a REST API for Querying Materials Databases

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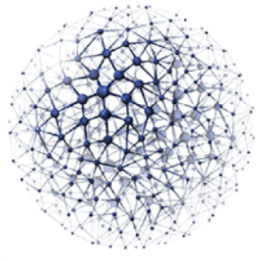
Shared Metadata and Data Formats for Big-Data Driven Materials Science
Berlin, 9 July 2019

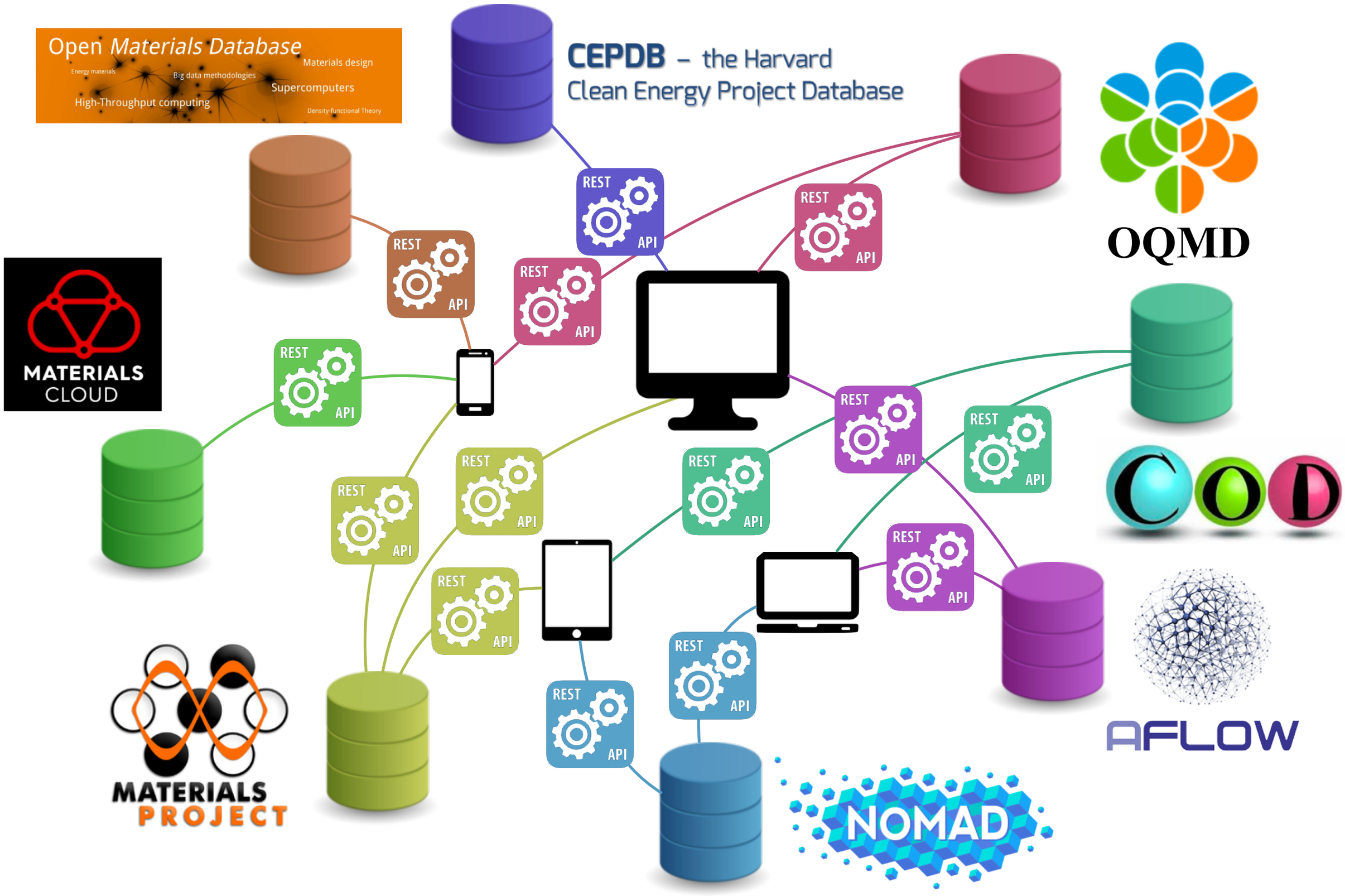
Many materials DB have become available online



OQMD

AFLOW

Each of these databases has its own user base and specific API



Query examples

- 

  http://www.crystallography.net/cod/result.php?formula=O2%20Si

- 

  http://www.materialsproject.org/rest/v2/materials/SiO2/vasp/structure?API_KEY=YOUR_API_KEY

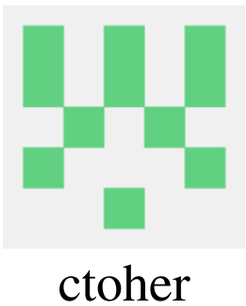
- 

  http://aflowlib.duke.edu/search/API/?species(Si,O),nspecies(2)

Query examples

gmrigna

I am trying to write a query for AFLOW for getting all the structures with the SiO2 formula.
I have tested:
http://aflowlib.duke.edu/search/API/?compound(SiO2)
but I ended up with "[]" which I do not think is the expected result from AFLOW.



ctoher

The query for SiO2 would be:
http://aflowlib.duke.edu/search/API/?compound(O2Si1)
AFLOW stores all material names alphabetically, and also includes the "1" after element symbols, so that SiO2 becomes O2Si1.

Note that currently, the compound keyword just does a simple string matching search, so just returns entries where the unit cell is SiO2, and not Si2O4, etc. To get all of the Si-O entries, it would be better to search by the elements themselves:
http://aflowlib.duke.edu/search/API/?species(Si,O),nspecies(2)

This returns the first 64 entries with just the elements Si and O. You can change the number/set of entries returned by using the "paging" keyword; e.g.:
http://aflowlib.duke.edu/search/API/?species(Si,O),nspecies(2),paging(2,100)
returns the second page of 100 entries.

Querying by formula #3

New issue

Closed **shyuep** opened this issue on Jun 22, 2017 · 5 comments

shyuep commented on Jun 22, 2017

I am trying to query the COD by formula. While I can execute the example in the wiki, I cannot run the following query.

```
select file from data where formula="Li"
```

Basically replacing the query to this does not work, though it seems it should based on the schema specified. Is there some trick to doing this?

