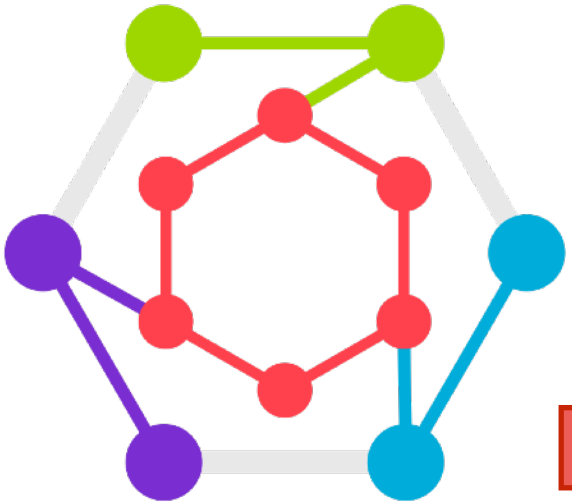


OPTIMADE: A Common REST API for Materials Databases Interoperability

Gian-Marco Rignanese

UCLouvain fnrs FREEDOM TO RESEARCH NOMAD MATERIALS PROJECT

1ères journées GDR IAMAT
Paris (France), 30 May - 1 June 2022

Materials advances are

one of the key drivers of innovation...

faster computers

more compact energy storage

more compact data storage

more efficient solar cells

How can one find materials with targeted properties in the information age?

good transparent conducting material

Google Search I'm Feeling Lucky

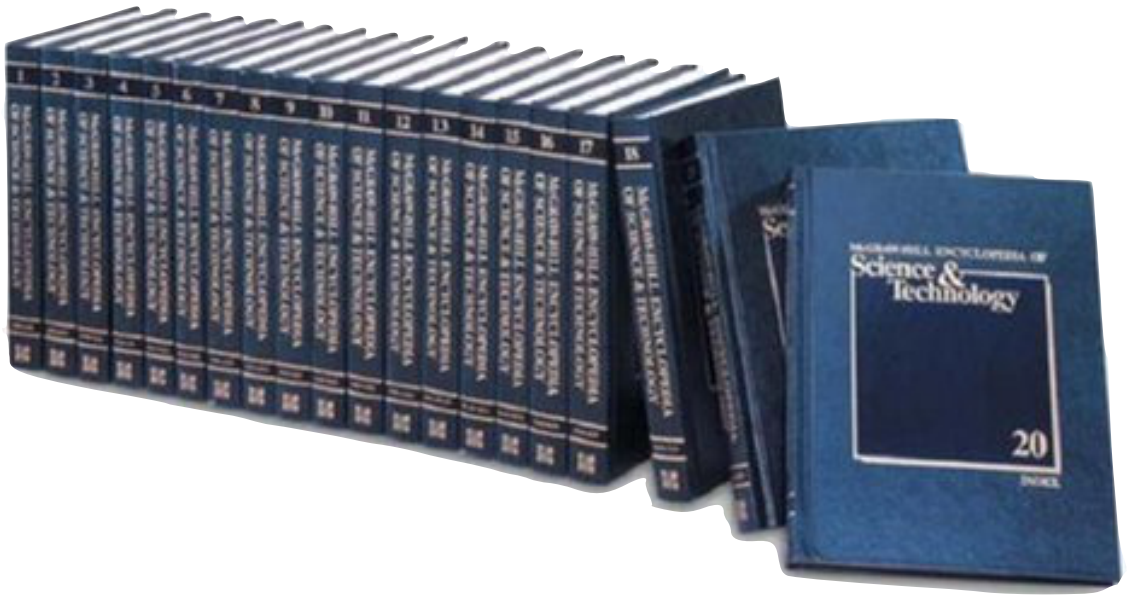
How can one find materials with targeted properties in the information age?

good stability & band gap > 3.2 eV & good carrier mobility

Google Search I'm Feeling Lucky

However, till recently, very little information was actually known about materials properties

- There are about 50,000 to 70,000 known inorganic compounds but
  - dielectric constants available only for ~300-400 compounds
  - elastic constants available only for ~200 compounds
  - band gaps available only for ~200 compounds
  - …

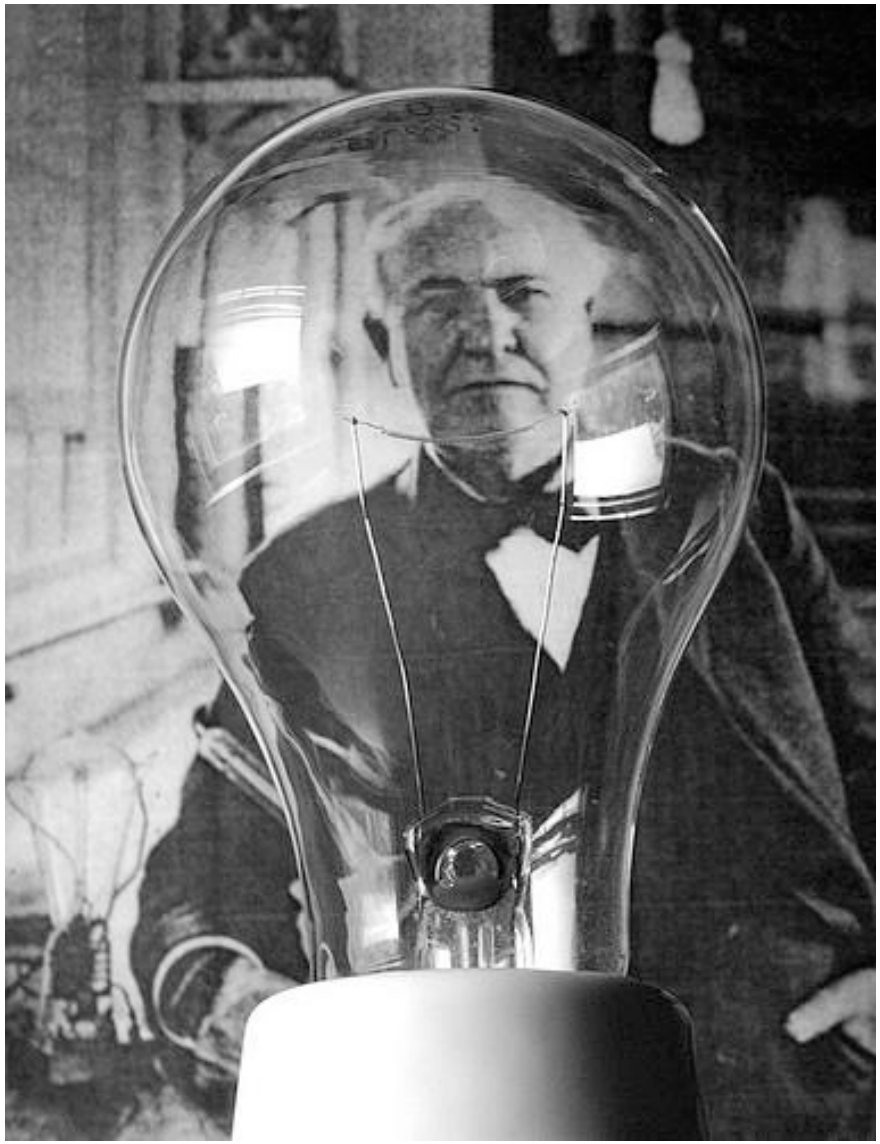


- For almost every property we are below 1% coverage

In fact, materials designers often operate almost in the dark!

Experimental materials design

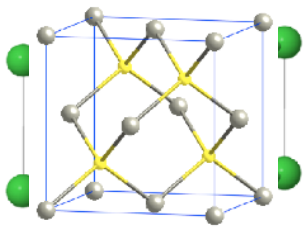
mainly proceeds by trial and error



Ab initio calculations have reached the required maturity for high-throughput materials screening

High-throughput *ab initio* materials design

Consider as many compounds as possible, typically $O(10^3) \rightarrow O(10^5)$



Data-Mining

$O(10^1) \rightarrow O(10^2)$ compounds

Thanks to such HT calculations,

many materials DB have become available online

JARVIS

COD

OQMD
The Open Quantum Materials Database

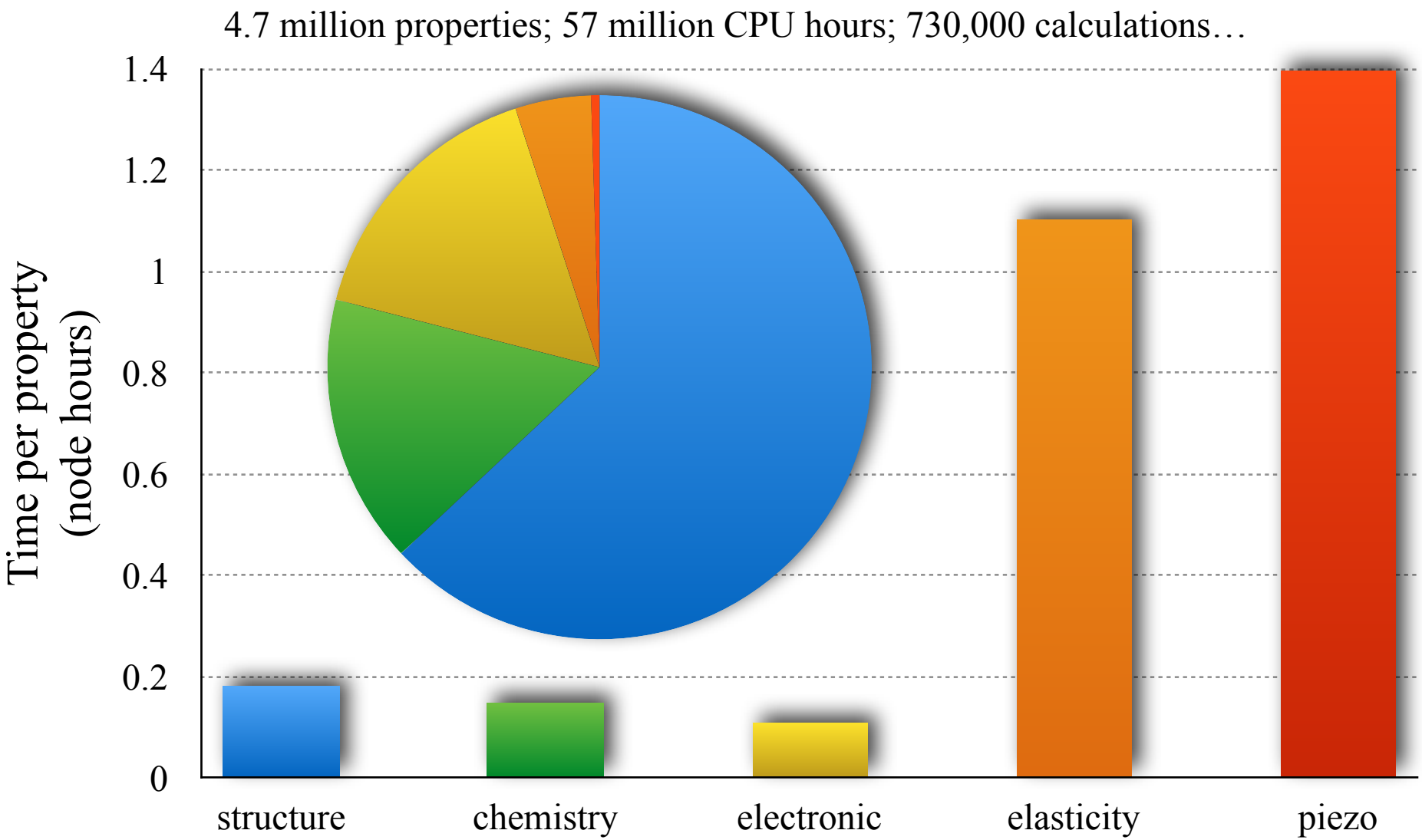
AFLOW

MATERIALS CLOUD

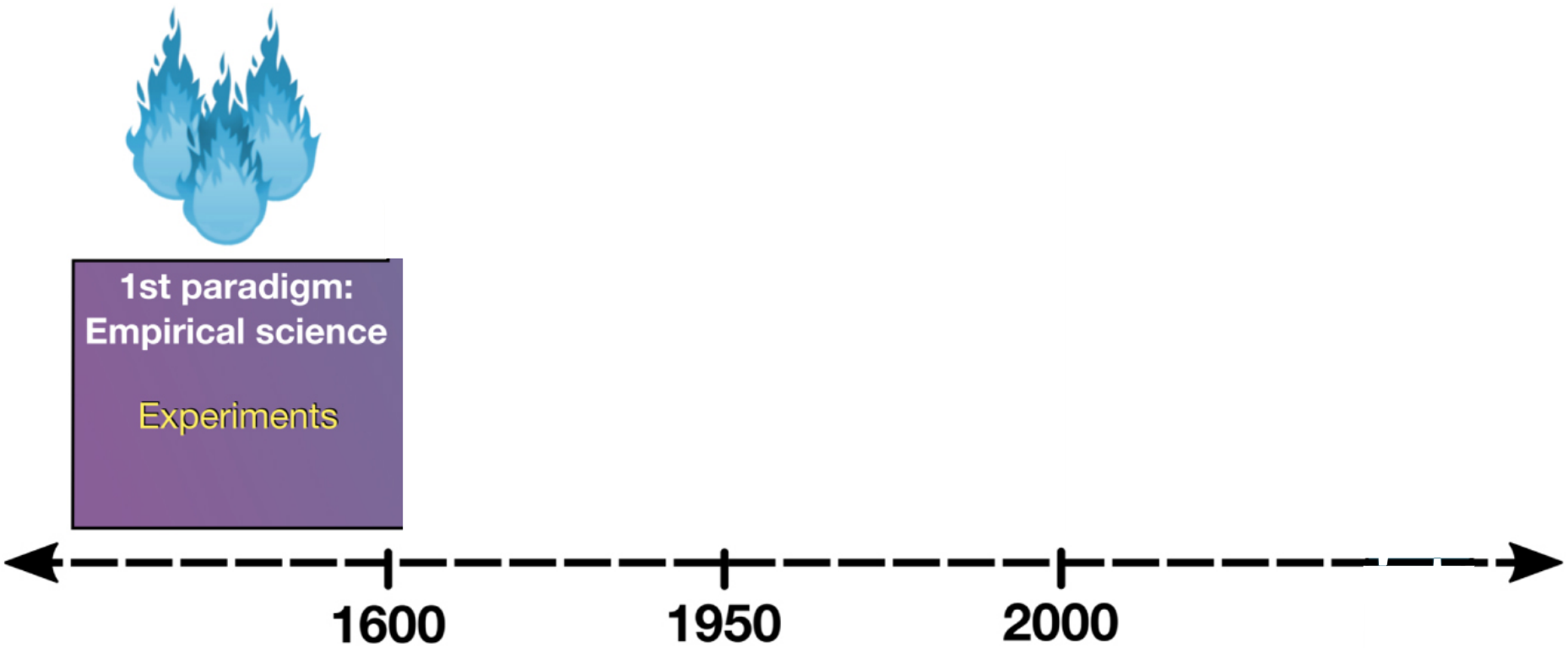
NOMAD

MATERIALS PROJECT

Predicting different properties requires very different computing time



(Big) data and machine learning are revolutionizing materials science



Materials design will require to take advantage of ALL the DB available online

JARVIS

COD

OQMD
The Open Quantum Materials Database

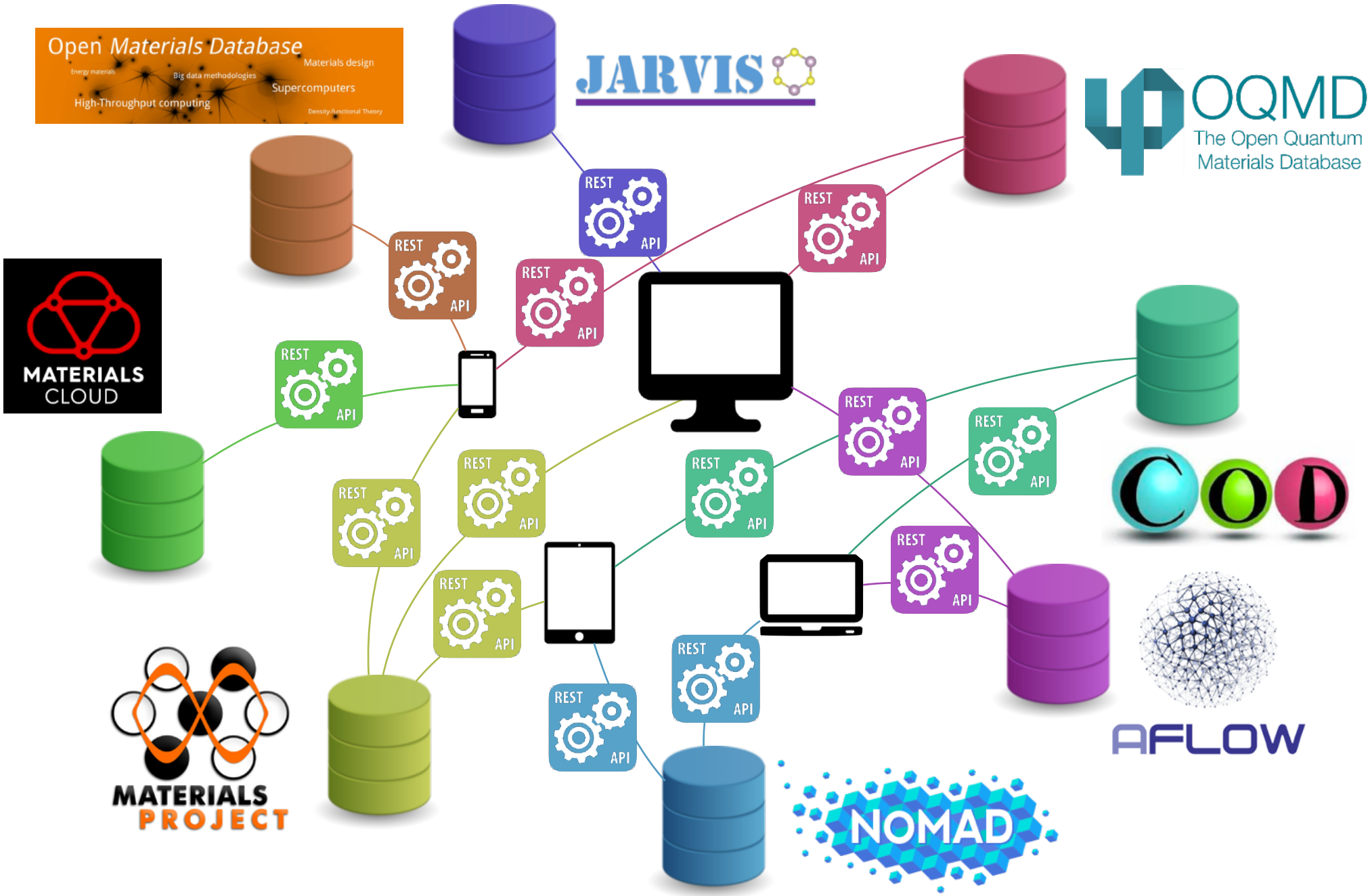
AFLOW

MATERIALS CLOUD

NOMAD

MATERIALS PROJECT

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

- 

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

- 

  http://aflow.org/API/aflux/?compound(SiO2)

  This returns no response...

