機器學習於材料資訊的應用
Machine Learning on Material Informatics

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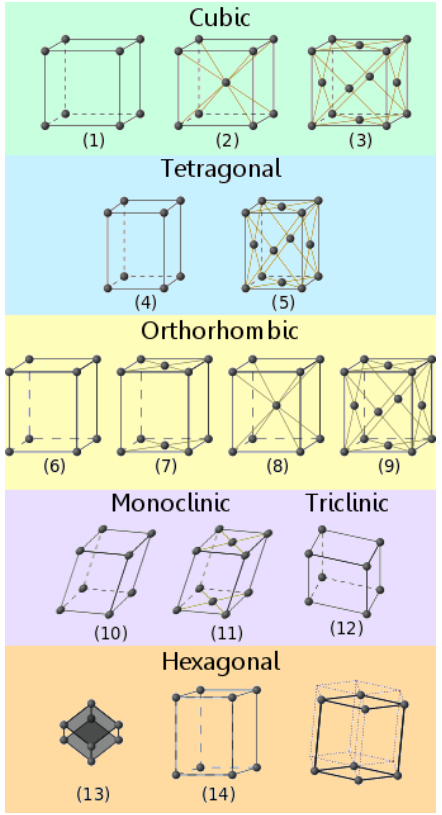
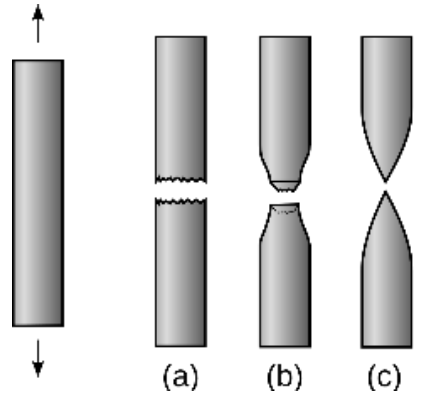
Data comes from Computational Materials Science

A new powerful approach to discover novel material

材料基因

Human Genome V.S. Material Genome

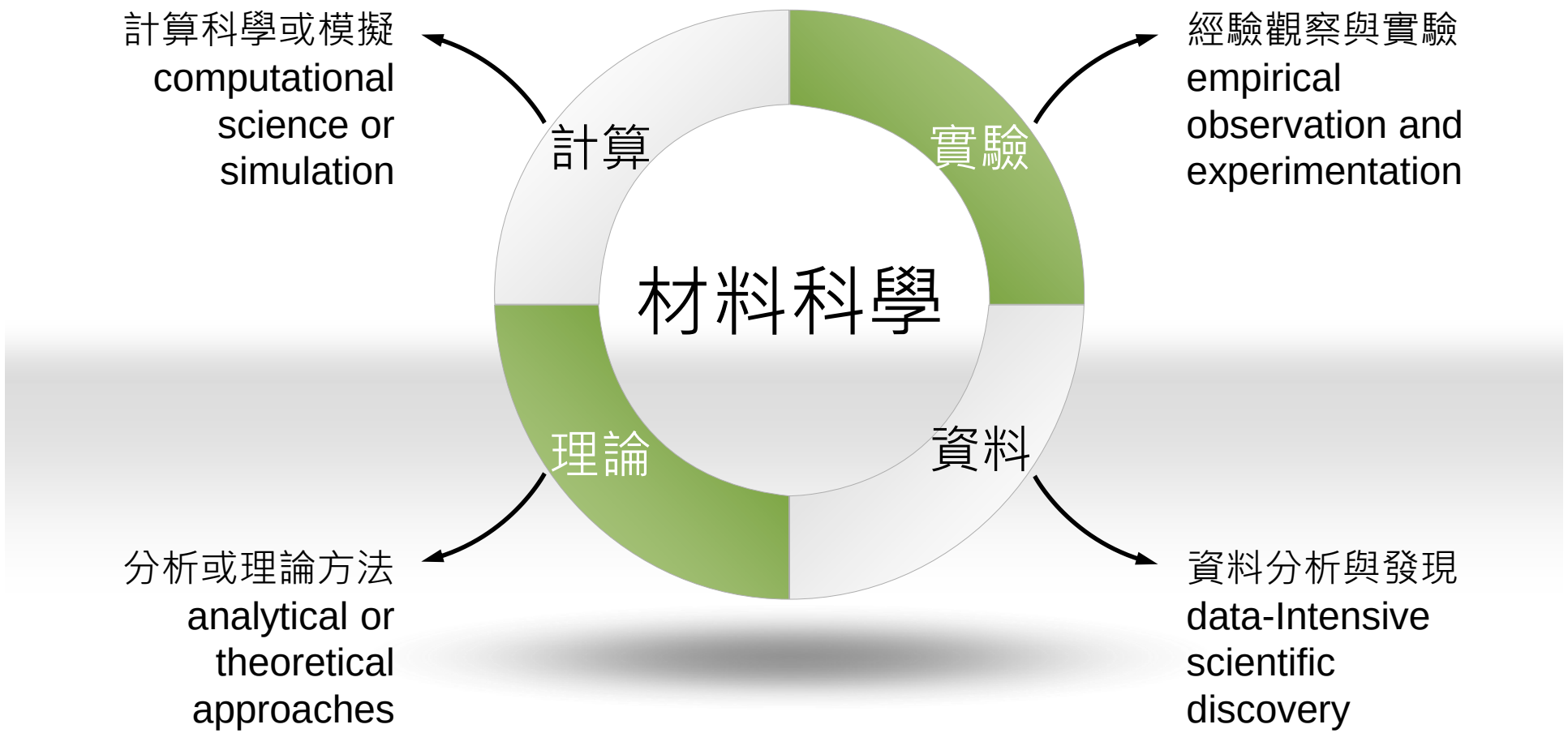




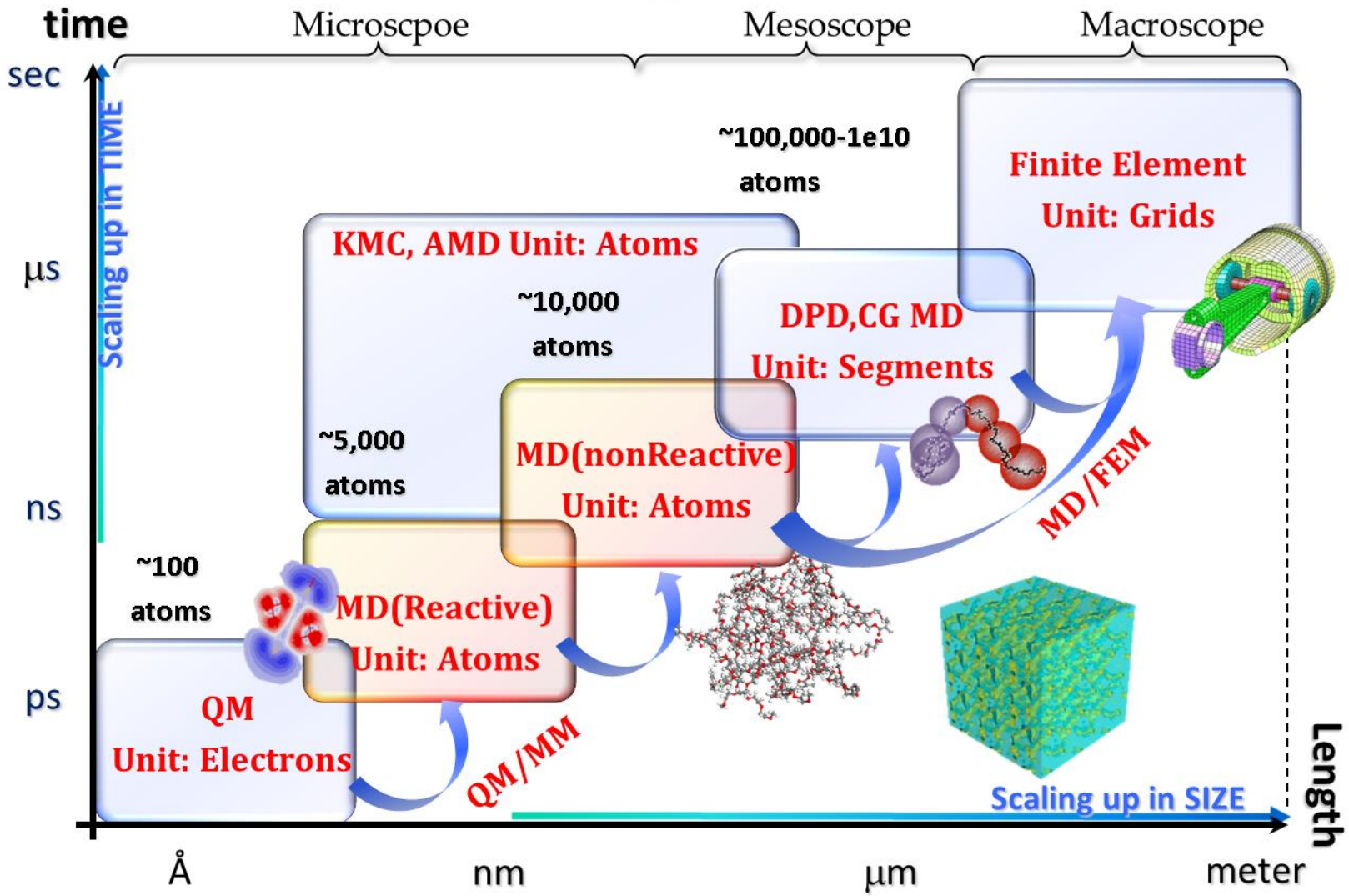
生物個體的外在表現叫作「表現型（phenotype）」，由內在的「基因型（genotype）」決定。改變表現型，首先要改變基因型。.

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。.