Also, I would highly recommend developing a REST API for the COD so that queries can be easily done via http only. Right now, one has to know the COD-ID to be able to download a cif file via http, but no other functionality is available.

shyuep commented on Jun 24, 2017 Author

I managed to figure out how to query by formula. It seems that the format of the formula is "- Li2 O -", which is somewhat strange. However, I still recommend that some form of REST API be implemented. E.g., http://www.crystallography.net/cod/cod_ids?formula="Li2 O" to get all the cod ids. Otherwise, querying for cod ids require the installation of mysql, which is rather unnecessary if all someone wanted to do is to get the cod ids.

Assignees

No one assigned

Labels

None yet

Projects

None yet

Milestone

No milestone

Notifications Customize

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3 participants

Response examples

- http://www.crystallography.net/cod/result.php?formula=O2%20Si

Search results

Result: there are 239 entries in the selection

Switch to the old layout of the page

Download all results as: list of COD numbers | list of CIF URLs | data in CSV format | archive of CIF files (ZIP)

Searching formula like 'O2 Si'

◀◀ First | ◀ Previous 20 | Page 1 of **12** | Next 20 ▶ | Last ▶▶ | Display 5 **20** 50 100 200 300 500 1000 entries per page

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
1010921	CIF	O2 Si	P 21 3	7.16; 7.16; 7.16 90; 90; 90	367.1	Barth, T F W The Cristobalite Structures. I. High-Cristobalite *American Journal of Science, Serie 5(1,1921-1938)*, **1932**, *23*, 350-356
1010938	CIF	O2 Si	P 41 21 2	4.964; 4.964; 6.92 90; 90; 90	170.5	Nieuwenkamp, W Die Kristallstruktur des Tief-Cristobalits Si O2 *Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)*, **1935**, *92*, 82-88
1010944	CIF	O2 Si	F d -3 m :1	7.12; 7.12; 7.12 90; 90; 90	360.9	Wyckoff, Ralph W. G. IX. Die Kristallstruktur von β-Crystobalit SiO~2~ (bei hohen Temperaturen stabile Form) *Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)*, **1925**, *62*, 189-200
1010954	CIF	O2 Si	F 41 3 2	7.12; 7.12; 7.12 90; 90; 90	360.9	Wyckoff, R W G The crystal structure of the high temperature form of Cristobalite (Si O2) *American Journal of Science, Serie 5(1,1921-1938)*, **1925**, *9*, 448-459
1011097	CIF	O2 Si	P 31 2 1	4.913; 4.913; 5.404 90; 90; 120	113	Wei, P. H. Die Bindung im Quarz *Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)*, **1935**, *92*, 355-362
1011159	CIF	O2 Si	P 32 2 1 S	4.91; 4.91; 5.4 90; 90; 120	112.7	Machatschki, F Kristallstruktur von Tiefquarz *Fortschritte der Mineralogie*, **1936**, *20*, 45-47
1011172	CIF	O2 Si	P 31 2 1	4.913; 4.913; 5.405 90; 90; 120	113	Brill, R; Hermann, C; Peters, C Studien ueber chemische Bindung mittels Fourieranalyse III. Die Bindung im Quarz *Naturwissenschaften*, **1939**, *27*, 676-677
1011176	CIF	O2 Si	P 32 2 1 S	4.9; 4.9; 5.4 90; 90; 120	112.3	Machatschki, F Die Kristallstruktur von Tiefquarz Si O2 und Aluminiumorthoarsenat Al As O4 *Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)*, **1936**, *94*, 222-230
1011200	CIF	O2 Si	P 62 2 2	5.013; 5.013; 5.47 90; 90; 120	119	Wyckoff, Ralph W. G. XXIX. Kriterien für hexagonale Raumgruppen und die Kristallstruktur von β-quarz *Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)*, **1926**, *63*, 507-537
1505106	CIF	O2 Si	P 1 21/n 1	13.382; 20.125; 19.89	5356	Schmidt, Wolfgang; Wilczok, Ursula; Weidenthaler, Claudia; Medenbach, Olaf; Goddard, Richard; Buth, Gernot; Cepak,

Response examples

- http://www.crystallography.net/cod/result.php?formula=O2%20Si&format=json


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Response examples

- http://www.materialsproject.org/rest/v2/materials/SiO2/vasp/structure


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0.3523788], "xyz": [5.8396584002119445, 0.0, 3.177431219788056], "label": "O", "properties": {"magmom": -0.0}}, {"species": [{"element":
"O", "occu": 1}], "abc": [0.6476212, 0.6476212, 0.0], "xyz": [5.8396584002119445, 5.8396584002119445, 0.0], "label": "O", "properties":
{"magmom": -0.0}}, {"species": [{"element": "O", "occu": 1}], "abc": [0.6476212, 0.3523788, 0.0], "xyz": [5.8396584002119445,
3.177431219788056, 0.0], "label": "O", "properties": {"magmom": -0.0}}, {"species": [{"element": "O", "occu": 1}], "abc": [0.3523788,
0.0, 0.3523788], "xyz": [3.177431219788056, 0.0, 3.177431219788056], "label": "O", "properties": {"magmom": -0.0}}, {"species":
[{"element": "O", "occu": 1}], "abc": [0.6476212, 0.0, 0.6476212], "xyz": [5.8396584002119445, 0.0, 5.8396584002119445], "label": "O",
```

Response examples

- http://aflowlib.duke.edu/search/API/?compound(O2Si1)


```
[{"compound":"O2Si1","auid":"aflow:cb11950759a0a497","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/FCC/O2Si1_ICSD_44271"}]
```


- http://aflowlib.duke.edu/search/API/?species(Si,O),nspecies(2)