Query examples

- 

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

- 

  http://aflow.org/API/aflux/?compound(O2Si1)

  This returns entries where the unit cell is SiO_2, but it does not return Si_2O_4 or simulation cells containing more formula units...

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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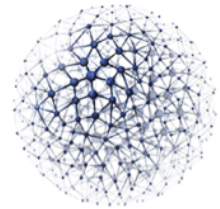
```

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"},
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{"compound":"O16Si8","auid":"aflow:390c258fcaa1a88b","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_170535","species":"O,Si","nspecies":"2"},
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{"compound":"O8Si4","auid":"aflow:1230ca6a3d7fea1d","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/ORC/O2Si1_ICSD_161310","species":"O,Si","nspecies":"2"},
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{"compound":"O4Si2","auid":"aflow:959caaad01f681df","aurl":"aflowlib.duke.edu:AFLOWDATA/ICSD_WEB/TET/O2Si1_ICSD_158532","species":"O,Si","nspecies":"2"},
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```

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:      "2020-04-30T07:18:43.634378"
version:         {…}
copyright:       "Materials Project, 2020"
```

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 lead 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, 2019, 2020, and 2021)

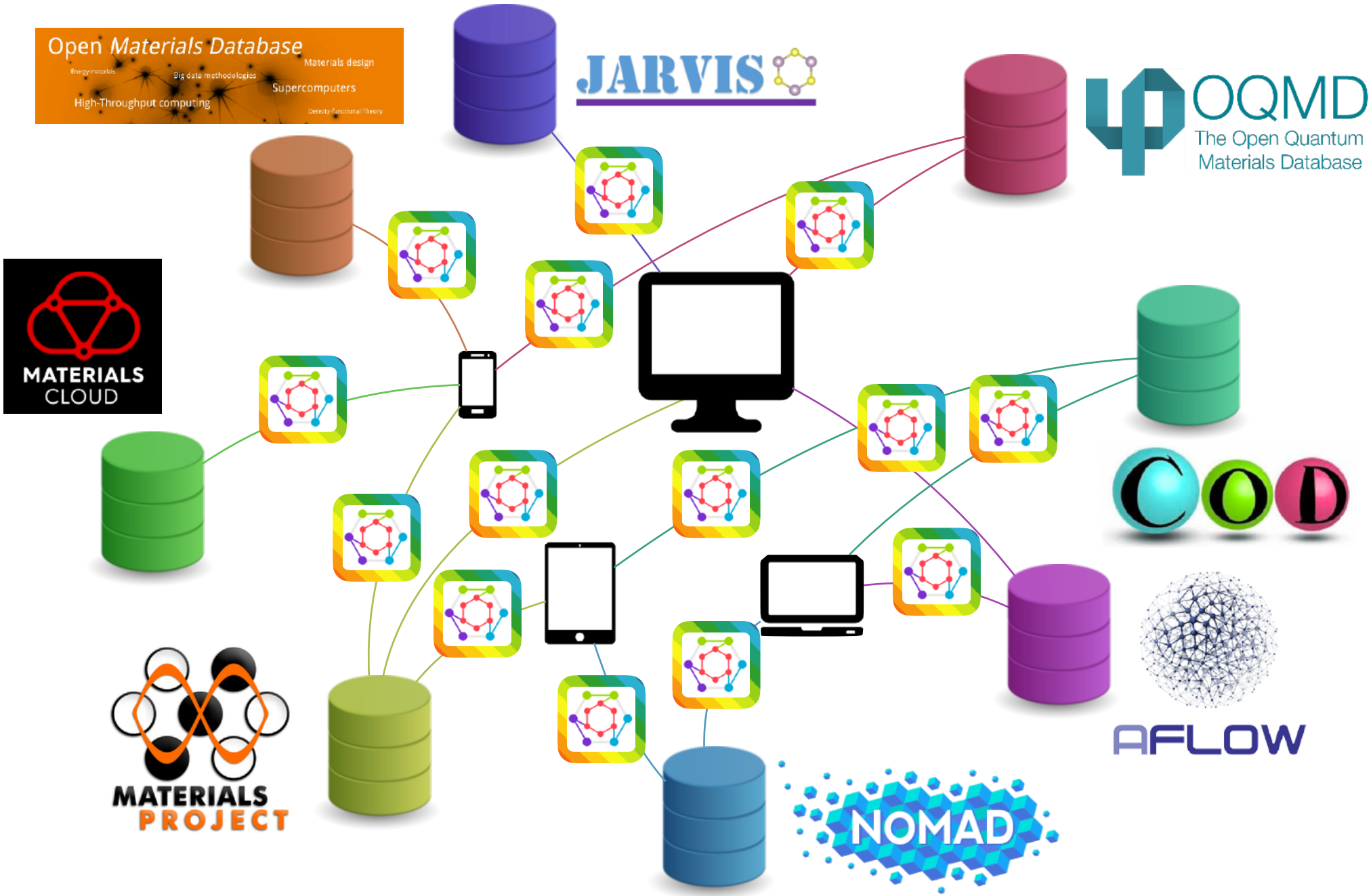






The users are now able to search

more materials DBs with the same query…



The users are now able to search

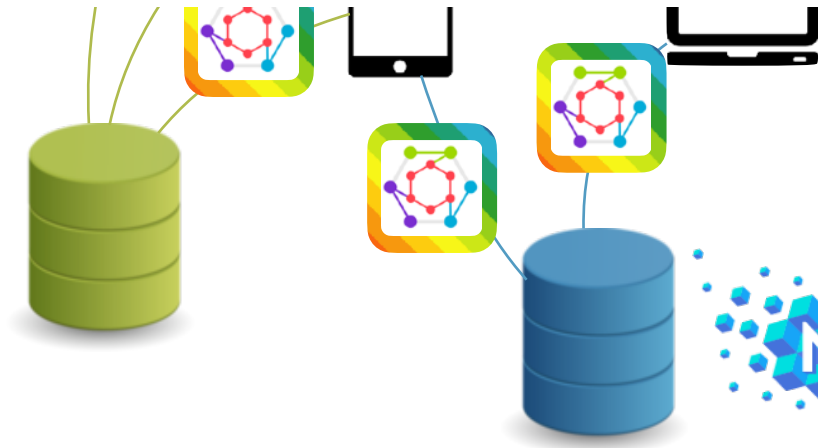
more materials DBs with the same query…

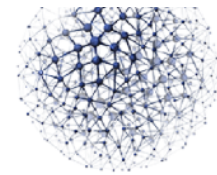
JARVIS

OQMD

Findable Accessible Interoperable Reusable

MATERIALS PROJECT





AFLOW

NOMAD

The users are now able to search more materials DBs with the same query…

- The philosophy of the OPTIMADE query is to enable the structural formula to be specified in a straightforward and intuitive manner.

- The query about SiO_2 can each be performed on standardized, versioned endpoints (**/v1/structures**) that permit a common filter format with well-defined terms (**?filter=chemical_formula_reduced="O2Si"**):

  <optimade_impl_url>/v1/structures?filter=chemical_formula_reduced="O2Si"

- Furthermore, the response format is exactly the same!

The users are now able to search more materials DBs with the same query…

- If we explore Group 14 compounds, we can write a simple query (1):

  /v1/structures?filter=elements HAS ANY "C", "Si", "Ge", "Sn", "Pb"

- We can further focus on binary materials (2):

  /v1/structures?filter=elements HAS ANY "C", "Si", "Ge", "Sn", "Pb" AND nelements=2

- We can discard one element (e.g., Pb) focusing on ternary materials (3):

  /v1/structures?filter=elements HAS ANY "C", "Si", "Ge", "Sn" AND NOT elements HAS "Pb"

  AND elements LENGTH 3

Provider	N_1	N_2	N_3
AFLOW	700,192	62,293	382,554
Crystallography Open Database (COD)	416,314	3,896	32,420
Theoretical Crystallography Open Database (TCOD)	2,631	296	660
Materials Cloud	886,518	801,382	103,075
Materials Project	27,309	3,545	10,501
Novel Materials Discovery Laboratory (NOMAD)	3,359,594	532,123	1,611,302
Open Database of Xtals (odbx)	55	54	0
Open Materials Database (*omdb*)	19,317	396	3,303
Open Quantum Materials Database (OQMD)	153,113	11,011	70,252

Further databases are known to have partial implementations of the OPTIMADE API, including JARVIS.

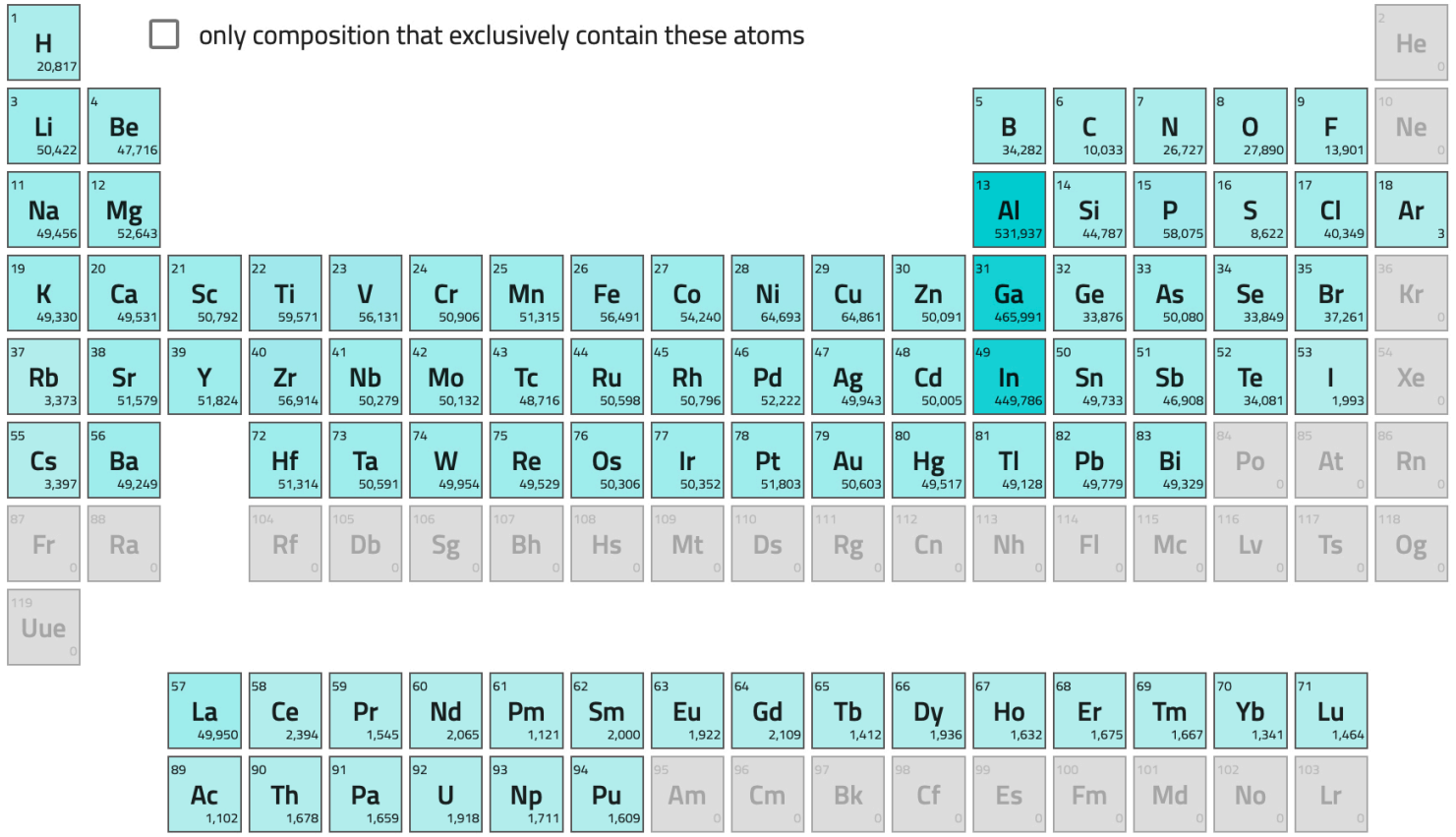
Computational data

ELEMENTS SYSTEM METHOD PROPERTIES UPLOADS Entries

Search with Optimade filter language

OPTIMADE elements HAS ANY "Al", "Ga", "In"

There are **1,394,894** entries left.



ENTRIES MATERIALS GROUPED ENTRIES DATASETS

1,394,894 entries

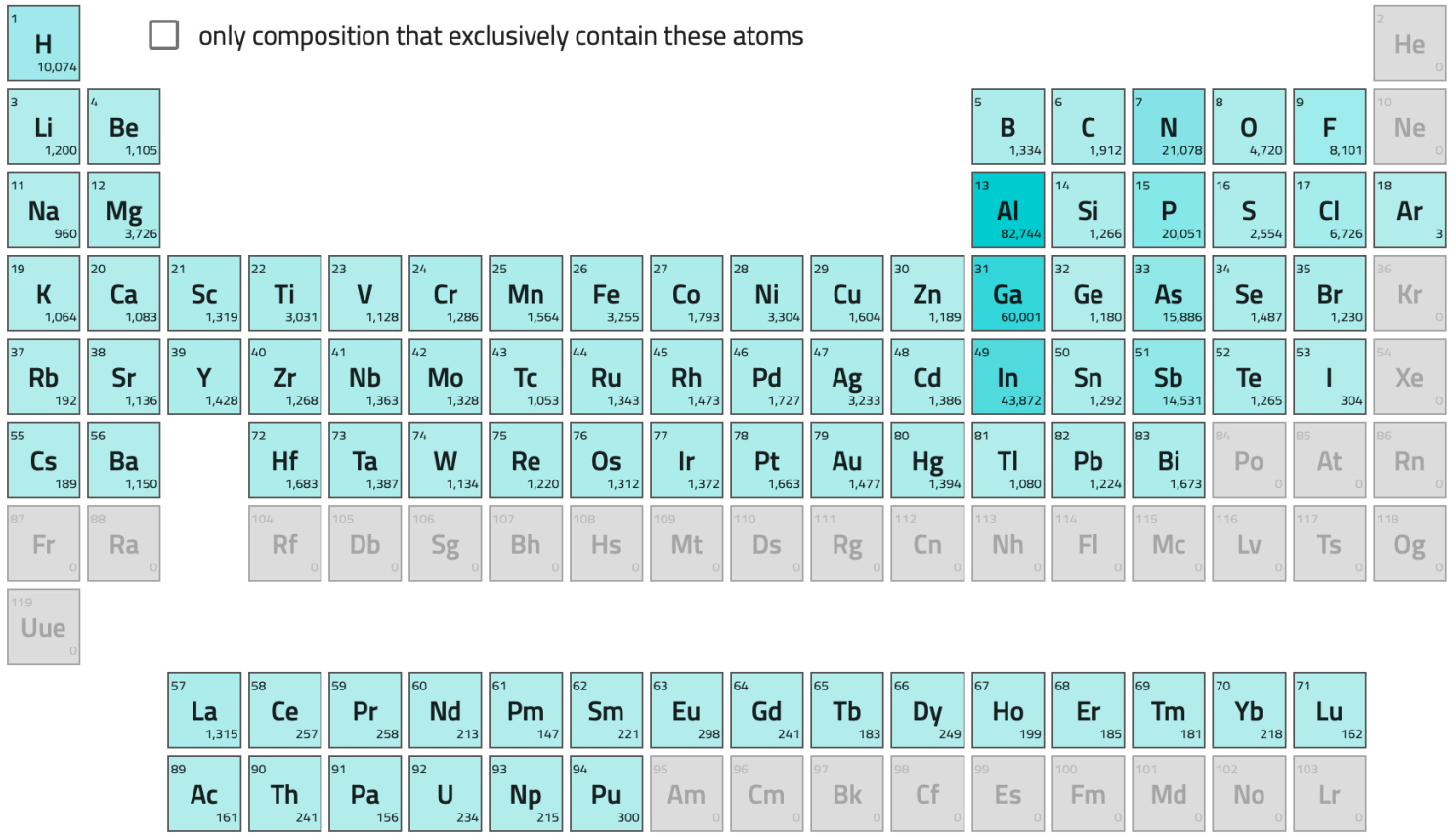
Computational data

ELEMENTS SYSTEM METHOD PROPERTIES UPLOADS Entries

Search with Optimade filter language

OPTIMADE elements HAS ANY "Al", "Ga", "In" AND nelements=2

There are **191,626** entries left.



ENTRIES MATERIALS GROUPED ENTRIES DATASETS

191,626 entries

NOMAD **Find and Download Data** LOGIN / REGISTER

SEARCH | UPLOAD | YOUR DATA | ENCYCLOPEDIA | METAINFO | ABOUT | TERMS | MORE

Computational data | ELEMENTS | SYSTEM | METHOD | PROPERTIES | UPLOADS | Entries

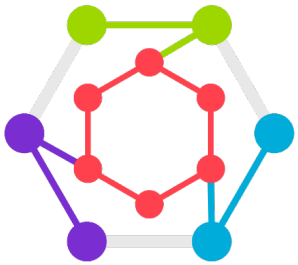
Search with Optimade filter language

OPTIMADE elements HAS ANY "Al", "Ga", "In" AND elements HAS ANY "N", "P", "As", "Sb" AND nelements=2

There are **71,546** entries left.

ENTRIES | MATERIALS | GROUPED ENTRIES | DATASETS

71,546 entries



OPTIMADE v1.0 (released July 2020)

- **REST API for common access to crystal structure databases**
  - Human-readable specification (~20k words)
  - Based on JSON API
  - Machine-readable OpenAPI 3.0 schema
- **Enables unified access to 25M crystal structures from 14 providers**
  - Federated providers list and discoverability mechanisms
  - API validation beyond OpenAPI through associated tooling
- **Features:**
  - Standardized representation for crystal structures, bibliographic references and links
  - Well-defined grammar/filter language
  - Introspective **/info** endpoint for extensibility
  - Strict response format, but data models are flexible where necessary

scientific data

OPEN

ARTICLE

OPTIMADE, an API for exchanging materials data

Casper W. Andersen *et al.*[#]

The Open Databases Integration for Materials Design (OPTIMADE) consortium has designed a universal application programming interface (API) to make materials databases accessible and interoperable. We outline the first stable release of the specification, v1.0, which is already supported by many leading databases and several software packages. We illustrate the advantages of the OPTIMADE API through worked examples on each of the public materials databases that support the full API specification.

[#]A full list of authors and their affiliations appears at the end of the paper.

/optimade/providers

OPTIMADE Providers Index Meta-Database

The list of OPTIMADE providers keeps track of all reserved database-specific prefixes and the URLs to the index databases of all OPTIMADE database providers that participate in the OPTIMADE network.

The list of providers is published in the form of a statically hosted OPTIMADE Index Meta-Database here:

- https://providers.optimade.org/

If you specifically seek the current list of providers for the latest version of the OPTIMADE specification, you can access it at this URL:

- https://providers.optimade.org/providers.json

If you seek the list of providers formatted according to a specific major version of the OPTIMADE specification, you can access it using this URL:

- https://providers.optimade.org/*<version>*/links

Where `<version>` designates a major version name of the OPTIMADE specification, e.g., `v1`.