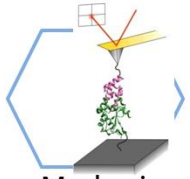
材料科學的分支


計算科學或模擬
computational science or simulation
經驗觀察與實驗
empirical observation and experimentation
計算
實驗
材料科學
理論
資料
分析或理論方法
analytical or theoretical approaches
資料分析與發現
data-Intensive scientific discovery

Multi-Scale Modeling for Materials Simulation

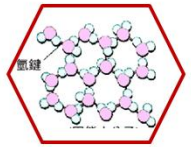


Properties you can get from calculation



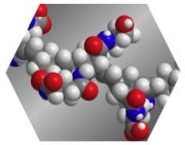
Mechanics

Elastic constant
Young's modus
Stress-strain
Hardness



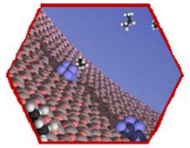
Thermodynamics

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



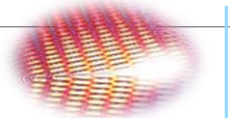
Structure

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



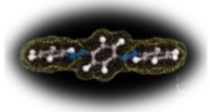
Dynamics

Diffusion coefficient
Viscosity (Green Kubo)
Auto-correlation function



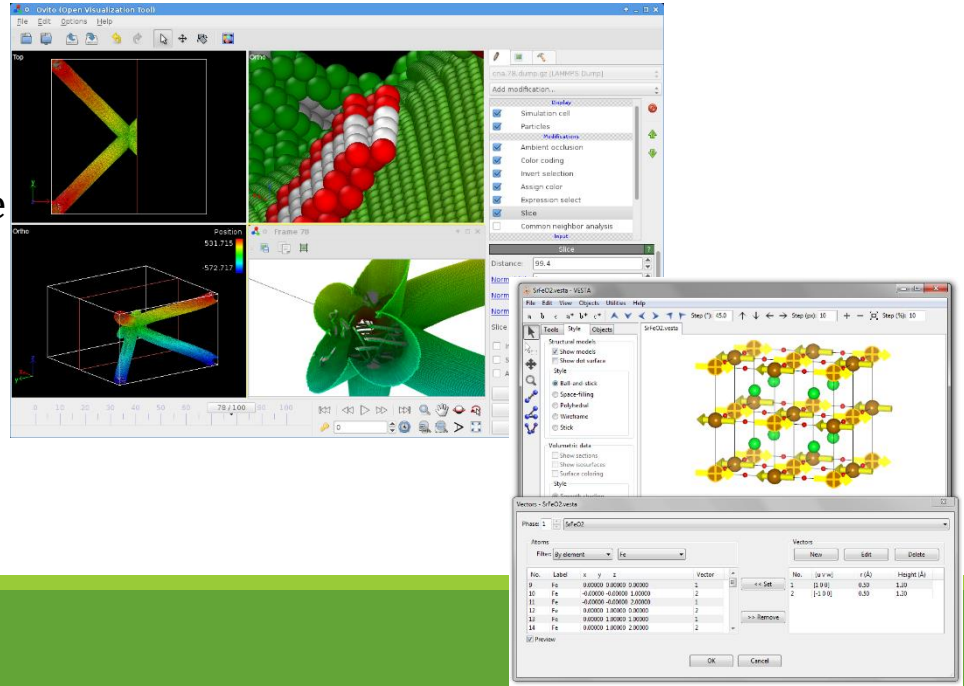
Optics

Birefringence
Dielectric constant
Abbe Number
Reflective Index

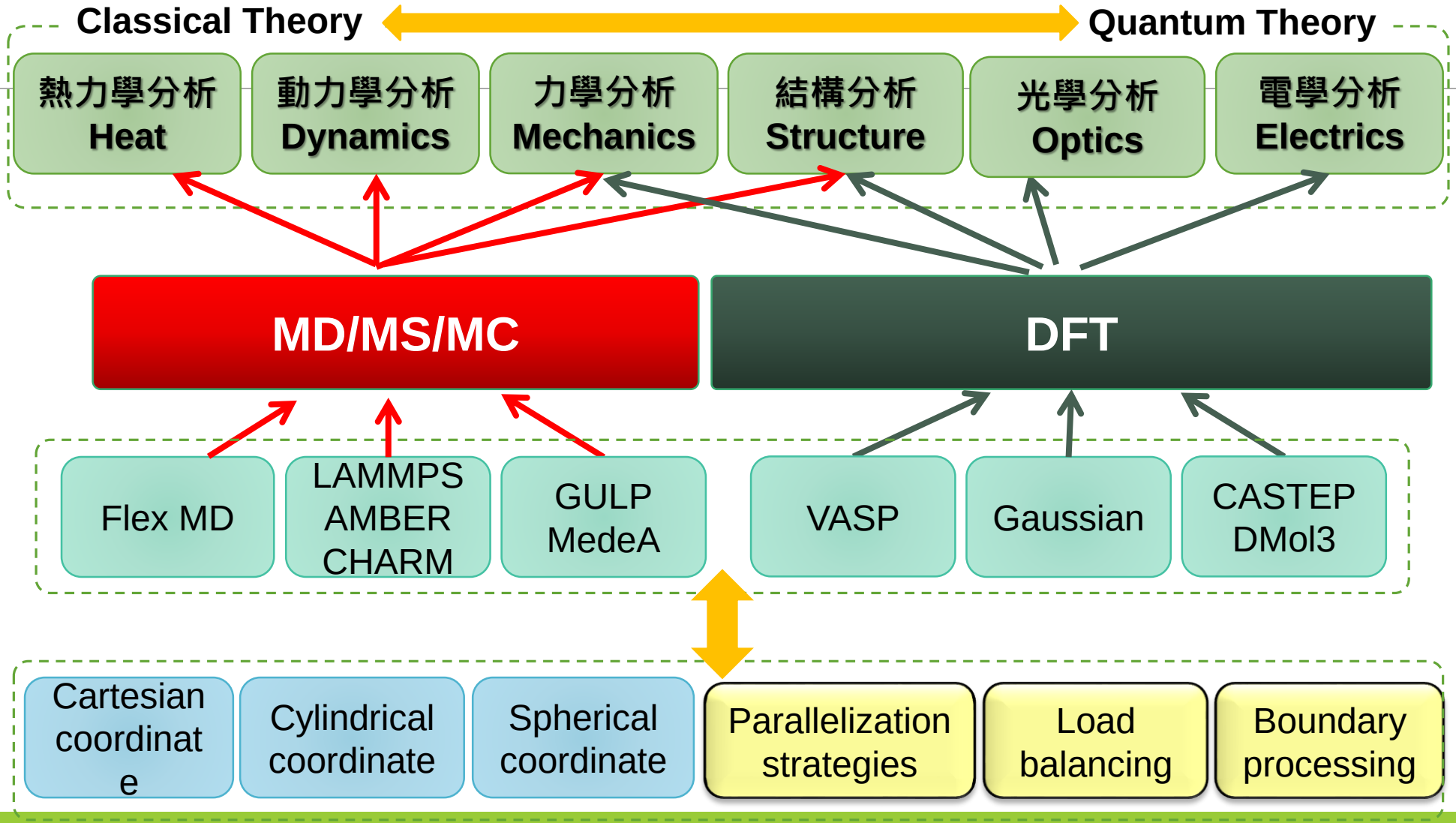


Electrics

Band structure/gap
Density of state



Molecular Modeling



Material Project

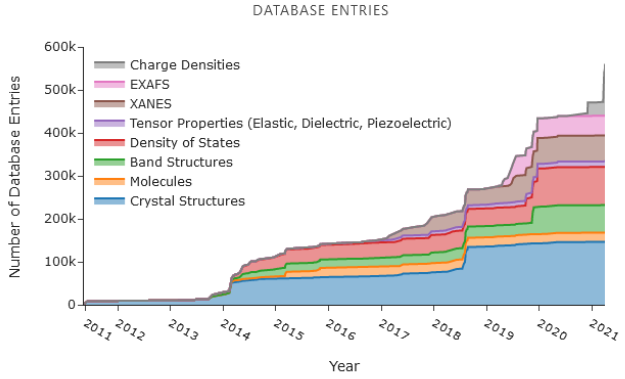
The Materials Project

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

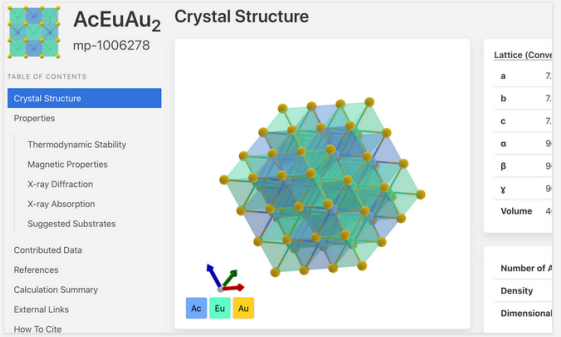
The Materials Project by the numbers

MATERIALS	REGISTERED USERS
154,718	300,000+
INTERCALATION ELECTRODES	**CITATIONS**
4,351	19,000+
MOLECULES	**CPU HOURS/YEAR**
24,989	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

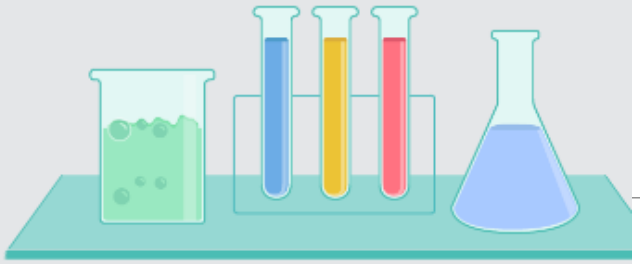
software

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

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.