```
[{"compound":"O16Si8","auid":"aflow:590a543e005fcdd0","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170533","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:fe6cb4a748ca8f04","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_75649","species":"O,Si","nspecies":"2"},
{"compound":"O48Si24","auid":"aflow:a461b6af4b750e1c","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_94091","species":"O,Si","nspecies":"2"},
{"compound":"O24Si12","auid":"aflow:3dd0d3cf29cc4b04","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_56684","species":"O,Si","nspecies":"2"},
{"compound":"O16Si8","auid":"aflow:390c258fcaa1a88b","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170535","species":"O,Si","nspecies":"2"},
{"compound":"O16Si8","auid":"aflow:a75642571911e18e","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170546","species":"O,Si","nspecies":"2"},
{"compound":"O16Si8","auid":"aflow:7ab784f658bc19f2","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170551","species":"O,Si","nspecies":"2"},
{"compound":"O32Si16","auid":"aflow:754d7c1cd7fbda3c","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170516","species":"O,Si","nspecies":"2"},
{"compound":"O48Si24","auid":"aflow:9234fc8908490437","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_153470","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:e38965ef50bb8383","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_51702","species":"O,Si","nspecies":"2"},
{"compound":"O16Si8","auid":"aflow:5776a1710b60ec68","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_52371","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:1230ca6a3d7fea1d","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_161310","species":"O,Si","nspecies":"2"},
{"compound":"O16Si8","auid":"aflow:cd572ec8afb4ca17","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170549","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:959caaad01f681df","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_158532","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:56a522816a93e6d2","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_44094","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:b2ea2a71662a72bd","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_75488","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:a35f25165b071cff","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_77455","species":"O,Si","nspecies":"2"},
{"compound":"O32Si16","auid":"aflow:f50fcdb9774379ef","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_170537","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:e5bab05610fe7bb9","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_158534","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:299991d2f1511af0","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_77453","species":"O,Si","nspecies":"2"},
{"compound":"O24Si12","auid":"aflow:ce56e3945cf72477","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_654474","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:92cb6fa4fd28ec7f","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_180899","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:1979ea531159ef9d","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_162632","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:82e5b5754426a3f1","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_40102","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:1467a7ac74faac62","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_30269","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:d2827ad42a60feb0","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_162615","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:25e045323e81c47f","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_40100","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:42c1d2f7ee203ab4","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_158530","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:5030145a4c52f6f8","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_77454","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:480fa53f47837b0f","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_77523","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:5e487cc16753b55f","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_155246","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:99bce9f359ed0e69","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_20604","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:ae065de2cb2efb4d","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_75740","species":"O,Si","nspecies":"2"},
{"compound":"O8Si4","auid":"aflow:a614499919eb5f27","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_47221","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:337b6a80c1cb295c","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_68163","species":"O,Si","nspecies":"2"},
{"compound":"O32Si16","auid":"aflow:1585e6302d35f389","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_171739","species":"O,Si","nspecies":"2"},
{"compound":"O4Si2","auid":"aflow:6cdd8fbc9e9762e3","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_647438","species":"O,Si","nspecies":"2"},
```

Response examples

JSON Raw Data Headers

Save Copy Collapse All


```
▶ 0:    {…}
▶ 1:    {…}
▶ 2:    {…}
▶ 3:    {…}
▶ 4:    {…}
▶ 5:    {…}
▶ 6:    {…}
▶ 7:    {…}
▶ 8:    {…}
▶ 9:    {…}
▶ 10:   {…}
▶ 11:   {…}
▶ 12:   {…}
▶ 13:   {…}
▶ 14:   {…}
▶ 15:   {…}
▶ 16:   {…}
▶ 17:   {…}
▶ 18:   {…}
▶ 19:   {…}
▶ 20:   {…}
▶ 21:   {…}
```


JSON Raw Data Headers

Save Copy Collapse All


```
▶ response:          […]
  valid_response:    true
  created_at:        "2019-07-07T06:55:03.238830"
▶ version:           {…}
  copyright:         "Materials Project, 2019"
```


JSON Raw Data Headers

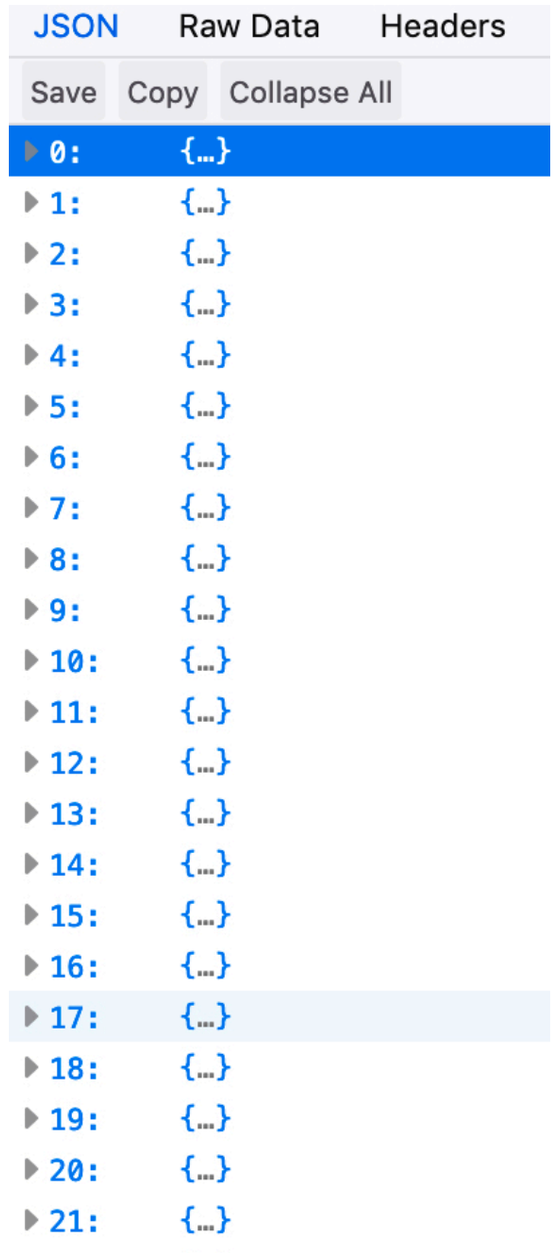
Save Copy Collapse All


