiDA (for Materials Cloud); Optimade API (common API to enable access to multiple databases)

Accessing online data: REST-API

- REST-API: Representational State Transfer Application Programming Interface
- In response to a client request, the API transfers a representation of the current state (e.g. current version of a section of a database) to the client
- Commonly used methods: GET (retrieve data from server), POST (post data to server)



Accessing online data: REST-API

Accessing online data: REST-API

- Use Python to submit GET request:

```
import modules for JSON, sys, os  
import json, sys, os  
from urllib.request import urlopen  
  
Import modules for urlopen  
Server path  
SERVER="https://" + <server> + "?"  
Search query  
QUERY=<query>  
URI  
EXAMPLE_URI = SERVER + QUERY  
Submit URI with query  
  
response=json.loads(urlopen(EXAMPLE_URI).read().decode("utf-8"))  
print(response)  
Read/decode JSON response  
Convert to dictionary-like object  
Print dictionary-like object
```

AFLUX: AFLOW Search API

`https://aflow.org/API/aflux/?<matchbook>, <directives>`

Search API Server

Query

Matchbook

- Materials keywords with arguments
- Keyword list is available from the help directive:

Directives

- Formatting instructions with arguments
- Available directives:
 - format: json (default) or html
 - paging: Controls number of entries and page displayed

[https://aflow.org/API/aflux/?help\(properties\)](https://aflow.org/API/aflux/?help(properties))

<https://aflow.org/API/aflux/?schema>

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

AFLUX: AFLOW Search API

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

| Logical operator | AFLUX syntax | Operator scope |
|----------------------|---------------------------|---------------------------|
| <block> (precedence) | "(" 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 |

AFLUX: AFLOW Search API

- Common keywords:

species: chemical species (usually element symbols)

nspecies: number of different species in compound

Egap: electronic band gap

spacegroup_relax: Space group of relaxed structure

aflow_prototype_label_relax: AFLOW prototype label (structure type) of relaxed structure

- Example: NaCl or KCl with an electronic band gap of at least 5 eV

`https://aflow.org/API/aflux/?species ((Na:K),Cl),nspecies(2),Egap(5*)`

server

(Na OR K) AND Cl

Number of
species == 2

Band gap
> 5eV

AFLUX: AFLOW Search API

- Data is returned in JSON format: JavaScript Object Notation
- JSON files can be read in and converted to Python dictionaries:

```
import json  
response_dict = json.load(response)
```

- Results are sorted in ascending order of first keyword in query
- Example: to sort in order of band gap:

[https://aflow.org/API/aflux/?Egap\(5*\),species\(\(Na:K\),Cl\),nSpecies\(2\)](https://aflow.org/API/aflux/?Egap(5*),species((Na:K),Cl),nSpecies(2))

AFLUX: AFLOW Search API

- Example: NaCl or KCl with an electronic band gap of at least 5eV

```
https://aflow.org/API/aflux/?species((Na:K),Cl),nspecies(2),  
Egap(5*)
```

```
import json, sys, os  
from urllib.request import urlopen
```

Import modules for JSON, sys, os
Import modules to open URLs

```
SERVER="https://aflow.org"  
API="/API/aflux??"
```

AFLOW server
AFLUX API

```
MATCHBOOK="species((Na:K),Cl),nspecies(2),Egap(5*)"
```

AFLUX matchbook

```
DIRECTIVES="$paging(0)"
```

AFLUX directives

```
SUMMONS=MATCHBOOK+","+DIRECTIVES
```

AFLUX query

```
response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))  
print(response)
```

Submit query, retrieve json, convert to Python dictionary
Print Python dictionary

AFLUX: AFLOW Search API

- Example: NaCl or KCl with an electronic band gap of at least 5eV

```
https://aflow.org/API/aflux/?species((Na:K),Cl),nspecies(2),Egap(5*)
```

Programmatically searching for data using AFLUX API: search for NaCl or KCl with an electronic band gap greater than 5eV

```
✓ 5s  ➡ https://aflow.org/API/aflux/?species((Na:K),Cl),nspecies(2),Egap(5*)
```

```
import json, sys, os
from urllib.request import urlopen

SERVER="https://aflow.org"
API="/API/aflux/?"
MATCHBOOK="species((Na:K),Cl),nspecies(2),Egap(5*)"
DIRECTIVES="$paging(0)"
SUMMONS=MATCHBOOK+","+DIRECTIVES

print(SERVER+API+SUMMONS)

response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))
print(response)
```

```
→ https://aflow.org/API/aflux/?species((Na:K),Cl),nspecies(2),Egap(5*),$paging(0)
[{'compound': 'Cl1K1', 'auid': 'aflow:04b2e3ac1bd9b49b', 'aurl': 'aflowlib.duke.edu:AFL0WDATA/ICSD_WEB/FCC/Cl1K1_ICSD_240523'},
```

AFLUX: AFLOW Search API

- Example: NaCl or KCl with an electronic band gap of at least 5eV
- Parse output: print chemical formula and band gap

```
response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))
for datum in response: ← Loop over entries in dictionary
    bandgap=[float(datum['Egap'])] ← Extract band gap
    compound=[str(x) for x in datum['compound'].split(",")]
    print ("{}, {}".format(compound, bandgap)) ← Extract compound
    ← Print data
```

AFLUX: AFLOW Search API

- Example: NaCl or KCl with an electronic band gap of at least 5eV
- Parse output: print chemical formula and band gap