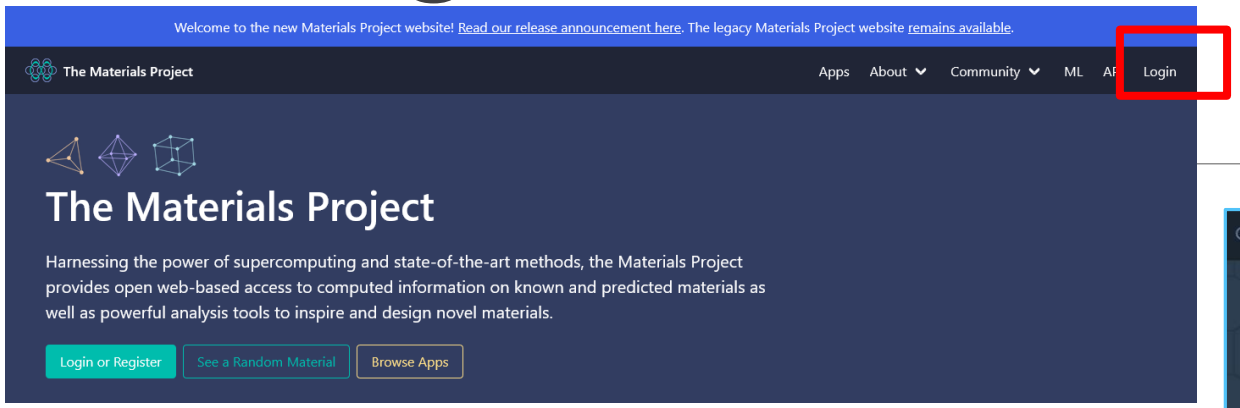
rank1 rank28 rank13

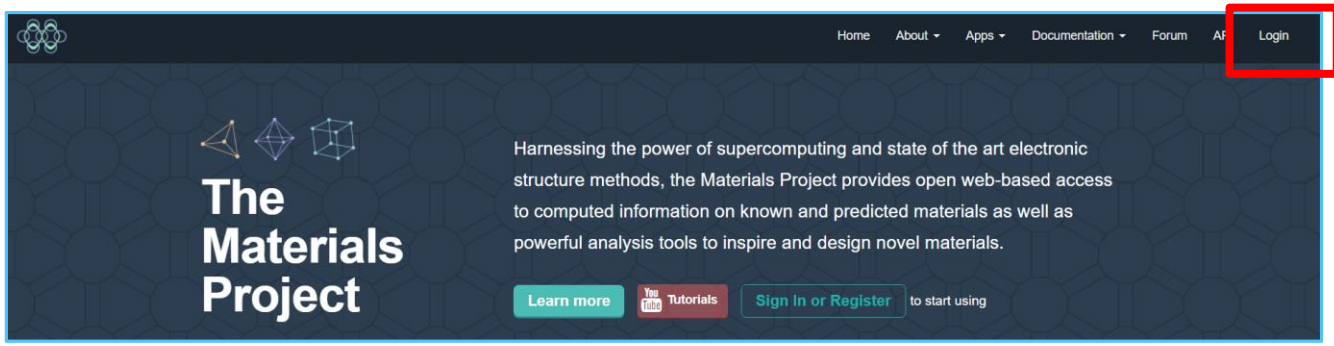


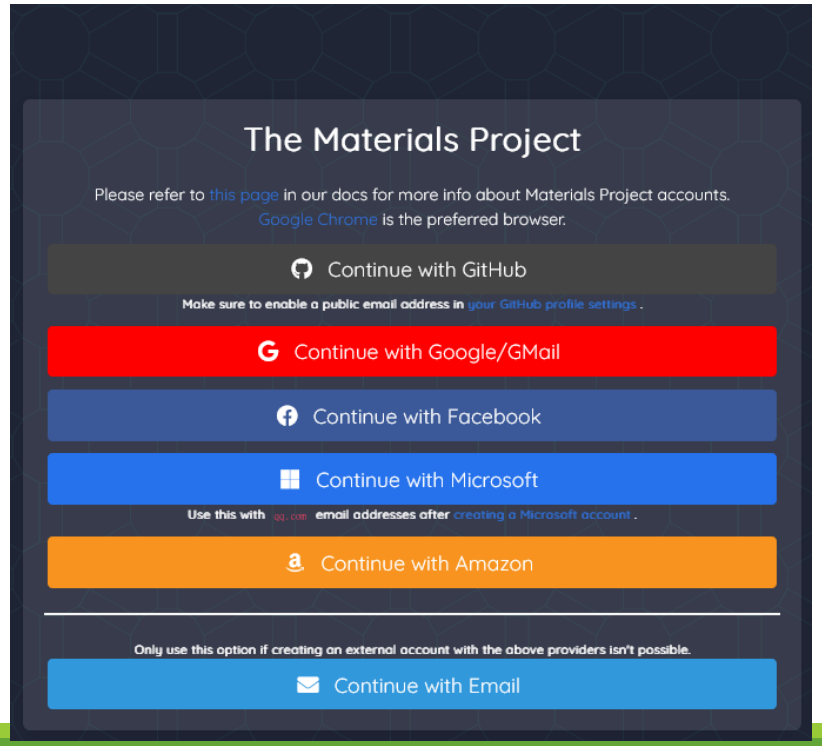
screening

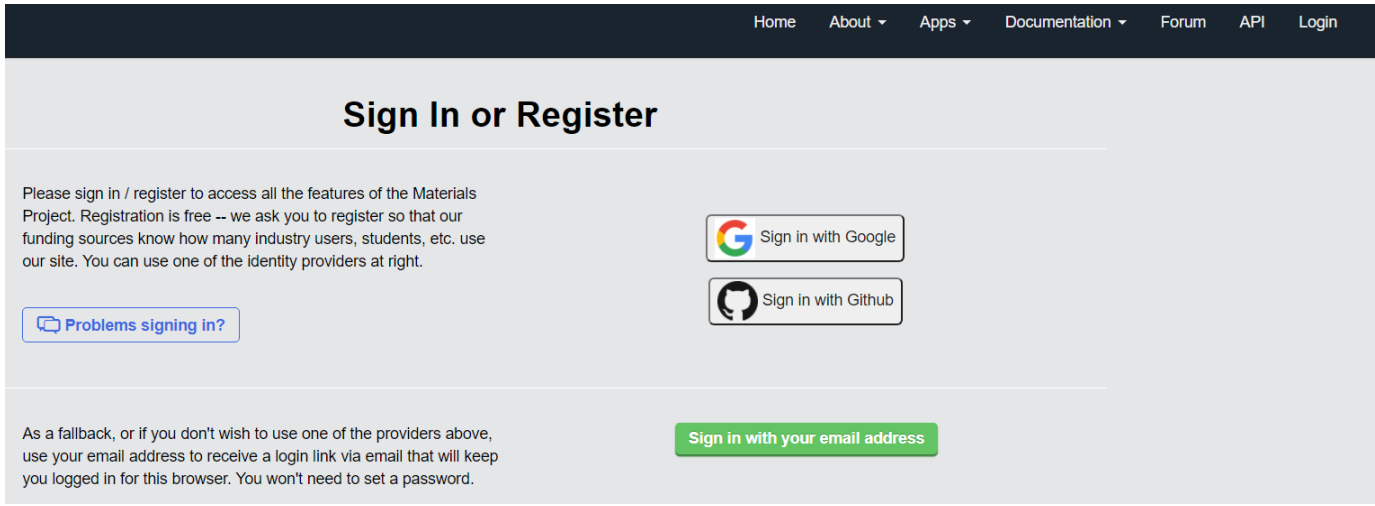
Computational materials science is now powerful enough that it can predict many properties of materials before those materials are ever synthesized in the lab. By scaling materials computations over supercomputing clusters, we have predicted several new battery materials which were made and tested in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