```
▶ 0:    {…}
▶ 1:    {…}
▶ 2:    {…}
▶ 3:    {…}
▶ 4:    {…}
▶ 5:    {…}
▶ 6:    {…}
▶ 7:    {…}
▶ 8:    {…}
▶ 9:    {…}
▶ 10:   {…}
▶ 11:   {…}
▶ 12:   {…}
▶ 13:   {…}
▶ 14:   {…}
▶ 15:   {…}
▶ 16:   {…}
▶ 17:   {…}
▶ 18:   {…}
▶ 19:   {…}
▶ 20:   {…}
▶ 21:   {…}
```

Response examples

JSON Raw Data Headers

Save Copy Collapse All



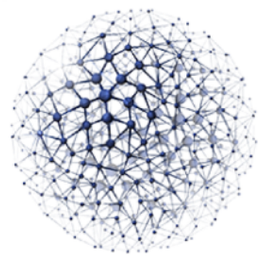
```
▶ 0:  {…}
▶ 1:  {…}
▶ 2:  {…}
▶ 3:  {…}
▶ 4:  {…}
▶ 5:  {…}
▶ 6:  {…}
▶ 7:  {…}
▶ 8:  {…}
▶ 9:  {…}
▶ 10:  {…}
▶ 11:  {…}
▶ 12:  {…}
▶ 13:  {…}
▶ 14:  {…}
▶ 15:  {…}
▶ 16:  {…}
▶ 17:  {…}
▶ 18:  {…}
▶ 19:  {…}
▶ 20:  {…}
▶ 21:  {…}
```

JSON Raw Data Headers

Save Copy Collapse All

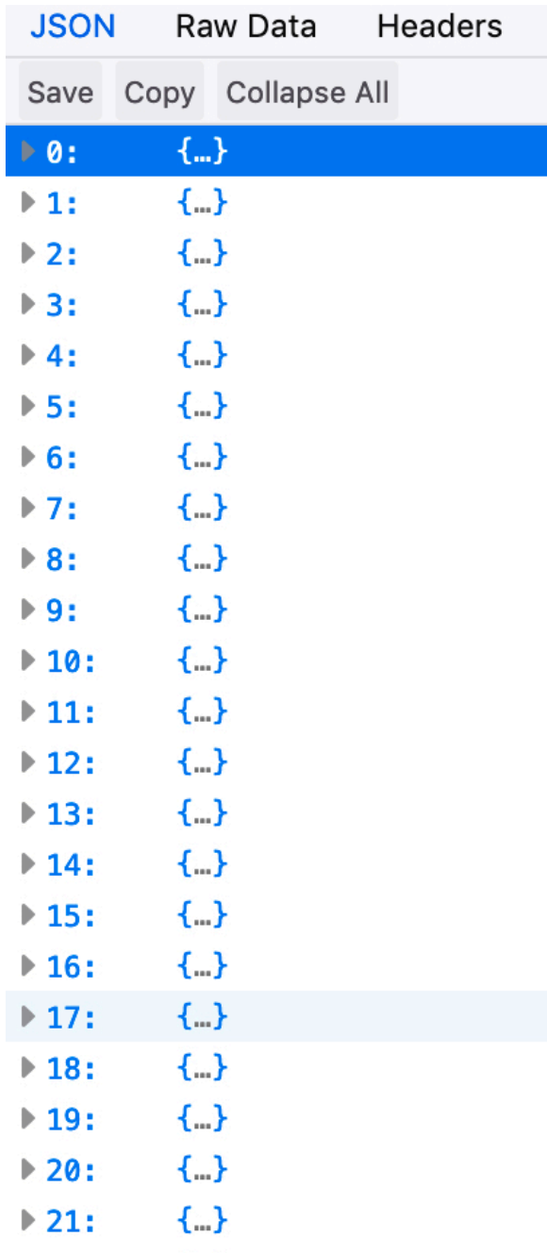
Raw Data

```
▼ response:
  ▶ 0:  {…}
  ▶ 1:  {…}
  ▶ 2:  {…}
  ▶ 3:  {…}
  ▶ 4:  {…}
  ▶ 5:  {…}
  ▶ 6:  {…}
  ▶ 7:  {…}
  ▶ 8:  {…}
  ▶ 9:  {…}
  ▶ 10:  {…}
  ▶ 11:  {…}
  ▶ 12:  {…}
  ▶ 13:  {…}
  ▶ 14:  {…}
  ▶ 15:  {…}
  ▶ 16:  {…}
  ▶ 17:  {…}
  ▶ 18:  {…}
  ▶ 19:  {…}
  ▶ 20:  {…}
  ▶ 21:  {…}
  ▶ 22:  {…}
  ▶ 23:  {…}
```



JSON Raw Data Headers

Save Copy Collapse All



```
▶ 0:  {…}
▶ 1:  {…}
▶ 2:  {…}
▶ 3:  {…}
▶ 4:  {…}
▶ 5:  {…}
▶ 6:  {…}
▶ 7:  {…}
▶ 8:  {…}
▶ 9:  {…}
▶ 10:  {…}
▶ 11:  {…}
▶ 12:  {…}
▶ 13:  {…}
▶ 14:  {…}
▶ 15:  {…}
▶ 16:  {…}
▶ 17:  {…}
▶ 18:  {…}
▶ 19:  {…}
▶ 20:  {…}
▶ 21:  {…}
```

Response examples

JSON Raw Data Headers

Save Copy Collapse All


```
0:
  file:          "1010921"
  a:             "7.16"
  siga:          null
  b:             "7.16"
  sigb:          null
  c:             "7.16"
  sigc:          null
  alpha:         "90"
  sigalpha:      null
  beta:          "90"
  sigbeta:       null
  gamma:         "90"
  siggamma:      null
  vol:           "367.1"
  sigvol:        null
  celltemp:      null
  sigcelltemp:   null
  diffrtemp:     null
  sigdiffrtemp:  null
  cellpressure:  null
  sigcellpressure: null
  diffrpressure: null
  sigdiffrpressure: null
  thermalhist:   null
  pressurehist:  null
  compoundsource: null
  nel:           "2"
  sg:            "P 21 3"
```


JSON Raw Data Headers

JSON Copy Collapse All


