

機器學習於材料資訊的應用

Machine Learning on Material Informatics

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Data comes from Computational Materials Science

A new powerful approach to
discover novel material

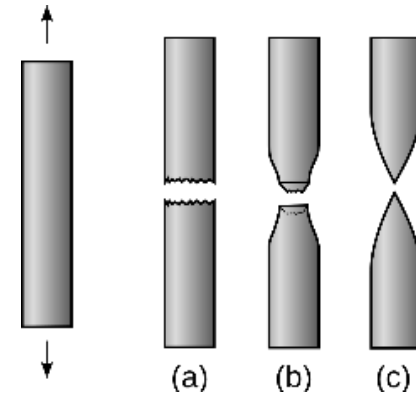
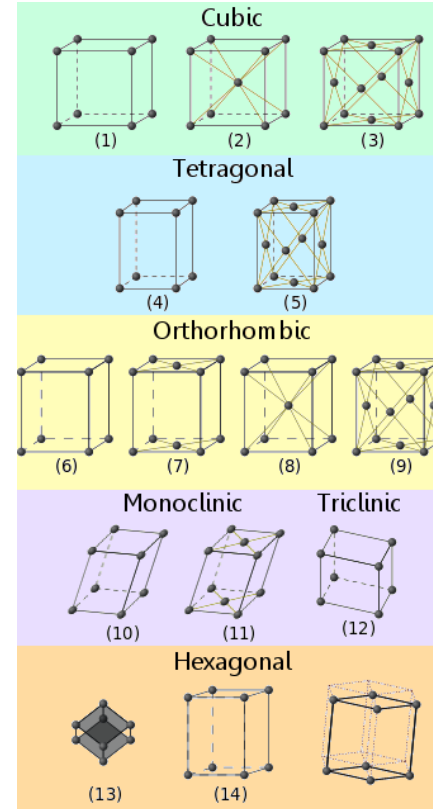