Parse JSON response: print chemical formula and electronic band gap

```
✓ 4s
  import json, sys, os
  from urllib.request import urlopen

  SERVER="https://afflow.org"
  API="/API/afflux/?"
  MATCHBOOK="species((Na:K),Cl),nspecies(2),Egap(5*)"
  DIRECTIVES="$paging(0)"
  SUMMONS=MATCHBOOK+","+DIRECTIVES

  response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))
  for datum in response:
    bandgap=[float(datum['Egap'])]
    compound=[str(x) for x in datum['compound'].split(",")]
    print ("{} , {}").format(compound, bandgap))

  ['Cl1K1'], [5.0487]
  ['Cl1K1'], [5.0534]
  ['Cl1K1'], [5.0547]
  ['Cl1K1'], [5.0529]
```

AFLUX: AFLOW Search API

- Directives: paging – control page number and number of entries per page: useful to limit amount of data returned at once to avoid overloading browser/computer
- “Page” is set of data returned at a time; “**paging(0)**” returns all data
- Paging takes two arguments: first is page number “**n**”, second is number of entries per page “**m**”: **paging(n,m)**
- Example: return first page with 10 entries per page: **paging(1,10)**
- Negative page number reverses sort order: **paging(-1,10)**

AFLUX: AFLOW Search API

- Example: NaCl or KCl with an electronic band gap of at least 5eV: first page of 10 entries

Paging: print first page of 10 entries per page

```
▶ import json, sys, os
  from urllib.request import urlopen

  SERVER="https://aflow.org"
  API="/API/aflux/?"
  MATCHBOOK="species((Na:K),Cl),nspecies(2),Egap(5*)"
  DIRECTIVES="$paging(1,10)"
  SUMMONS=MATCHBOOK+","+DIRECTIVES

  response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))
  for datum in response:
    bandgap=[float(datum['Egap'])]
    compound=[str(x) for x in datum['compound'].split(",")]
    print ("{}, {}".format(compound, bandgap))

⇒ ['Cl1K1'], [5.0427]
  ['Cl1K1'], [5.0482]
  ['Cl1K1'], [5.0422]
```

AFLUX: AFLOW Search API

- Example: search for materials containing C, Si, Ge, Sn, but not Pb:

```
<API>/?species( (C:Si:Ge:Sn) , !Pb) , $paging(1,64)
```

C or Si or Ge or Sn

NOT Pb

First page of 64 entries

Search for materials containing C, Si, Ge or Sn but not Pb

```
[2] import json, sys, os
18s   from urllib.request import urlopen

      SERVER="https://aflow.org"
      API="/API/aflux/?"
      MATCHBOOK="species((C:Si:Ge:Sn),!Pb)"
      DIRECTIVES="$paging(1,10)"
      SUMMONS=MATCHBOOK+" "+DIRECTIVES

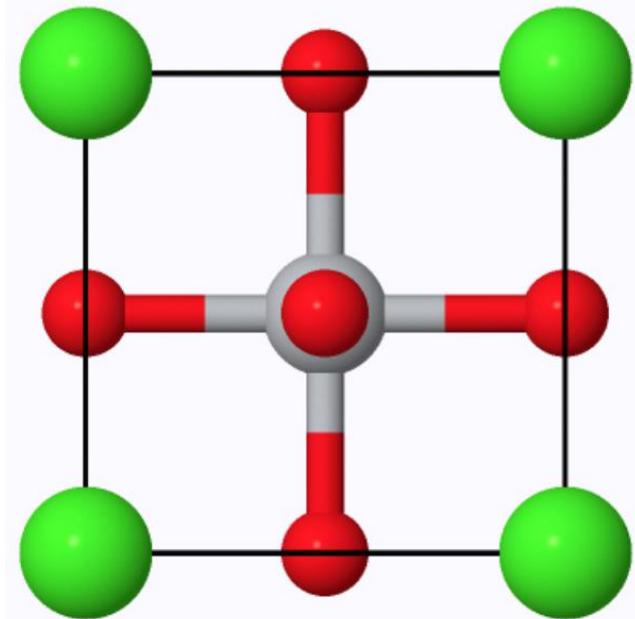
      print(SERVER+API+SUMMONS)

      response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))
      print(response)

https://aflow.org/API/aflux/?species\(\(C:Si:Ge:Sn\),!Pb\),\$paging\(1,10\)
[{'compound': 'Ag1Al1Au1Sn1', 'auid': 'aflow:4389c382c27f3f50', 'aurl': 'aflowlib.duke.edu:AFL0WDATA/LIB4_RAW/AgAlAuSn:PAW_PBE/ABCD_cF16_216_c_d_b_a.ABCD',
```

AFLUX: Structure Type Search

- Prototype labels:



Perovskite structure:

ABC₃_cP5_221_a_b_c

Pearson
Composition

Space group

Wyckoff positions

- Search for NaCl in rocksalt structure:
prototype label is “AB_cF8_225_a_b”

```
<API>/?species(Na,Cl),nspecies(2),  
aflow_prototype_label_relax(AB_cF8_225_a_b)
```

Search for NaCl in rocksalt structure: prototype label is AB_cF8_225_a_b

```
3s import json, sys, os  
from urllib.request import urlopen  
  
SERVER="https://aflow.org"  
API="/API/aflux/?"  
MATCHBOOK="species(Na,Cl),nspecies(2),aflow_prototype_label_relax(AB_cF8_225_a_b)"  
DIRECTIVES="$paging(0)"  
response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))  
print(response)  
  
[{"compound": "Cl1Na1", "auid": "aflow:39ab5e62afdb5ac0", "aurl": "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/FCC/Cl1Na1_ICSD_622369"},
```

Mehl et al., Comput. Mater. Sci. **136**, S1-S828 (2017);
Hicks et al., Comput. Mater. Sci. **161**, S1-S1011 (2019);
Hicks et al., npj Comput. Mater. **7**, 30 (2021).