```
response:
  0:
    material_id:        "mp-600033"
    structure:
      @module:          "pymatgen.core.structure"
      @class:           "Structure"
      charge:           null
      lattice:
        matrix:         […]
        a:              9.01708962
        b:              9.01708962
        c:              9.01708962
        alpha:          90
        beta:           90
        gamma:          90
        volume:         733.160668139128
      sites:
        0:
          species:
            0:
              element:  "Si"
              occu:     1
          abc:
            0:          0.25
            1:          0.5
            2:          0
          xyz:
            0:          2.254272405
```


JSON Raw Data Headers

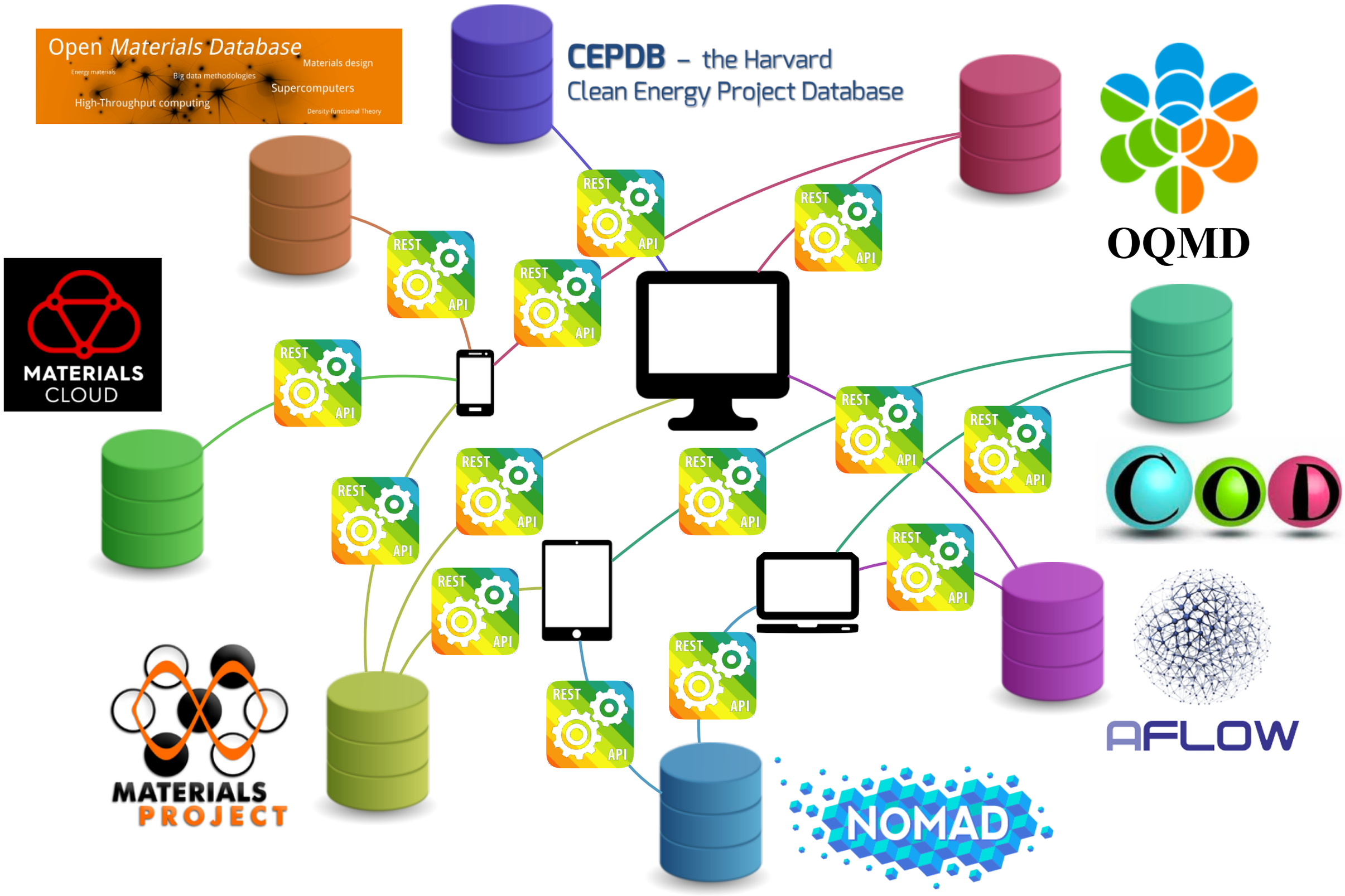
Save Copy Collapse All Expand All