材料基因

Human Genome V.S. Material Genome

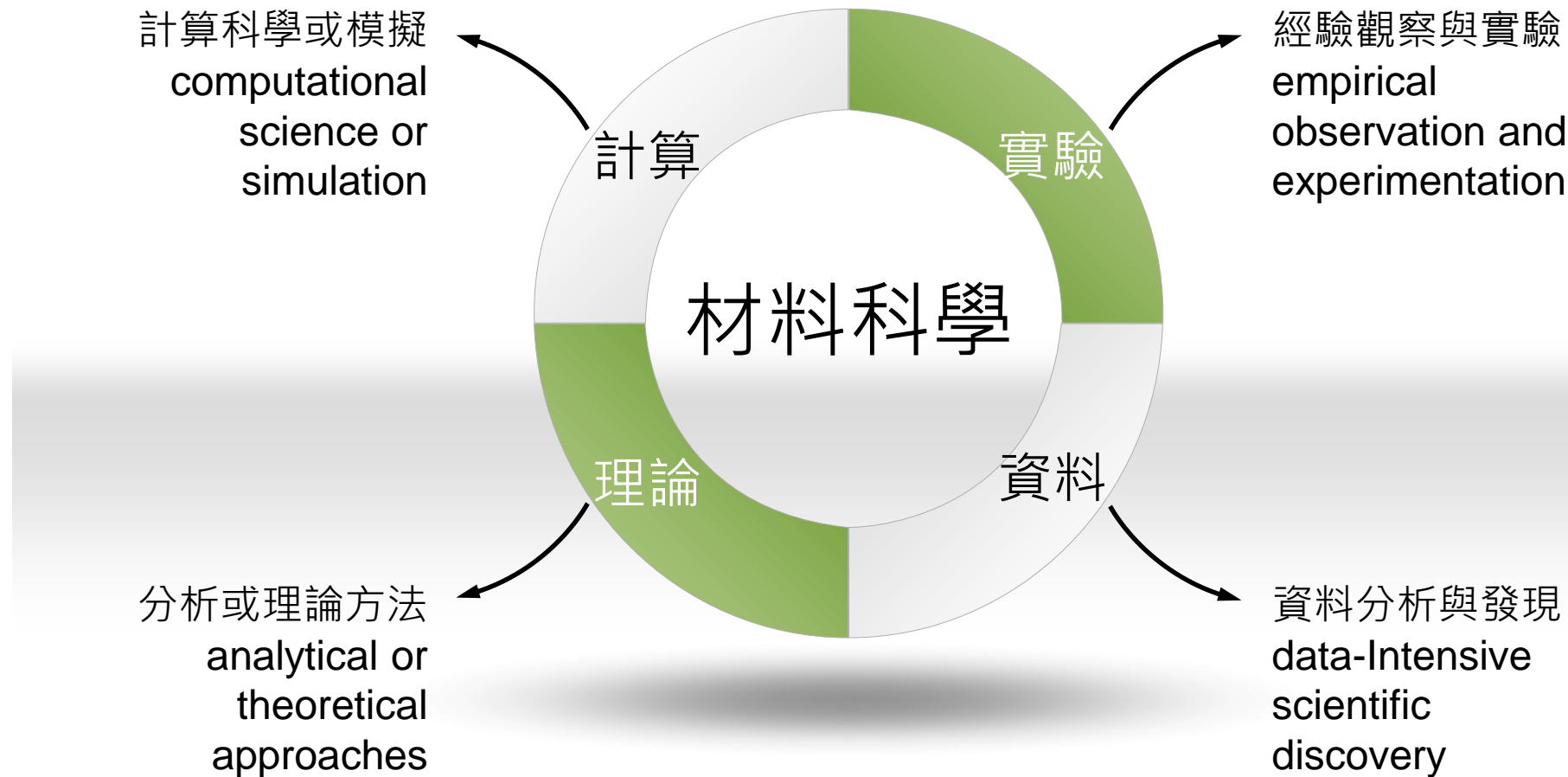


生物個體的外在表現叫作「表現型 (phenotype)」，由內在的「基因型 (genotype)」決定。改變表現型，首先要改變基因型。

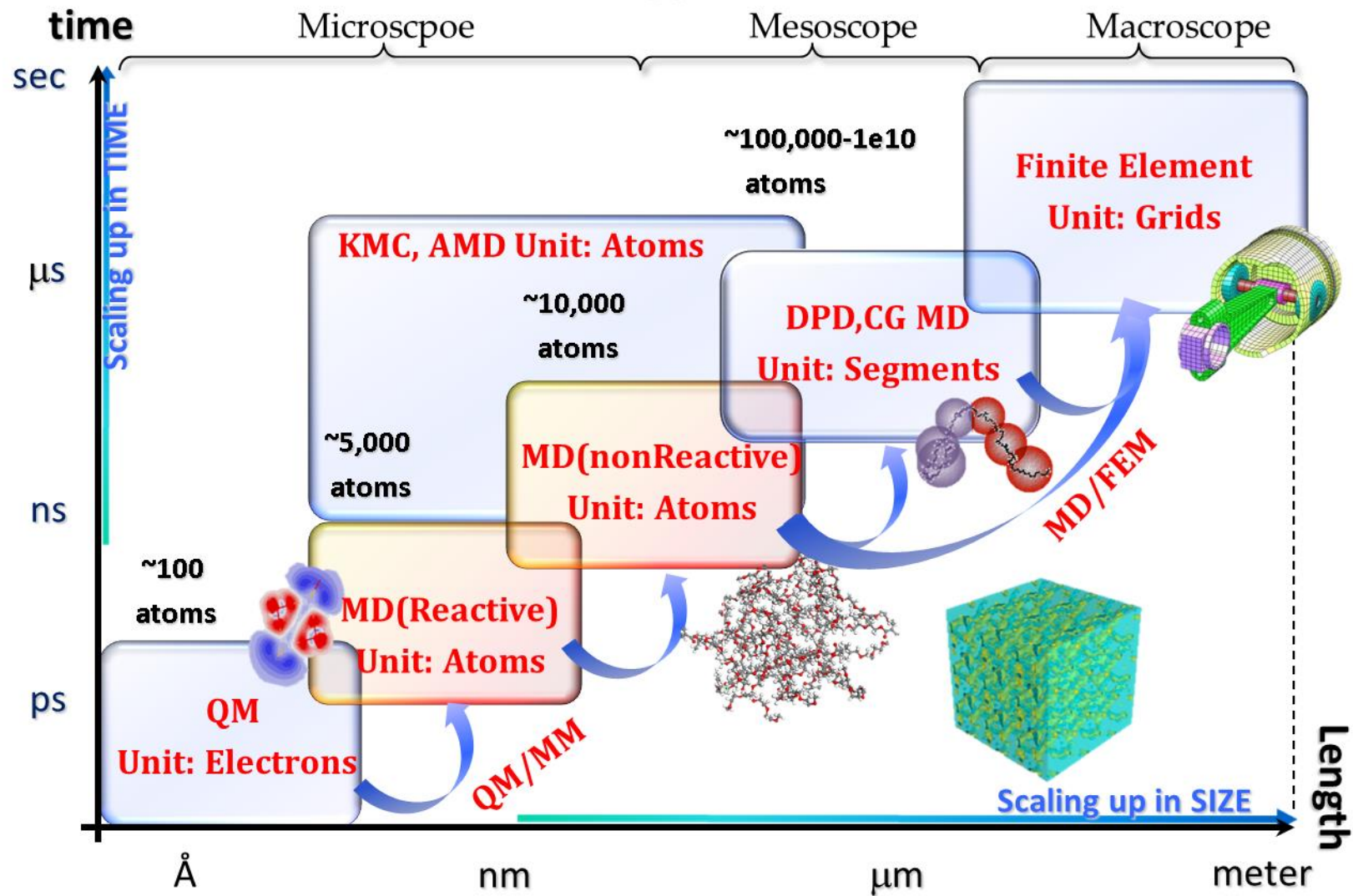


材料在巨觀尺度表現出來的材料特性是由微觀尺度下的原子組態所決定的。要改變材料特性，首先要改變微觀的原子組態。

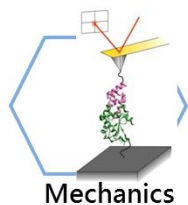
材料科學的分支



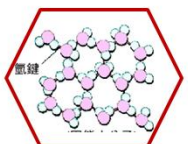
Multi-Scale Modeling for Materials Simulation



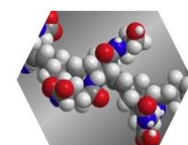
Properties you can get from calculation



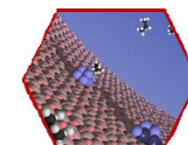
Elastic constant
Young's modulus
Stress-strain
Hardness



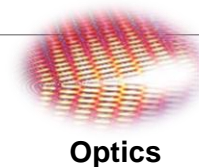
Glass transition temperature
Coefficient of Thermal expansion
Thermal conductivity(Green Kubo)
Phonon density
Solubility Parameters



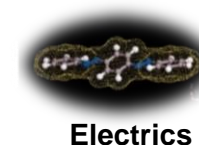
Radius distribution function
Bond length, angle, dihedral angle
Gyration Radius
Atomic shear strain



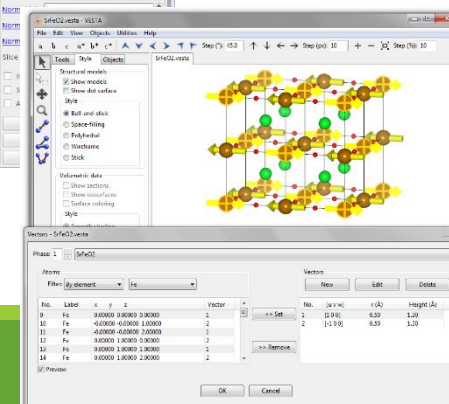
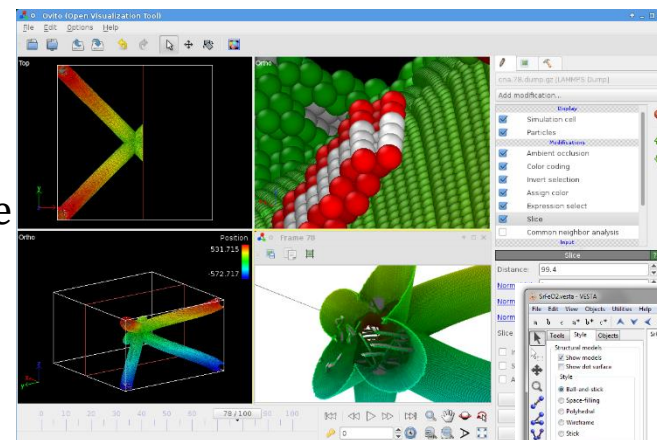
Diffusion coefficient
Viscosity (Green Kubo)
Auto-correlation function



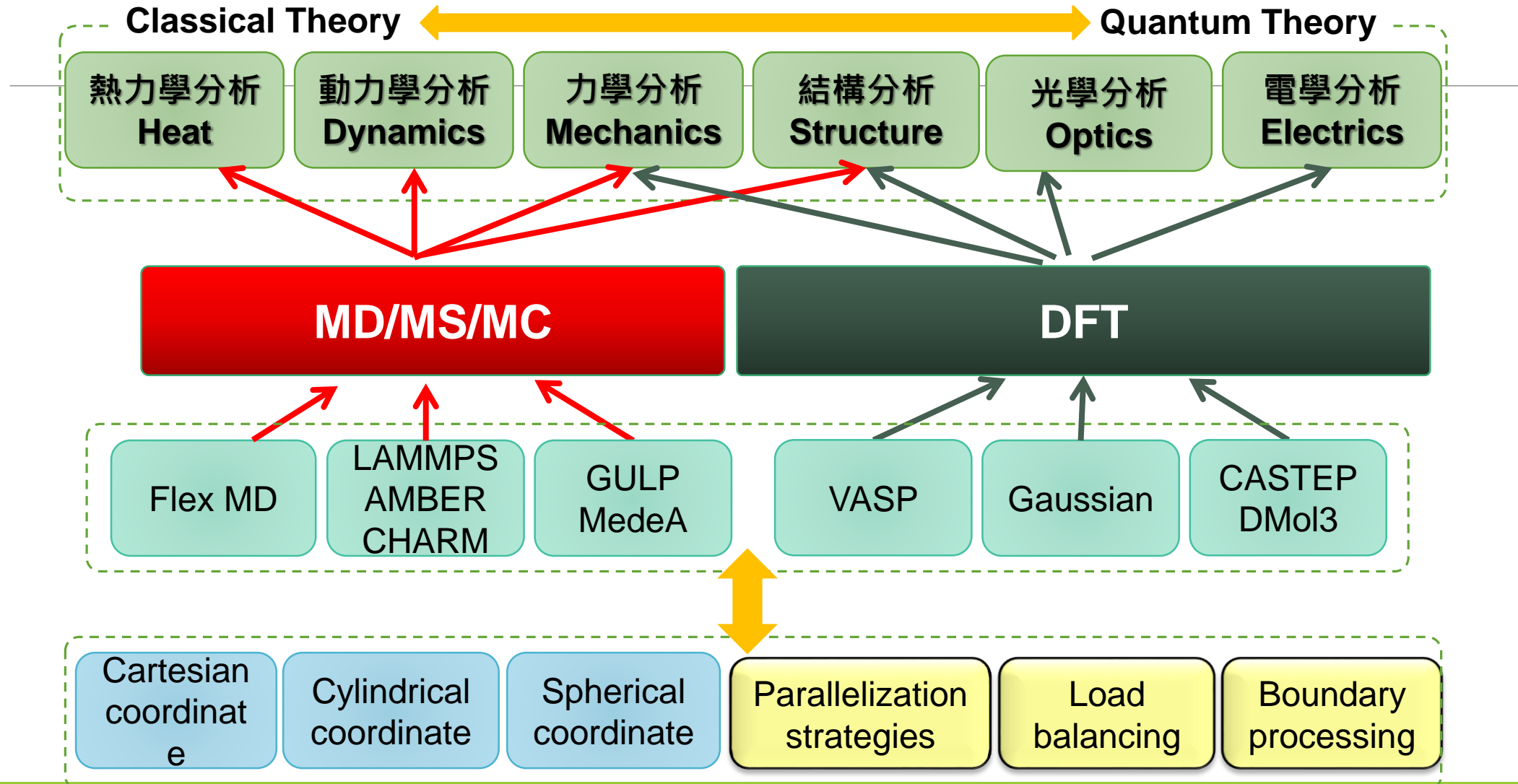
Birefringence
Dielectric constant
Abbe Number
Reflective Index



Band structure/gap
Density of state



Molecular Modeling



Material Project



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](#)[See a Random Material](#)[Browse Apps](#)

The Materials Project by the numbers

MATERIALS

154,718

REGISTERED USERS

300,000+

INTERCALATION ELECTRODES

4,351

CITATIONS

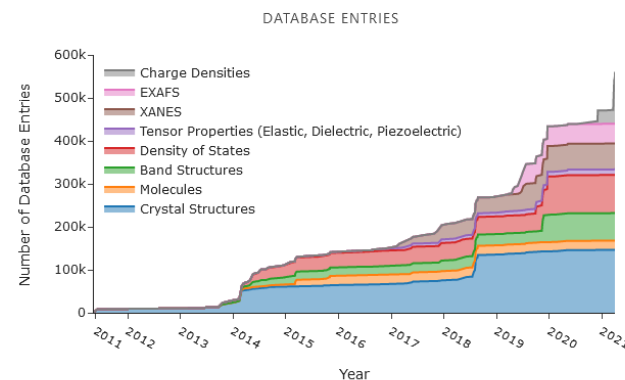
19,000+

MOLECULES

24,989

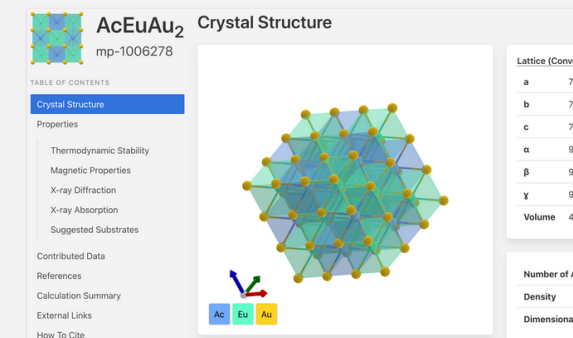
CPU HOURS/YEAR

100 million



View detailed computed information about any material.