Repository organization

The OPTIMADE providers repository is hosted here: https://github.com/Materials-Consortia/providers

The repository is organized this way:

- `/src/links/<version>/providers.json` is the current providers.json file formatted according to OPTIMADE version `<version>` and any later version that uses a format that is backward compatible with this version.
- `/src/info/<version>/info.json` is the proper response to the info endpoint formatted according to OPTIMADE version `<version>` and any later version that uses a format that is backward compatible with this version.
- `/_redirect` specify http rewrites to map index meta-database URLs `/<version>/info` and `/<version>/links` to the corresponding files under `src/`, as well as `/providers.json`.

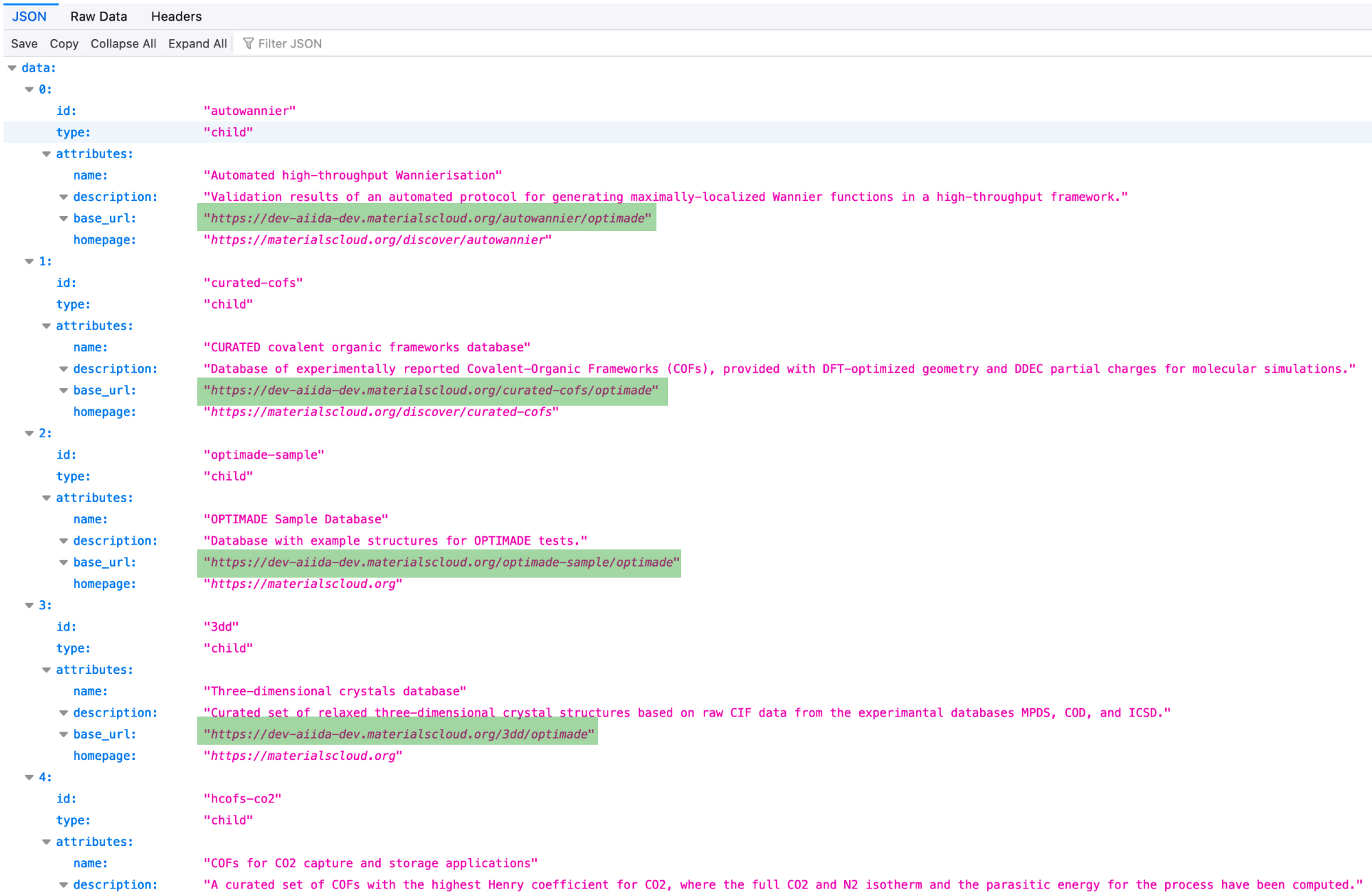
/optimade/providers

JSON Raw Data Headers

Save Copy Collapse All Expand All Filter JSON


```
data:
  0:
    type:          "provider"
    id:            "aiida"
    attributes:
      name:        "AiiDA"
      description: "Automated Interactive Infrastructure and Database for Computational Science (AiiDA)"
      base_url:    null
      homepage:    "http://www.aiida.net"
  1:
    type:          "provider"
    id:            "aflow"
    attributes:
      name:        "aflow.org"
      description: ""
      base_url:    null
      homepage:    null
  2:
    type:          "provider"
    id:            "cod"
    attributes:
      name:        "Crystallography Open Database"
      description: "Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals,
      base_url:    "https://www.crystallography.net/cod/optimade"
      homepage:    "https://www.crystallography.net/cod"
  3:
    type:          "provider"
    id:            "exmpl"
    attributes:
```

/optimade/links



OPTIMADE-Client

OPTIMADE
Open Databases Integration
for Materials Design

Currently valid OPTIMADE API version: `v1.0.0`

Client version: `2020.11.22`

Source code: GitHub

Help improve the application: Report a bug | Suggest a feature/change

This is a friendly client to search through databases and other implementations exposing an OPTIMADE RESTful API. To get more information about the OPTIMADE API, please see the offical web page. All providers are retrieved from the OPTIMADE consortium's list of providers.

Note: The structure property `assemblies` is currently not supported. Follow the issue on GitHub to learn more.

▸ FAQ

My modules

filter= Start typing...

COD v1.0.0 · SSS v1.0.1 · 2DS v1.0.1 · 2DT v1.0.1 · AOT v1.0.1 · TDC v1.0.1 · AHT v1.0.1 · CUR v1.0.1 · OPT v1.0.1 · STO v1.0.1 · PMO v1.0.1 · SSL v1.0.1

MP v1.0.1 · MPDS v1.0.0 · odbx v1.0.1 · OMD v1.0.0 · TOQ v1.0.0 · TCO v1.0.0

A GitHub repository is available

Open Databases Integration for Materials Design

The Open Databases Integration for Materials Design (OPTIMADE) makes the materials databases interoperational by developing a common REST API.

http://www.optimade.org

GitHub

Repositories 11 | Packages | People 36 | Teams | Projects | Settings

optimade-python-tools

Tools for implementing and consuming OPTiMaDe APIs in Python

Python | MIT | 13 | 10 | 18 (3 issues need help) | 4 | Updated 9 hours ago

optimade-validator-action

GitHub Actions action to validate OPTiMaDe implementations using the validator from Materials-Consortia/optimade-python-tools

Shell | MIT | 2 | 1 | 1 | 0 | Updated yesterday

materials-consortia.github.io

OPTiMaDe website

JavaScript | 3 | 0 | 3 | 1 | Updated 7 days ago

OPTIMADE-Filter

OPTiMaDe filter language parser in Perl

Perl | LGPL-3.0 | 1 | 0 | 0 | 0 | Updated 7 days ago

Top languages

Python | Shell | JavaScript | Java | Makefile

Most used topics

Loading...

People >

jmol-commits Mailing List for Jmol

An interactive viewer for three-dimensional chemical structures.

Brought to you by: aherraez, egonw, hansonr, migueljmol, and 2 others

jmol-commits — Automatic notifications from the CVS repository

[Jmol-commits] SF.net SVN: jmol:[22399] trunk/Jmol/src/org/jmol

From: <ha...@us...> - 2022-04-14 04:51:57

```
Revision: 22399
          http://sourceforge.net/p/jmol/code/22399
Author:   hansonr
Date:     2022-04-14 04:51:53 +0000 (Thu, 14 Apr 2022)
Log Message:
-----------
Jmol.___JmolVersion="14.32.48" //  also 15.2.48

new feature: Optimade reader
 - https://github.com/Materials-Consortia/OPTIMADE/blob/master/optimade.rst
 - requires qualifier Optimade:: because there is no identifying characteristic of the return
 - example: load Optimade::https://optimade.materialsproject.org/v1/structures?filter=nelements=6&page_limit=1
```

RESEARCH ARTICLE

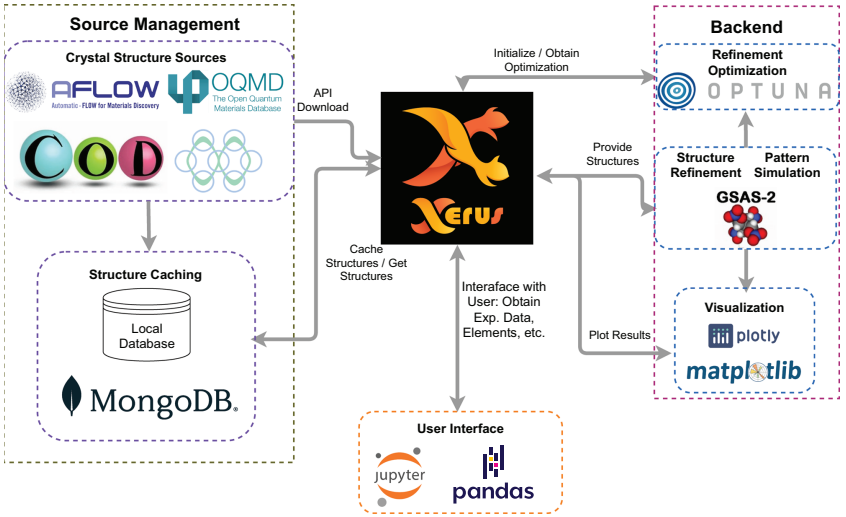
ADVANCED THEORY AND SIMULATIONS
www.advtheorysimul.com

XERUS: An Open-Source Tool for Quick XRD Phase Identification and Refinement Automation

Pedro Baptista de Castro, Kensei Terashima,* Miren Garbine Esparza Echevarria, Hiroyuki Takeya, and Yoshihiko Takano**

DOI: 10.1002/adts.202100588

Adv. Theory Simul. **2022**, 2100588



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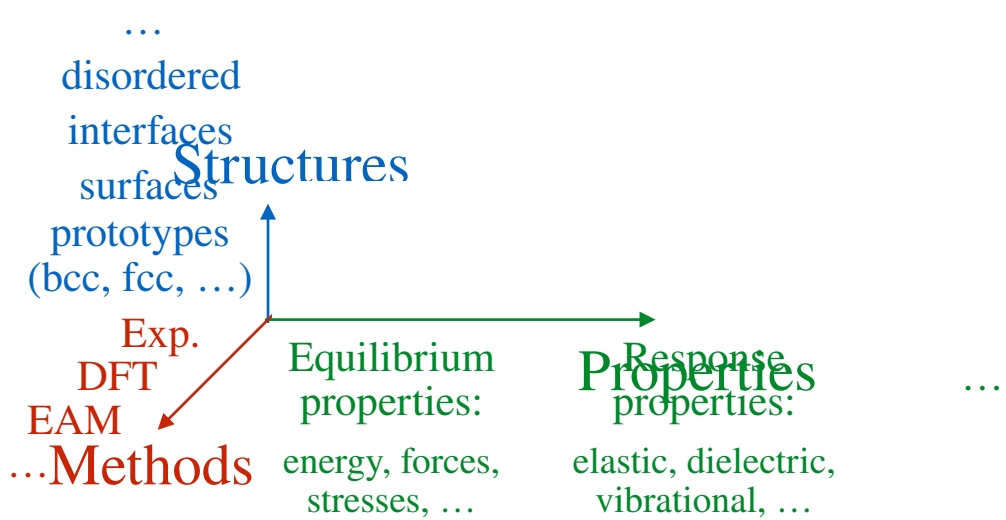
master Xerus / Xerus / queriers / Go to file Add file ...

pedrobcst Added support for multiple uses querying at same time (experimental..) 7c55464 on Apr 15 History

..		
__init__.py	v1	6 months ago
aflow.py	Added missing header and timeout to OPTIMADE	last month
cod.py	Fix typos from conflict (#15)	2 months ago
mp.py	Set a timeout for requests to avoid infinite hanging	2 months ago
multiquery.py	Added support for multiple uses querying at same time (experimental..)	last month
optimade.py	Added missing header and timeout to OPTIMADE	last month
oqmd.py	Set a timeout for requests to avoid infinite hanging	2 months ago
tcif.py	Added support for multiple uses querying at same time (experimental..)	last month

Opportunities



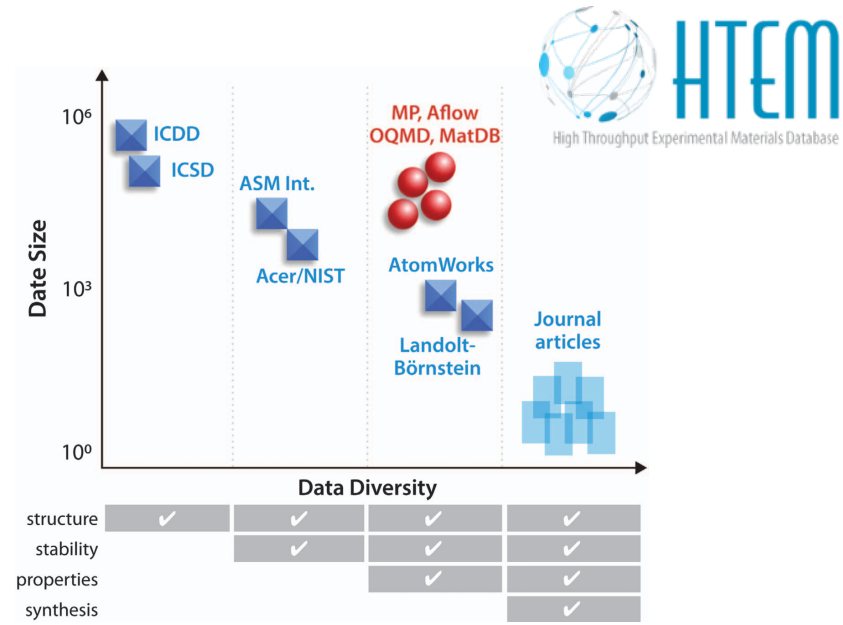
cecam supports OPTIMADE

Centre Européen de Calcul Atomique et Moléculaire

- 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.
- A post-doctoral fellow will be hired for an initial period of 12 months to work on specific tasks dedicated to *expanding the current developments in OPTIMADE to classical molecular dynamics or bio-simulations*
- Longer-term actions:
  - *creating a service to integrate and interrogate efficiently the different databases*
  - *creating and maintaining a dictionary of metadata*

Opportunities

ANSYS
GRANTA
MPDS Materials Platform for Data Science
PAULING FILE Inorganic Materials Database
NIMS
MatNavi NIMS Materials Database
AtomWork Adv.



[Zakutayev *et al.*, Sci. Data **5**,180053 (2018)]

Structures

… disordered interfaces surfaces prototypes (bcc, fcc, …)

Methods

Exp. DFT EAM …

Equilibrium properties: energy, forces, stresses, …

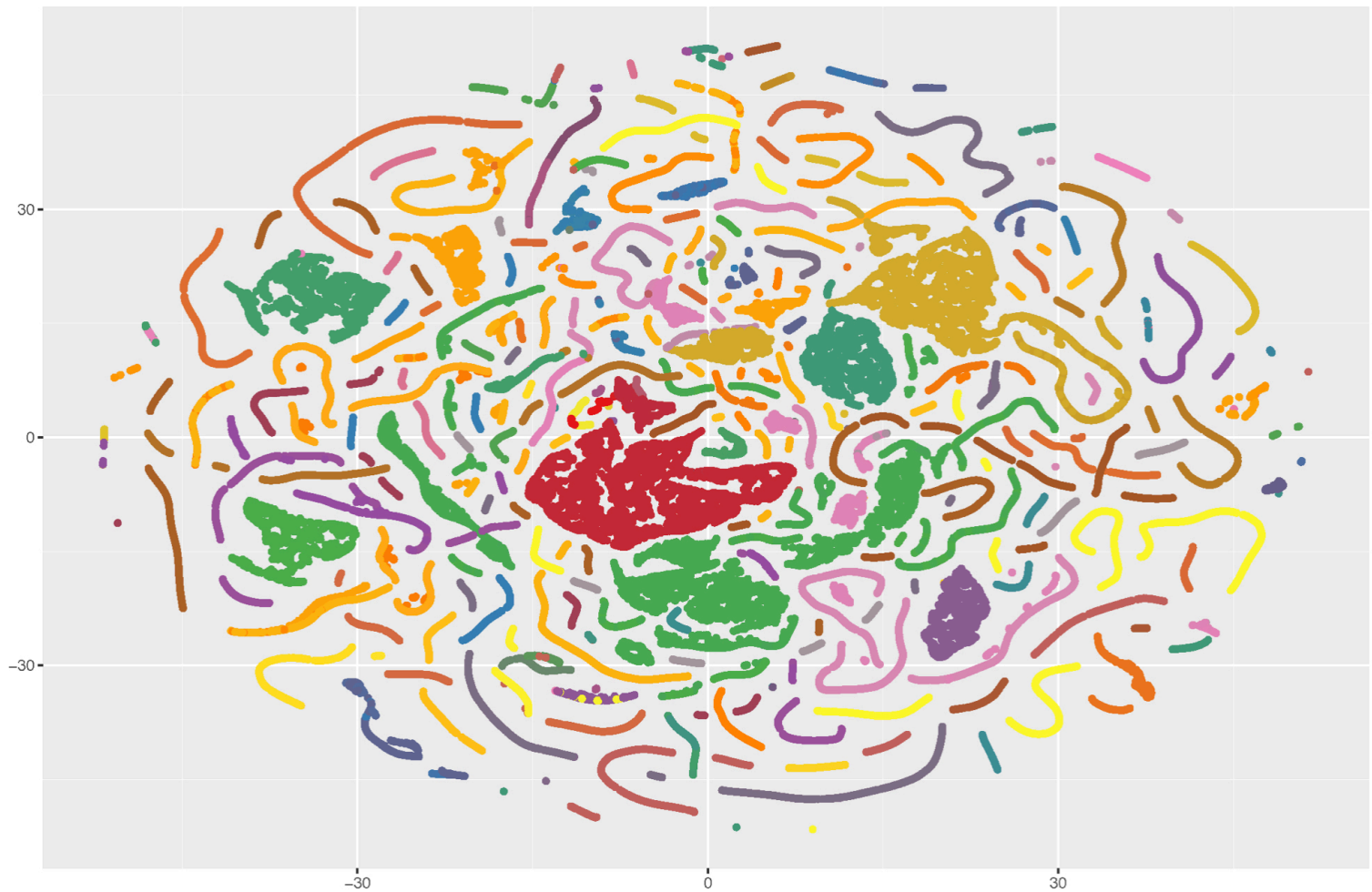
Response properties: elastic, dielectric, vibrational, …

…

Properties

HTEM Content

Public version of HTEM DB features composition (37093), structure (47213), optical (26577), and electrical (12849) properties of thin films synthesized using combinatorial methods. It currently contains 1307 sample libraries with 57597 thin film samples, across a wide range of materials (oxides, nitrides, sulfide, intermetallics).