Login



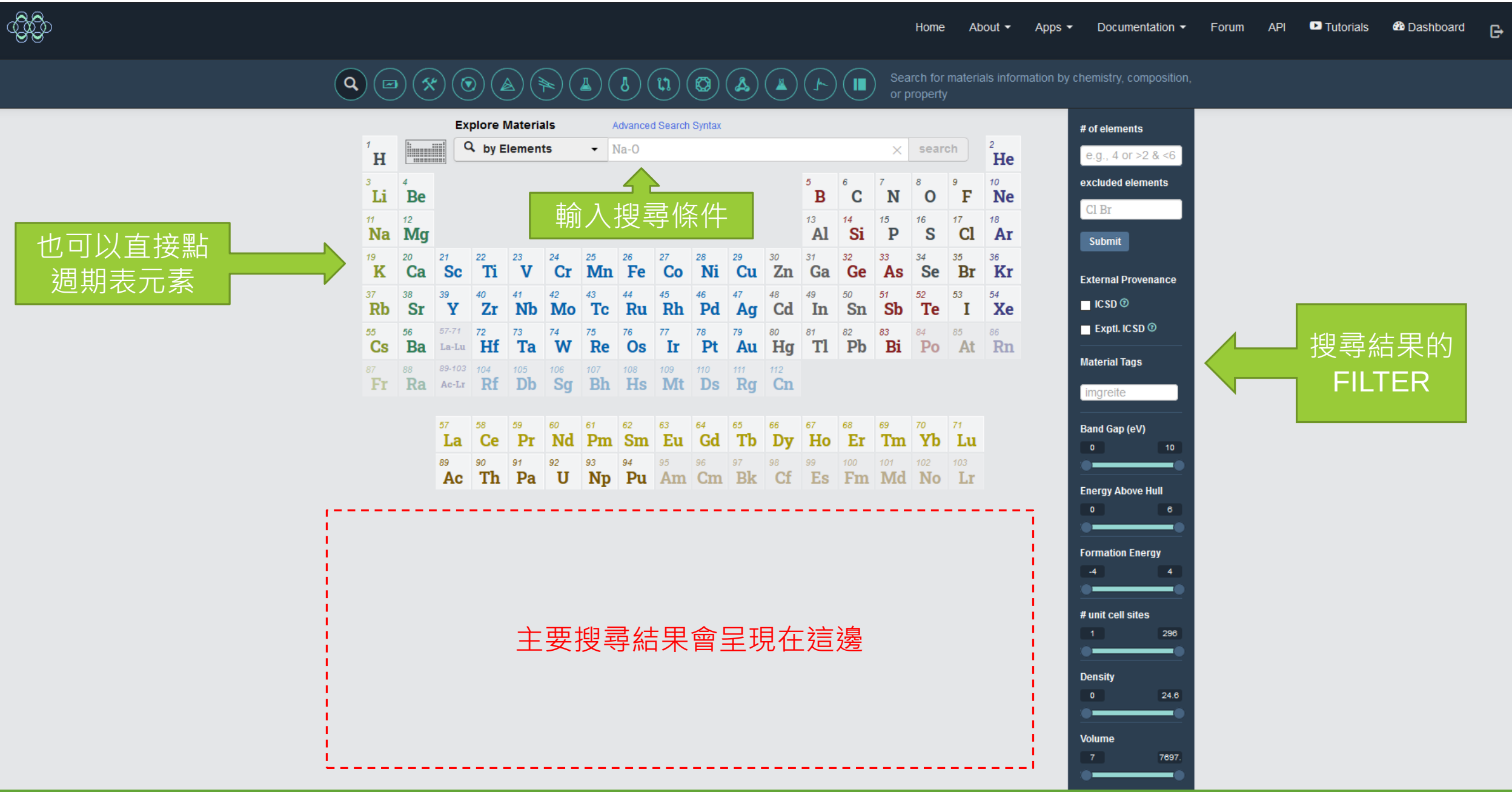






https://materialsproject.org/

https://legacy.materialsproject.org/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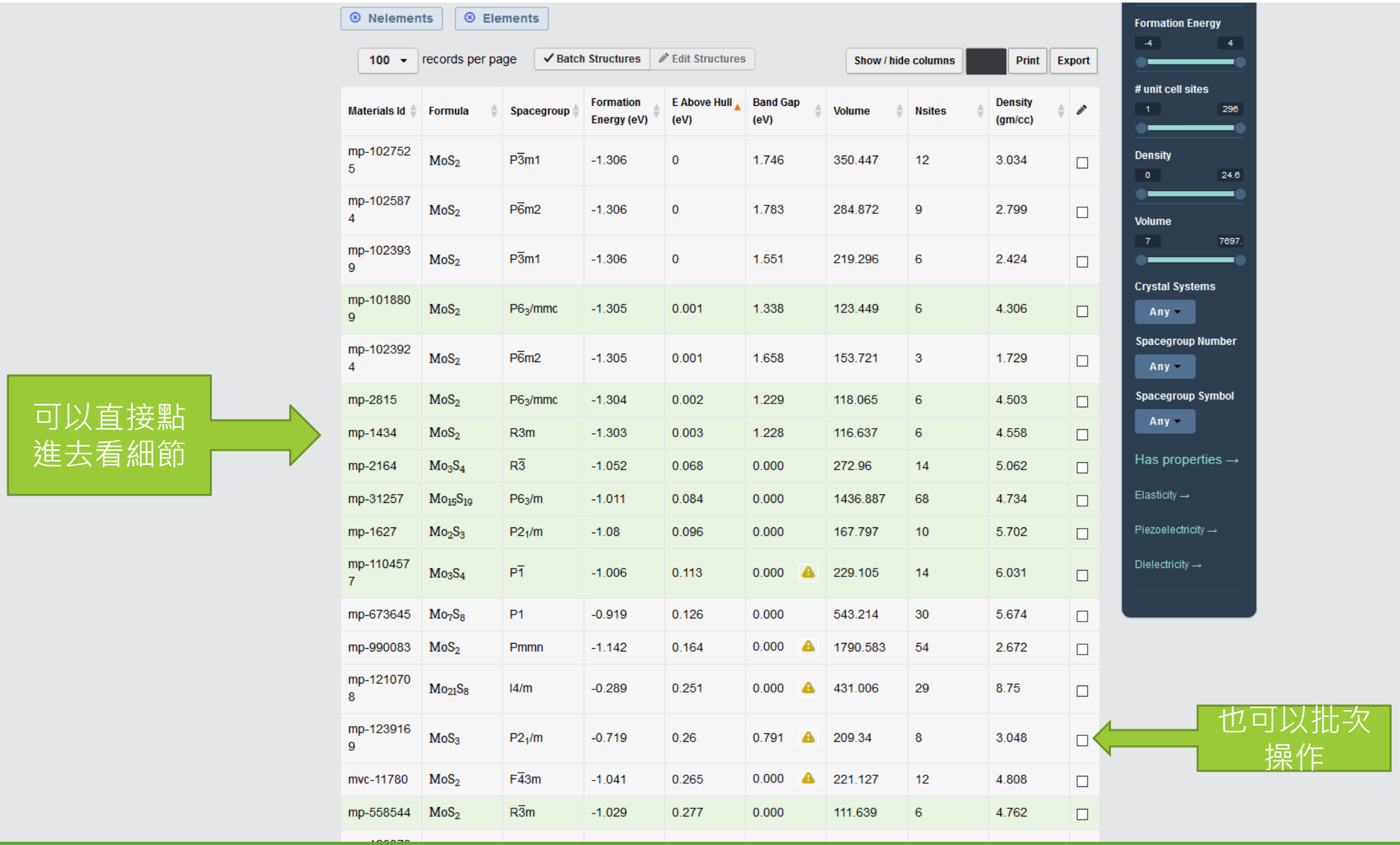
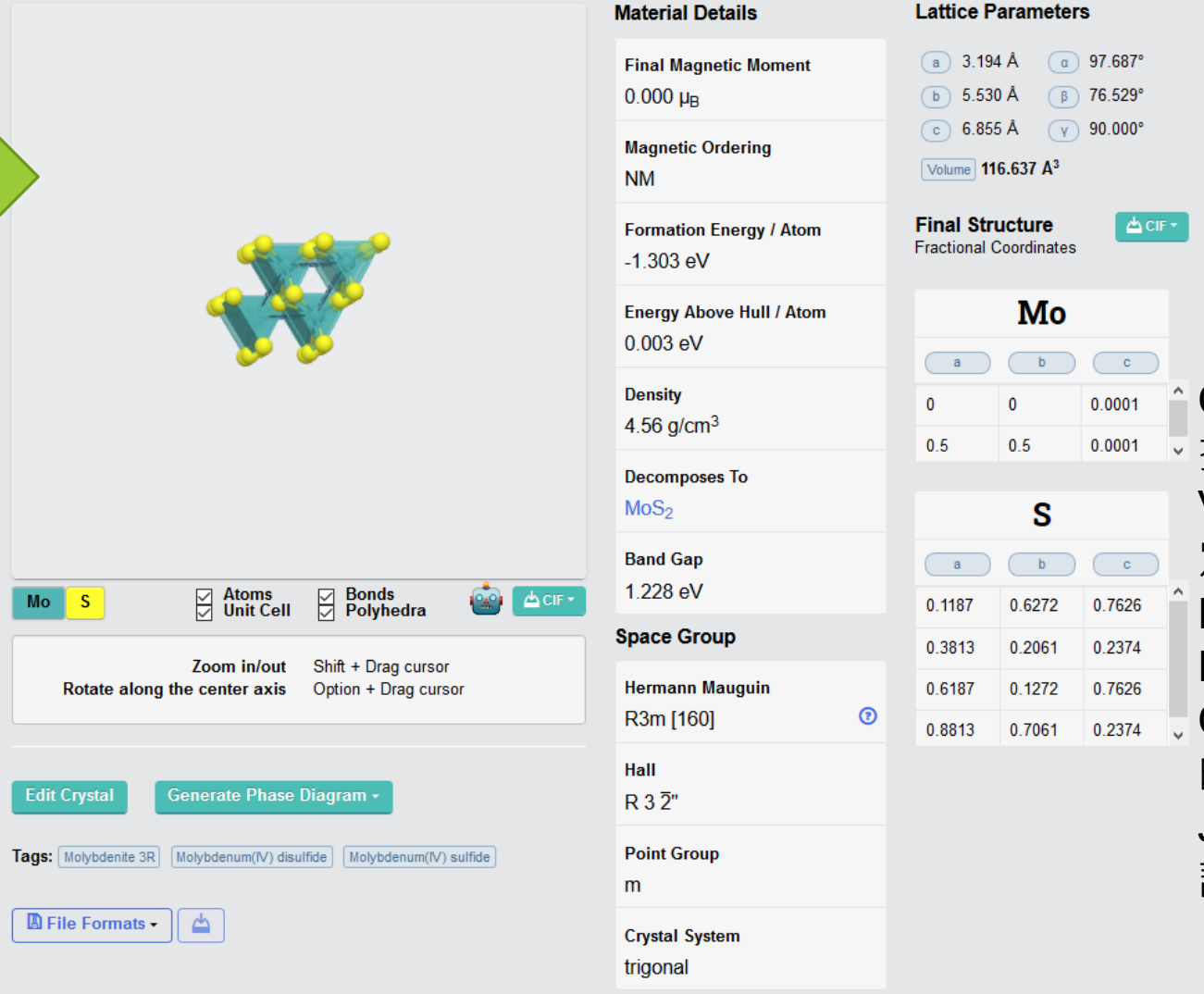
也可以直接點週期表元素
# of elements
e.g., 4 or >2 & <6
excluded elements
Cl Br
Submit
External Provenance
ICSD
Exptl. ICSD
Material Tags
imgreite
Band Gap (eV)
Energy Above Hull
Formation Energy
unit cell sites
Density
Volume
搜尋結果的FILTER
主要搜尋結果會呈現在這邊