Every material in our database has a detailed page displaying all of its computed properties. By providing materials researchers with the information they need to design better, the Materials Project aims to accelerate innovation in materials research. [See a random material.](#)

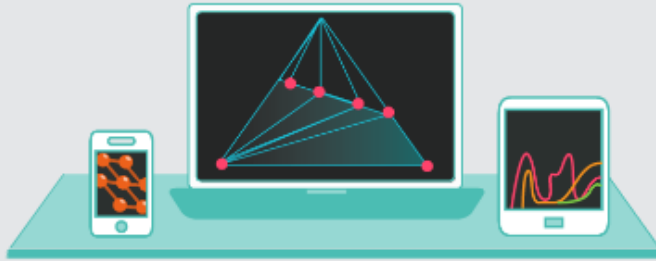


Supercomputing

Supercomputing clusters at national laboratories provide the infrastructure that enables our computations, data, and algorithms to run at unparalleled speed. We principally use the Lawrence Berkeley National Laboratory's [NERSC](#) Scientific Computing Center and Computational Research Division, but we are also active with Oak Ridge's [OLCF](#) Argonne's [ALCF](#) and San Diego's [SDSC](#)



About Material Project



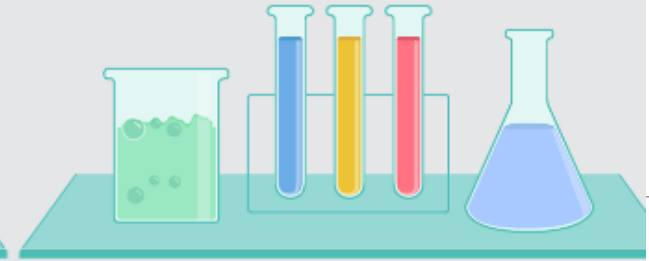
software

By computing properties of all known materials, the Materials Project aims to remove guesswork from materials design in a variety of applications. Experimental research can be targeted to the most promising compounds from computational data sets. Researchers will be able to data-mine scientific trends in materials properties. By providing materials researchers with the information they need to design better, the Materials Project aims to accelerate innovation in materials research.



supercomputers

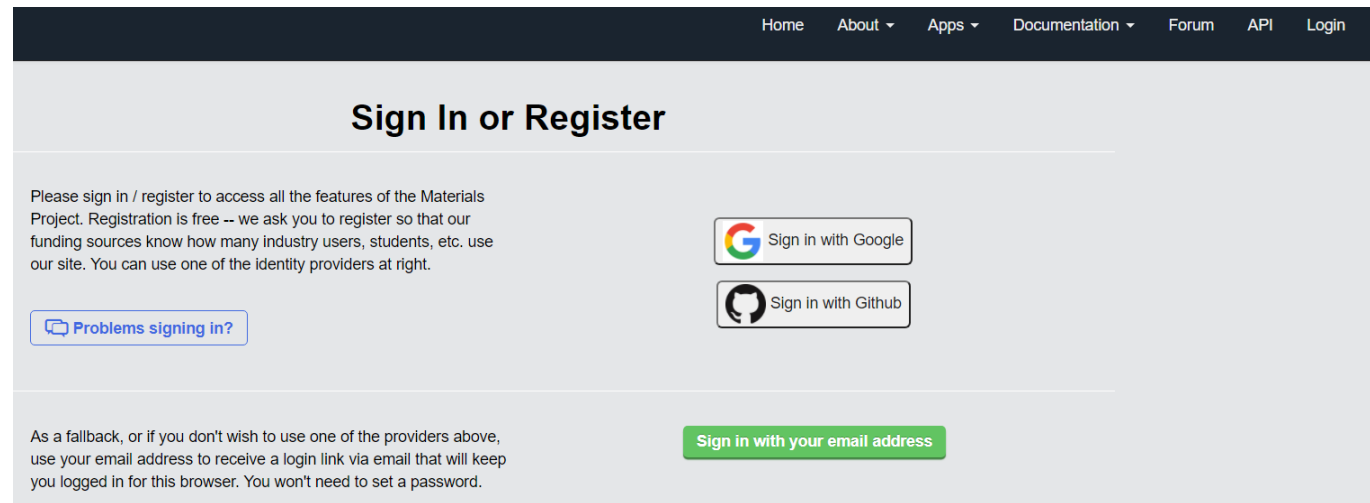
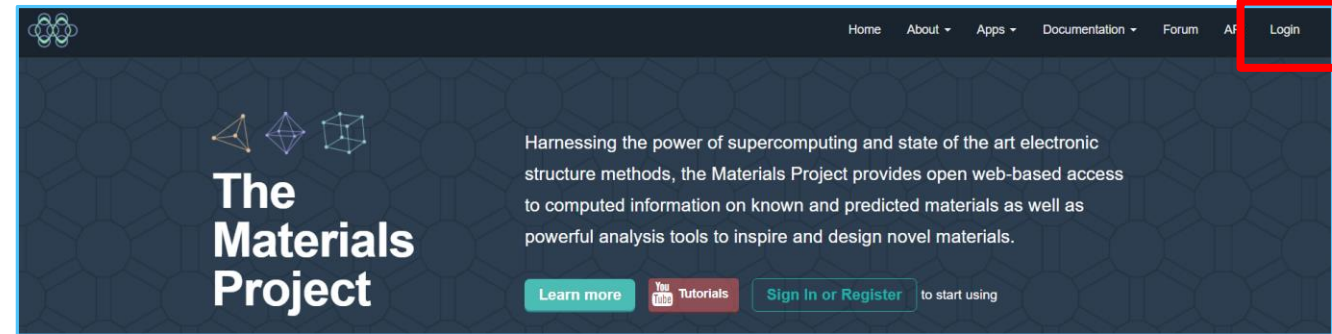
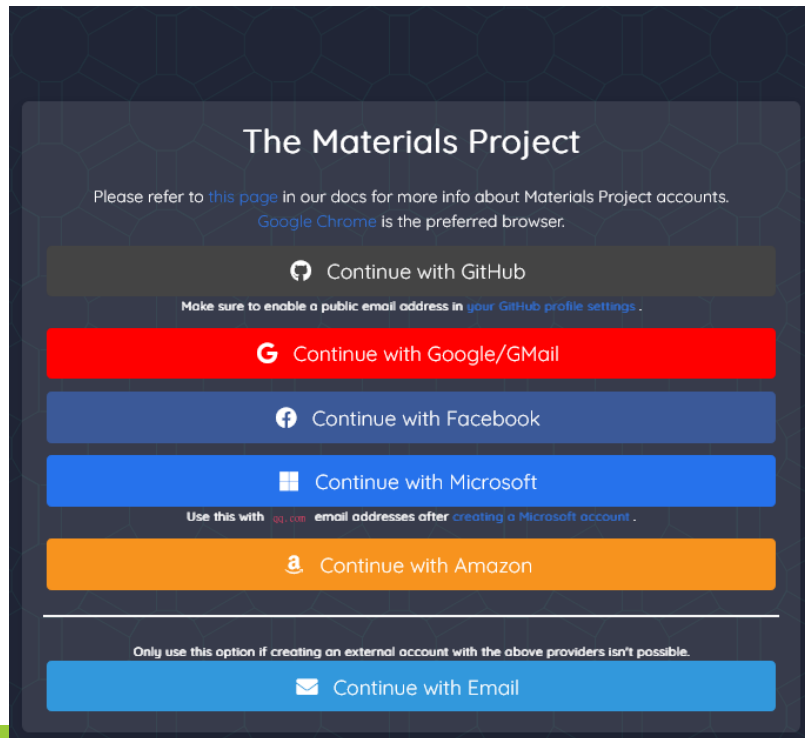
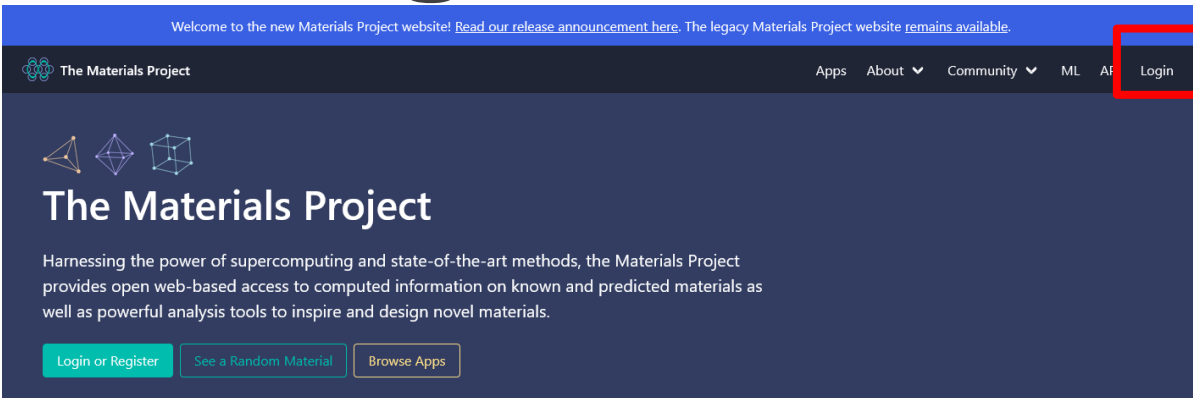
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screening