API

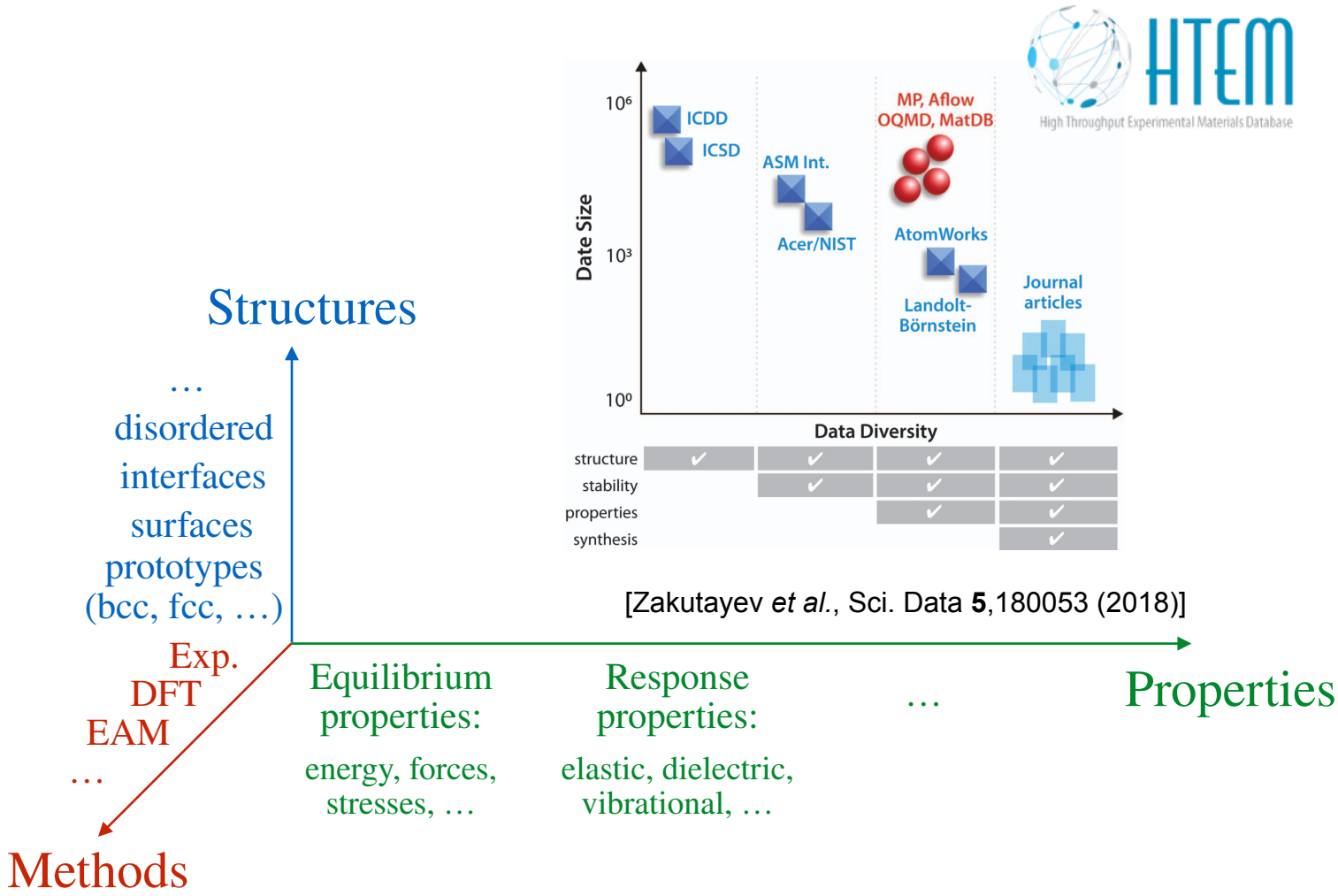
Comporting with an open-data ethos, all data in the HTEM DB is available via a RESTful JSON-based API to allow programmatic access. This is the same API that serves as a backend for this website. Those who choose to utilize the API can download data in full to create their own visualizations and analyses beyond what is available here.

Base URI: https://htem-api.nrel.gov/api

API Documentation: https://htem-api.nrel.gov/

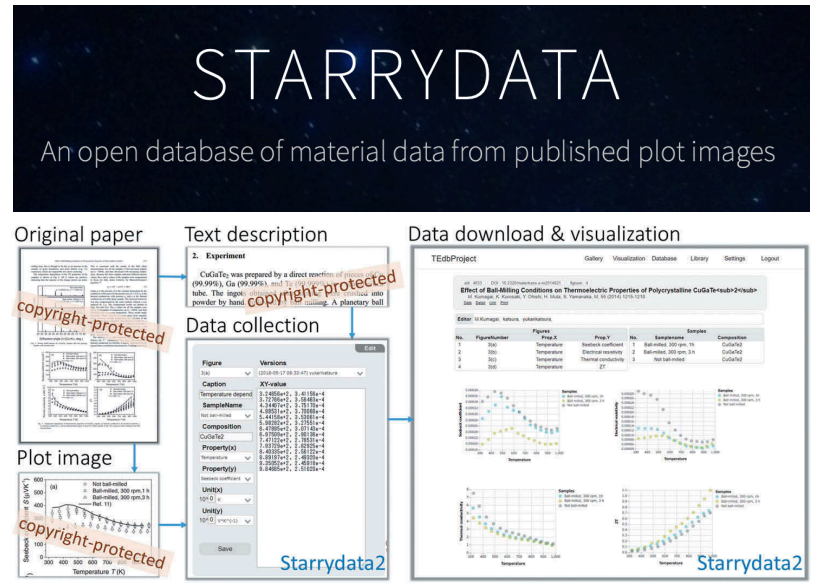
If you use our data in your research, please cite its use following the instructions in our How to Cite page.

Opportunities



[Zakutayev *et al.*, Sci. Data **5**,180053 (2018)]

Opportunities



[Y. Katsura *et al.*, Sci. Technol. Adv. Mater. **20**, 511 (2019)]

STARRYDATA

An open database of material data from published plot images

STARRYDATA API

Posted on September 13, 2018 by starrydata in Uncategorized

We have implemented APIs for Starrydata web system.

You can get all data associated to specific paper/figure/sample by the following URIs.

JSON DATA FOR A SPECIFIC PAPERID(='SID')/FIGUREID/SAMPLEID

https://www.starrydata2.org/api/paper/(paperid)
https://www.starrydata2.org/api/figure/(figureid)
https://www.starrydata2.org/api/sample/(sampleid)

A SPECIFIC ELEMENT OF AN ENTRY

https://www.starrydata2.org/api/paper/(paperid)/title

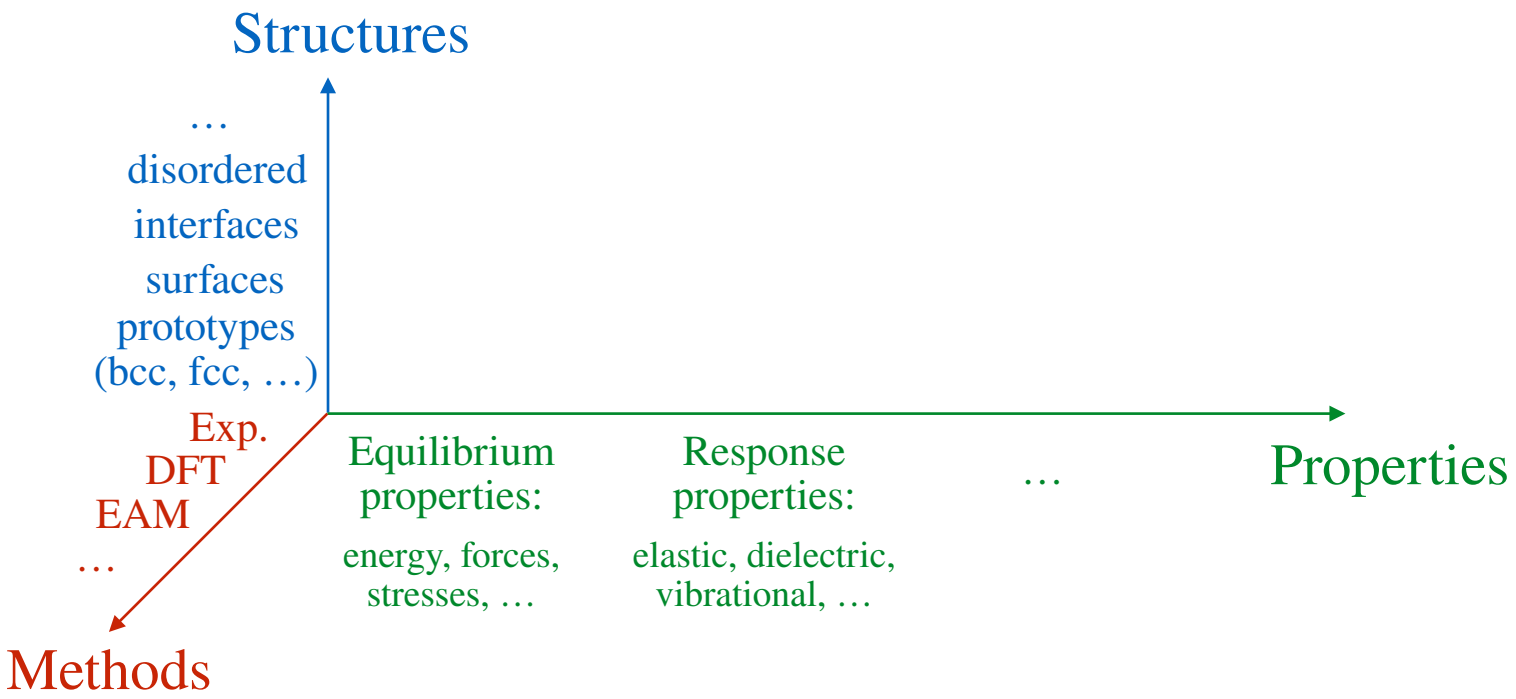
https://www.starrydata2.org/api/sample/(sampleid)/composition

A LIST OF PAPERIDS/FIGUREIDS/SAMPLEIDS THAT CONTAIN SPECIFIC ATOMS IN THE SAMPLE COMPOSITIONS

https://www.starrydata2.org/api/paper/search?atom=Bi,Te
https://www.starrydata2.org/api/figure/search?atom=Bi,Te
https://www.starrydata2.org/api/sample/search?atom=Bi,Te
https://www.starrydata2.org/api/search/search?atom=Bi,Te
(for a gathered list of paperids, figureids, sampleids)
The default is AND search.
OR search can be done by writing 'Bi,Te,or'

Opportunities

- OPTIMADE would clearly benefit from semantically enabling the system using an **ontology**, both for search as well as for integrating information from the underlying databases.



What's next for OPTIMADE?

- **Semantic interoperability through an ontology**
  - "An Ontology for the Materials Design Domain", arXiv:2006.07712 (H. Li, R. Armiento, and P. Lambrix)
  - Fostering links and synergy with:
    - European Materials Modelling Ontology (EMMO)
    - Work that has already been done in the IUCr (International Union of Crystallography) about the CIF standard (CIF2)
  - https://github.com/Materials-Consortia/ontology
- **Expanding to classical molecular dynamics and bio-simulations**

  Platform for fitting machine-learned interatomic potentials
  - Workshop in 30 May-3 June 2021 at CECAM + Digital

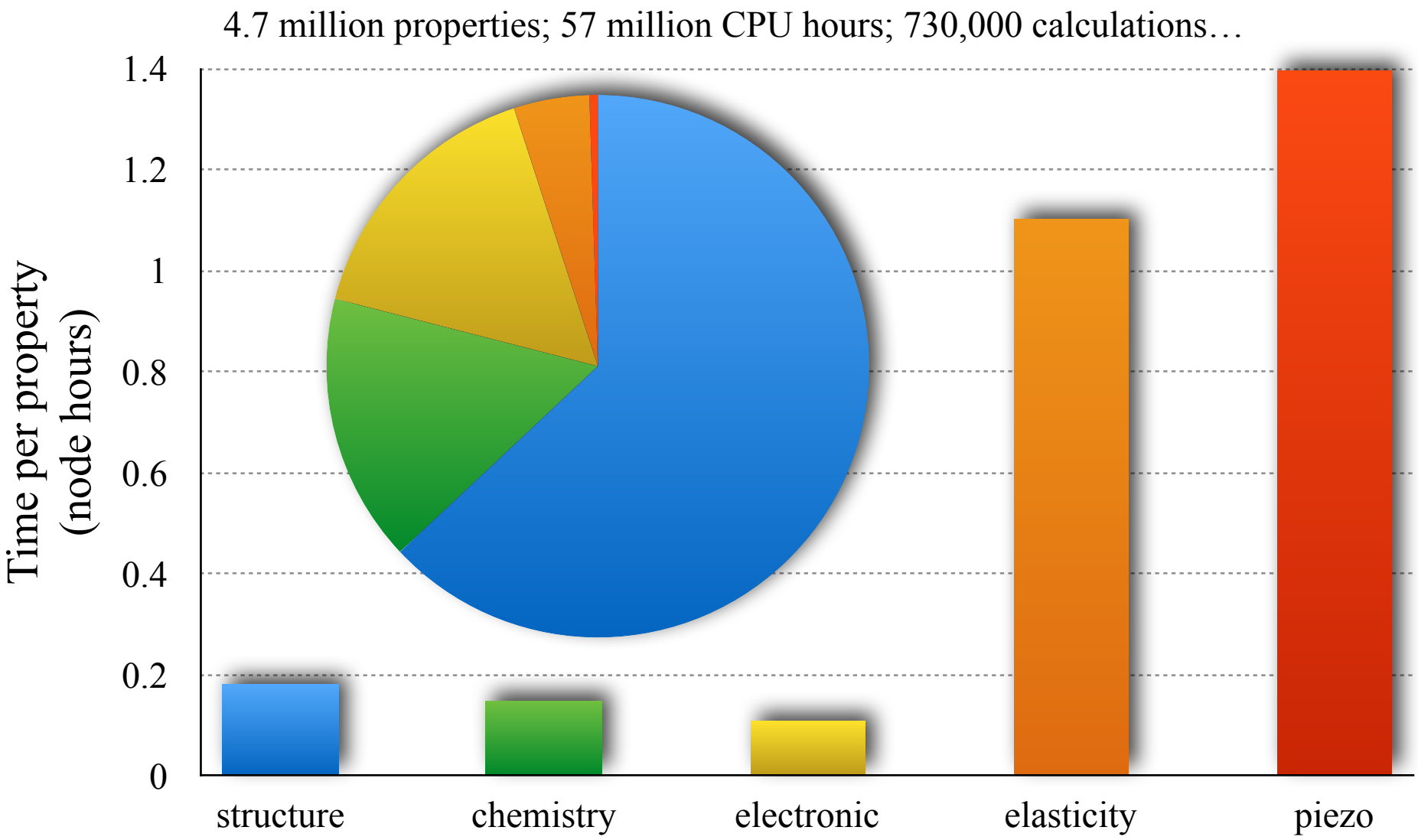
    https://www.cecam.org/workshop-details/1120

    Contacts: gian-marco.rignanese@uclouvain.be

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

The amount of data available in the DBs depends on the computing time for each property



For reducing the computational cost,

machine learning may be very handy

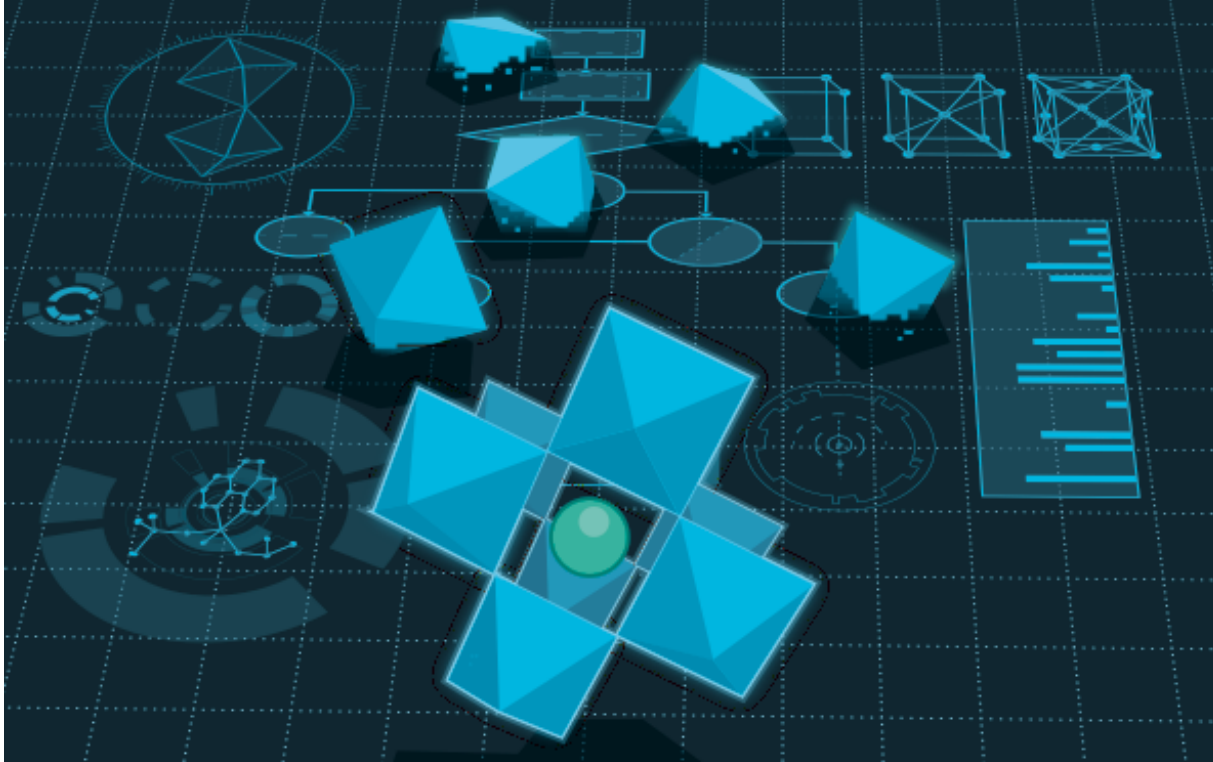
NEWS FEATURE

[N. Nosengo, Nature **566,** 475 (2016)]

THE MATERIAL CODE

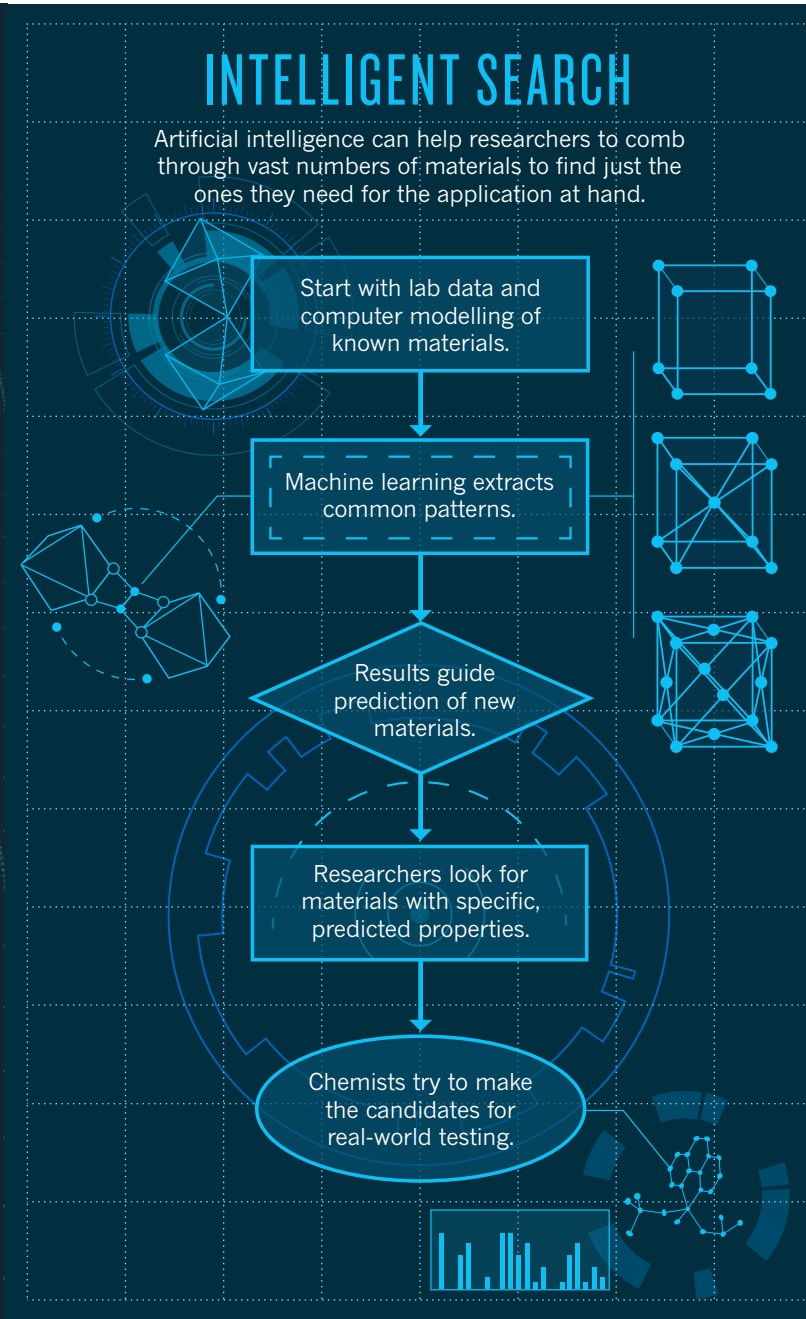
Machine-learning techniques could revolutionize how materials science is done.