可以直接點進去看細節

也可以批次操作

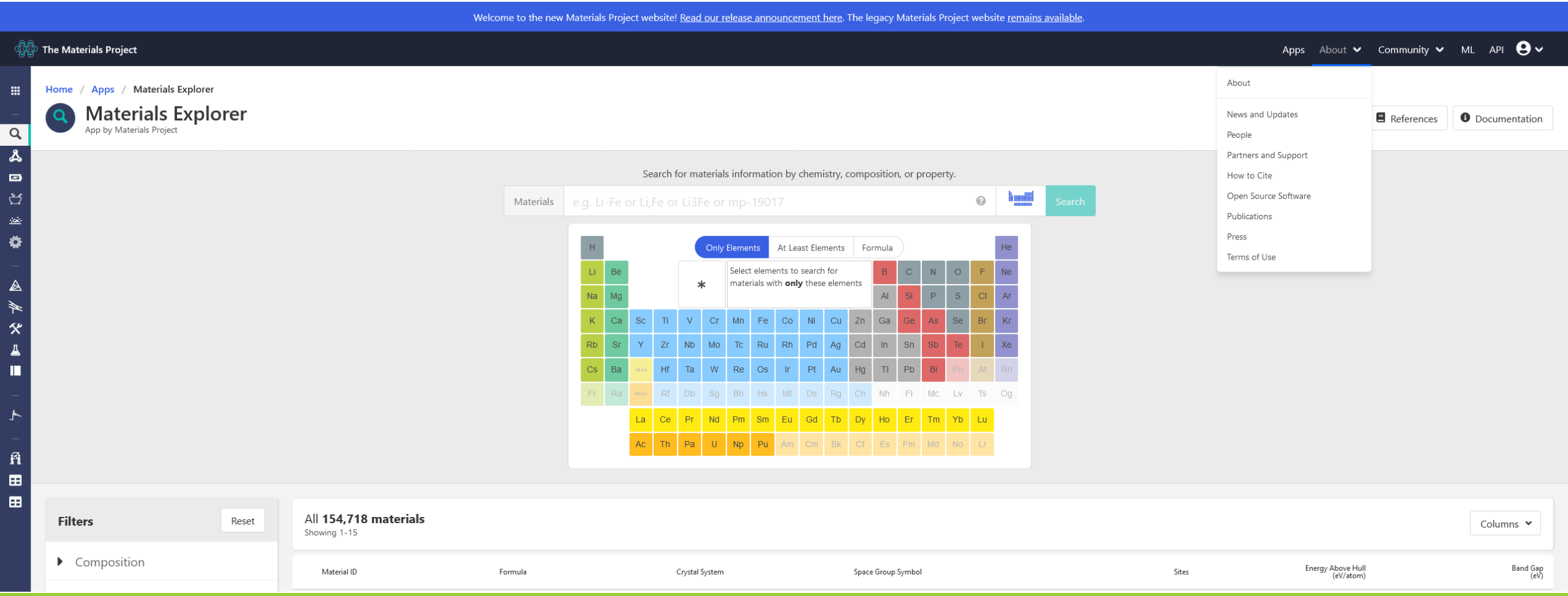
將結構視覺化的區域



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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API
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Materials Explorer
App by Materials Project
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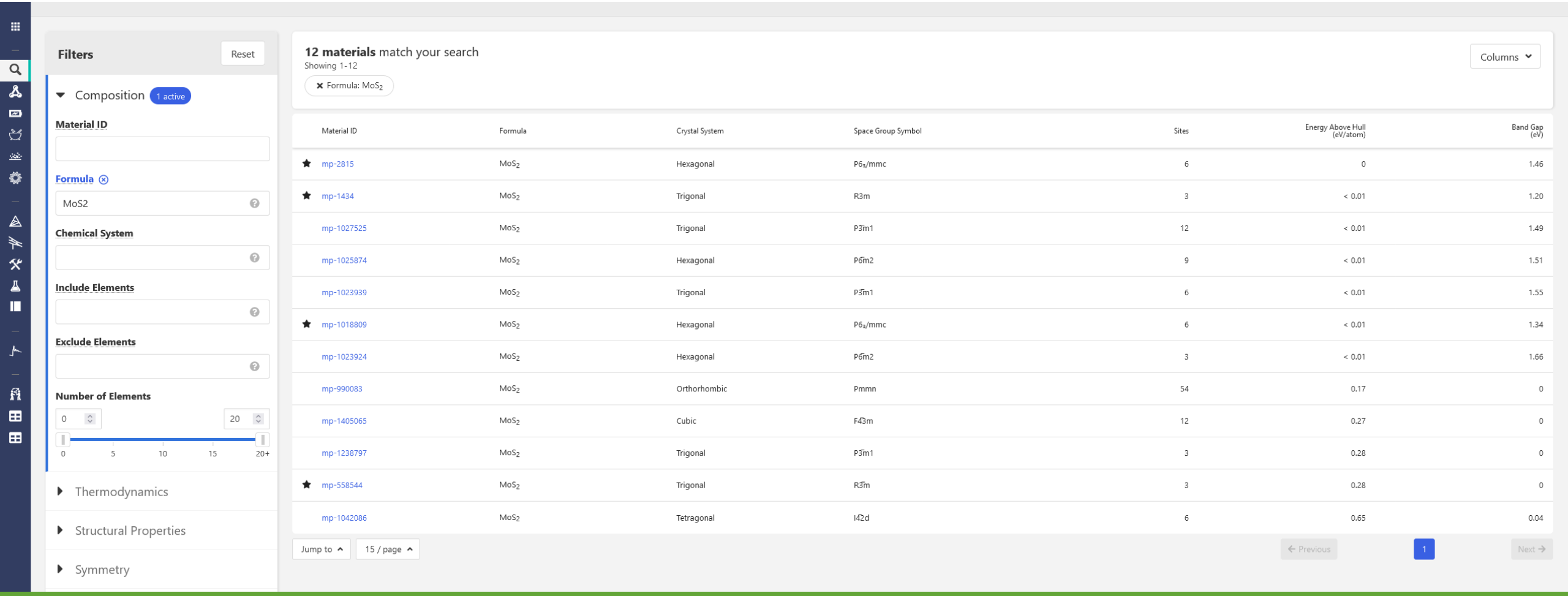
News and Updates
People
Partners and Support
How to Cite
Open Source Software
Publications
Press
Terms of Use
References
Documentation
Search for materials information by chemistry, composition, or property.
Materials
e.g. Li-Fe or Li,Fe or Li3Fe or mp-19017
Search
Only Elements
At Least Elements
Formula
Select elements to search for materials with only these elements
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
0
5
10
15
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 MoS2 Hexagonal P6₃/mmc 6 0 1.46
mp-1434 MoS2 Trigonal R3m 3 < 0.01 1.20
mp-1027525 MoS2 Trigonal P3̄m1 12 < 0.01 1.49
mp-1025874 MoS2 Hexagonal P6̄m2 9 < 0.01 1.51
mp-1023939 MoS2 Trigonal P3̄m1 6 < 0.01 1.55
mp-1018809 MoS2 Hexagonal P6₃/mmc 6 < 0.01 1.34
mp-1023924 MoS2 Hexagonal P6̄m2 3 < 0.01 1.66
mp-990083 MoS2 Orthorhombic Pmmn 54 0.17 0
mp-1405065 MoS2 Cubic F4̄3m 12 0.27 0
mp-1238797 MoS2 Trigonal P3̄m1 3 0.28 0
mp-558544 MoS2 Trigonal R3̄m 3 0.28 0
mp-1042086 MoS2 Tetragonal I4̄2d 6 0.65 0.04
Jump to
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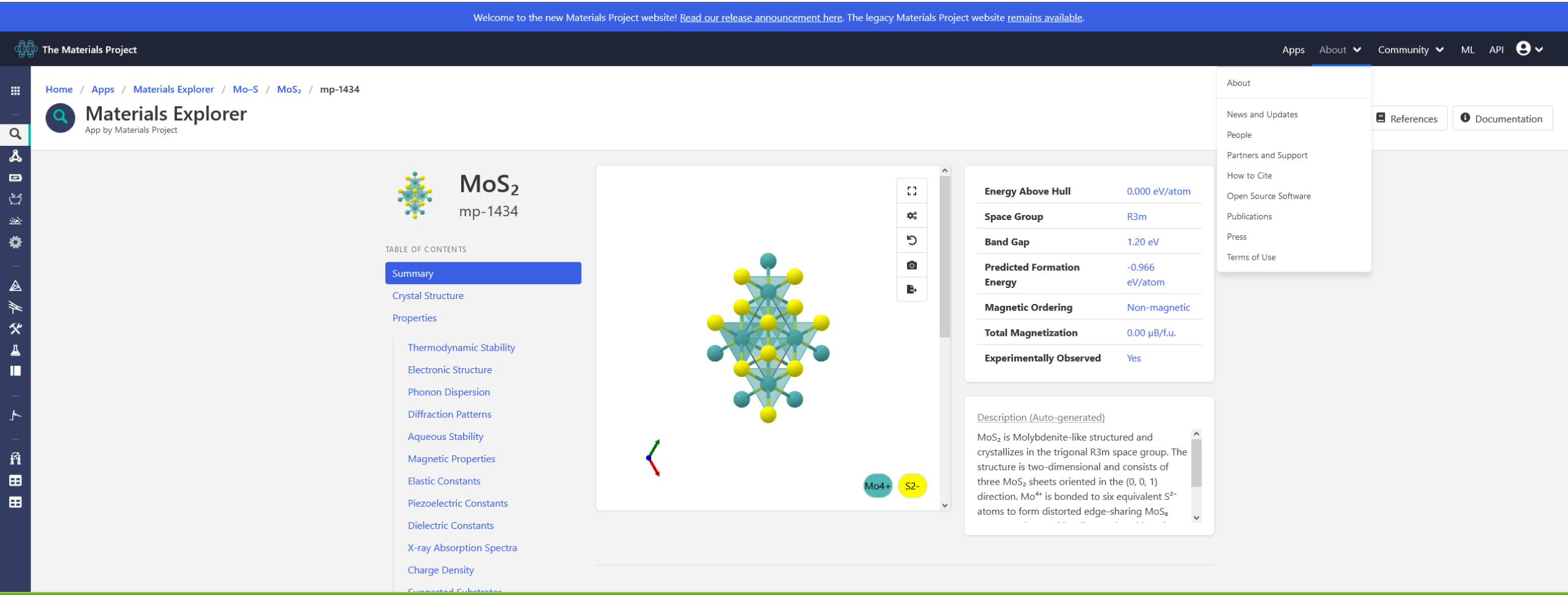
1
Next