AFLUX: AFLOW Search API

- Example: use AFLOW-specific keywords to search for lead-free cubic halide perovskites with a band gap greater than 3 eV

```
<API>/?species( (F:Cl:Br:I) , !Pb) , nspecies(3) ,  
aflow_prototype_label_relax(ABC3_cP5_221_a_b_c) , Egap(3*)
```

Search for lead-free halide perovskites with band-gap greater than 3eV

```
[5] import json, sys, os  
18s   from urllib.request import urlopen  
  
 SERVER="https://aflow.org"  
 API="/API/aflux/?"  
 MATCHBOOK="species((F:Cl:Br:I),!Pb),nspecies(3),aflow_prototype_label_relax(ABC3_cP5_221_a_b_c),Egap(3*)"  
 DIRECTIVES="$paging(0)"  
 SUMMONS=MATCHBOOK+","+DIRECTIVES  
  
 response=json.loads(urlopen(SERVER+API+SUMMONS).read().decode("utf-8"))  
 print(response)  
  
[{'compound': 'Ag1Be1F3', 'auid': 'aflow:aa197e3461543939', 'aurl': 'aflowlib.duke.edu:AFLOWDATA/LIB3_RAW/AgBe_svF/T0009.ABC:LDAU2',
```

- Can also use “Halogens” to search for group of elements

```
<API>/?species(Halogens, !Pb) , nspecies(3) ,  
aflow_prototype_label_relax(ABC3_cP5_221_a_b_c) , Egap(3*)
```

AFLOW Search Page: Exercises

1. Use the AFLUX API to find the VRH bulk moduli (“ael_bulk_modulus_vrh”) for materials containing Ti in the AFLOW database. What is the material with the highest bulk modulus? What is the space group of this material? Is it a metal or an insulator (“Egap_type”)?
2. Use the AFLUX API to find the electronic band gaps (“Egap”) for all rocksalt structure (“AB_cF8_225_a_b”) alkali halide (“AlkaliMetals”, “Halogens”) materials in the AFLOW database. How many entries are returned?

Materials Project API

- Materials Project uses MPRester API
- Special client needs to be downloaded and installed (not available through Colab):
`pip install mp-api`
`from mp_api.client import MPRester`
- Materials Project uses a “document-based” database (MongoDB); data is returned as document objects
- Materials Project API also requires an API key (related to your login/registration on MP website)
- To use pip in Colab: `!pip install mp-api`

Materials Project API

- MP API key available at: <https://next-gen.materialsproject.org/api>

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API Key

Your API Key

<your-API-key-here>

To make any request to the Materials Project API, you must use an API key. Your API key is generated for you automatically upon registering with the Materials Project website and is synced with the email you used to register.

Remember to keep your API key safe and to not share it with anyone you do not trust.

If you are logged in, you can always access your API key from this page or from your [dashboard](#).

If you intend heavy API usage, you can give us a heads up by sending a message to heavy.api.use@materialsproject.org. This is not required, but may help us if we see unusual load on our servers. For large and/or long-running queries, we ask that you please make a local copy and only retrieve the data once.

- MP API key will be alphanumeric string unique to your account on Materials Project

Materials Project API

- MPRester API usage example: search for Si-O compounds with band gap between 0.5 and 1.0 eV:

```
with MPRester("<your_api_key_here>") as mpr:
```

```
    docs = mpr.summary.search(elements=["Si", "O"], band_gap=(0.5, 1.0))
```

Compositions with Si and O

Band gap between 0.5eV and 1.0eV

- This will return all data associated with the entries satisfying this query. To restrict returned data to specific attributes, use “fields”:

```
with MPRester("<your_api_key_here>") as mpr:
```

```
    docs = mpr.summary.search(elements=["Si", "O"], band_gap=(0.5, 1.0),  
        fields=["material_id", "band_gap", "volume"])
```

Return only this data

Materials Project API

```
▶ !pip install mp-API
from mp_api.client import MPRester

with MPRester("<your-api-key-here>") as mpr:
    docs = mpr.summary.search(elements=["Si", "O"], band_gap=(0.5, 1.0), fields=["material_id", "band_gap", "volume"])
    print(docs)

[{"volume": 1013.9709061448139, "material_id": MPID(mp-1224617), "band_gap": 0.8252000000000002, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}, {"volume": 695.498126677145, "material_id": MPID(mp-1227528), "band_gap": 0.7827999999999999, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}, {"volume": 946.9207311486335, "material_id": MPID(mp-1224625), "band_gap": 0.9364999999999999, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}, {"volume": 1881.884702293924, "material_id": MPID(mp-686232), "band_gap": 0.5483, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}, {"volume": 995.8436795717986, "material_id": MPID(mp-1203093), "band_gap": 0.7426, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}, {"volume": 2313.151551863883, "material_id": MPID(mp-1229169), "band_gap": 0.6122000000000001, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}, {"volume": 957.6037554914742, "material_id": MPID(mp-1173853), "band_gap": 0.9215, "fields_not_requested": ["builder_meta", "nsites", "elements", "nelements", "composition", "composition_reduced", "formula_pretty", "formula_anonymous", "chemsys", "density", "density_atomic", "symmetry", "property"]}]
```