BY NICOLA NOSENGO

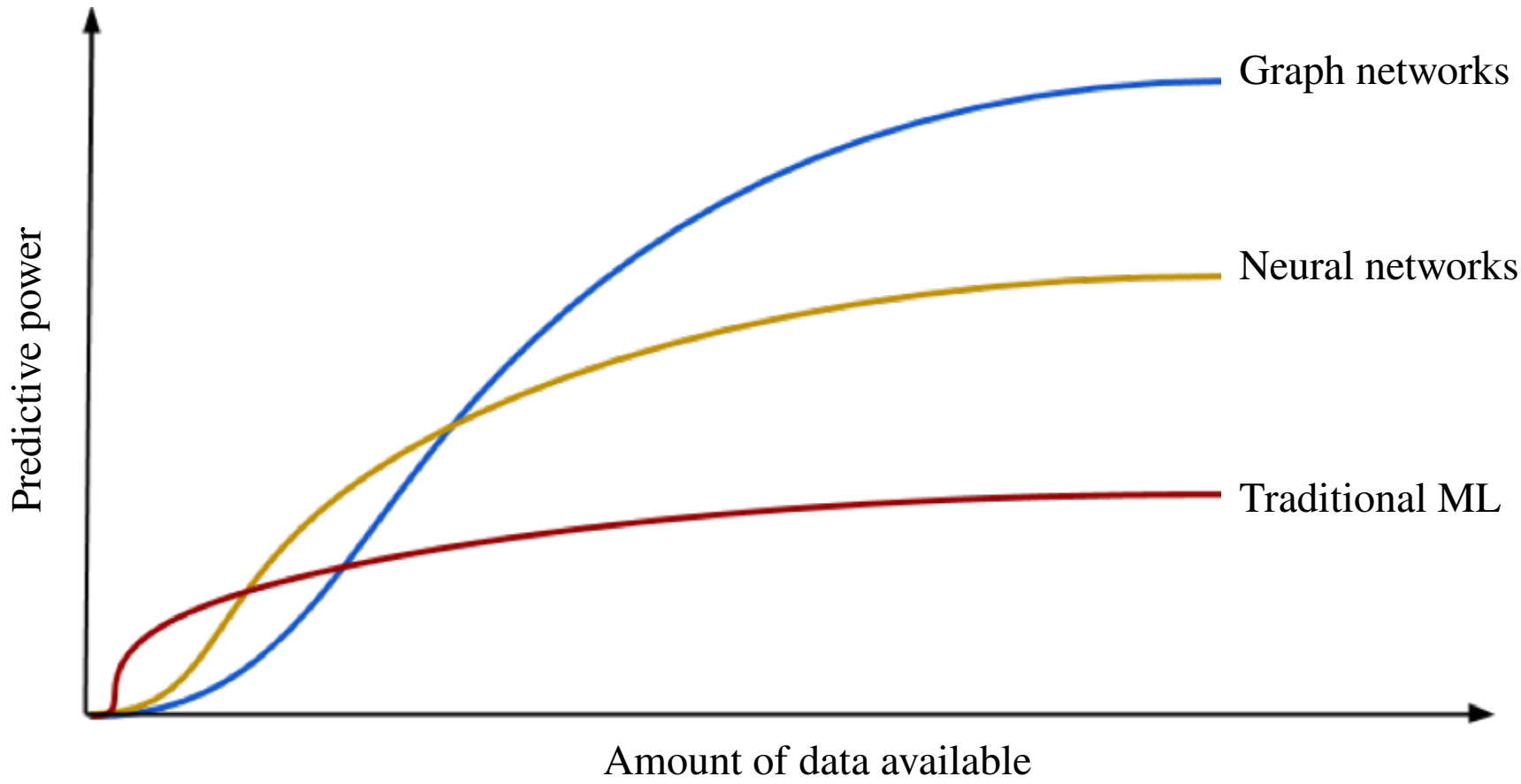


INTELLIGENT SEARCH

Artificial intelligence can help researchers to comb through vast numbers of materials to find just the ones they need for the application at hand.



The predictive power of the model depends on the amount of data available

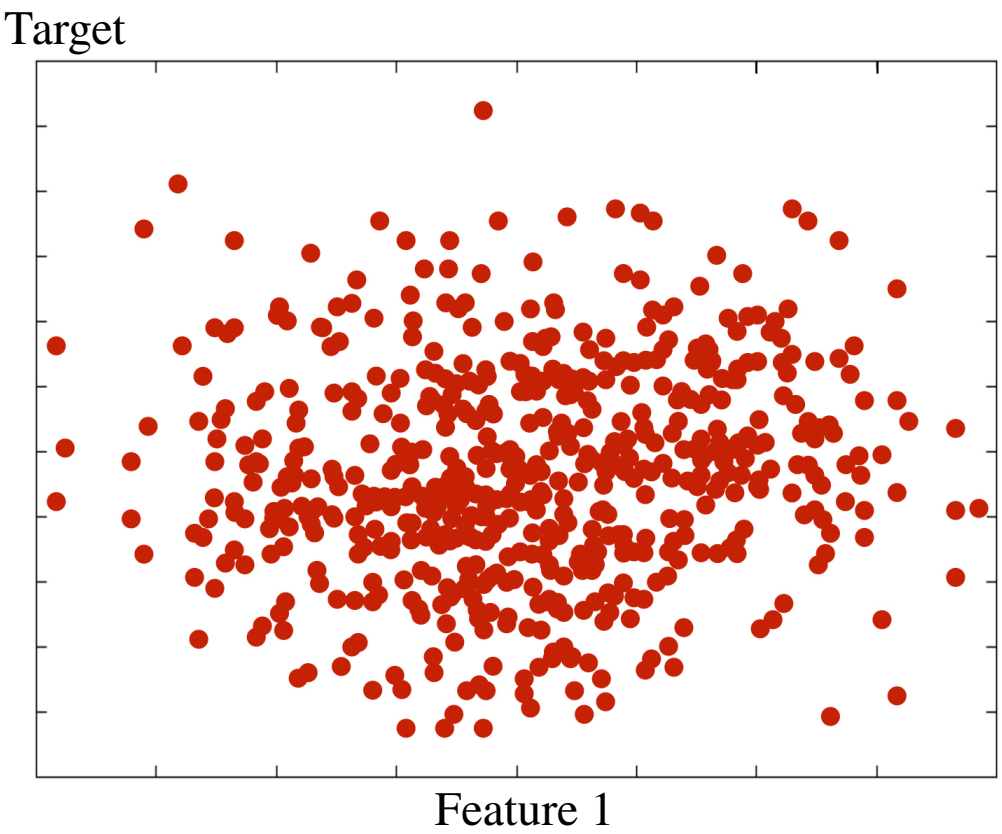


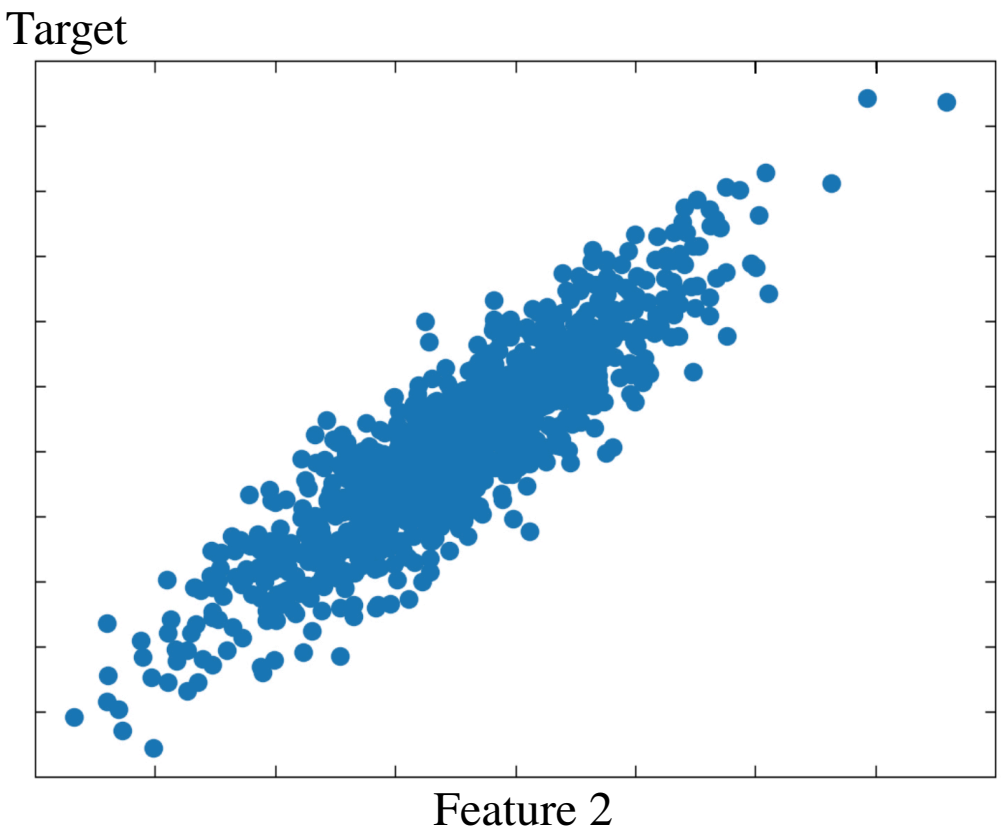
Computationally demanding material properties are precisely those with little available data

Material Optimal Descriptor Network (MODNet)

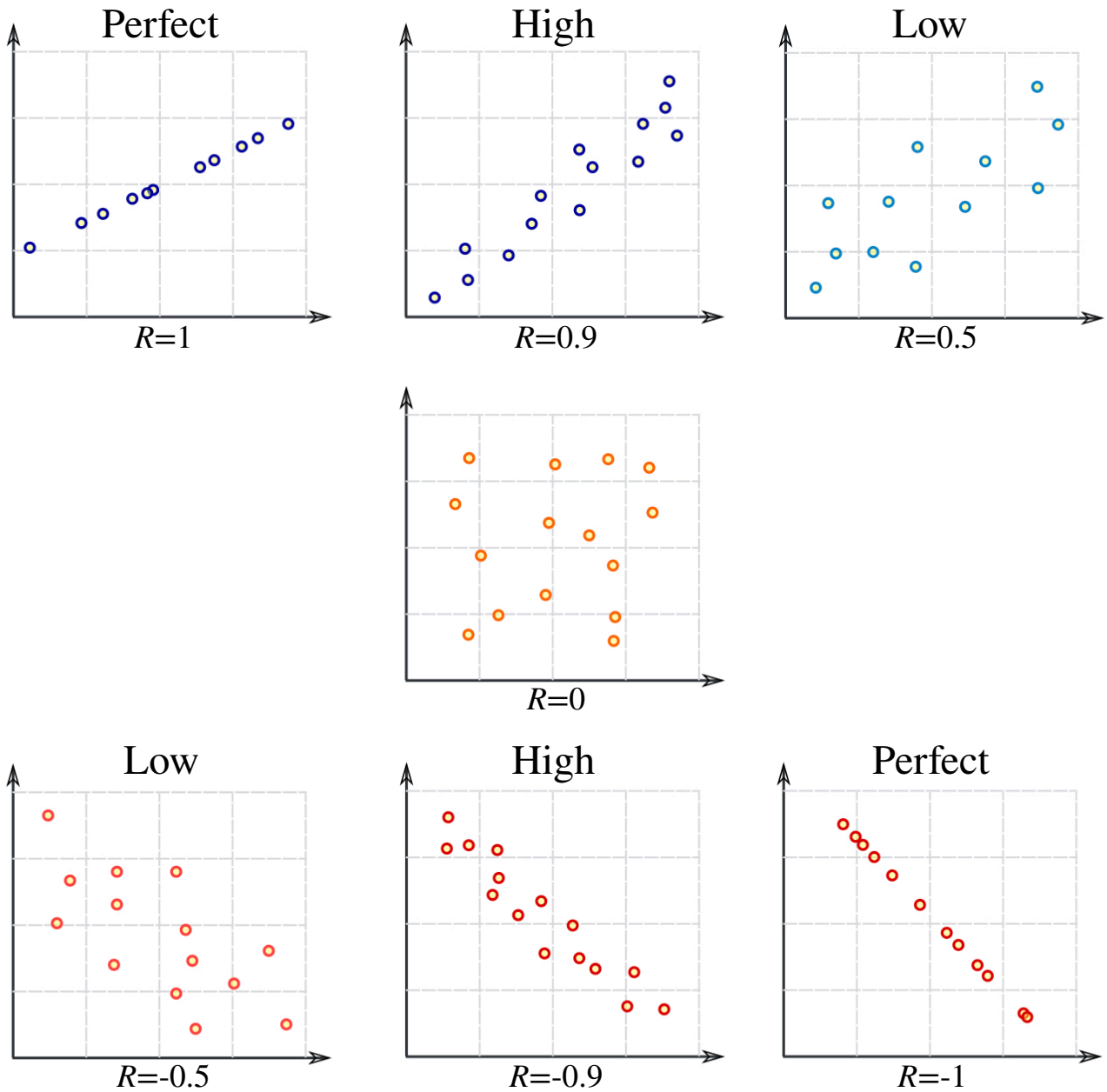
- Concept: feedforward neural network with an optimal set of descriptors.
- Idea: **Feature selection** by **relevance-redundancy algorithm**
  - Prior physical knowledge and constraints are taken into account by adopting physically-meaningful features.
  - This reduces the optimization space without relying on a massive amount of data.
- Bonus: **Novel architecture** that learns on **multiple properties**

To be relevant, the selected features should present some kind of interrelation with the target property



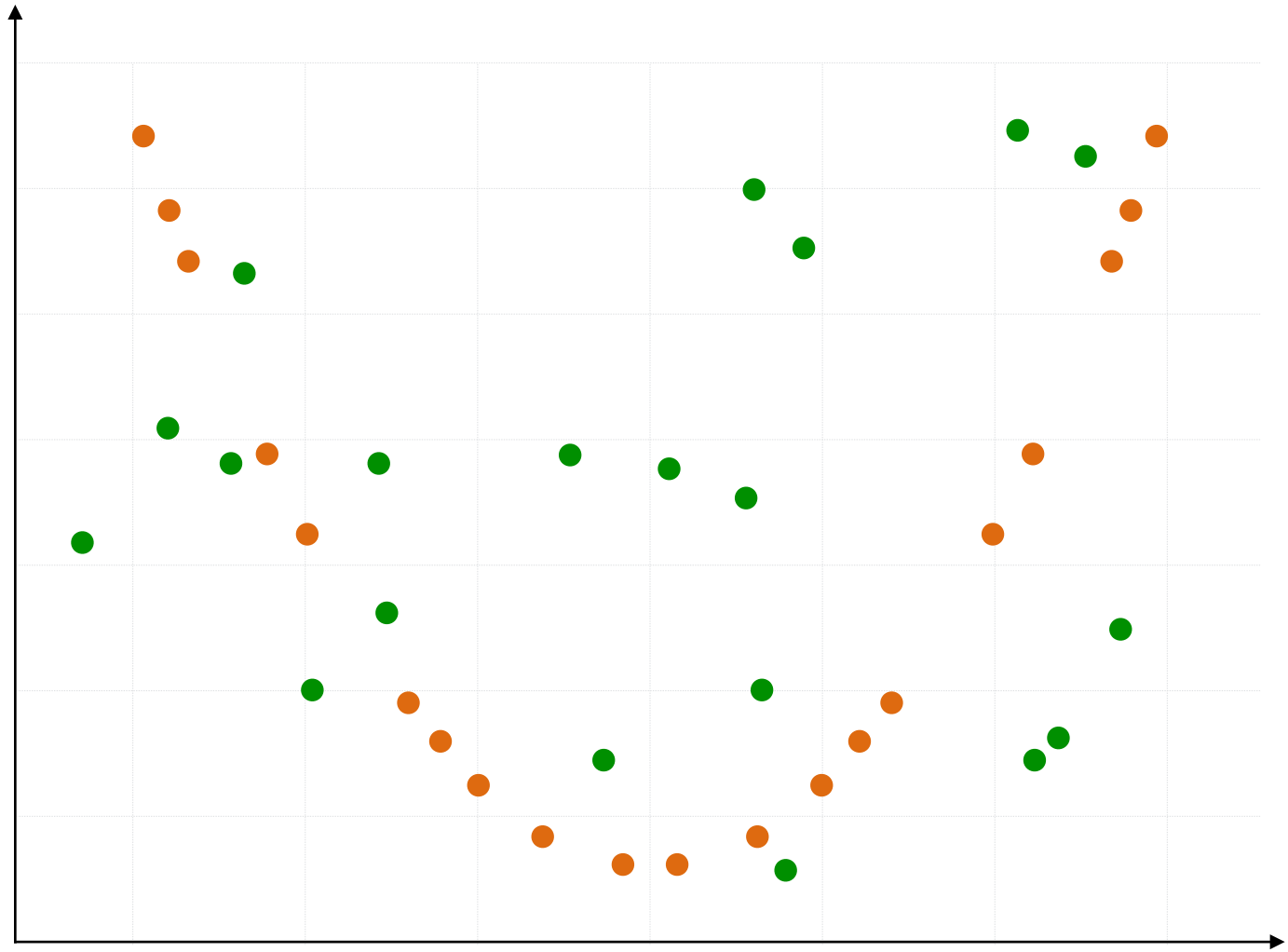


Pearson correlation coefficient is a measure of the interrelation between two variables



Pearson correlation coefficient

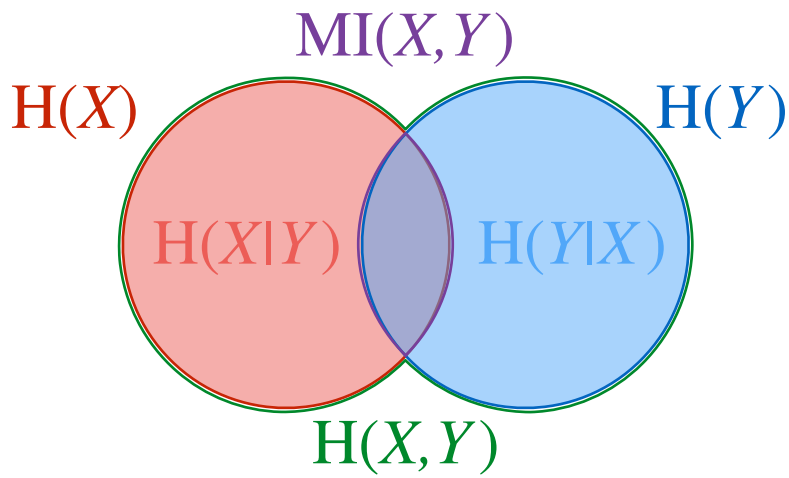
presents, however, a series of limitations

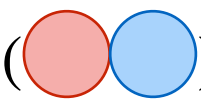
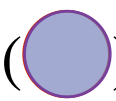


$R=0$

In MODNet, feature selection is based on the Normalized Mutual Information (NMI)

- The **mutual information** (MI) of two random variables is a measure of the mutual dependence between the two variables.
  It quantifies the "amount of information" (entropy) obtained about one random variable through observing the other random variable.