New Portal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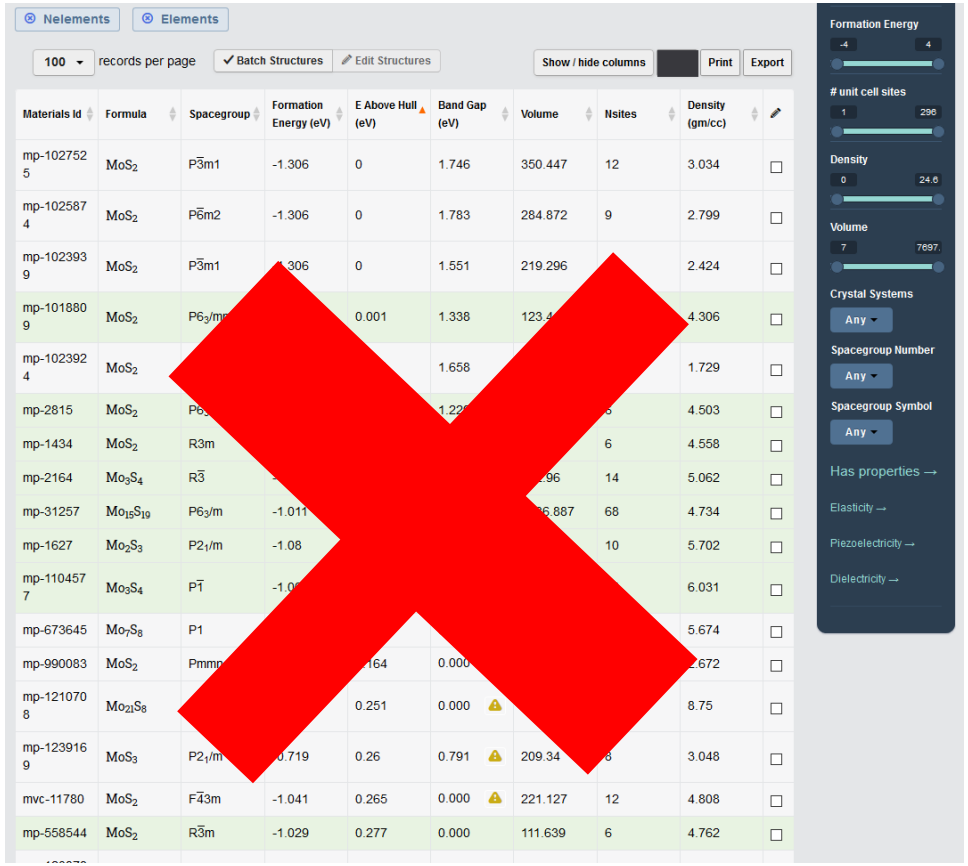
Piezoelectric Constants
Dielectric Constants
X-ray Absorption Spectra
Charge Density
Mo4+
S2-
Energy Above Hull 0.000 eV/atom
Space Group R3m
Band Gap 1.20 eV
Predicted Formation Energy -0.966 eV/atom
Magnetic Ordering Non-magnetic
Total Magnetization 0.00 μB/f.u.
Experimentally Observed Yes
Description (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

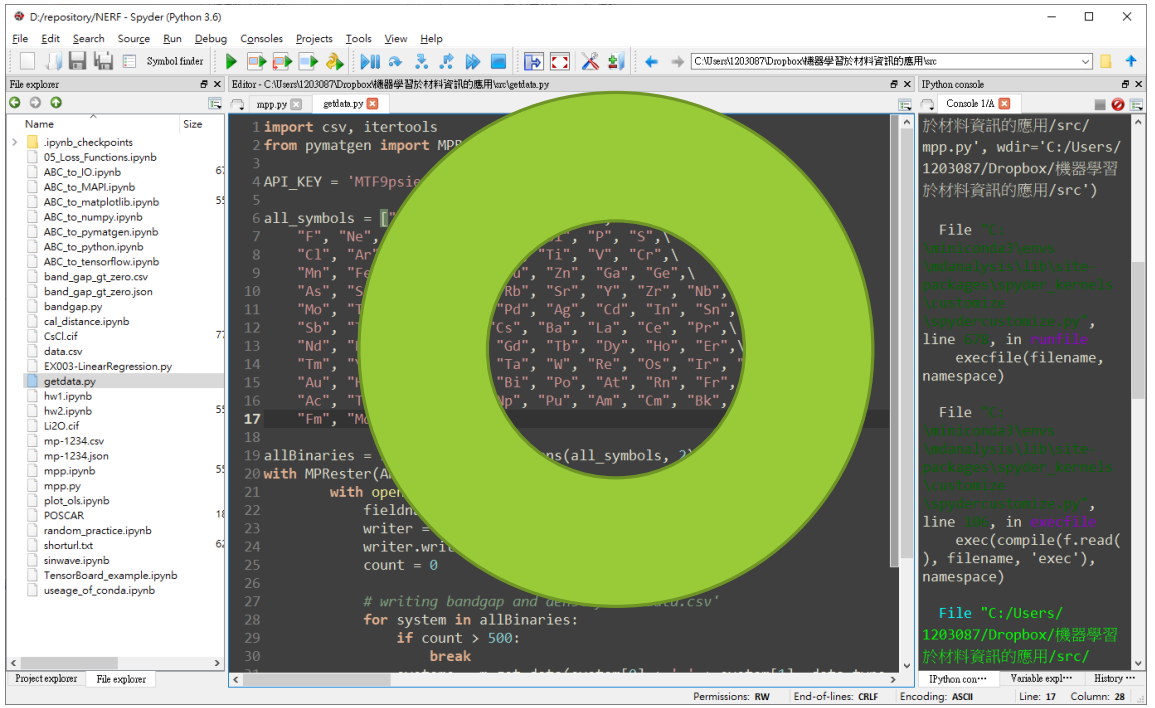
Get Data

手動下載



自動化下載

open Materials Application Programming Interface (API)



Open Source Software

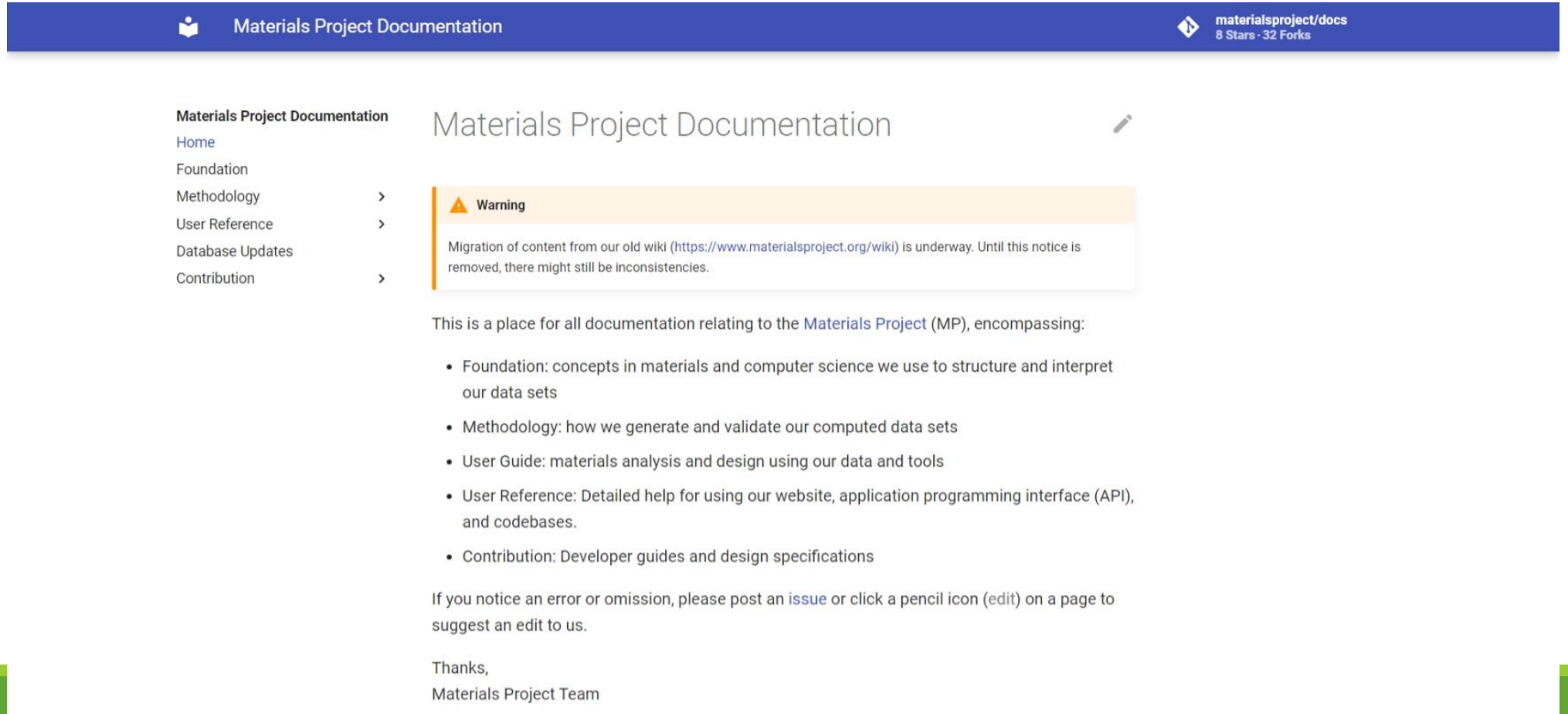
- Pymatgen open source Python library for materials analysis
- Crystal Toolkit web app framework from the Materials Project which is now forming the basis of the Materials Project website
- FireWorks defining, managing, and executing scientific workflows
- Custodian job management framework that perform 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