Materials Project API

- Important keywords:
`elements`: chemical elements in composition
`band_gap`: electronic band gap
`material_id`: Materials Project ID for material
`volume`: cell volume
- Can also download all data for a particular entry using its MP ID:
`with MPRester("<your_api_key_here>") as mpr:`
 `data = mpr.materials.get_data_by_id("mp-22862")`
- More information: <https://docs.materialsproject.org/downloading-data/how-do-i-download-the-materials-project-database>

Optimade: Common Materials Search API

- Rapid expansion of Materials Databases and APIs creates issues with having to learn a new API for each database
- Therefore, efforts are being made to implement common APIs and standards
- Optimade Common API is an API developed by the Optimade consortium:
<https://www.optimade.org/>
- Current full Optimade specification:
<https://github.com/Materials-Consortia/OPTIMADE/blob/master/optimade.rst>

C. Anderson et al., Sci. Data **8**, 217 (2021).

Optimade: Common Materials Search API

- Databases supporting Optimade include: optimade.org/providers-dashboard/
 - AFLOW: aflow.org/API/optimade/v1
 - Alexandria: alexandria.icams.rub.de/pbe/v1/
 - Computational Materials Repository: <https://cmrdb.fysik.dtu.dk>
 - COD: Crystallography Open Database: crystallography.net/cod/optimade
 - Jarvis: jarvis.nist.gov
 - NoMaD: nomad-lab.eu/prod/rae/optimade/
 - Materials Cloud: materialscloud.org/optimade/
 - Materials Platform for Data Science: api.mpds.io
 - Materials Project: optimade.materialsproject.org
 - OQMD: oqmd.org/optimade/
- Full current list is available at: optimade.org/providers-dashboard/

Optimade: Common Materials Search API

- Optimade supports several logical operators:
 - Basic Boolean operations: “AND”, “OR”, “NOT”
 - Numeric and string comparisons: “<”, “>”, “=”, “<=”, “>=”, “!=”
 - Substring comparisons: “CONTAINS”, “STARTS WITH”, “ENDS WITH”
 - List comparisons: “HAS”, “HAS ALL”, “HAS ANY” “HAS ONLY”, “LENGTH”
- Optimade keywords:
 - “**elements**”: list of elements to query
 - “**nelements**”: number of elements
- Optimade endpoints: **structures, calculations**

C. Anderson et al., Sci. Data **8**, 217 (2021).

Optimade: Common Materials Search API

- Optimade query URI has the following structure:

```
<scheme>://<authority>/<path>/<endpoint>?filter=<query>
```

server endpoint query

- Example: Optimade API on AFLOW, search for materials containing Ti:
 - Server scheme/authority/path: <https://aflow.org/API/optimade/v1/>
 - Structures endpoint: **structures**
 - Query: **elements HAS “Ti”**
 - Full URI:
[https://aflow.org/API/optimade/v1/structures?filter=elements HAS “Ti”](https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20%22Ti%22)

C. Anderson et al., Sci. Data 8, 217 (2021).

Optimade: Common Materials Search API

JSON Raw Data Headers

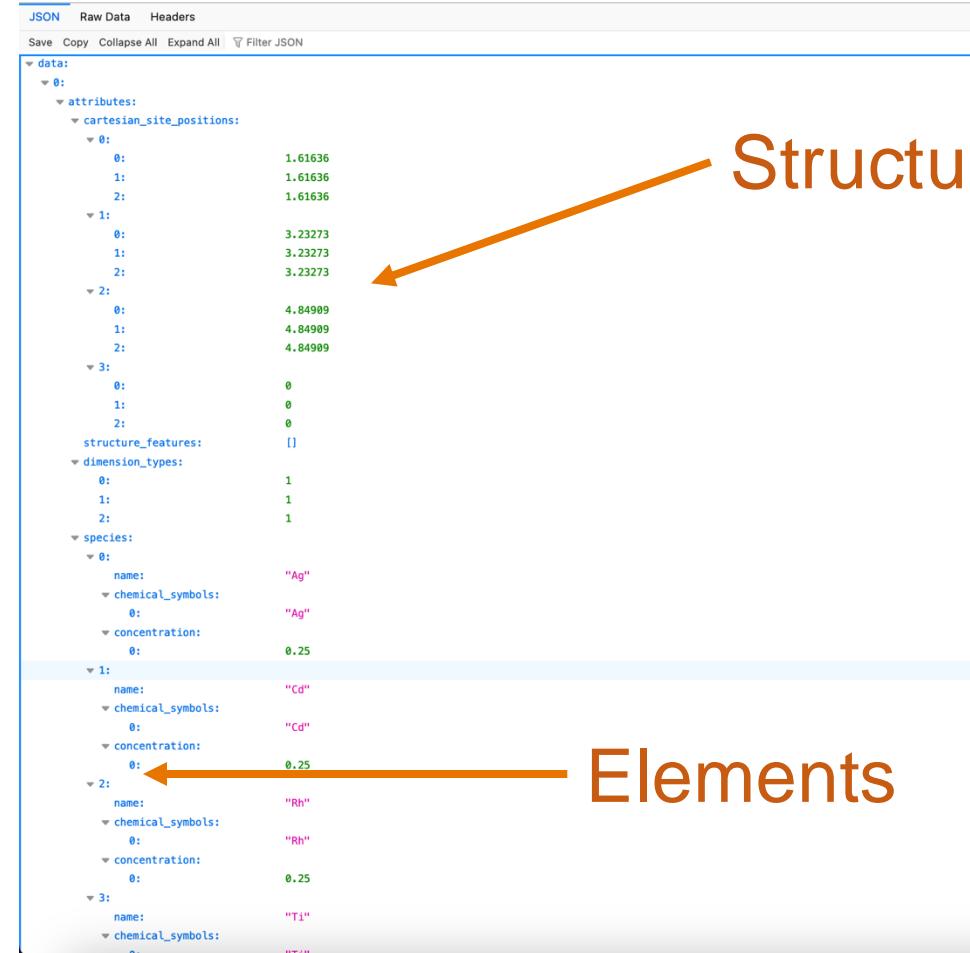
Save Copy Collapse All Expand All Filter JSON