Computational materials science is now powerful enough that it can predict many properties of materials before those materials are ever synthesized in the lab. By scaling materials computations over supercomputing clusters, we have predicted several new battery materials which were made and tested in the lab. Recently, we have also identified new transparent conducting oxides and thermoelectric materials using this approach.

Login





Search for materials information by chemistry, composition, or property

Explore Materials

Advanced Search Syntax

1 H	<div>by Elements</div> <div>Na-O</div> <div>search</div>																2 He	
3 Li	4 Be																	10 Ne
11 Na	12 Mg																	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
55 Cs	56 Ba	57-71 La-Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
87 Fr	88 Ra	89-103 Ac-Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn							
57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu				
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr				

輸入搜尋條件

也可以直接點
週期表元素

搜尋結果的
FILTER

主要搜尋結果會呈現在這邊

of elements

e.g., 4 or >2 & <6

excluded elements

Cl Br

Submit

External Provenance

ICSD

Exptl. ICSD

Material Tags

imgreite

Band Gap (eV)

0

10

Energy Above Hull

0

6

Formation Energy

-4

4

unit cell sites

1

298

Density

0

24.6

Volume

7

7697

Nelements		Elements							
100 records per page		Batch Structures		Edit Structures		Show / hide columns		Print	Export
Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	Volume	Nsites	Density (gm/cc)	
mp-1027525	MoS ₂	P $\bar{3}$ m1	-1.306	0	1.746	350.447	12	3.034	<input type="checkbox"/>
mp-1025874	MoS ₂	P $\bar{6}$ m2	-1.306	0	1.783	284.872	9	2.799	<input type="checkbox"/>
mp-1023939	MoS ₂	P $\bar{3}$ m1	-1.306	0	1.551	219.296	6	2.424	<input type="checkbox"/>
mp-1018809	MoS ₂	P6 ₃ /mmc	-1.305	0.001	1.338	123.449	6	4.306	<input type="checkbox"/>
mp-1023924	MoS ₂	P $\bar{6}$ m2	-1.305	0.001	1.658	153.721	3	1.729	<input type="checkbox"/>
mp-2815	MoS ₂	P6 ₃ /mmc	-1.304	0.002	1.229	118.065	6	4.503	<input type="checkbox"/>
mp-1434	MoS ₂	R3m	-1.303	0.003	1.228	116.637	6	4.558	<input type="checkbox"/>
mp-2164	Mo ₃ S ₄	R $\bar{3}$	-1.052	0.068	0.000	272.96	14	5.062	<input type="checkbox"/>
mp-31257	Mo ₁₅ S ₁₉	P6 ₃ /m	-1.011	0.084	0.000	1436.887	68	4.734	<input type="checkbox"/>
mp-1627	Mo ₂ S ₃	P2 ₁ /m	-1.08	0.096	0.000	167.797	10	5.702	<input type="checkbox"/>
mp-1104577	Mo ₃ S ₄	P $\bar{1}$	-1.006	0.113	0.000	229.105	14	6.031	<input type="checkbox"/>
mp-673645	Mo ₇ S ₈	P1	-0.919	0.126	0.000	543.214	30	5.674	<input type="checkbox"/>
mp-990083	MoS ₂	Pmmn	-1.142	0.164	0.000	1790.583	54	2.672	<input type="checkbox"/>
mp-1210708	Mo ₂₁ S ₈	I4/m	-0.289	0.251	0.000	431.006	29	8.75	<input type="checkbox"/>
mp-1239169	MoS ₃	P2 ₁ /m	-0.719	0.26	0.791	209.34	8	3.048	<input type="checkbox"/>
mvc-11780	MoS ₂	F $\bar{4}$ 3m	-1.041	0.265	0.000	221.127	12	4.808	<input type="checkbox"/>
mp-558544	MoS ₂	R $\bar{3}$ m	-1.029	0.277	0.000	111.639	6	4.762	<input type="checkbox"/>

Formation Energy

-4 4

unit cell sites

1 296

Density

0 24.6

Volume

7 7697

Crystal Systems

Any

Spacegroup Number

Any

Spacegroup Symbol

Any

Has properties →

Elasticity →

Piezoelectricity →

Dielectricity →

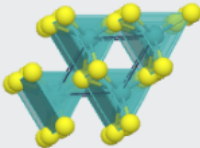
可以直接點
進去看細節

也可以批次
操作

將結構視覺化
的區域

MATERIAL: **MoS₂** ID: **mp-1434** DOI: **10.17188/1190621** [Show Help Guides](#)

[Electronic Structure](#) [X-Ray Diffraction](#) [X-Ray Absorption](#) [Substrates](#) [Elasticity](#) [Piezoelectricity](#) [Dielectric Properties](#)
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Material Details

- Final Magnetic Moment: 0.000 μ_B
- Magnetic Ordering: NM
- Formation Energy / Atom: -1.303 eV
- Energy Above Hull / Atom: 0.003 eV
- Density: 4.56 g/cm³
- Decomposes To: [MoS₂](#)
- Band Gap: 1.228 eV

Lattice Parameters

a	3.194 Å	α	97.687°
b	5.530 Å	β	76.529°
c	6.855 Å	γ	90.000°
Volume	116.637 Å ³		

Final Structure [CIF](#)
Fractional Coordinates

Mo		
a	b	c
0	0	0.0001
0.5	0.5	0.0001

S		
a	b	c
0.1187	0.6272	0.7626
0.3813	0.2061	0.2374
0.6187	0.1272	0.7626
0.8813	0.7061	0.2374

Space Group

Hermann Mauguin
R3m [160]

Hall
R 3 $\bar{2}$

Point Group
m

Crystal System
trigonal

Mo **S** ☒ Atoms Unit Cell ☒ Bonds Polyhedra [CIF](#)

Zoom in/out Rotate along the center axis Shift + Drag cursor Option + Drag cursor

[Edit Crystal](#) [Generate Phase Diagram](#)

Tags: [Molybdenite 3R](#) [Molybdenum\(IV\) disulfide](#) [Molybdenum\(IV\) sulfide](#)

[File Formats](#) [Download](#)

下載資料
的地方

CIF:晶體結構的標準檔案交換格式

VASP:執行VASP計算的設定檔案(不包含最重要的POTCAR)

POSCAR:原子的座標輸入

CSSR: unit cell 定義和原子的fractional coordinates.

JSON:JSON格式的所有資訊

New Portal

Welcome to the new Materials Project website! [Read our release announcement here](#). The legacy Materials Project website [remains available](#).

Search for materials information by chemistry, composition, or property.