```
0:
  compound:     "O16Si8"
  auid:         "aflow:590a543e005fcdd0"
  aurl:         "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/O
  species:      "O,Si"
  nspecies:     "2"
1:
  compound:     "O8Si4"
  auid:         "aflow:fe6cb4a748ca8f04"
  aurl:         "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/O
  species:      "O,Si"
  nspecies:     "2"
2:
  compound:     "O48Si24"
  auid:         "aflow:a461b6af4b750e1c"
  aurl:         "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/O
  species:      "O,Si"
  nspecies:     "2"
3:
  compound:     "O24Si12"
  auid:         "aflow:3dd0d3cf29cc4b04"
  aurl:         "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/O
  species:      "O,Si"
  nspecies:     "2"
4:
  compound:     "O16Si8"
  auid:         "aflow:390c258fcaa1a88b"
  aurl:         "aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/O
  species:      "O,Si"
```

Discussions are going on to define a common API

- The initial release was developed by the participants of the workshops "Open Databases Integration for Materials Design" held at:
  - the Lorentz Center (October 2016)
  - the CECAM (June 2018 & June 2019)

The users will be able to search more materials DBs with the same query…



Query & response example

- http://www.crystallography.net/cod/optimade/structures/?filter=chemical_formula="SiO2"

{"data":[{"links":{"self":"http://www.crystallography.net/cod/1010921.cif"},"type":"structure","modification_date":"2017-02-28T05:33:56Z","id":"1010921","attributes":{"_cod_text":"Barth, T F W\nThe Cristobalite Structures. I. High-Cristobalite\nAmerican Journal of Science, Serie 5(1,1921-1938)\n23\n(1932)\n350-356","_cod_beta":"90","_cod_b":"7.16","_cod_authors":"Barth, T F W","_cod_unreduced_formula":"O2 Si","_cod_formula":"- O2 Si -","_cod_file":"1010921","local_id":"1010921","_cod_sg":"P 21 3","_cod_nel":"2","_cod_gamma":"90","_cod_journal":"American Journal of Science, Serie 5(1,1921-1938)","_cod_a":"7.16","_cod_sgHall":"P 2ac 2ab 3","_cod_chemname":"Silicon oxide","_cod_alpha":"90","_cod_svnrevision":"130149","nelements":"2","immutable_id":"http://www.crystallography.net/cod/1010921.cif@130149","last_modified":"2017-02-28T05:33:56Z","_cod_firstpage":"350","_cod_mineral":"Cristobalite high","_cod_year":"1932","_cod_title":"The Cristobalite Structures. I. High-Cristobalite","_cod_cellformula":"- O16 Si8 -","_cod_date":"2017-02-28","_cod_Zprime":"0.666667","_cod_flags":"has coordinates","_cod_Z":"8","_cod_calcformula":"- O2 Si -","_cod_time":"05:33:56","_cod_volume":"23","_cod_vol":"367.1","_cod_lastpage":"356","_cod_c":"7.16"}},{"attributes":{"last_modified":"2017-02-28T05:33:56Z","nelements":"2","immutable_id":"http://www.crystallography.net/cod/1010938.cif@130149","_cod_mineral":"Cristobalite low","_cod_firstpage":"82","_cod_year":"1935","_cod_title":"Die Kristallstruktur des Tief-Cristobalits Si O2","_cod_nel":"2","_cod_gamma":"90","_cod_alpha":"90","_cod_svnrevision":"130149","_cod_a":"4.964","_cod_sgHall":"P 4abw 2nw","_cod_journal":"Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)","_cod_chemname":"Silicon oxide","_cod_authors":"Nieuwenkamp, W","_cod_unreduced_formula":"O2 Si","_cod_b":"4.964","_cod_sg":"P 41 21 2","local_id":"1010938","_cod_file":"1010938","_cod_formula":"- O2 Si -","_cod_compoundsource":"from Eschwege, Germany","_cod_sigb":"0.005","_cod_text":"Nieuwenkamp, W\nDie Kristallstruktur des Tief-Cristobalits Si O2\nZeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)\n92\n(1935)\n82-88","_cod_siga":"0.005","_cod_beta":"90","_cod_vol":"170.5","_cod_c":"6.92","_cod_lastpage":"88","_cod_volume":"92","_cod_sigc":"0.005","_cod_time":"05:33:56","_cod_calcformula":"- O2 Si -","_cod_Z":"4","_cod_flags":"has coordinates","_cod_date":"2017-02-28","_cod_cellformula":"- O8 Si4 -","_cod_Zprime":"0.5"},"id":"1010938","modification_date":"2017-02-28T05:33:56Z","type":"structure","links":{"self":"http://www.crystallography.net/cod/1010938.cif"}},{"id":"1010944","attributes":{"_cod_time":"18:32:58","_cod_calcformula":"- O2 Si