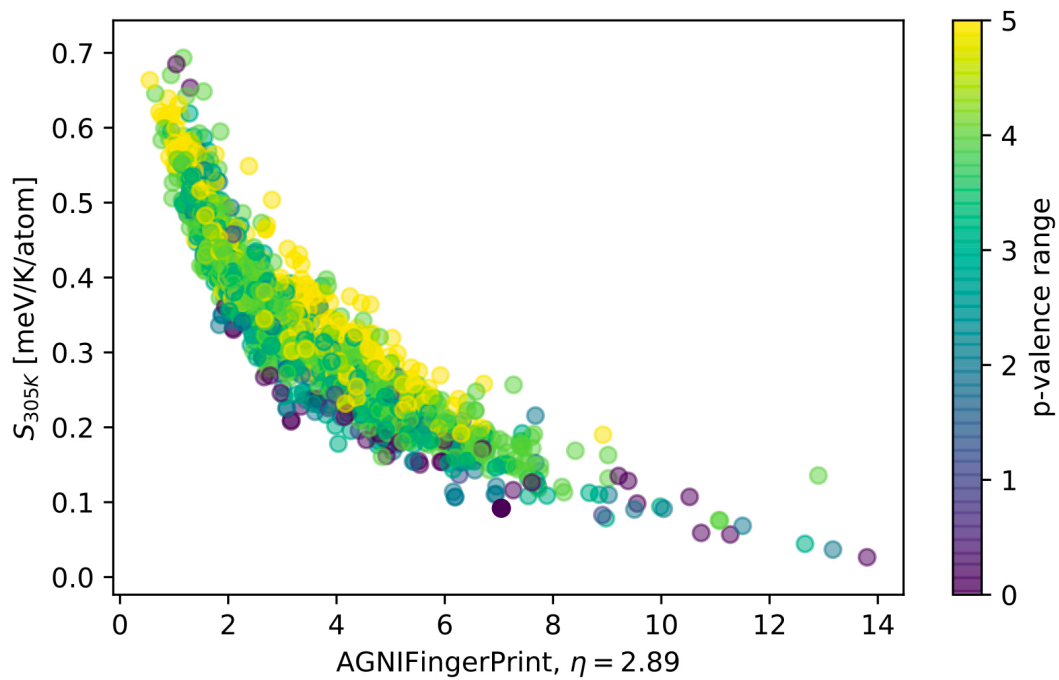


- Their Normalized Mutual Information $\mathrm{NMI}(X, Y) = \dfrac{\mathrm{MI}(X, Y)}{(\mathrm{H}(X) + \mathrm{H}(Y))/2}$ is bounded between 0 () and 1 ()

[P.-P. De Breuck *et al.*, npj Computational Materials **7**, 83(2021)]

The feature *f* having the highest NMI with the target variable *y* will be chosen the first one

- This provides some understanding of the underlying physics.
  Indeed, it pinpoints the most important and complementary variables.
- For instance, the vibrational entropy is found to be strongly related to
  - the inter-atomic bond length
  - the valence range of the constituent elements (ionicity of the bond).



[P.-P. De Breuck *et al.*, npj Computational Materials **7**, 83(2021)]

For the next chosen features, redundancy should also be avoided

- To this end, we define a relevance and redundancy *RR* score: given
  - a subset of selected features $\mathscr{F}_s$ extracted from the set $\mathscr{F}$
  - another feature f

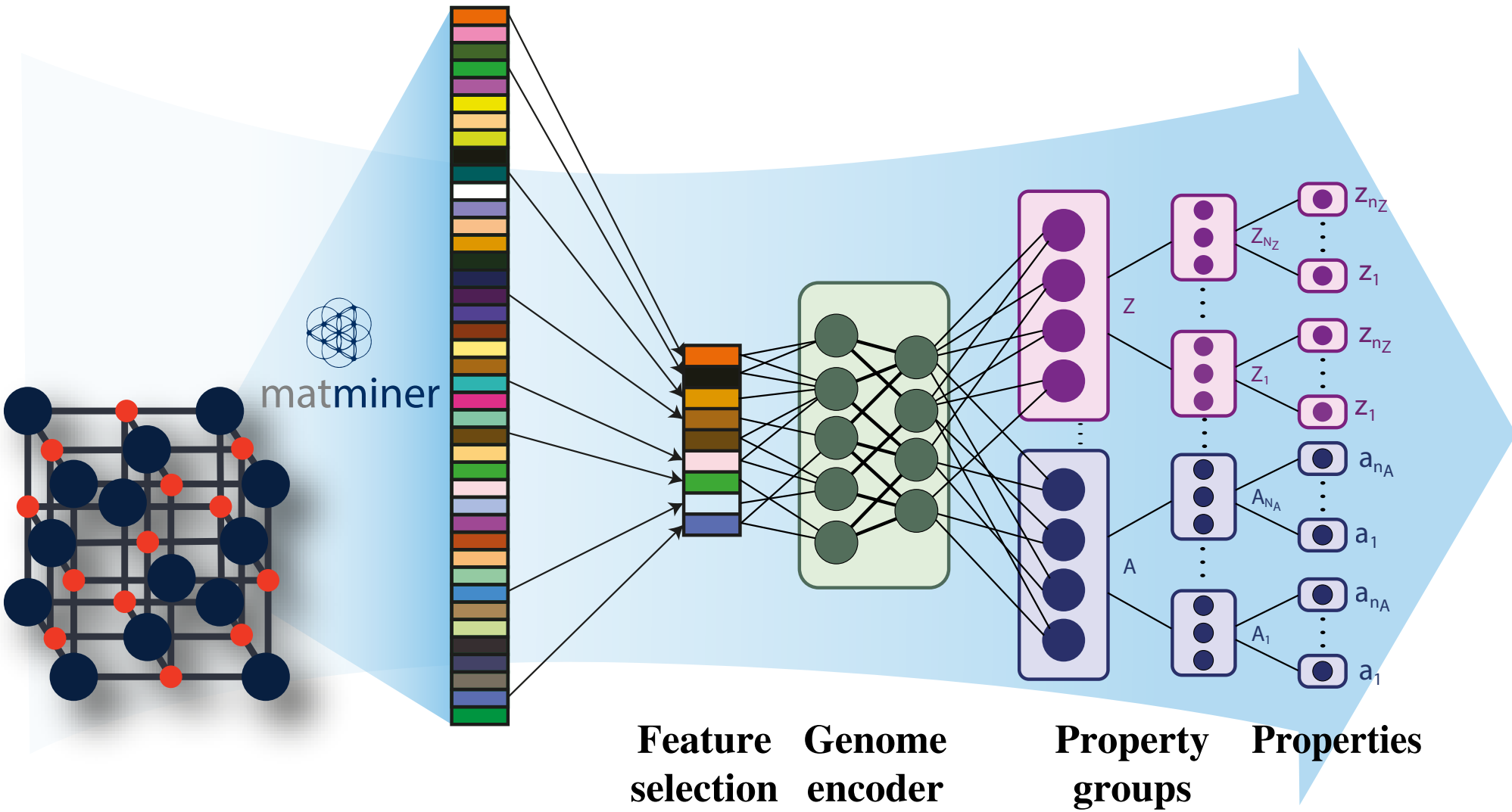
$$RR(f) = \frac{\mathrm{NMI}(f, y)}{\left[\max_{f_s \in \mathscr{F}_s} \left(\mathrm{NMI}(f, f_s)\right)\right]^p + c}$$

  where p and c are determine the relevance/redundancy balance.

- In practice, varying p and c dynamically seems to work better, as redundancy is a bigger issue with a small amount of features.

- The selection proceeds until the number of features reaches a threshold (fixed arbitrarily or, better, optimized to minimize the model error).

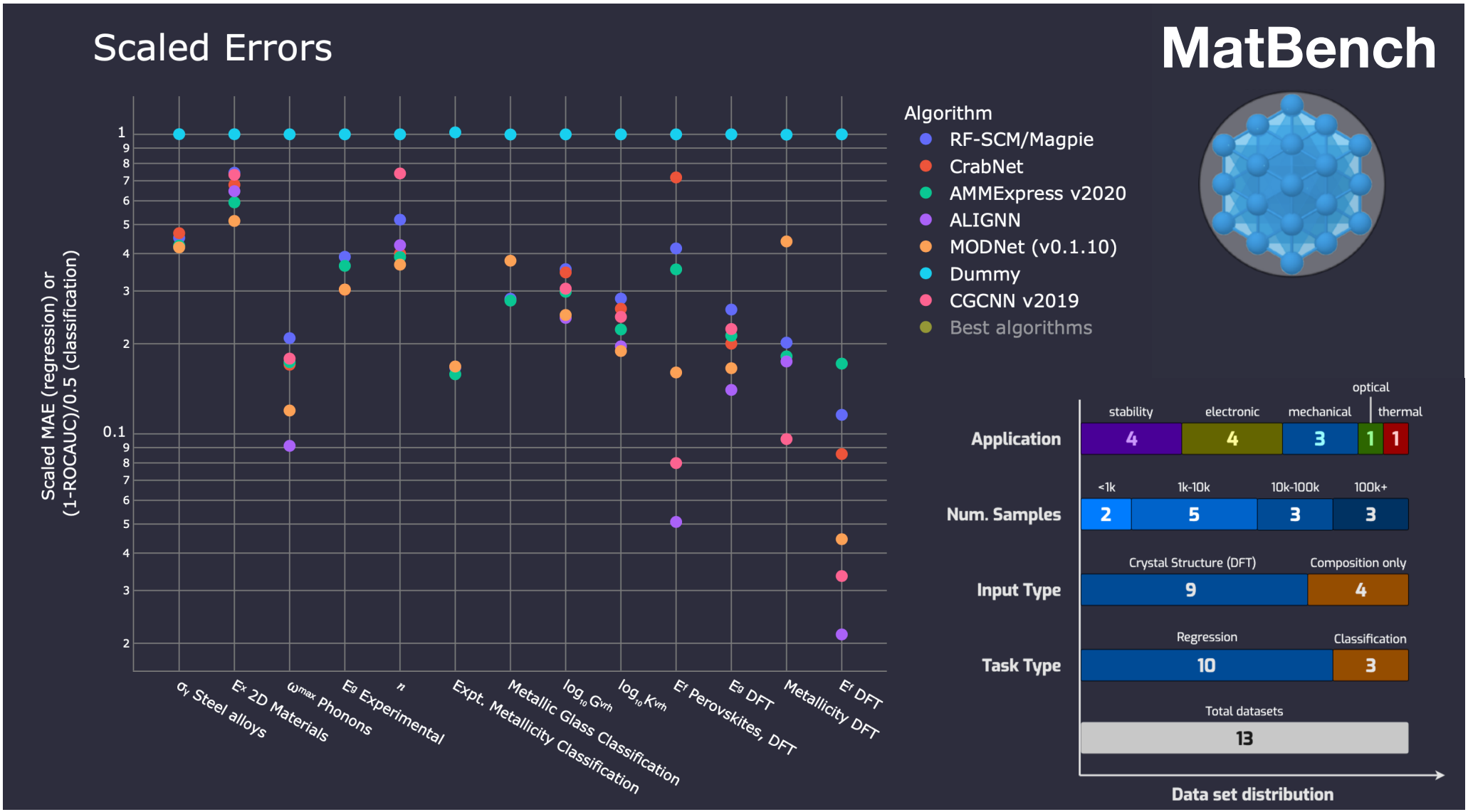
MODNet introduces the possibility of learning on multiple properties simultaneously



[P.-P. De Breuck *et al.*, npj Computational Materials **7**, 83(2021)]

MODNet performs very well

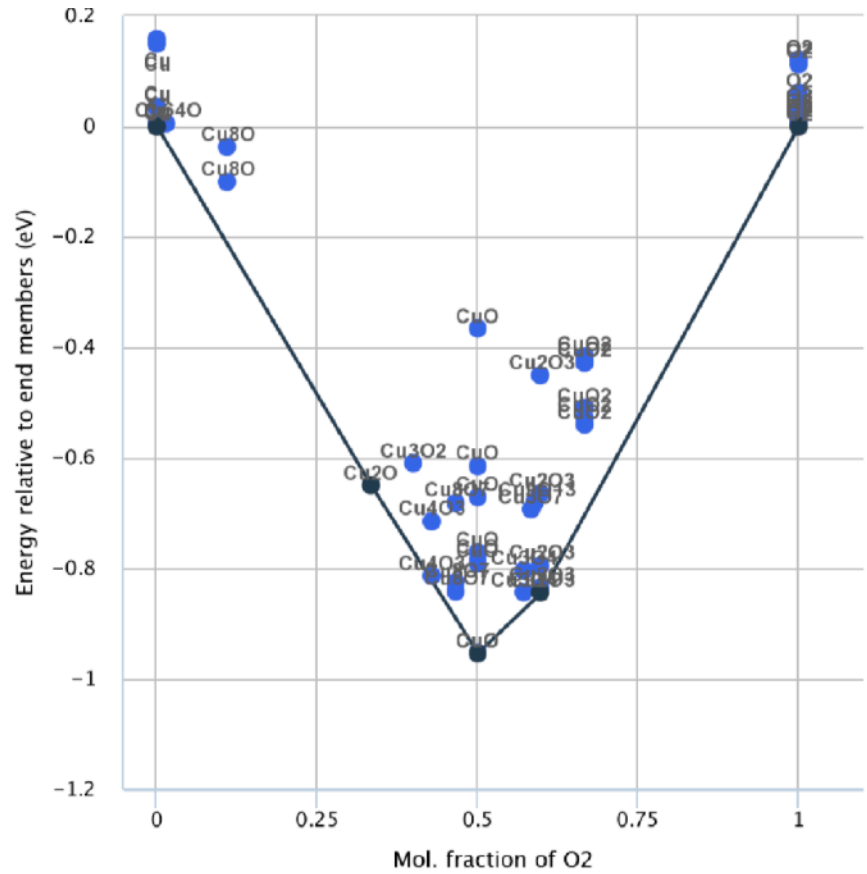
on the curated MatBench test suite



[A. Dunn *et al.*, npj Comput. Mater **6**, 138 (2020); https://github.com/hackingmaterials/matbench]

How can we predict the phase stability of polymorphs at different temperatures?

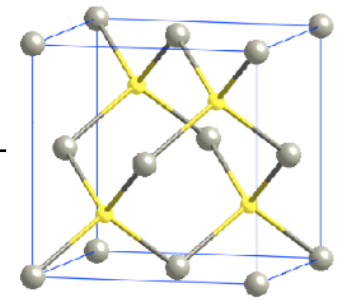
- At T=0K: for exemple, the Cu-O system



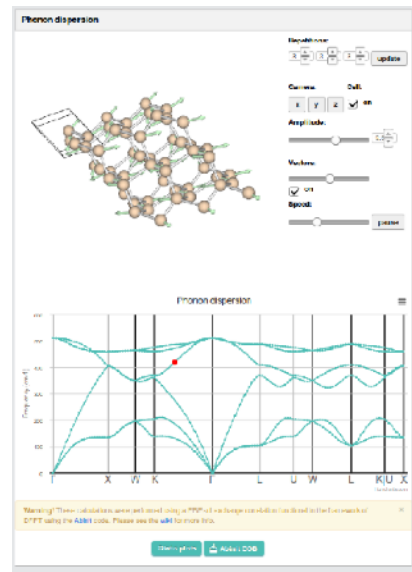
- At T>0K, the vibrational entropy needs to be taken into account. This can be done by DFPT but it is very demanding.