Materials e.g. Li-Fe or Li₂Fe or Li₃Fe or mp-19017 Search

H

Only Elements

At Least Elements

Formula

He

Li	Be	<div> <div>*</div> <div>Select elements to search for materials with only these elements</div> </div>																B	C	N	O	F	Ne									
Na	Mg																	Al	Si	P	S	Cl	Ar									
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr															
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe															
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn															
Fr	Ra	Ac-Ar	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og															
																		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
																		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

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- Terms of Use

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Filters

Reset

► Composition

All 154,718 materials

Showing 1-15

Columns ▼

Material ID	Formula	Crystal System	Space Group Symbol	Sites	Energy Above Hull (eV/atom)	Band Gap (eV)
-------------	---------	----------------	--------------------	-------	-----------------------------	---------------

New Portal

Filters

Reset

▼ Composition 1 active

Material ID

Formula

MoS₂

Chemical System

Include Elements

Exclude Elements

Number of Elements

0 20

► Thermodynamics

► Structural Properties

► Symmetry

12 materials match your search

Showing 1-12

✕ Formula: MoS₂

Columns

Material ID	Formula	Crystal System	Space Group Symbol	Sites	Energy Above Hull (eV/atom)	Band Gap (eV)
★ mp-2815	MoS ₂	Hexagonal	P6 ₃ /mmc	6	0	1.46
★ mp-1434	MoS ₂	Trigonal	R3m	3	< 0.01	1.20
mp-1027525	MoS ₂	Trigonal	P3̄m1	12	< 0.01	1.49
mp-1025874	MoS ₂	Hexagonal	P6̄m2	9	< 0.01	1.51
mp-1023939	MoS ₂	Trigonal	P3̄m1	6	< 0.01	1.55
★ mp-1018809	MoS ₂	Hexagonal	P6 ₃ /mmc	6	< 0.01	1.34
mp-1023924	MoS ₂	Hexagonal	P6̄m2	3	< 0.01	1.66
mp-990083	MoS ₂	Orthorhombic	Pmmn	54	0.17	0
mp-1405065	MoS ₂	Cubic	F4̄3m	12	0.27	0
mp-1238797	MoS ₂	Trigonal	P3̄m1	3	0.28	0
★ mp-558544	MoS ₂	Trigonal	R3̄m	3	0.28	0
mp-1042086	MoS ₂	Tetragonal	I4̄2d	6	0.65	0.04

Jump to

15 / page

← Previous

1

Next →

New Portal

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The Materials Project

Apps

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Community ▾

ML

API



[Home](#) / [Apps](#) / [Materials Explorer](#) / [Mo-S](#) / [MoS₂](#) / [mp-1434](#)



Materials Explorer

App by Materials Project



MoS₂
mp-1434

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[Electronic Structure](#)

[Phonon Dispersion](#)

[Diffraction Patterns](#)

[Aqueous Stability](#)

[Magnetic Properties](#)

[Elastic Constants](#)

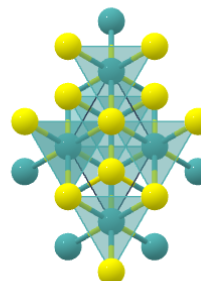
[Piezoelectric Constants](#)

[Dielectric Constants](#)

[X-ray Absorption Spectra](#)

[Charge Density](#)

[Supported Substrates](#)



Mo4+

S2-

Energy Above Hull	0.000 eV/atom
Space Group	R3m
Band Gap	1.20 eV
Predicted Formation Energy	-0.966 eV/atom
Magnetic Ordering	Non-magnetic
Total Magnetization	0.00 μB/f.u.
Experimentally Observed	Yes

Description (Auto-generated)

MoS₂ is Molybdenite-like structured and crystallizes in the trigonal R3m space group. The structure is two-dimensional and consists of three MoS₂ sheets oriented in the (0, 0, 1) direction. Mo⁴⁺ is bonded to six equivalent S²⁻ atoms to form distorted edge-sharing MoS₆ octahedra.

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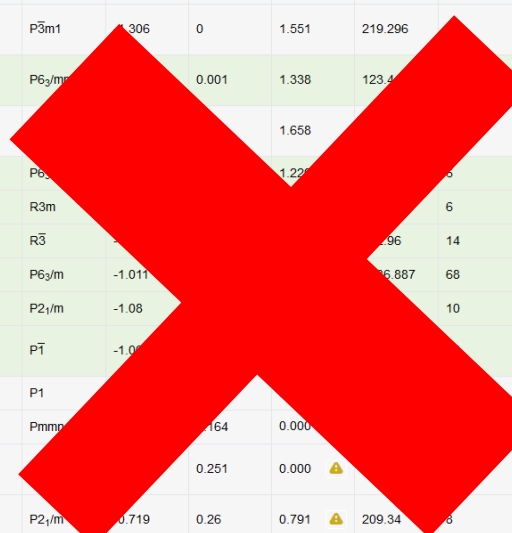
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[Documentation](#)

Get Data

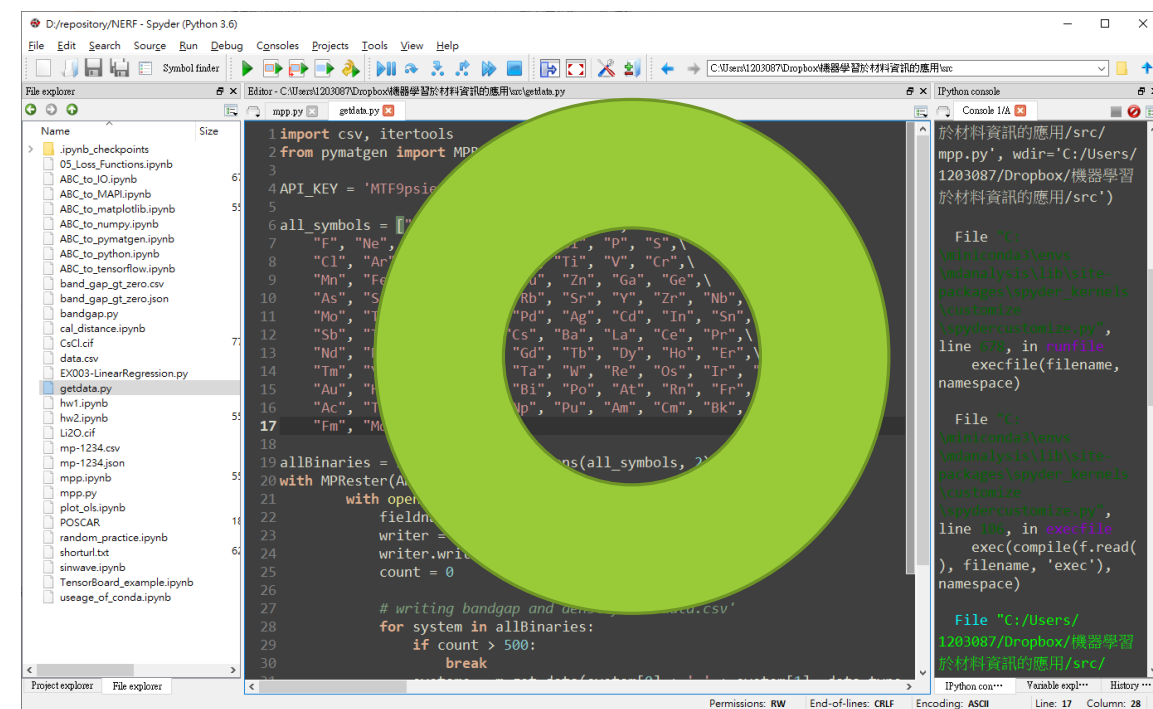
手動下載



Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	Volume	Nsites	Density (gm/cc)
mp-1027525	MoS ₂	P3m1	-1.306	0	1.746	350.447	12	3.034
mp-1025874	MoS ₂	P6m2	-1.306	0	1.783	284.872	9	2.799
mp-1023939	MoS ₂	P3m1	-1.306	0	1.551	219.296		2.424
mp-1018809	MoS ₂	P6 ₃ /mm2	-1.306	0.001	1.338	123.4		4.306
mp-1023924	MoS ₂				1.658			1.729
mp-2815	MoS ₂	P6 ₃ /mm2			1.22			4.503
mp-1434	MoS ₂	R3m					6	4.558
mp-2164	Mo ₃ S ₄	R3				96	14	5.062
mp-31257	Mo ₁₅ S ₁₉	P6 ₃ /m	-1.011			6.887	68	4.734
mp-1627	Mo ₂ S ₃	P2 ₁ /m	-1.08				10	5.702
mp-1104577	Mo ₃ S ₄	P1	-1.0					6.031
mp-673645	Mo ₇ S ₉	P1						5.674
mp-990083	MoS ₂	Pmmn		0.164	0.000			2.672
mp-1210708	Mo ₂₁ S ₈			0.251	0.000			8.75
mp-1239169	MoS ₃	P2 ₁ /m	0.719	0.26	0.791	209.34	8	3.048
mp-11780	MoS ₂	F43m	-1.041	0.265	0.000	221.127	12	4.808
mp-558544	MoS ₂	R3m	-1.029	0.277	0.000	111.639	6	4.762