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

TABLE OF CONTENTS

- The Materials Project API
- API Key
- Accessing Data
- Documentation
- Additional APIs
- Getting Help

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:

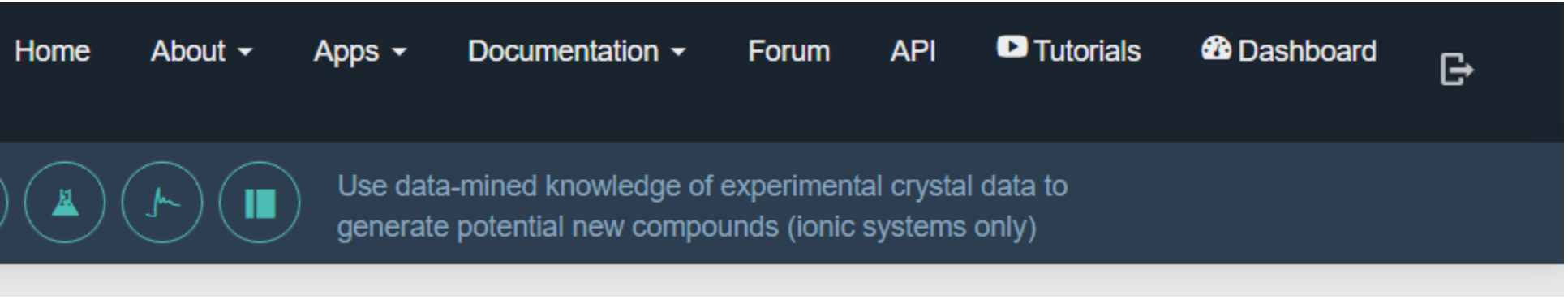
1. You can use our first-party supported Python client. This is the recommend route. During the pre-release of the new website, this has to be installed manually via github.com/materialsproject/api.

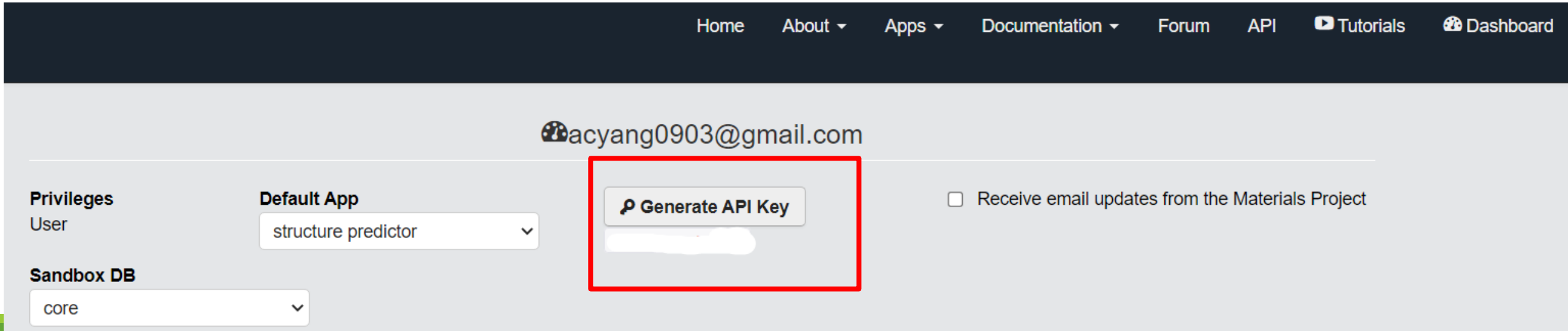
```
from mp_api.client import MPRester
```

   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	`pip install mp-api` (may be available in *pymatgen* at a later date)	`pip install pymatgen`
Python client import code	`from mp_api.client import MPRester`	`from pymatgen.ext.matproj import MPRester`
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 elemments, 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":
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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],
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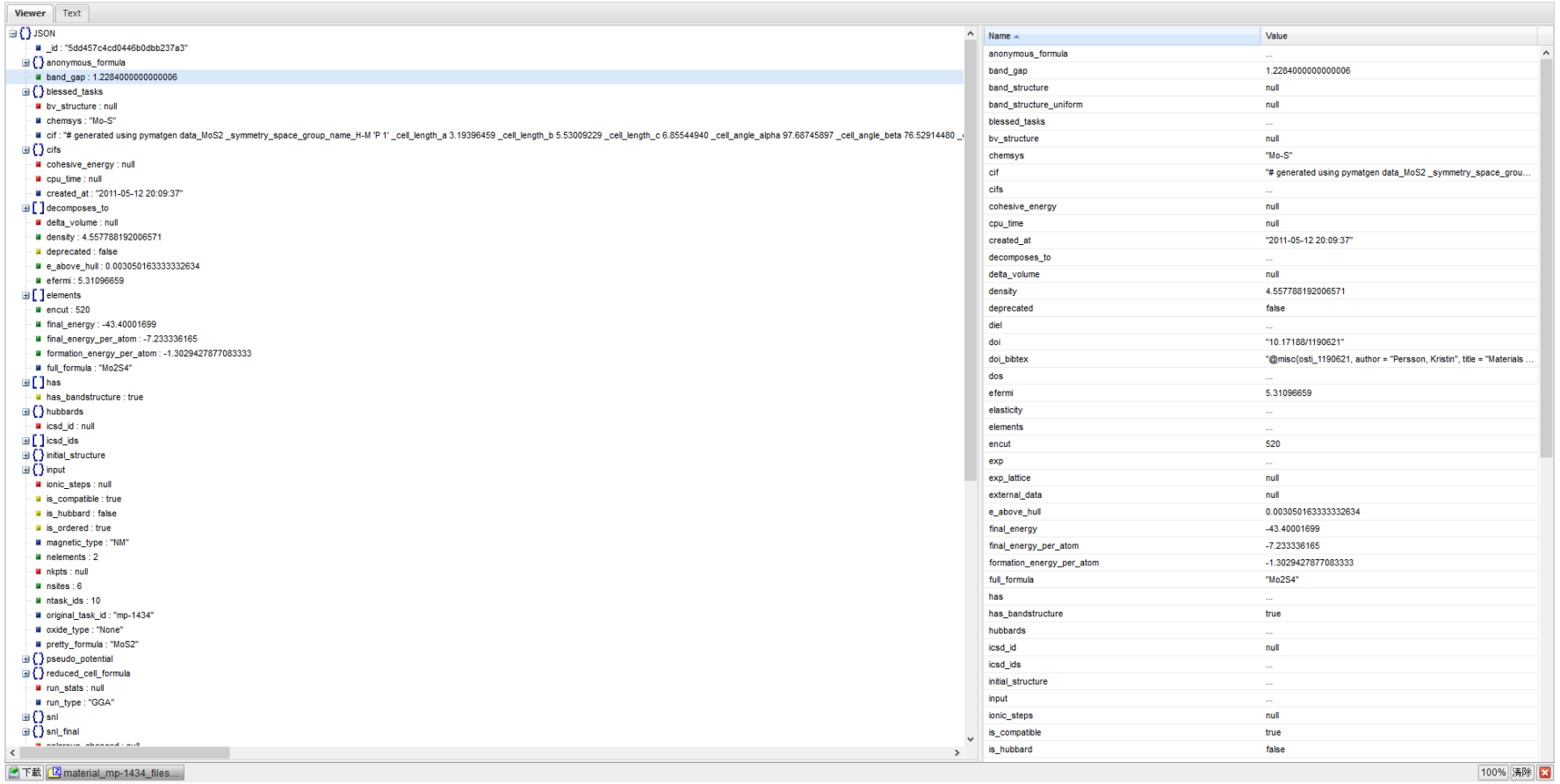
earth element"], "nsites": 6}, "piezo": null, "diel": null, "deprecated": false, "full_formula": "Lu2Al4"}], "valid_response": true, "created_at": "2021-05-31T20:46:37.838142", "version": {"db": "2021_05_13",
"pymatgen": "2022.0.8", "rest": "2.0"}, "copyright": "Materials Project, 2021"}

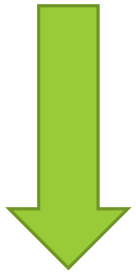
Online jsonviewer
http://jsonviewer.stack.hu/