▶ data: [...] ← Materials data

meta:
query:
representation: "/v1/structures?filter=elements%20HAS%20ONLY%20%22Ti%22"
api_version: "1.0.0"
schema: "<https://schemas.optimade.org/openapi/v1.0.0/optimade.json>"
time_stamp: "2024-02-25T01:35:40Z"
more_data_available: true
provider:
name: "AFLLOW"
description: "Automatic-FLOW (AFLLOW) Computational Materials Data Repository"
prefix: "aflow"
homepage: "<https://aflow.org>"
implementation:
name: "aflow-optimade-ng"
version: "ada0d743"
source_url: "<https://aflow.org/install-aflow>"
maintainer:
email: "optimade@aflowlib.duke.edu"
issue_tracker: "<https://groups.io/g/aflow>"
_aflux_aflux_query: "[http://aflow.org/API/aflux/?auid,aflowlib_date,composition,compound,natoms,nspecies,positions_cartesian,species,stoichiometry,paging\(1,100\),format\(json\)](http://aflow.org/API/aflux/?auid,aflowlib_date,composition,compound,natoms,nspecies,positions_cartesian,species,stoichiometry,paging(1,100),format(json))"
data_available: 3530330 ← Links
data_returned: 3530330 ← Total data available
links:
first: 'https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20ONLY%20%22Ti%22&page_number=1&page_limit=100'
next: 'https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20ONLY%20%22Ti%22&page_number=2&page_limit=100'

Optimade: Common Materials Search API

- Example: Optimade API on AFLOW, search for materials containing Ti:
[https://aflow.org/API/optimade/v1/structures?filter=elements HAS "Ti"](https://aflow.org/API/optimade/v1/structures?filter=elements HAS 'Ti')



The screenshot shows a JSON API response from the Optimade API on AFLOW. The response is a list of materials, each represented by a 'data' object. The 'data' object contains various attributes such as 'cartesian_site_positions', 'structure_features', 'dimension_types', and 'species'. The 'species' attribute is expanded to show individual elements with their names ('Ag', 'Cd', 'Rh', 'Ti') and chemical symbols ('Ag', 'Cd', 'Rh', 'Ti'). Two orange arrows point from the text 'Structural data' and 'Elements' to the respective parts of the JSON structure.

```
JSON Raw Data Headers
Save Copy Collapse All Expand All Filter JSON

data:
  0:
    attributes:
      cartesian_site_positions:
        0:
          0: 1.61636
          1: 1.61636
          2: 1.61636
        1:
          0: 3.23273
          1: 3.23273
          2: 3.23273
        2:
          0: 4.84989
          1: 4.84989
          2: 4.84989
        3:
          0: 0
          1: 0
          2: 0
      structure_features: []
    dimension_types:
      0: 1
      1: 1
      2: 1
    species:
      0:
        name: "Ag"
        chemical_symbols:
          0: "Ag"
        concentration:
          0: 0.25
      1:
        name: "Cd"
        chemical_symbols:
          0: "Cd"
        concentration:
          0: 0.25
      2:
        name: "Rh"
        chemical_symbols:
          0: "Rh"
        concentration:
          0: 0.25
      3:
        name: "Ti"
        chemical_symbols:
          0: "Ti"
```

Optimade: Common Materials Search API

- Optimade syntax contains reserved characters: e.g. spaces, quotation marks
- These need to be escaped with some browsers and with Python urllib library to avoid errors
- Replace space with "%20"; replace quotation marks with "%22"
- Example: Optimade API on AFLOW, search for materials containing Ti:
<https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20%22Ti%22>



Replace space with %20
Replace " with %22

Optimade: Common Materials Search API

- Example: Using Python to query AFLOW using Optimade API, search for materials containing Ti:

[https://aflow.org/API/optimade/v1/structures/?filter=elements HAS “Ti”](https://aflow.org/API/optimade/v1/structures/?filter=elements HAS ‘Ti’)