自動化下載

open Materials Application Programming Interface (API)



```
1 import csv, itertools
2 from pymatgen import MP
3
4 API_KEY = 'MTF9psie'
5
6 all_symbols = [
7     "F", "Ne",
8     "Cl", "Ar",
9     "Mn", "Fe",
10    "As", "S",
11    "Pd", "Ag", "Cd", "In", "Sn",
12    "Sb", "T",
13    "Nd", "H",
14    "Ta", "W", "Re", "Os", "Ir",
15    "Au", "Hg", "Pt", "Pb", "Bi", "Po", "At", "Rn", "Fr",
16    "Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk",
17    "Fm", "Md",
18
19 allBinaries = [
20     with MPRester(A
21         with open
22         fieldn
23         writer =
24         writer.writ
25         count = 0
26
27     # writing bandgap and density to a csv file
28     for system in allBinaries:
29         if count > 500:
30             break
```

Open Source Software


- ❑ [Pymatgen](#) open source Python library for materials analysis
- ❑ [Crystal Toolkit](#) web app framework from the Materials Project which is now forming the basis of the Materials Project website
- ❑ [FireWorks](#) defining, managing, and executing scientific workflows
- ❑ [Custodian](#) job management framework that perform error checking, job management and error recovery
- ❑ [Atomate](#) provides "recipes" for performing complex materials science computations.
- ❑ [Emmet](#) is a toolkit of packages designed to build the Materials API.
- ❑ [Maggma](#) a framework to build complex data transformation pipelines from files to a REST API
- ❑ [MPContribs](#) provides API to contribute computational data to Materials Project.


Material Project

- Material Project提供了兩個工具供材料科學家使用他們的資料庫:
 - Materials Application Programming Interface (MAPI) ，資料釋出的協定。
 - Python Materials Genomics (pymatgen) materials analysis package ，分析的工具包。
- MAPI透過REpresentational State Transfer (REST)架構，方便使用者透過http requests存取資料。
- 在RESTful架構, 所有資訊都是整合至**resources**, 而**resources**也都透過 uniform resource identifier (URI)來指定網站上資料庫中的位置.
- Pymatgen (Python Materials Genomics)是一個針對材料科學的open-source Python library，特別是和Material Project高度整合。

MAPI DOC

□ Materials Project Documentation

 Materials Project Documentation

 materialsproject/docs
8 Stars · 32 Forks

Materials Project Documentation

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Materials Project Documentation



 **Warning**

Migration of content from our old wiki (<https://www.materialsproject.org/wiki>) is underway. Until this notice is removed, there might still be inconsistencies.

This is a place for all documentation relating to the [Materials Project](#) (MP), encompassing:

- Foundation: concepts in materials and computer science we use to structure and interpret our data sets
- Methodology: how we generate and validate our computed data sets
- User Guide: materials analysis and design using our data and tools
- User Reference: Detailed help for using our website, application programming interface (API), and codebases.
- Contribution: Developer guides and design specifications

If you notice an error or omission, please post an [issue](#) or click a pencil icon (edit) on a page to suggest an edit to us.

Thanks,
Materials Project Team

API keys

- 註冊登入後，可以到dashboard查看你的API KEY。
- 不要共用API KEY，如果有外流就重新產生一把。
- All MP https requests must supply API key as:
 - A x-api-key header, e.g., {'X-API-KEY': 'YOUR_API_KEY'} (recommended method)
 - As a GET (e.g., ?API_KEY=YOUR_API_KEY) or POST variable, e.g., {'API_KEY': 'YOUR_API_KEY'}
- 以GET方式，向Material Project網站要求material id 1234 的資源。

https://www.materialsproject.org/rest/v2/materials/mp-1234/vasp?API_KEY=YOUR_API_KEY

Find Your API-KEY



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API Key



Your API Key

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.

Accessing Data

To use the API, you have three options:

1. You can use our first-party supported Python client. This is the recommend route. During the pre-release of the new website, this has to be installed manually via github.com/materialsproject/api.

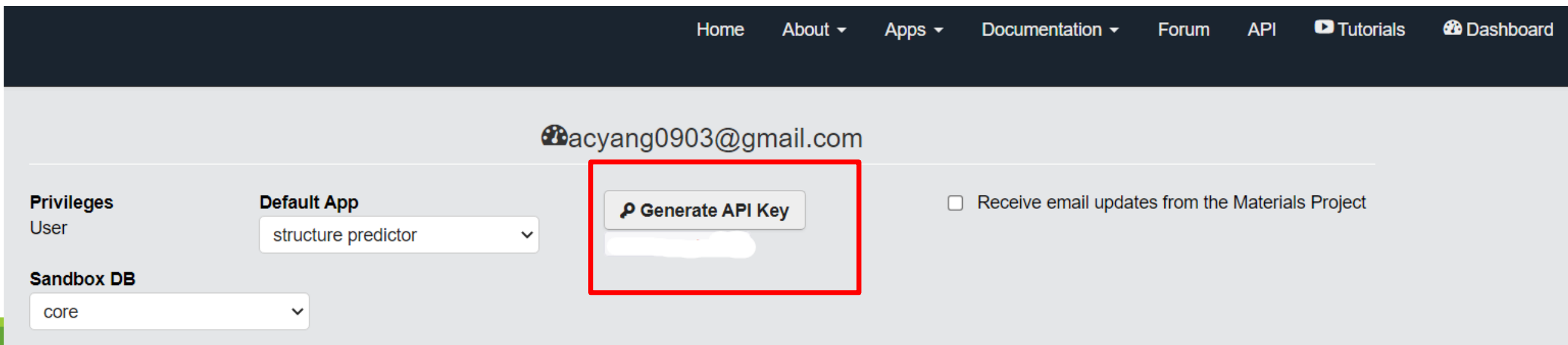
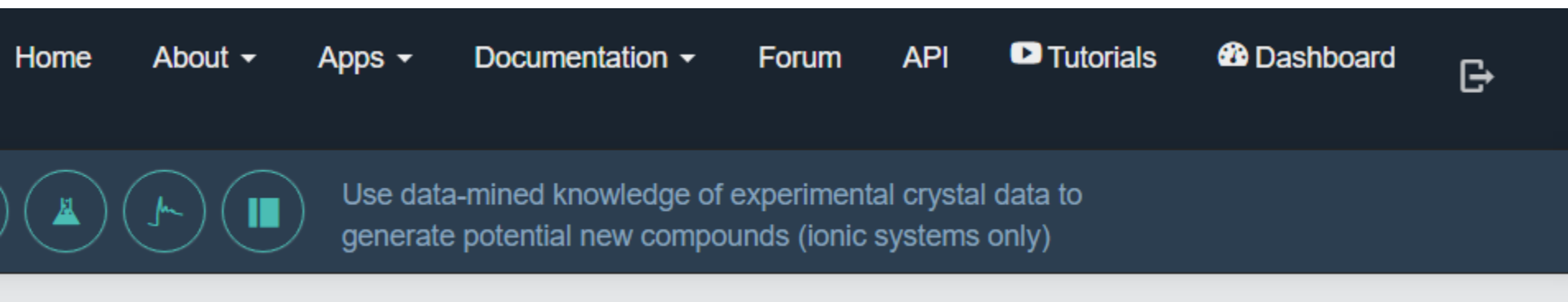
```
from mp_api.client import MPRester
```

This may ultimately replace the legacy MPRester available in [pymatgen](#).

2. You can demo the API interactively at api.materialsproject.org. Click the "Authorize" button, paste in your API key, and then click the appropriate section to try out a query.
3. Since this is a REST API, and offers a fully-compliant OpenAPI specification, it's possible to use the API with many libraries in many languages and environments, including JavaScript, MATLAB, Mathematica, etc. However, we do not offer first-party support for explaining how to do this, and you will have to follow the specification yourself.

Data Documents

Find Your API-KEY



Comparison of new API to legacy API

Comparison of new API to legacy API

This table summarizes the differences between the new and legacy APIs for existing users.