An automatic workflow was developed

Autoparal



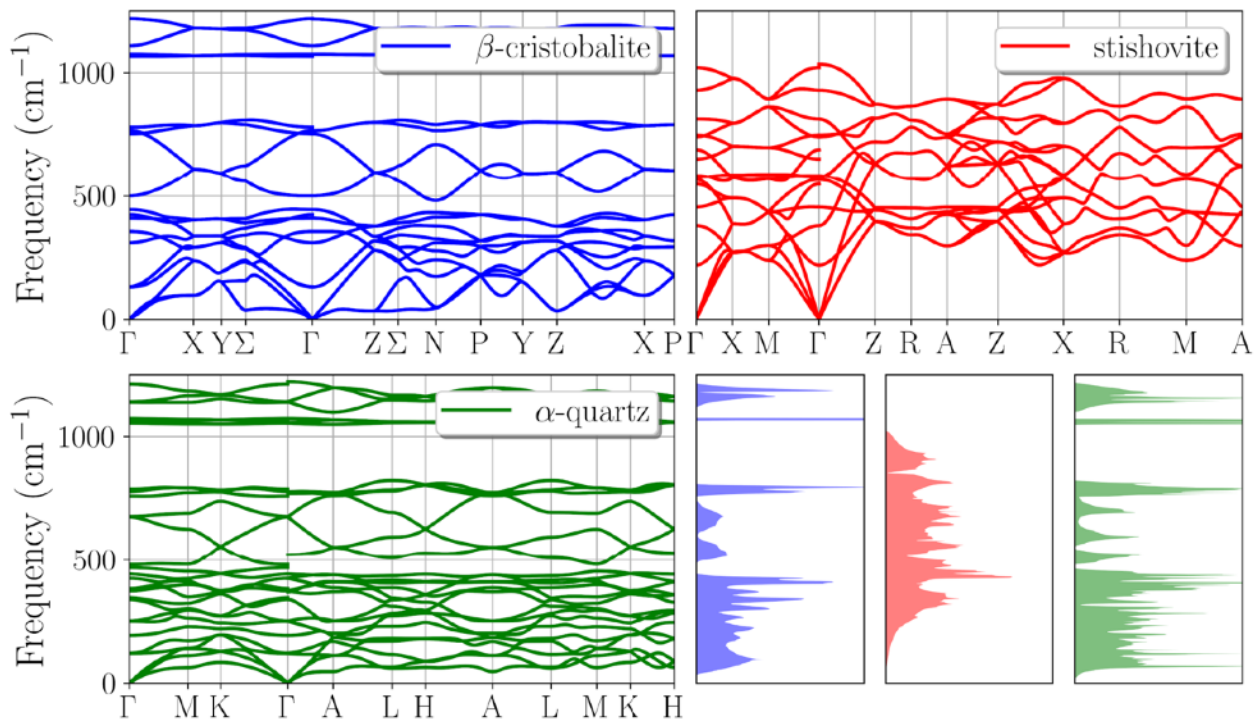
- Automatic parallel configuration
- Automatic error handling
- Perturbations fully parallelized
- Store the results on a Database



The vibrational properties were calculated for 1521 semiconductors

- The dataset includes:
  - phonon band structure
  - LO-TO splitting
  - phonon DOS
  - Born effective charges
  - dielectric tensor
  - derived quantities:

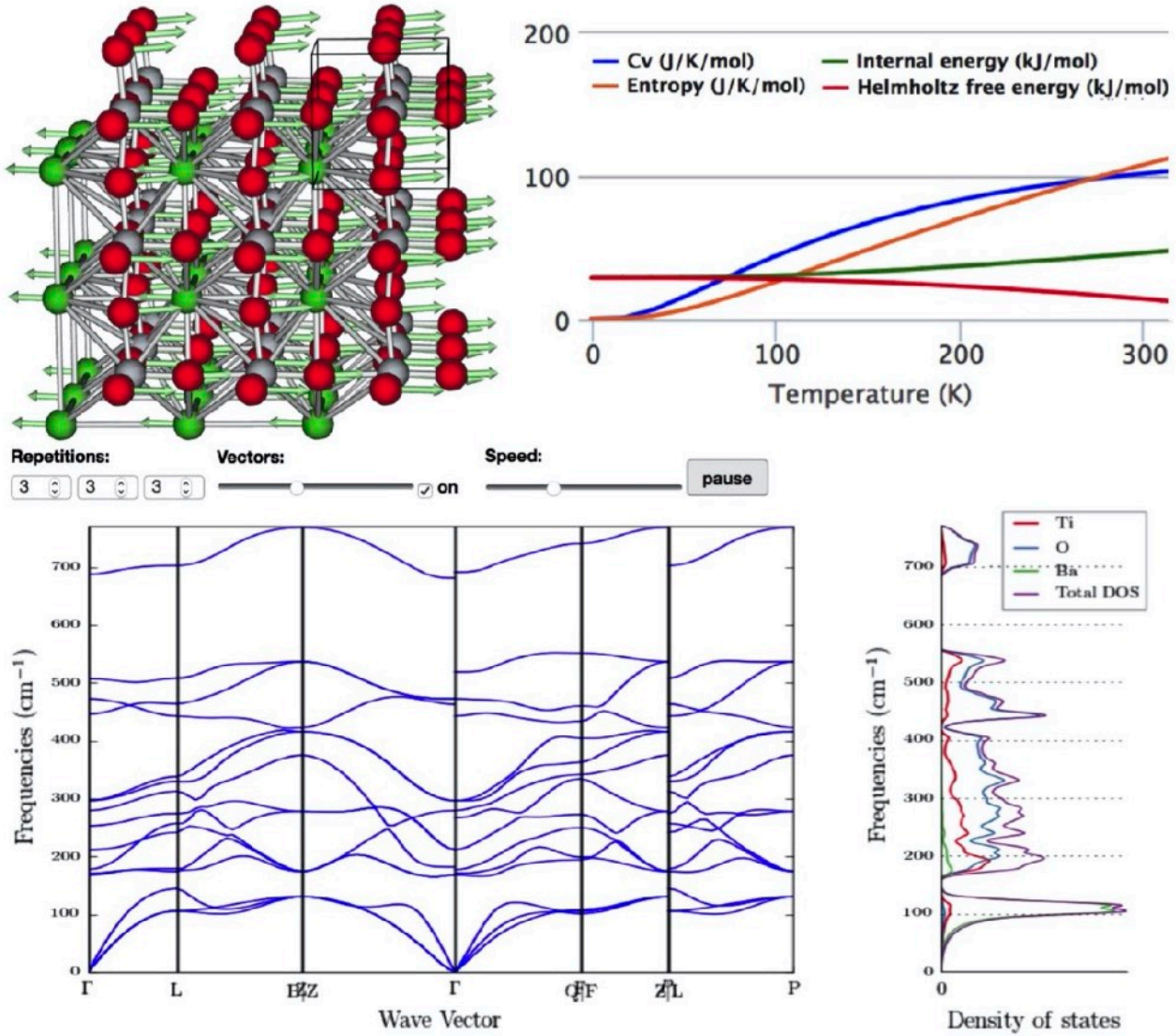
    ΔF, ΔE_{ph} , C_v and S
- The dataset is openly available!



SCIENTIFIC DATA

G. Petretto, S. Dwaraknath, H.P.C. Miranda, D. Winston, M. Giantomassi, M.J. van Setten, X. Gonze, K.A. Persson, G. Hautier, and G.-M. Rignanese, Sci. Data **5**, 180065 (2018).

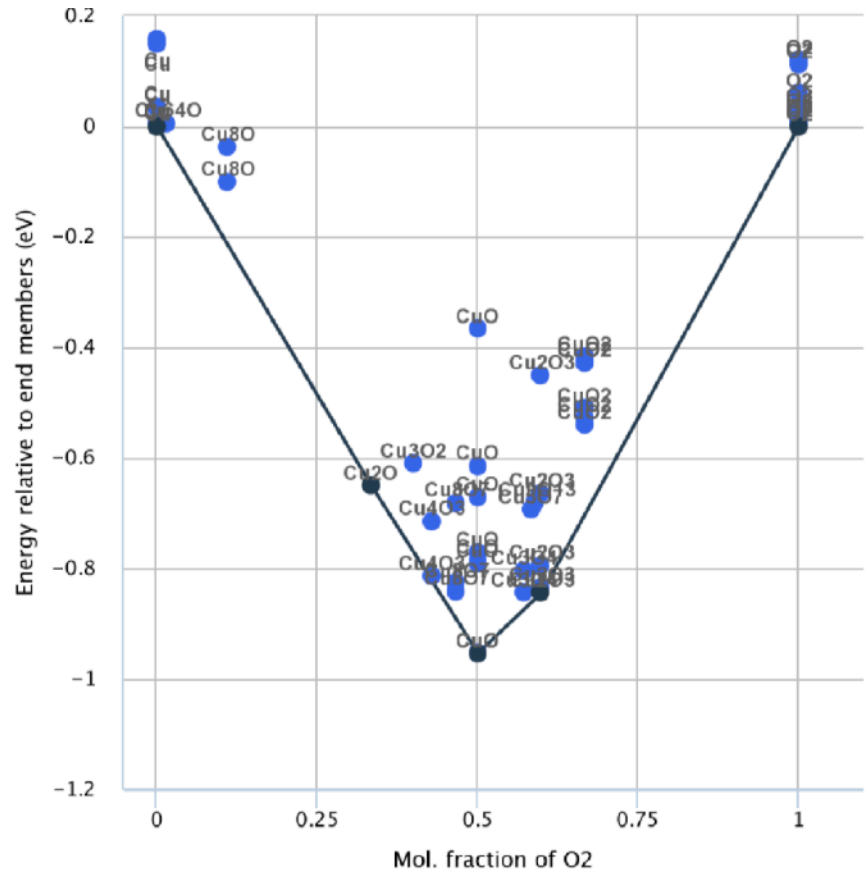
The vibrational properties are available on the Materials Project website



… but only for those 1521 semiconductors

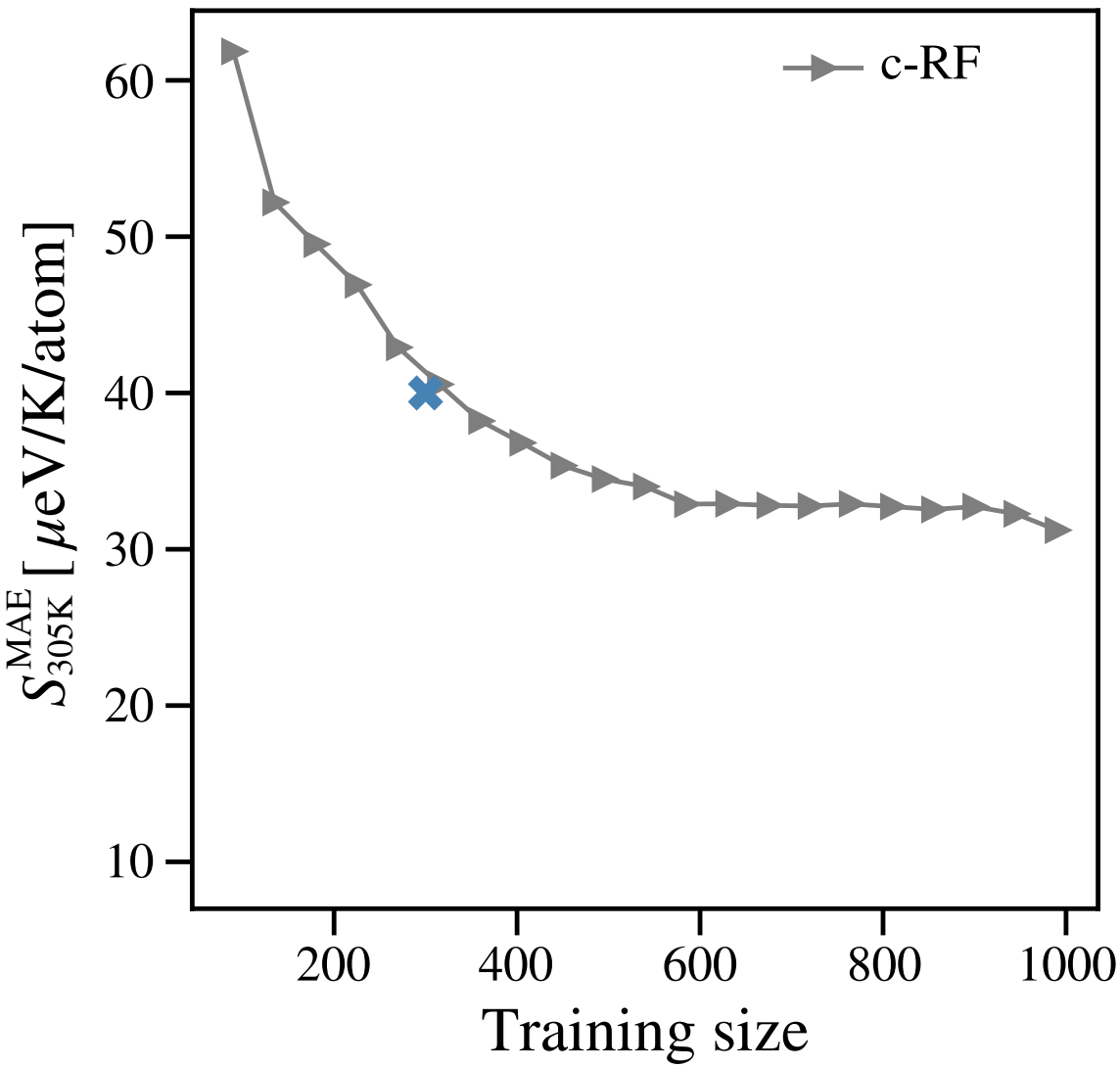
How can we predict the phase stability of polymorphs at different temperatures?

- At T=0K: for exemple, the Cu-O system



- At T>0K, the vibrational entropy needs to be taken into account.
  Let's use machine learning.

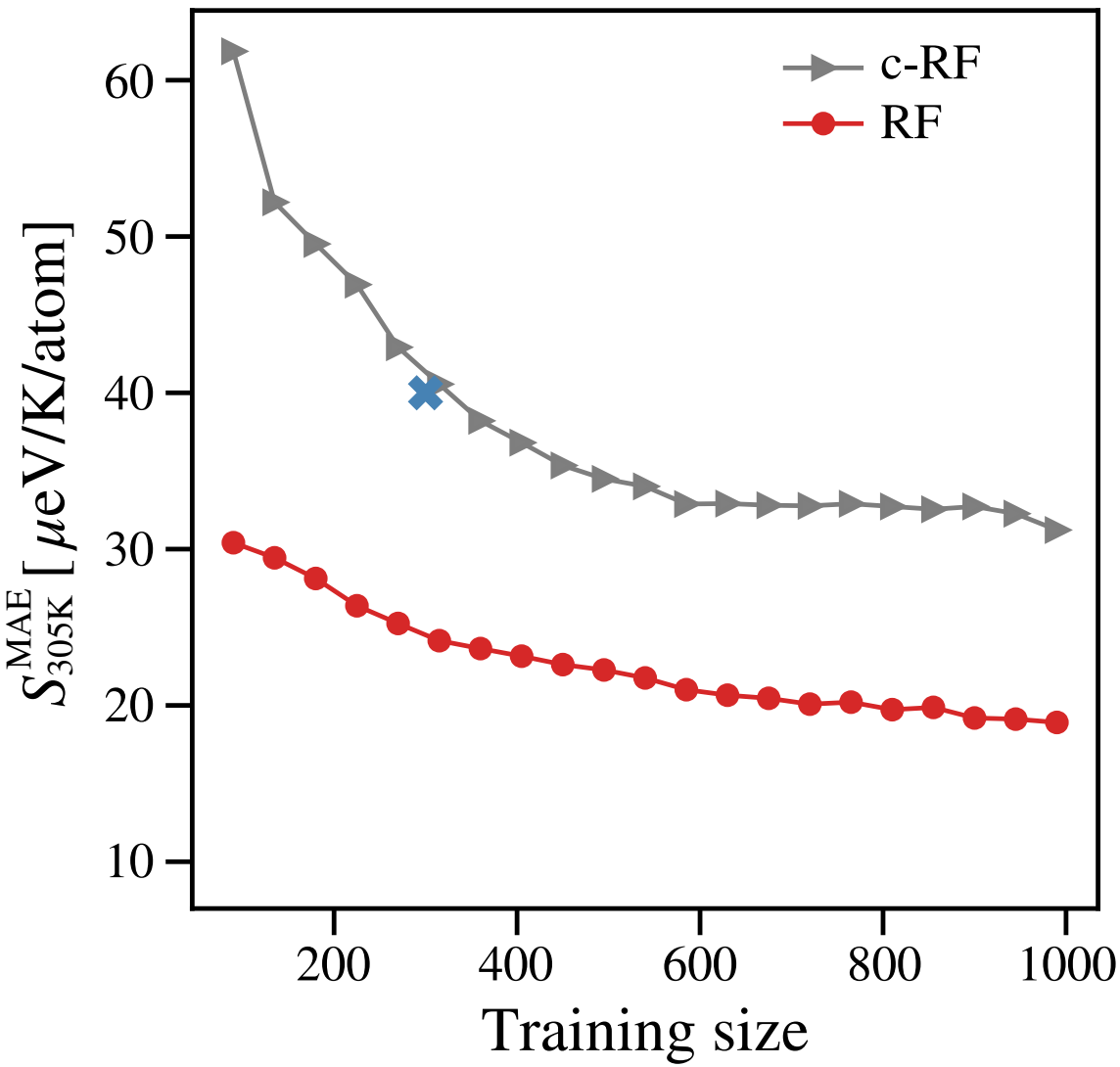
Early attempts with ML were based on RF using only chemical composition features



[F. Legrain *et al.*, Chem. Mater. **29**, 6220 (2017)]