Integration with pymatgen

The Materials API

pymatgen

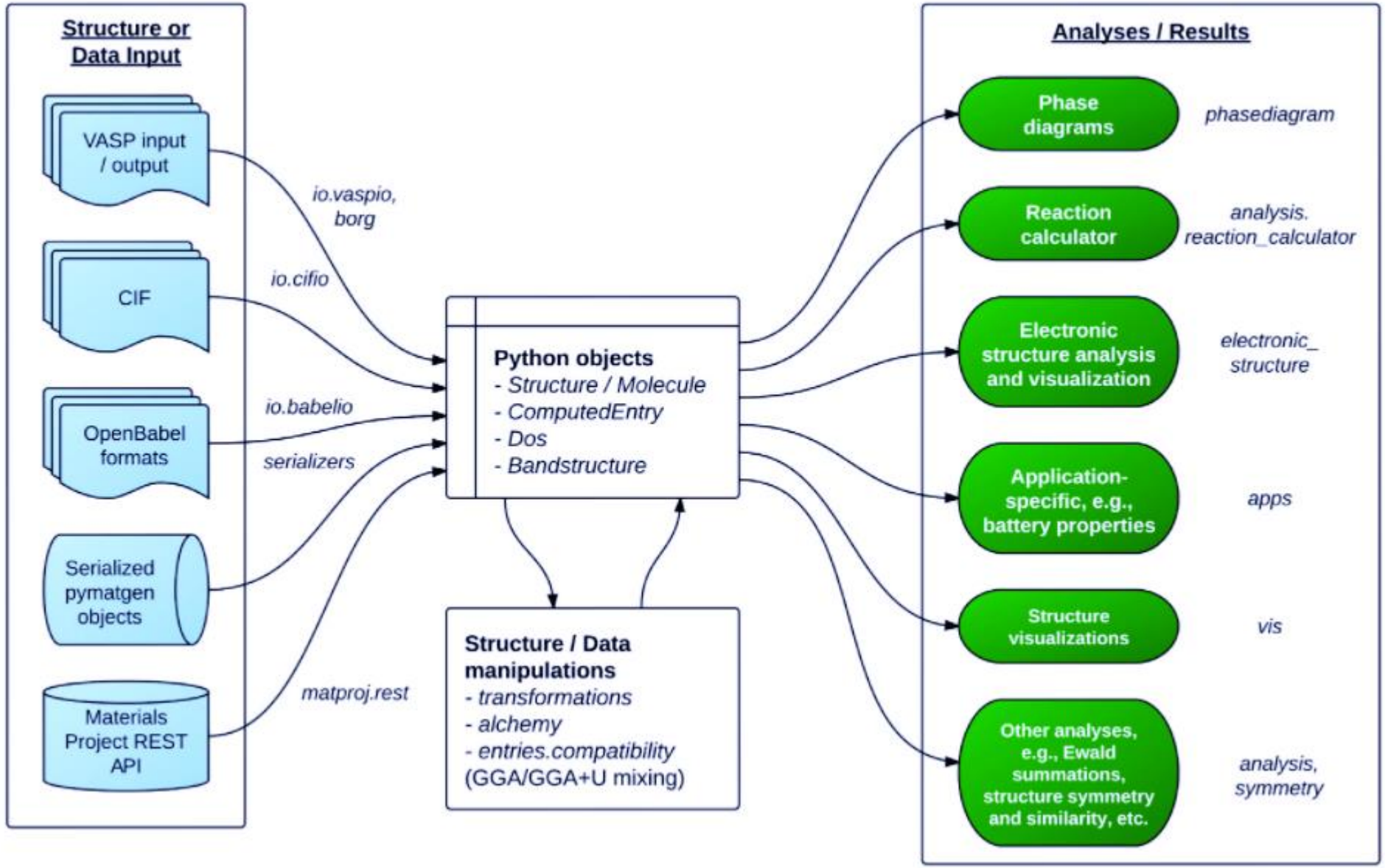


Powerful Materials Analytics Tool

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

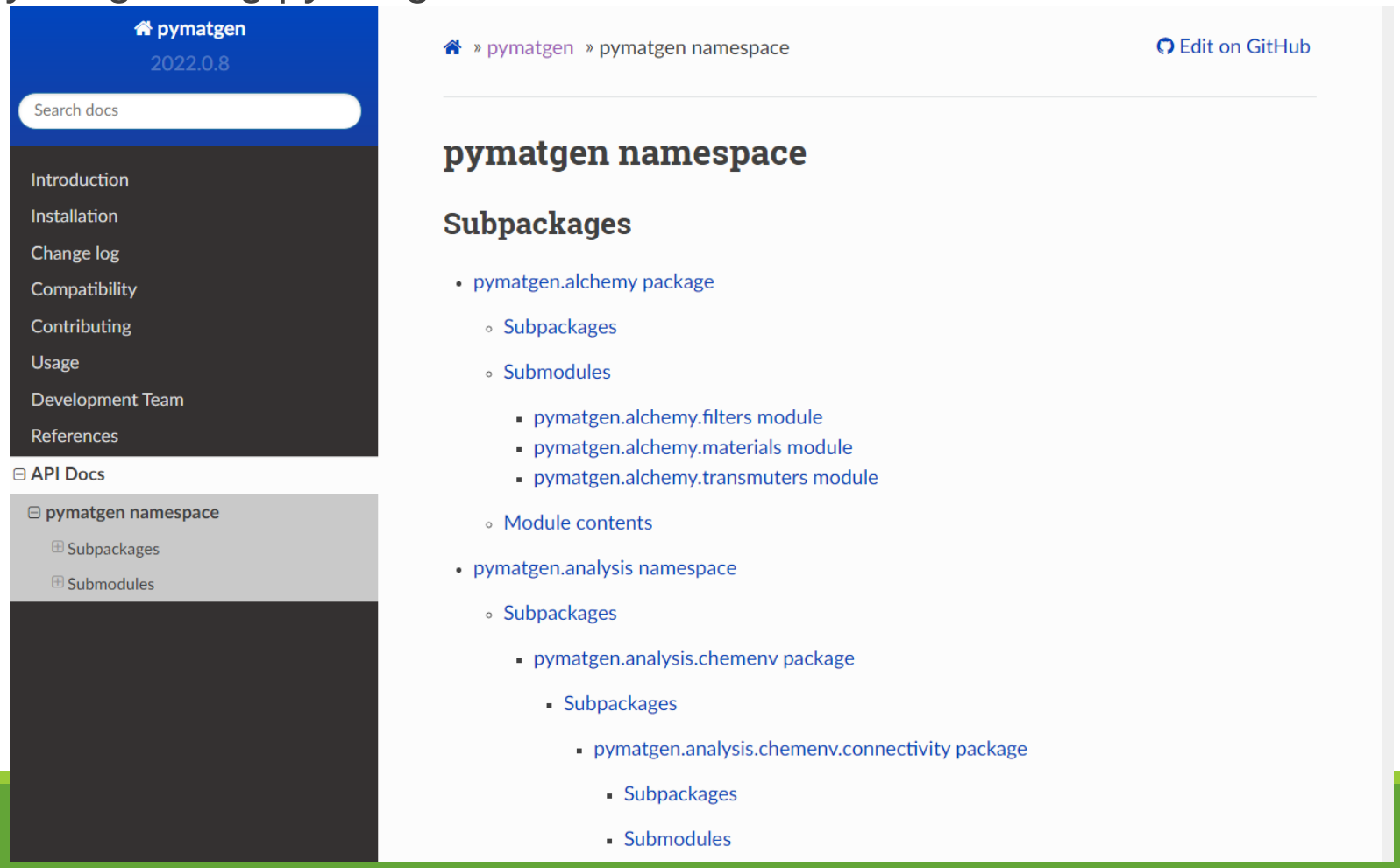


Compatibility of pymatgen v2022.0.0

```
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



pymatgen namespace

- pymatgen.alchemy
- pymatgen.analysis
- pymatgen.apps
- pymatgen.cli
- pymatgen.command_line
- pymatgen.core
- pymatgen.electronic_structure
- pymatgen.entries
- pymatgen.ext

pymatgen namespace

- pymatgen.io
- pymatgen.optimization
- pymatgen.phonon
- pymatgen.symmetry
- pymatgen.transformations
- pymatgen.util
- pymatgen.vis

pymatgen.core

- pymatgen.core.bonds module
- pymatgen.core.composition module
- pymatgen.core.ion module
- pymatgen.core.lattice module
- pymatgen.core.libxcfunc module
- pymatgen.core.molecular_orbitals module
- pymatgen.core.operations module
- pymatgen.core.periodic_table module

pymatgen.core

- pymatgen.core.sites module
- pymatgen.core.spectrum module
- pymatgen.core.structure module
- pymatgen.core.surface module
- pymatgen.core.tensors module
- pymatgen.core.trajectory module
- pymatgen.core.units module
- pymatgen.core.xcfunc module

pymatgen.ext

- pymatgen.ext.cod module
- pymatgen.ext.crystalsai module
- pymatgen.ext.jhu module
- pymatgen.ext.matproj module
- pymatgen.ext.optimade module

pymatgen.electronic_structure

- pymatgen.electronic_structure.bandstructure module
- pymatgen.electronic_structure.boltztrap module
- pymatgen.electronic_structure.boltztrap2 module
- pymatgen.electronic_structure.cohp module
- pymatgen.electronic_structure.core module
- pymatgen.electronic_structure.dos module
- pymatgen.electronic_structure.plotter module

pymatgen.io

- pymatgen.io.abinit
- pymatgen.io.cp2k
- pymatgen.io.exciting
- pymatgen.io.feff
- pymatgen.io.lammps
- pymatgen.io.lobster
- pymatgen.io.qchem
- pymatgen.io.vasp

pymatgen.io

- pymatgen.io.adf module
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- pymatgen.io.ase module
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- pymatgen.io.cube module

pymatgen.io

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pymatgen.io

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- pymatgen.io.xyz module

pymatgen.analysis

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- pymatgen.analysis.eos module
- pymatgen.analysis.ewald module

pymatgen.analysis

- pymatgen.analysis.excitation module
- pymatgen.analysis.find_dimension module
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- pymatgen.analysis.functional_groups module
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- pymatgen.analysis.local_env module
- pymatgen.analysis.molecule_matcher module

pymatgen.analysis

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pymatgen.analysis

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- pymatgen.analysis.transition_state module
- pymatgen.analysis.wulff module
- pymatgen.analysis.xps module