	New API	Legacy API
Currently recommended for	Early adopters	Everyone else
Base URL	api.materialsproject.org	materialsproject.org/rest/v2
Documentation	api.materialsproject.org/docs	mapidoc
Specification	OpenAPI-compliant specification available	None available
Support	Our new API will be supported for the foreseeable future once released	Will be available for at least one year after new API is finalized
Data Updates	Will receive new data updates included latest and most accurate data	Will be frozen at database release v2021.03.13
API Key	Available below	Available at legacy.materialsproject.org/open
Python client installation	<code>pip install mp-api</code> (may be available in <i>pymatgen</i> at a later date)	<code>pip install pymatgen</code>
Python client import code	<code>from mp_api.client import MPRestler</code>	<code>from pymatgen.ext.matproj import MPRestler</code>
MPContribs integration for user contributed data	Yes	No

Uniform Resource Identifier (URI) design

Preamble URL

Request type Unique Identifier Data type

`https://www.materialsproject.org/rest/v2/{request_type}/{identifier}/{parameters}`

1. preamble(前言、開場白)

就是個網址而已，聲明這是一個https REST request，v2 表明這是version 2 of the MAPI。

`https://www.materialsproject.org/rest/v2/`

2. request_type

指名你request的是哪種操作或資訊，除了"materials"之外還有"tasks", "battery", "reaction", "mpquery" and "api_check"。

3. identifier

根據request_type可以有不同的identifier，像是material id(e.g., mp-1234), formula(e.g. Fe₂O₃), chemical system("-" separated list of elements, e.g., Li-Fe-O), or task id。

4. parameters

根據request_type和identifier決定的參數，視情況可能會有多個parameters。

像是vasp表示的是computational data，exp表示的是experimental data。

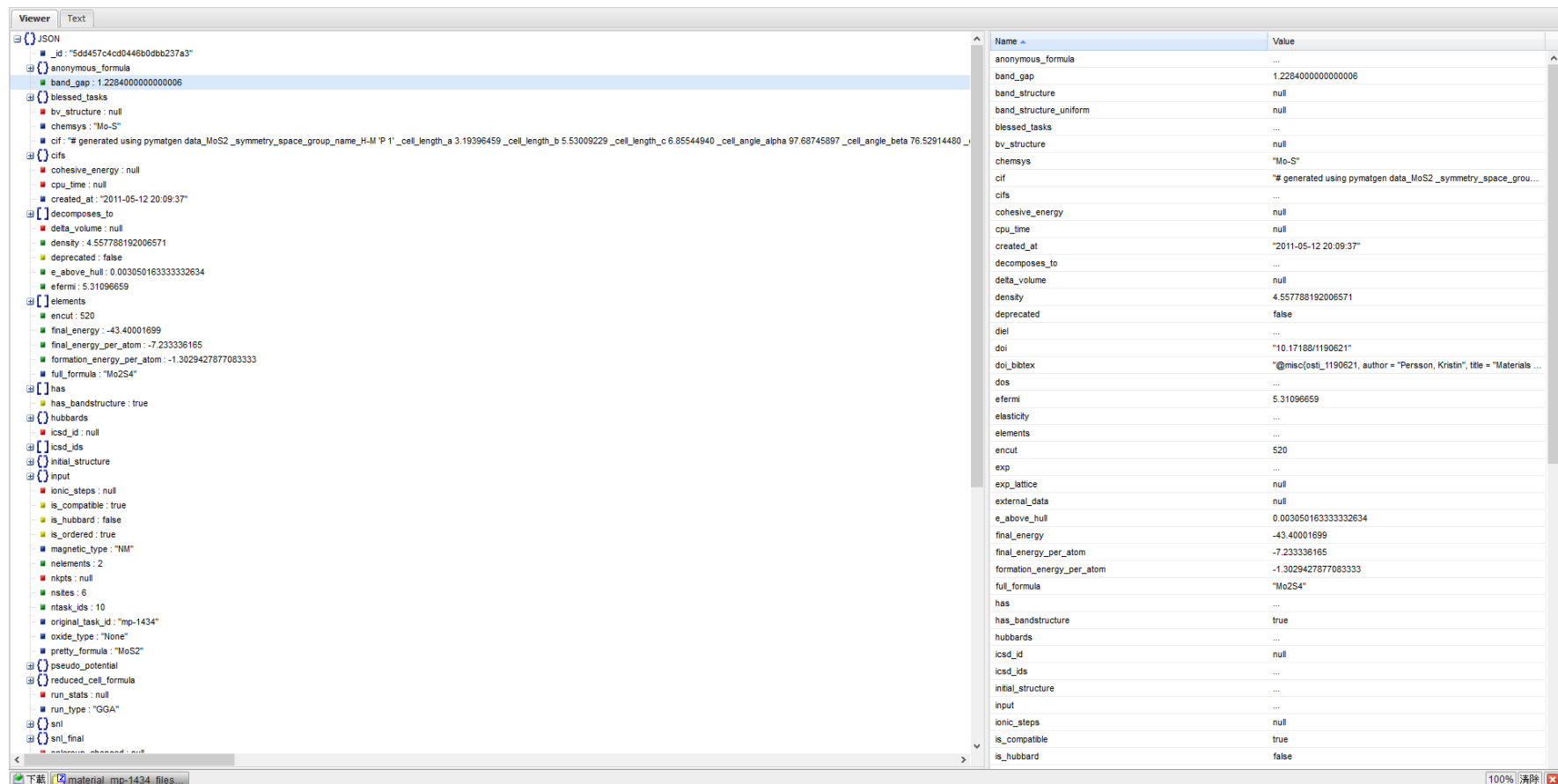
而vasp/energy表示的是computational data中的energy性質。

Sample JSON output

- 現階段回傳的物件都是以JavaScript Object Notation (JSON)回傳，目前還未支援XML。
- 直接在網址列輸入http request，會接在網頁呈現。
- 可以另存網頁得到JSON檔案。

```
{
  "response": [
    {
      "energy": -26.91801468,
      "energy_per_atom": -4.48633578,
      "volume": 116.92379066659765,
      "formation_energy_per_atom": -0.48230172,
      "nsites": 6,
      "unit_cell_formula": {
        "Lu": 2.0,
        "Al": 4.0
      },
      "pretty_formula": "LuAl2",
      "is_hubbard": false,
      "elements": ["Lu", "Al"],
      "nelements": 2,
      "e_above_hull": 0,
      "hubbards": {},
      "is_compatible": true,
      "spacegroup": {
        "symprec": 0.1,
        "source": "spglib",
        "symbol": "Fd-3m",
        "number": 227,
        "point_group": "m-3m",
        "crystal_system": "cubic",
        "hall": "F 4d 2 3 -1d",
        "task_ids": [
          "mp-940234",
          "mp-925833",
          "mp-940654",
          "mp-1234",
          "mp-1258536",
          "mp-1438947",
          "mp-1678516",
          "mp-1803625",
          "mp-1593631"
        ],
        "band_gap": 0.0,
        "density": 6.502480539556319,
        "icsd_id": null,
        "icsd_ids": [
          608375,
          57958,
          608376,
          608372,
          608371,
          608370
        ],
        "cif": "# generated using pymatgen\\ndata_LuAl2\\n_symmetry_space_group_name_H-M 'P 1'\\n_cell_length_a 5.48873961\\n_cell_length_b 5.48873961\\n_cell_length_c 5.48873961\\n_cell_angle_alpha 60.00000000\\n_cell_angle_beta 60.00000000\\n_cell_angle_gamma 60.00000000\\n_symmetry_Int_Tables_number 1\\n_chemical_formula_structural LuAl2\\n_chemical_formula_sum 'Lu2 Al4'\\n_cell_volume 116.92379067\\n_cell_formula_units_Z 2\\nloop\\n_symmetry_equiv_pos_site_id\\n_symmetry_equiv_pos_as_xyz\\n 1 'x, y, z'\\nloop\\n_atom_site_type_symbol\\n_atom_site_label\\n_atom_site_symmetry_multiplicity\\n_atom_site_fract_x\\n_atom_site_fract_y\\n_atom_site_fract_z\\n_atom_site_occupancy\\n Lu Lu0 1 0.25000000 0.25000000 0.25000000 1\\n Lu Lu1 1 0.00000000 0.00000000 0.00000000 1\\n Al Al2 1 0.62500000 0.12500000 0.62500000 1\\n Al Al3 1 0.62500000 0.62500000 0.12500000 1\\n Al Al4 1 0.12500000 0.62500000 0.62500000 1\\n Al Al5 1 0.62500000 0.62500000 0.62500000 1\\n",
        "total_magnetization": 0.00022485,
        "material_id": "mp-1234",
        "oxide_type": "None",
        "tags": [
          "Aluminium lutetium (2/1)"
        ],
        "elasticity": {
          "G_Reuss": 61.0,
          "G_VRH": 61.0,
          "G_Voigt": 62.0,
          "G_Voigt_Reuss_Hill": 61.0,
          "K_Reuss": 82.0,
          "K_VRH": 82.0,
          "K_Voigt": 82.0,
          "K_Voigt_Reuss_Hill": 82.0,
          "elastic_anisotropy": 0.04,
          "elastic_tensor": [
            [174.0, 36.0, 36.0, 0.0, 0.0, 0.0],
            [36.0, 174.0, 36.0, 0.0, 0.0, 0.0],
            [36.0, 36.0, 174.0, 0.0, 0.0, 0.0],
            [0.0, 0.0, 0.0, 57.0, 0.0, 0.0],
            [0.0, 0.0, 0.0, 0.0, 57.0, 0.0],
            [0.0, 0.0, 0.0, 0.0, 0.0, 57.0]
          ],
          "homogeneous_poisson": 0.2,
          "poisson_ratio": 0.2,
          "universal_anisotropy": 0.04,
          "elastic_tensor_original": [
            [173.8039399290068, 36.29190678313171, 36.29190678313171, 0.0, 0.0, 0.0],
            [36.29190678313171, 173.8039399290068, 36.29190678313171, 0.0, 0.0, 0.0],
            [36.29190678313171, 36.29190678313171, 173.8039399290068, 0.0, 0.0, 0.0],
            [0.0, 0.0, 0.0, 56.801403605413576, 0.0, 0.0],
            [0.0, 0.0, 0.0, 0.0, 56.801403605413576, 0.0],
            [0.0, 0.0, 0.0, 0.0, 0.0, 56.801403605413576]
          ],
          "compliance_tensor": [
            [6.2, -1.1, -1.1, 0.0, -0.0, 0.0],
            [-1.1, 6.2, -1.1, -0.0, 0.0, -0.0],
            [-1.1, -1.1, 6.2, -0.0, -0.0, 0.0],
            [0.0, -0.0, -0.0, 17.6, 0.0, -0.0],
            [-0.0, 0.0, -0.0, 0.0, 17.6, -0.0],
            [0.0, -0.0, 0.0, -0.0, -0.0, 17.6]
          ],
          "warnings": [
            "Contains a rare earth element"
          ],
          "nsites": 6,
          "piezo": null,
          "diel": null,
          "deprecated": false,
          "full_formula": "Lu2Al4"}],
      "valid_response": true,
      "created_at": "2021-05-31T20:46:37.838142",
      "version": {
        "db": "2021_05_13",
        "pymatgen": "2022.0.8",
        "rest": "2.0",
        "copyright": "Materials Project, 2021"
      }
    }
  ]
}
```