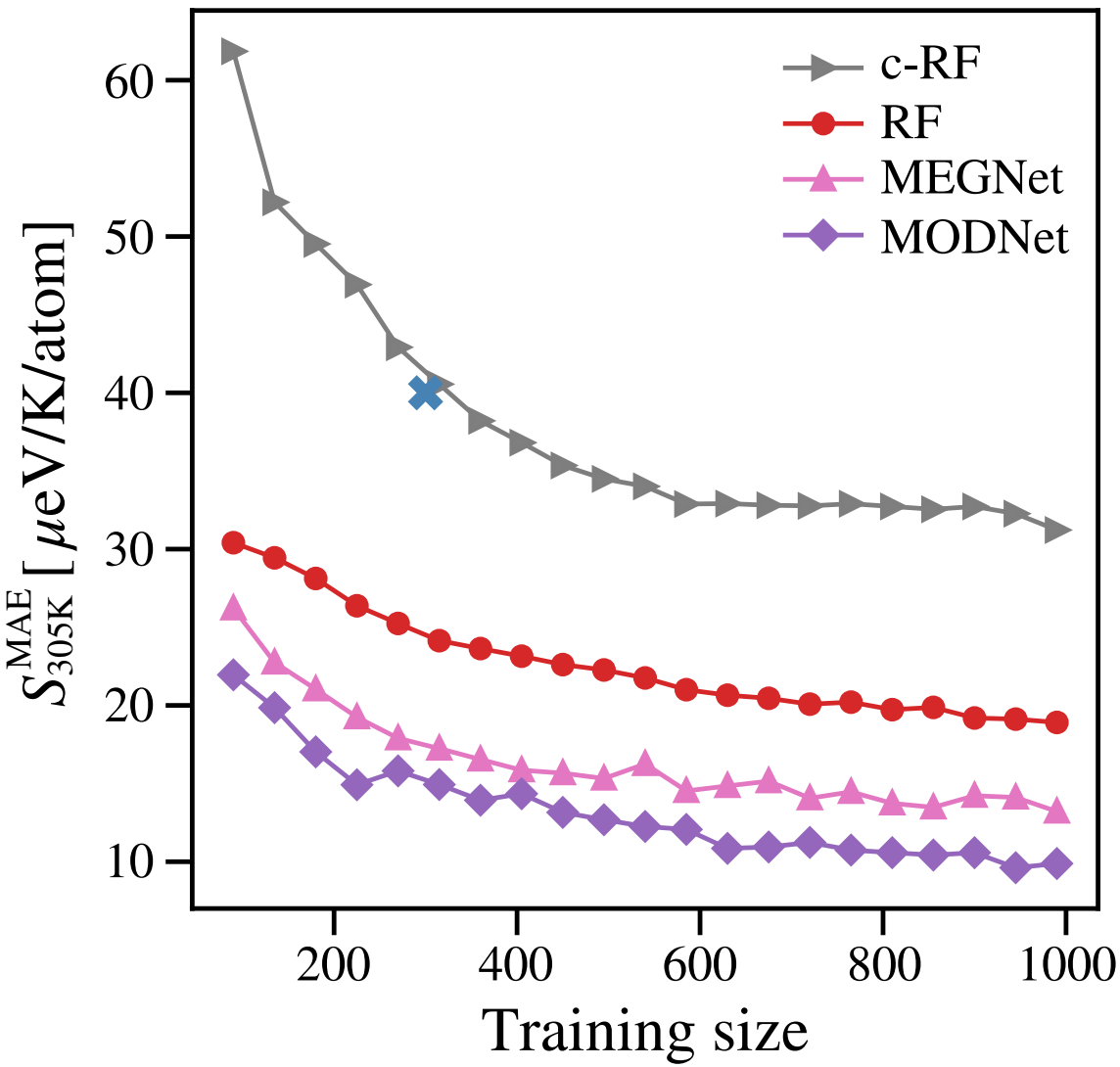
Including structural features

clearly improves the predicting power



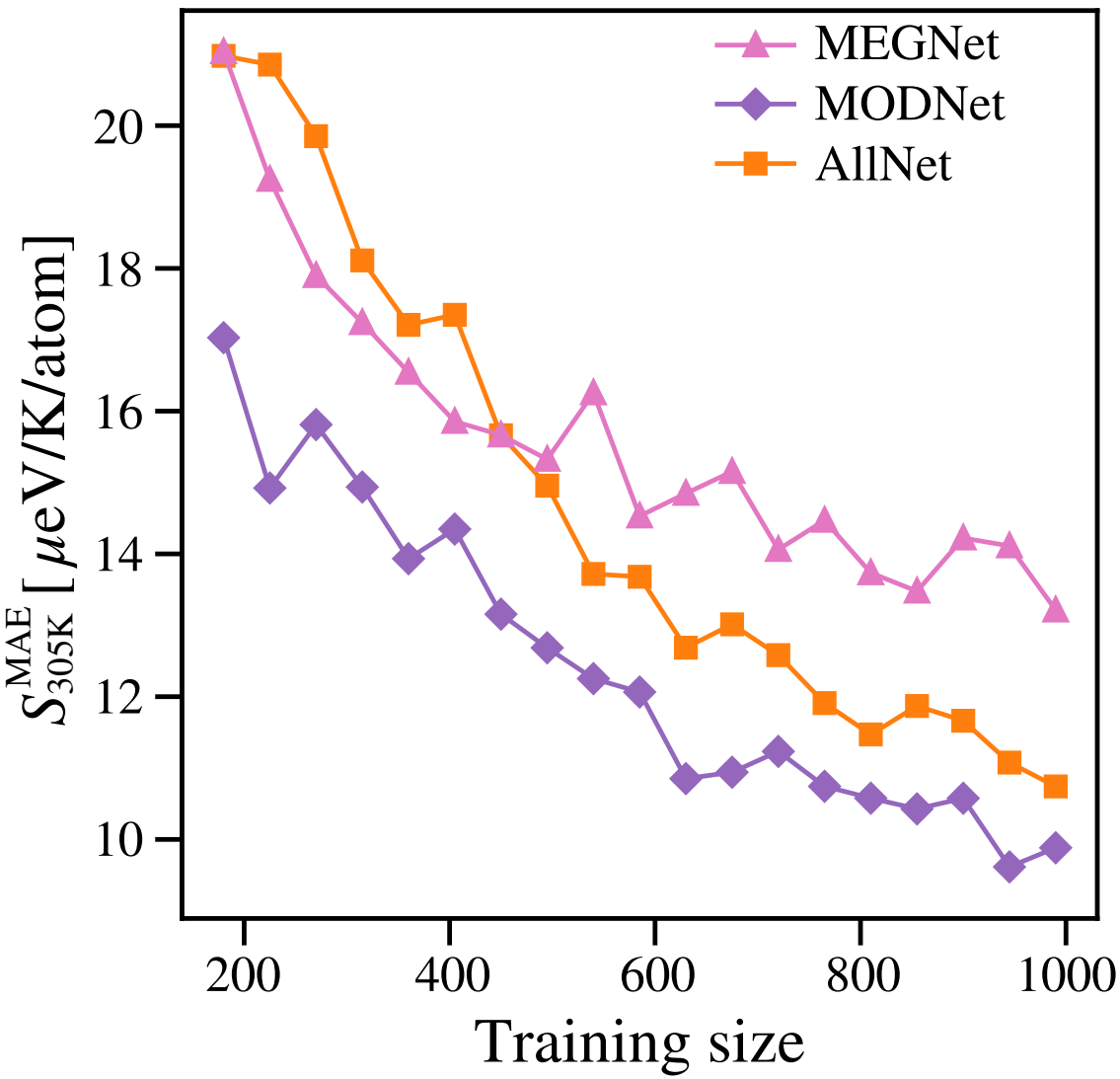
NB: Performing feature selection on the input space has no effect on the results as a RF intrinsically selects optimal features while learning.

Neural-network models perform better than RF approaches whatever the size of the data set



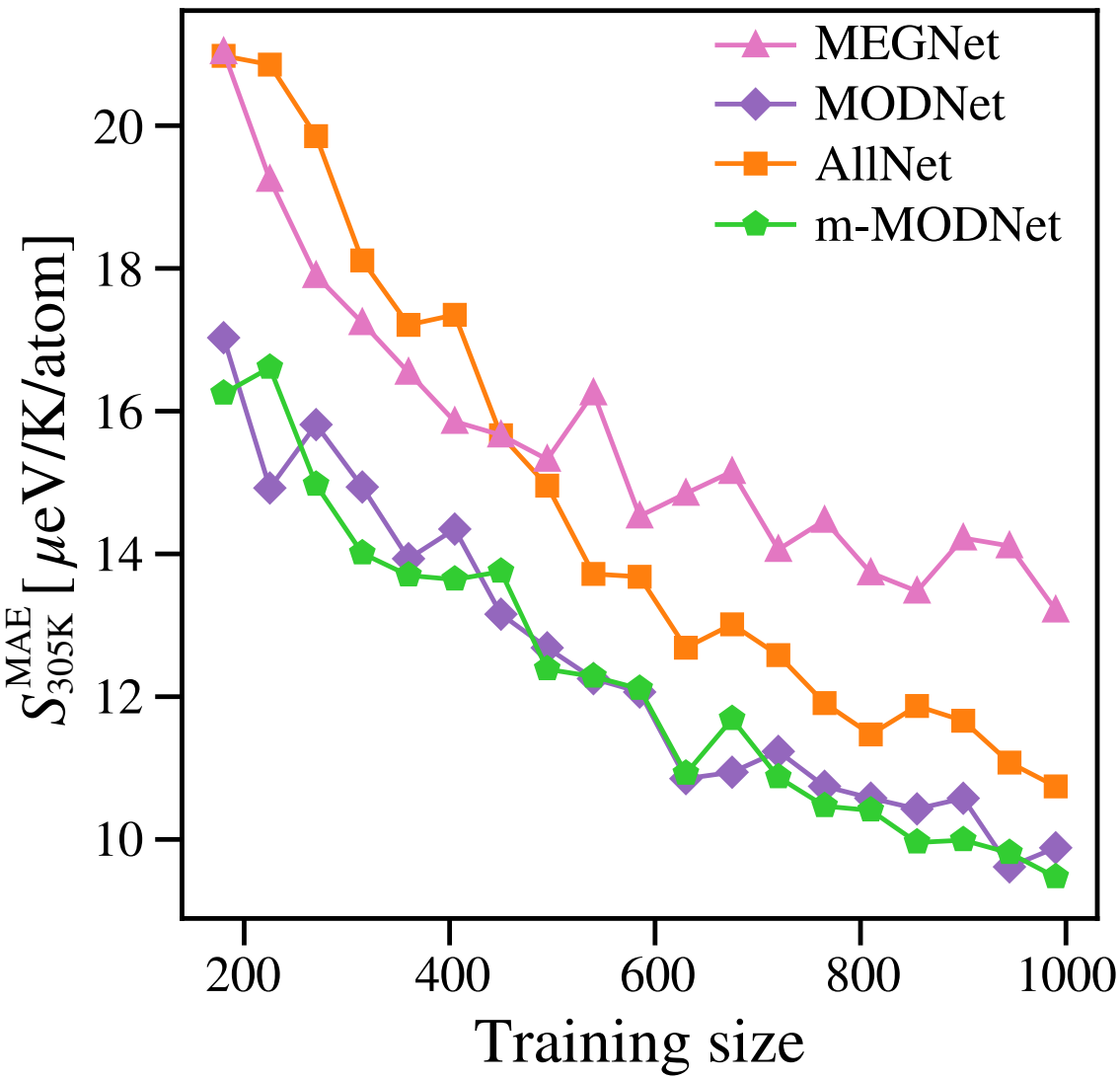
[P.-P. De Breuck *et al.*, npj Computational Materials **7**, 83(2021)]

Feature selection is really important especially for small training size



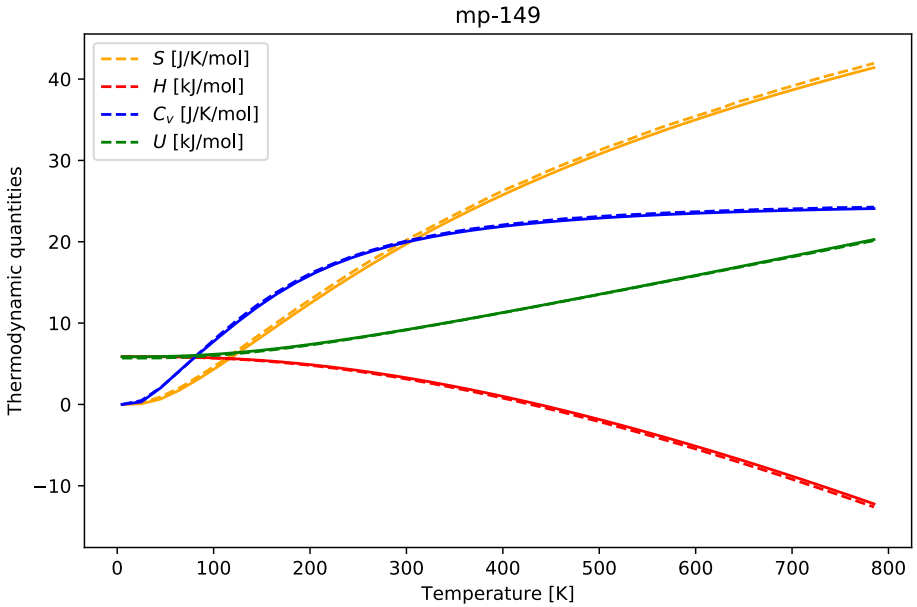
[P.-P. De Breuck *et al.*, npj Computational Materials **7**, 83(2021)]

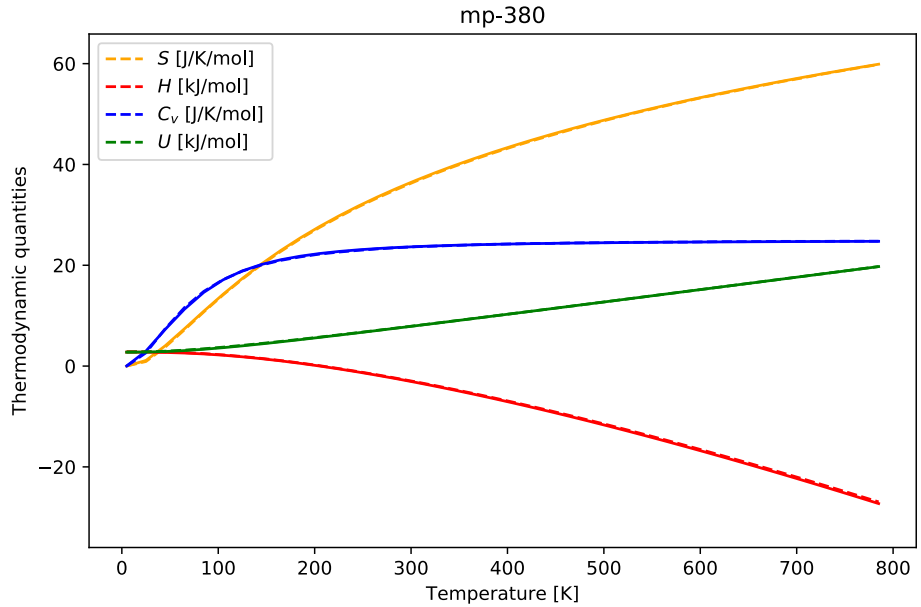
The joint-learning approach (m-MODNet) shows on average a slight improve in accuracy

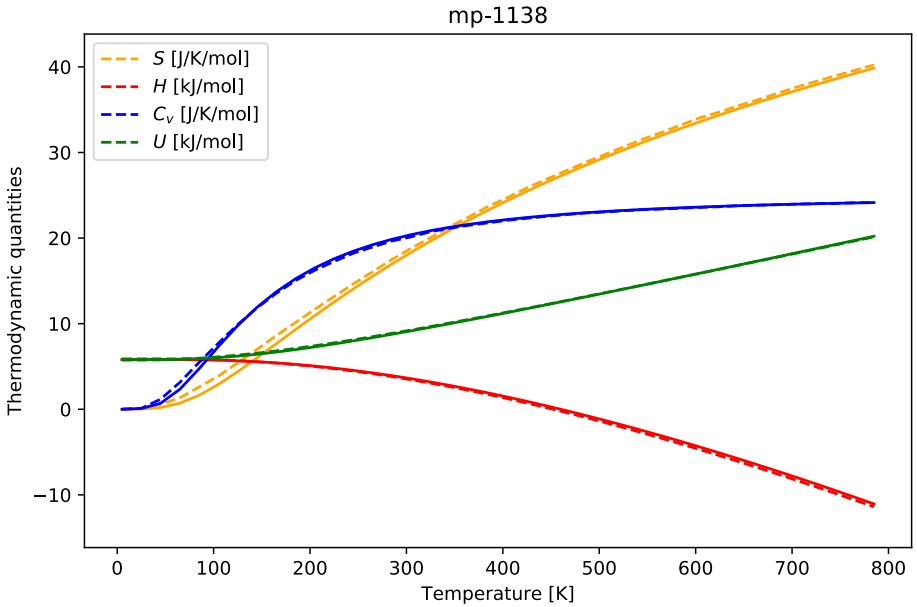


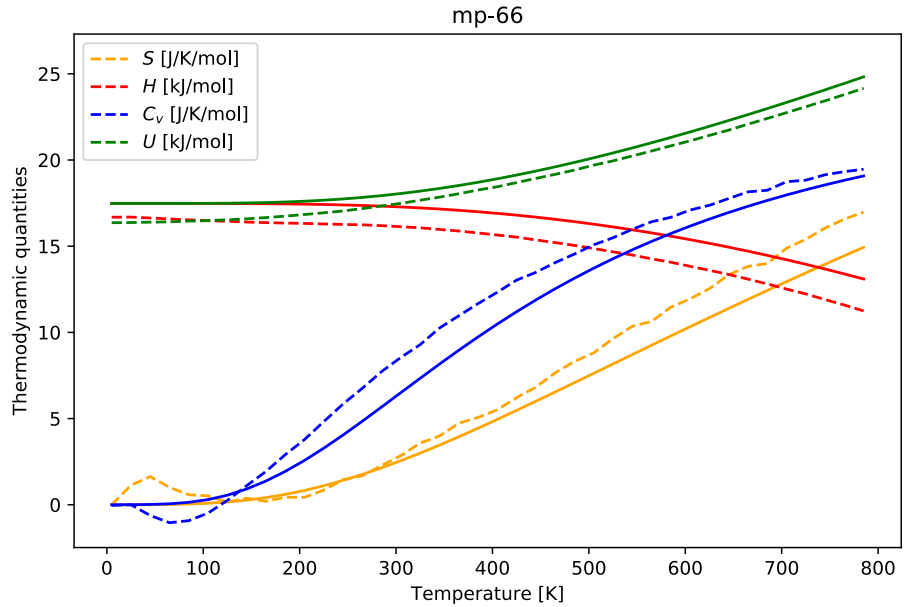
and provides a single model for multiple properties

In particular, it is possible to obtain curves of the thermodynamic properties vs. temperature

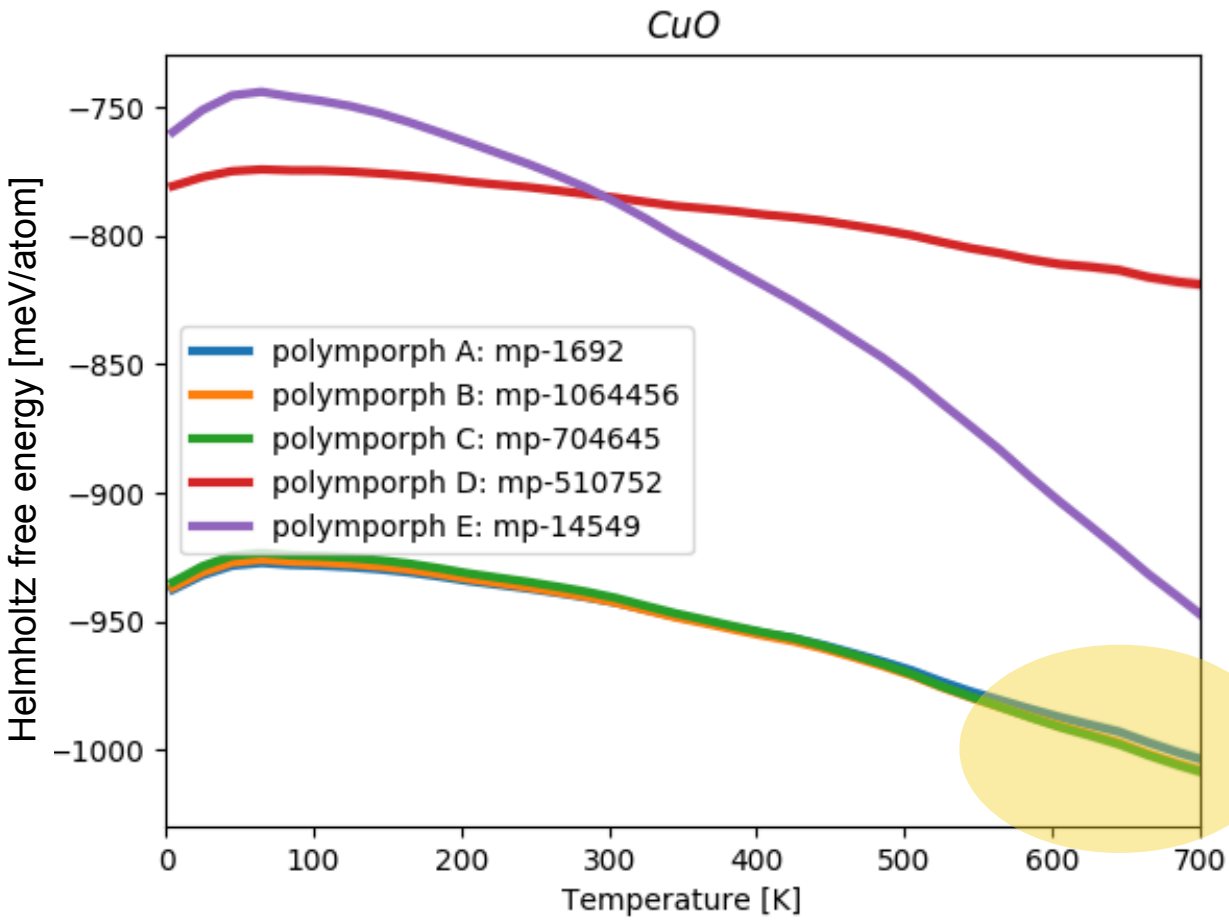








Thanks to this approach, we can build temperature dependent stability graphs



Accuracy