-","_cod_doi":"10.1524/zkri.1925.62.1.189","_cod_sigc":"0.01","_cod_issue":"1-6","_cod_vol":"360.9","_cod_lastpage":"200","_cod_c":"7.12","_cod_volume":"62","_cod_Zprime":"0.0416667","_cod_date":"2017-09-01","_cod_cellformula":"- O16 Si8 -","_cod_Z":"8","_cod_flags":"has coordinates","_cod_svnrevision":"200079","_cod_alpha":"90","_cod_sgHall":"F 4d 2 3 -1d","_cod_a":"7.12","_cod_journal":"Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)","_cod_chemname":"Silicon dioxide -
Î²","_cod_nel":"2","_cod_gamma":"90","_cod_year":"1925","_cod_firstpage":"189","_cod_mineral":"Cristobalite high","_cod_title":"IX. Die Kristallstruktur von Î²-Crystobalit SiO~2~ (bei hohen Temperaturen stabile Form)","ne
Ralph W. G
\n(1925)\n
G.","_cod_
{"id":"101
O2)","last_
5(1,1921-1
Si -","loc
Cristobali
\n448-459"
-","_cod_t
{"self":"h
coordinate
O2 Si -","
H.","_cod_b":"4.913","_cod_beta":"90","_cod_text":"Wei, P. H.\nDie Bindung im Quarz\nZeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)\n92\n(1935)
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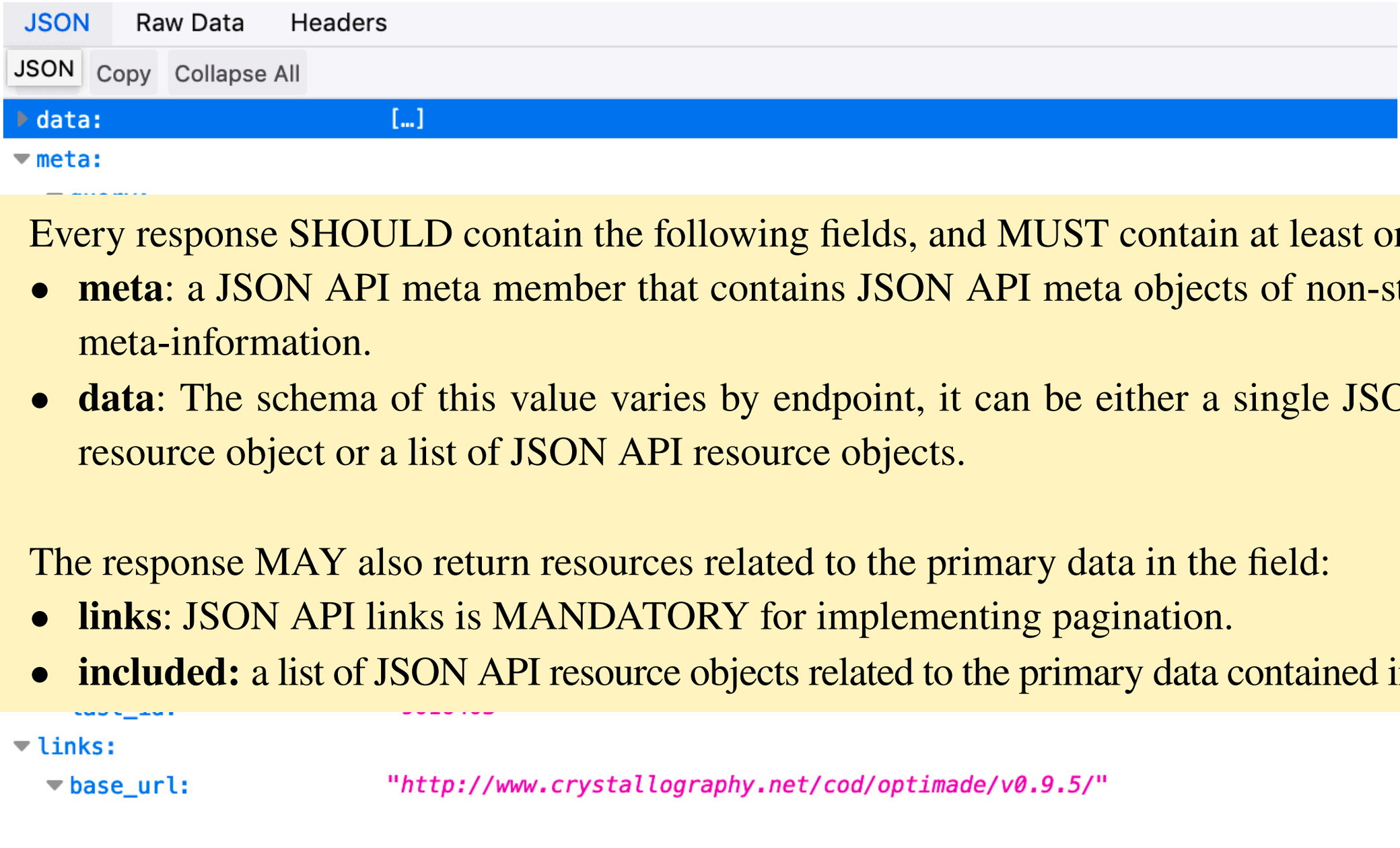
Die Bindung im Quarz\nNaturwissenschaften\n27\n(1939)\n676-677\",\"_cod_formula\":\"- O2 Si -\",\"_cod_file\":\"1011172\",\"local_id\":\"1011172\",\"_cod_sg\":\"P 31 2 1\",\"_cod_b\":\"4.913\",\"_cod_unreduced_formula\":\"O2 Si\",\"_cod_authors\":\"Brill, R; Hermann, C; Peters, C\"}},{\"modification_date\":\"2017-02-27T23:17:43Z\",\"type\":\"structure\",\"links\":{\"self\":\"http://www.crystallography.net/cod/1011176.cif\"},\"attributes\":{\"_cod_time\":\"23:17:43\",\"_cod_calcformula\":\"- O2 Si -\",\"_cod_vol\":\"112.3\",\"_cod_c\":\"5.4\",\"_cod_lastpage\":\"230\",\"_cod_volume\":\"94\",\"_cod_date\":\"2017-02-27\",\"_cod_cellformula\":\"- O6 Si3 -\",\"_cod_Z\":\"3\",\"_cod_flags\":\"has coordinates\",\"_cod_gamma\":\"120\",\"_cod_nel\":\"2\",\"_cod_svnrevision\":\"77586\",\"_cod_alpha\":\"90\",\"_cod_journal\":\"Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)\",\"_cod_a\":\"4.9\",\"_cod_chemname\":\"Silicon oxide - $-alpha\",\"nelements\":\"2\",\"immutable_id\":\"http://www.crystallography.net/cod/1011176.cif@77586\",\"last_modified\":\"2017-02-27T23:17:43Z\",\"_cod_firstpage\":\"222\",\"_cod_year\":\"1936\",\"_cod_mineral\":\"Quartz low\",\"_cod_title\":\"Die Kristallstruktur von Tiefquarz Si O2 und Aluminiumorthoarsenat Al As O4\",\"_cod_text\":\"Machatschki, F\nDie Kristallstruktur von Tiefquarz Si O2 und Aluminiumorthoarsenat Al As O4\nZeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977)\n94\n(1936)\n222-230\",\"_cod_beta\":\"90\",\"_cod_authors\":\"Machatschki, F\",\"_cod_unreduced_formula\":\"O2 Si\",\"_cod_b\":\"4.9\",\"local_id\":\"1011176\",\"_cod_sg\":\"P 32 2 1 S\",\"_cod_file\":\"1011176\",\"_cod_formula\":\"- O2 Si -\"},\"id\":\"1011176\"},{\"modification_date\":\"2017-09-01T18:55:58Z\",\"links\":{\"self\":\"http://www.crystallography.net/cod/1011200.cif\"},\"type\":\"structure\",\"attributes\":{\"_cod_Z\":\"3\",\"_cod_flags\":\"has coordinates\",\"_cod_Zprime\":\"0.25\",\"_cod_date\":\"2017-09-01\",\"_cod_cellformula\":\"- O6 Si3 -\",\"_cod_lastpage\":\"537\",\"_cod_vol\":\"119\",\"_cod_c\":\"5.47\",\"_cod_issue\":\"1-6\",\"_cod_volume\":\"63\",\"_cod_time\":\"18:55:58\",\"_cod_calcformula\":\"- O2 Si

This document defines a JSON response format that complies with the **JSON API** v1.0 specification. All endpoints of an API implementation MUST be able to provide responses in the JSON format specified below and MUST respond in this format by default.

Query & response example

- http://www.crystallography.net/cod/optimade/structures/?filter=chemical_formula="SiO2"



Query & response example

- http://www.crystallography.net/cod/optimade/structures/?filter=chemical_formula="SiO2"

Identifiers that start with an underscore are specific to a database provider, and MUST be on the format of a database-provider-specific prefix as defined in Appendix 1.

This standard refers to database-specific prefixes. These are assigned and included in this standard. The presently assigned prefixes are:

- _exmpl_: used for examples, not to be assigned to a real database
- _aflow_: aflow.org
- _cam_: Cambridge databases
- _cod_: crystallography open database
- _mcloud_: materialscloud.org
- _mp_: materialsproject.org
- _nmd_: nomad laboratory
- _omdb_: open materials database
- _oqmd_: open quantum materials database
- _pcod_: predicted crystallography open database
- _tcod_: theoretical crystallography open database

A GitHub repository has been created

Materials-Consortia

http://www.optimade.org

Repositories 7 | Packages | People 34 | Teams | Projects | Settings

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OPTiMaDe

Specification of a common REST API for access to materials databases

Makefile 14 11 37 2 Updated 3 hours ago

optimade-python-tools

Tools for implementing and consuming OPTiMaDe APIs in Python

Python MIT 9 4 8 4 Updated 4 days ago

OPTiMaDe-FilterParser

OPTiMaDe filter language parser in Perl

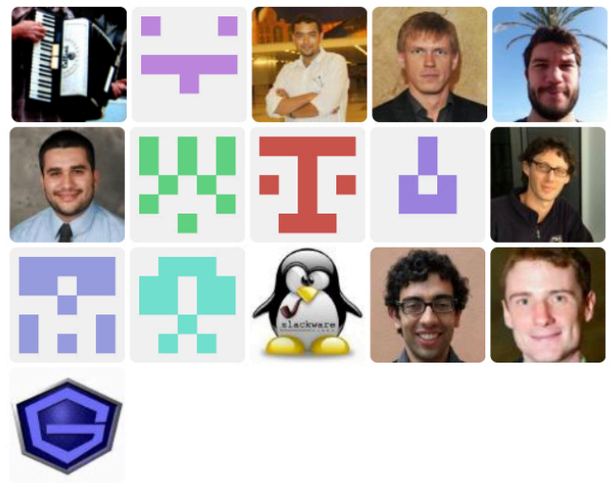
Makefile LGPL-3.0 0 0 0 0 Updated 7 days ago

Top languages

Python Makefile Shell

JavaScript Java

People 34 >

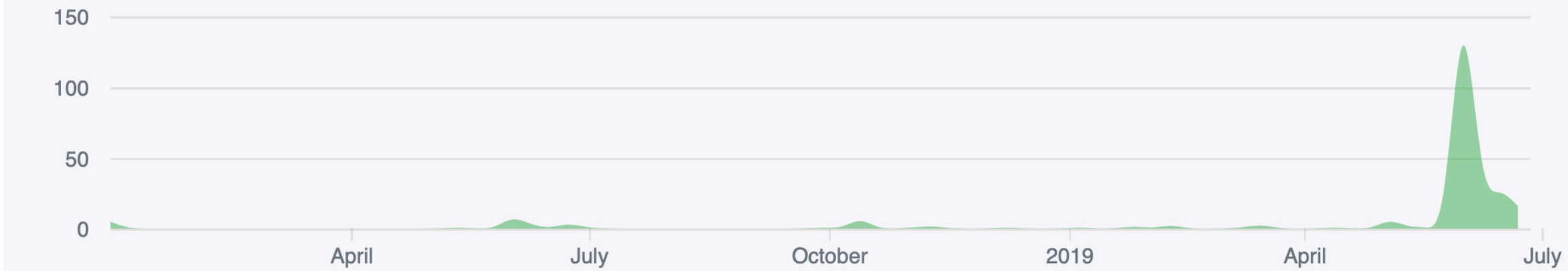


The GitHub repository is very active…

Jan 7, 2018 – Jul 5, 2019

Contributions: **Commits** ▾

Contributions to develop, excluding merge commits



The GitHub repository is very active…

Materials-Consortia / OPTiMaDe

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Specification of a common REST API for access to materials databases http://www.optimade.org/

Edit

Manage topics

404 commits | 5 branches | 1 release | 1 environment | 15 contributors

Branch: develop | New pull request | Create new file | Upload files | Find File | Clone or download

CasperWA Merge pull request #150 from rartino/queryable ... Latest commit bb4c86b 4 days ago

.github	Fixing some capitalization	23 days ago
dependencies/Debian-8.6	Grammar documentation checks (#10)	7 months ago
tests	Fix a few more broken tests. I'm unsure how I missed them.	12 days ago
.gitignore	Merge remote-tracking branch 'upstream/develop' into sorting-pagination	23 days ago
.travis.yml	Travis CI setup (#62)	2 months ago
.words.lst	Reverting back "Ångström" -> "ångström".	23 days ago
AUTHORS	Fixing some capitalization	23 days ago
GNUmakefile	Fixing mkcomdepend and grammatica dependencies (#54)	6 months ago
README.md	Merge branch 'develop' into merge_master_in_develop	17 days ago
optimade.md	Updated in response to review comments: fix TOC formatting, add ID ex...	4 days ago

List of contributors (in alphabetical order)

Casper Andersen, Thomas Archer, Rossella Aversa, Rickard Armiento, Evgeny Blokhin, Gareth Conduit, Davide Di Stefano, Alexander Dorsk, Claudia Draxl, Shyam Dwaraknath, Suleyman Er, Matthew Evans, Adam Fekete, Marco Fornari, Matteo Giantomassi, Abhijith Gopakumar, Marco Govoni, Saulius Gražulis, Geoffroy Hautier, Vinay Hedge, Georg Huhs, Jens Hummelshoej, Karsten W. Jacobsen, Ankit Kariryaa, Boris Kozinsky, Snehal Kumbhar, Nicola Marzari, Andrius Merkys, Fawzi Mohamed, Andrew Morris, Arash Mostofi, Nicolas Mounet, Corey Oses, Guido Petretto, Thomas Purcell, Giovanni Pizzi, Francesco Ricci, Gian-Marco Rignanese, Matthias Scheffler, Markus Scheidgen, Daniel Speckhard, Leopold Talirz, Cormac Toher, Daniele Tomerini, Martin Uhrin, Pierre Villars, David Waroquiers, Donald Winston, Chris Wolverton, Yibin Xu, Xiaoyu Yang

cecam supports OPTiMaDe

- During the “CECAM brainstorming meeting on Data Driven Science”, which took place at CECAM Headquarters (25 and 26 of March 2019), it was decided that the CECAM would support the OPTiMaDe initiative.
- One full time post-doctoral fellow will be hired for an <u>initial period of 12 months</u> to work on specific tasks dedicated to
  - *expanding the current developments in OPTiMaDe to classical molecular dynamics or bio-simulations*
- <u>Longer-term actions:</u>
  - c*reating a service to integrate and interrogate efficiently the different databases*
  - *creating and maintaining a dictionary of metadata*