<http://jsonviewer.stack.hu/>



Integration with pymatgen

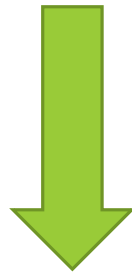


The Materials API



pymatgen

pymatgen

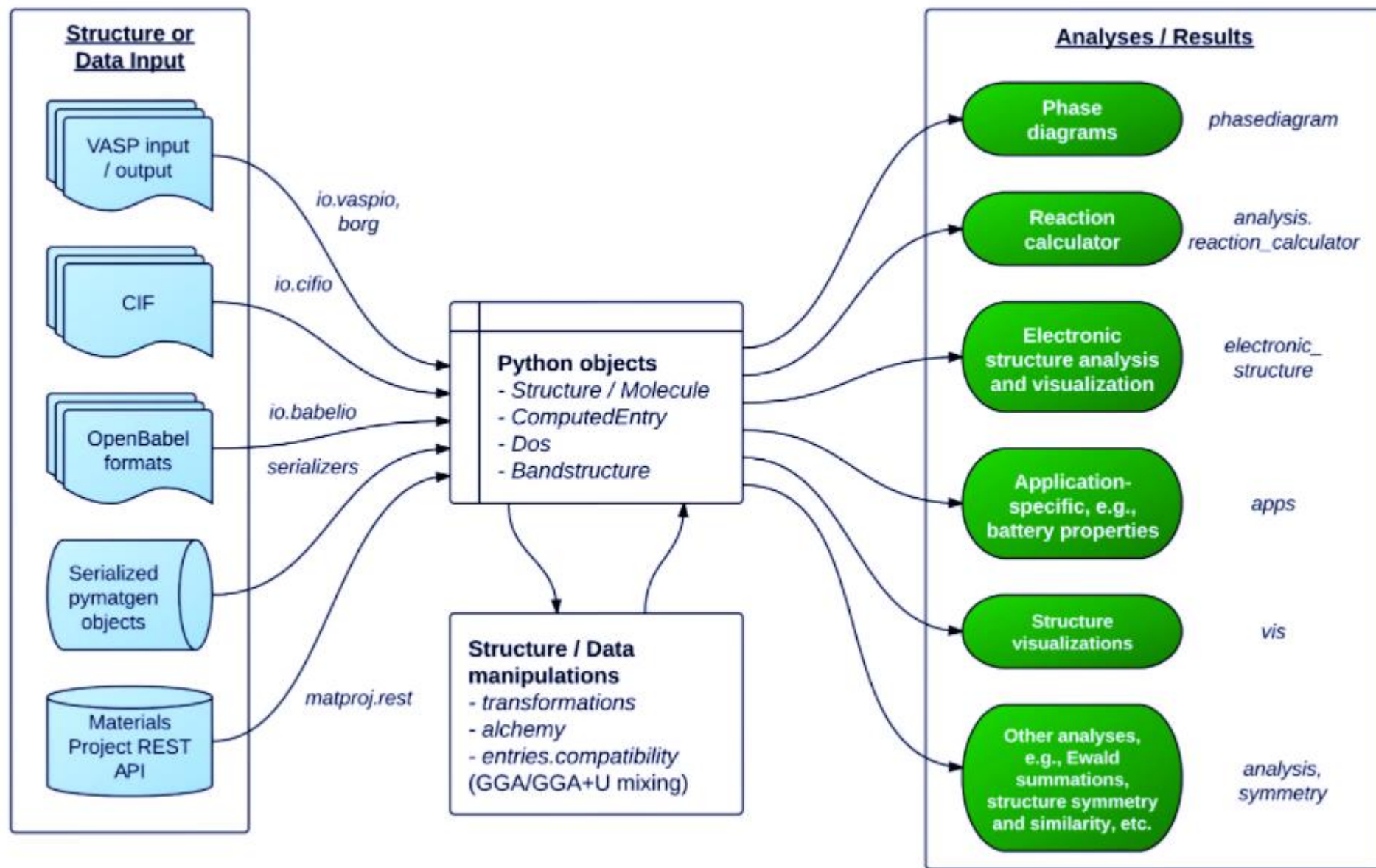


**Powerful Materials
Analytics Tool**

Introduction to Pymatgen

- 提供Element, Site, Molecule, Structure objects多種class，方便用戶進一步操作。
- 支援VASP, ABINIT, CIF, Gaussian, XYZ等多種檔案格式
- 提供多種分析模組phase diagrams, Pourbaix diagrams, diffusion analyses, reactions, Electronic structure, density of states和band structure。
- 和Materials Project REST API, Crystallography Open Database and other external data sources的API整合。
- As of 2023, pymatgen only supports Python 3.7 and above latest version is **v2023.5.31**

typical workflow for pymatgen



Compatibility of pymatgen v2022.0.0

```
from pymatgen import Composition # now "from pymatgen.core.composition import Composition"
from pymatgen import Lattice # now "from pymatgen.core.lattice import Lattice"
from pymatgen import SymmOp # now "from pymatgen.core.operations import SymmOp"
from pymatgen import DummySpecie, DummySpecies, Element, Specie, Species # now "from
pymatgen.core.periodic_table ..."
from pymatgen import PeriodicSite, Site # now "from pymatgen.core.sites ..."
from pymatgen import IMolecule, IStructure, Molecule, Structure # now "from
pymatgen.core.structure ..."
from pymatgen import ArrayWithUnit, FloatWithUnit, Unit # now "from pymatgen.core.units ..."
from pymatgen import Orbital, Spin # now "from pymatgen.electronic_structure.core ..."
from pymatgen import MPRester # now "from pymatgen.ext.matproj ..."
```

Pymatgen API DOC

□ <https://pymatgen.org/pymatgen.html>

The screenshot displays the Pymatgen API documentation website. The left sidebar features a navigation menu with links to Introduction, Installation, Change log, Compatibility, Contributing, Usage, Development Team, and References. Below this is a section for API Docs, which is currently expanded to show the pymatgen namespace, including Subpackages and Submodules. The main content area shows the pymatgen namespace page, which includes a search bar, a breadcrumb trail (home » pymatgen » pymatgen namespace), and an 'Edit on GitHub' link. The page title is 'pymatgen namespace', and the section is 'Subpackages'. The content lists two main subpackages: 'pymatgen.alchemy package' and 'pymatgen.analysis namespace'. The 'pymatgen.alchemy package' section includes links to its Subpackages (pymatgen.alchemy.filters module, pymatgen.alchemy.materials module, and pymatgen.alchemy.transmuters module) and its Module contents. The 'pymatgen.analysis namespace' section includes links to its Subpackages (pymatgen.analysis.chemenv package) and Submodules (pymatgen.analysis.chemenv.connectivity package).

pymatgen
2022.0.8

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pymatgen namespace

- Subpackages
- Submodules

» pymatgen » pymatgen namespace

Edit on GitHub

pymatgen namespace

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pymatgen.io

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pymatgen.analysis

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