Programmatically retrieving data using the Optimade Common API

Search AFLOW for materials with element Ti

```
[2] import json, sys, os
    from urllib.request import urlopen

    SERVER='https://aflow.org'
    API='/API/optimade/v1/structures?'
    FILTER='filter=elements%20HAS%20%22Ti%22'

    print(SERVER+API+FILTER)

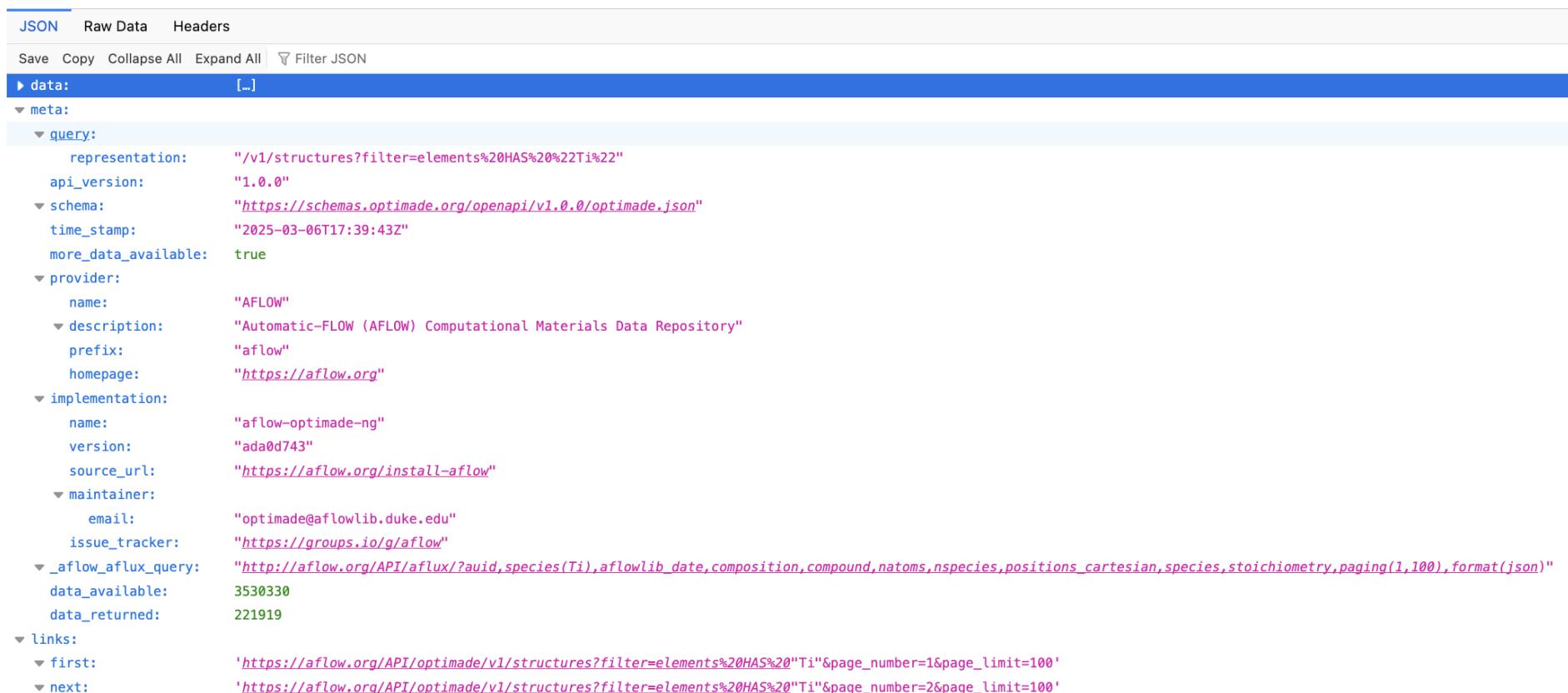
    response=json.loads(urlopen(SERVER+API+FILTER).read().decode("utf-8"))
    print(response)

https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20%22Ti%22
{'data': [{}'attributes': {'cartesian_site_positions': [[1.61636, 1.61636, 1.61636], [3.23273, 3.23273, 3.23273], [4.84909, 4.84909, 4.84909], [0, 0, 0]]},
```

Optimade: Common Materials Search API

- Example: Using Python to query AFLOW using Optimade API, search for materials containing Ti:

[https://aflow.org/API/optimade/v1/structures/?filter=elements HAS "Ti"](https://aflow.org/API/optimade/v1/structures/?filter=elements HAS \)



The screenshot shows a JSON viewer interface with the following details:

- Header tabs: JSON, Raw Data, Headers.
- Toolbar: Save, Copy, Collapse All, Expand All, Filter JSON.
- JSON Structure:
 - data:** [...] (highlighted in blue)
 - meta:**
 - query:**
 - representation: "/v1/structures?filter=elements%20HAS%20%22Ti%22"
 - api_version: "1.0.0"
 - schema:** "https://schemas.optimade.org/openapi/v1.0.0/optimade.json"
 - time_stamp: "2025-03-06T17:39:43Z"
 - more_data_available: true
 - provider:**
 - name: "AFLOW"
 - description:** "Automatic-FLOW (AFLOW) Computational Materials Data Repository"
 - prefix: "aflow"
 - homepage: "https://aflow.org"
 - implementation:**
 - name: "aflow-optimade-ng"
 - version: "ada0d743"
 - source_url: "https://aflow.org/install-aflow"
 - maintainer:**
 - email: "optimade@aflowlib.duke.edu"
 - issue_tracker: "https://groups.io/g/aflow"
 - _aflow_aflux_query:** "http://aflow.org/API/aflux/?auid,species(Ti),aflowlib_date,composition,compound,natoms,nspecies,positions_cartesian,species,stoichiometry,paging(1,100),format(json)"
 - data_available:** 3530330
 - data_returned:** 221919
 - links:**
 - first:** "https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20%22Ti%22&page_number=1&page_limit=100"
 - next:** "https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20%22Ti%22&page_number=2&page_limit=100"

Optimade: Common Materials Search API

- Example: Using Python to query NOMAD using Optimade API, search for materials containing Ti and O only:

[https://nomad-lab.eu/prod/rae/optimade/structures?filter=elements HAS ONLY "Ti", "O"](https://nomad-lab.eu/prod/rae/optimade/structures?filter=elements HAS ONLY \)

Search Nomad for materials containing only Ti and O

```
✓ 2s ⏎ import json, sys, os
    from urllib.request import urlopen

    SERVER='https://nomad-lab.eu'
    API='/prod/rae/optimade/structures?'
    FILTER='filter=elements%20HAS%20ONLY%20%22Ti%22'

    print(SERVER+API+FILTER)

    response=json.loads(urlopen(SERVER+API+FILTER).read().decode("utf-8"))
    print(response)

→ https://nomad-lab.eu/prod/rae/optimade/structures?filter=elements%20HAS%20ONLY%20%22Ti%22
{'data': [{id: 'kA1ZbAWVgKlBpBU4FzWgbglu1gbJ', type: 'structures', attributes: {immutable_id: 'kA1ZbAWVgKlBpBU4FzWgbglu1gbJ',
```

Optimade: Common Materials Search API

- Example: Using Python to query NOMAD using Optimade API, search for materials containing Ti and O only:

<https://nomad-lab.eu/prod/rae/optimade/structures?filter=elements HAS ONLY "Ti", "O">

JSON Raw Data Headers

Save Copy Collapse All Expand All (slow) Filter JSON

▶ data: [...]

▼ meta:

- ▶ query: {...}
- api_version: "1.0.1"
- more_data_available: true
- time_stamp: "2024-02-25T01:51:54Z"
- data_returned: 904
- ▶ provider: {...}
- data_available: 10000
- ▶ implementation: {...}
- included: []
- ▶ links: {...}

JSON Raw Data Headers

Save Copy Collapse All Expand All (slow) Filter JSON

data:

0:

- id: "kA1zbAWgK1BpBU4FzWgbglu1gbJ"
- type: "structures"
- attributes:
 - immutable_id: "kA1zbAWgK1BpBU4FzWgbglu1gbJ"
 - last_modified: "2022-04-25T14:08:37Z"
 - elements: 2
 - elements_ratios:
 - chemical_formula_descriptive: "0108Ti108"
 - chemical_formula_reduced: "0108Ti108"
 - chemical_formula_hill: "0108Ti108"
 - chemical_formula_anonymous: "A108B108"
 - dimension_types:
 - nperiodic_dimensions: 3
 - lattice_vectors: [...]
 - cartesian_site_positions:
 - nsites: 216
 - species: [...]
 - species_at_sites:
 - structure_features:
 - _nmd_dft_crystal_system: "unavailable"
 - _nmd_dft_quantities: [...]
 - _nmd_calc_hash: "7GGNECBYVPFg4I8mnIPPCBXZYATY"
 - _nmd_files:
 - _nmd_dft_system: "unavailable"
 - _nmd_only_atoms: "0Ti"
 - _nmd_dft_code_name: "FHI-aims"
 - _nmd_dft_spacegroup: -1
 - _nmd_raw_id: "E700D13F-9E44-44A0-AA8B-BEF975FE47F9"
 - _nmd_nomad_version: "0.10.11"
 - _nmd_external_id: null
 - _nmd_dft_n_geometries: 1
 - _nmd_last_edit: null
 - _nmd_dft_basis_set: "numeric AOs"
 - _nmd_external_db: null

Total data
returned for this
request

Optimade: Common Materials Search API

- Example: search AFLOW for materials containing C, Si, Ge, Sn, but not Pb:

```
<API>/?filter=elements HAS ANY "C", "Si", "Ge", "Sn" AND  
NOT elements HAS "Pb"
```

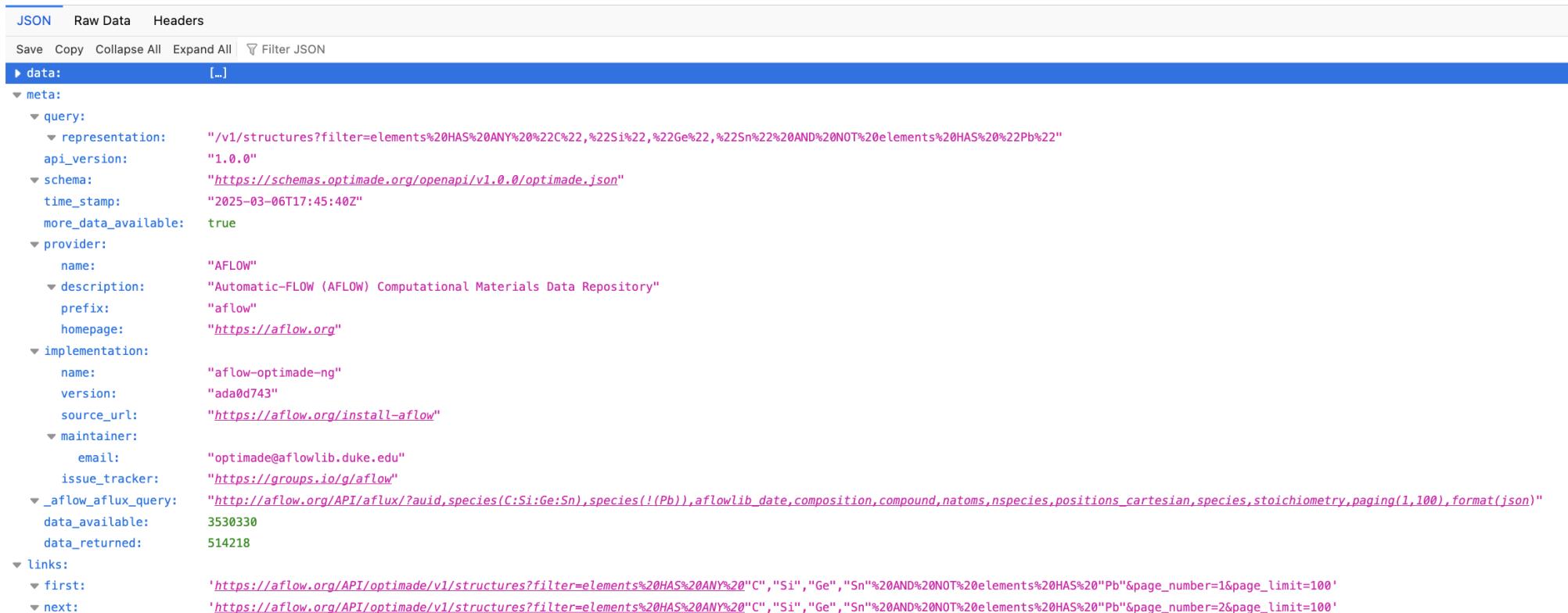
Search AFLOW for materials with C or Si or Ge or Sn but not Pb

```
✓ 41s  play  
import json, sys, os  
from urllib.request import urlopen  
  
SERVER='https://aflow.org'  
API='/API/optimade/v1/structures?'  
FILTER='filter=elements%20HAS%20ANY%20%22C%22,%22Si%22,%22Ge%22,%22Sn%22%20AND%20NOT%20elements%20HAS%20%22Pb%22'  
  
print(SERVER+API+FILTER)  
  
response=json.loads(urlopen(SERVER+API+FILTER).read().decode("utf-8"))  
print(response)  
  
https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20ANY%20%22C%22,%22Si%22,%22Ge%22,%22Sn%22%20AND%20NOT%20elements%20HAS%20%22Pb%22  
{'links': {'base_url': {'href': 'http://aflow.org/API/optimade'}, 'meta': {'_aflow_db_version': '1.0'}}, '_aflow_base_url':
```

Optimade: Common Materials Search API

- Example: search AFLOW for materials containing C, Si, Ge, Sn, but not Pb:

```
<API>/?filter=elements HAS ANY "C", "Si", "Ge", "Sn" AND  
NOT elements HAS "Pb"
```



The screenshot shows a JSON viewer interface with the following structure:

- JSON Raw Data Headers**: Buttons at the top.
- Save Copy Collapse All Expand All Filter JSON**: Actions below the headers.
- data: []**: The main data object.
- meta:** A collapsed section under **data:**.
- query:** A collapsed section under **meta:**.
- representation:** `"/v1/structures?filter=elements%20HAS%20ANY%20%22C%22,%22Si%22,%22Ge%22,%22Sn%22%20AND%20NOT%20elements%20HAS%20%22Pb%22"`
- api_version:** `"1.0.0"`
- schema:** `"https://schemas.optimade.org/openapi/v1.0.0/optimade.json"`
- time_stamp:** `"2025-03-06T17:45:40Z"`
- more_data_available:** `true`
- provider:** A collapsed section under **meta:**.
- name:** `"AFLOW"`
- description:** `"Automatic-FLOW (AFLOW) Computational Materials Data Repository"`
- prefix:** `"aflow"`
- homepage:** `"https://aflow.org"`
- implementation:** A collapsed section under **meta:**.
- name:** `"aflow-optimade-ng"`
- version:** `"ada0d743"`
- source_url:** `"https://aflow.org/install-aflow"`
- maintainer:** A collapsed section under **meta:**.
- email:** `"optimade@aflowlib.duke.edu"`
- issue_tracker:** `"https://groups.io/g/aflow"`
- _aflux_aflux_query:** `"http://aflow.org/API/aflux/?auid,species(C:Si:Ge:Sn),species(!(Pb)),aflowlib_date,composition,compound,natoms,nspecies,positions_cartesian,species,stoichiometry,paging(1,100),format(json)"`
- data_available:** `3530330`
- data_returned:** `514218`
- links:** A collapsed section under **meta:**.
- first:** `'https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20ANY%20%C","%22Si%22,%22Ge%22,%22Sn%20AND%20NOT%20elements%20HAS%20%22Pb%22&page_number=1&page_limit=100'`
- next:** `'https://aflow.org/API/optimade/v1/structures?filter=elements%20HAS%20ANY%20%C","%22Si%22,%22Ge%22,%22Sn%20AND%20NOT%20elements%20HAS%20%22Pb%22&page_number=2&page_limit=100'`

AFLOW Search Page: Exercises

1. Use the Optimade API to find binary ($n\text{elements}=2$) materials containing Al in the AFLOW database. How many entries are returned?
2. Use the Optimade API to find materials containing Li but not Na in the NOMAD database. How many entries are returned?
3. Use the Optimade API to find ternary materials containing Nb in the NOMAD database. How many entries are returned?

Conclusions

- Computational and experimental materials data is becoming widely available online
- Data can be retrieved both through web portals as well as programmatically using REST-APIs
- Several databases have their own search APIs, enabling the programmatic submission of complex search queries and data retrieval
- Optimade Common API enables access to several materials databases, including aflow.org, materialsproject.org, nomad-lab.eu, oqmd.org, materialscloud.org, etc.

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- Patrick Huck, Anubhav Jain, Kristin Persson et al. (LBNL): Materials Project
- Markus Scheidgen, Claudia Draxl et al. (Humboldt Universität zu Berlin): NOMAD



AFLUX
Automatic - FLOW for Materials Discovery

