The Materials Project

Combining science and informatics to accelerate materials innovation

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Traditional Materials Development

\(~20\) years

\($$$$\)
Data-driven Materials Development

\(~2X\) years

\($$$$\)
$E \psi(r) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r)$
The Materials Project is an open initiative to make the calculated information of all known inorganic materials publicly available to researchers to accelerate materials innovation.
Python + MongoDB infrastructure

ICSD + Predictions

FireWorks
Workflow Engine

mongoDB

Processed information

pymatgen
Materials Analytics

Apps

The Materials API (RESTful)

Computing resources

Raw data
Defines core **extensible** Python objects for materials data representation.

Provides a **robust and well-documented** set of structure and thermodynamic analysis tools relevant to many applications.

Establishes an **open platform** for researchers to collaboratively develop sophisticated analyses of materials data.
pymatgen is managed via GitHub.

Licensed under the MIT license.

Available on the Python Package Index
FireWorks

Custom “set it and forget it” workflow manager

Transparently manages job allocations across multiple supercomputing resources

Supports complex non-linear workflows.
Inorganic Crystal Database
≈ 50,000 unique materials

> 30,000 materials calculated
> 3000 bandstructures
≈ 400 battery materials
≈ 10 million CPU hours

NERSC
The Materials API

An open platform for accessing materials data based on REpresentational State Transfer (REST) principles.

Flexible and scalable to cater to large number of users, with different access privileges.

Simple to use and code agnostic.
Identifier, typically a formula (Fe2O3), id (1234) or chemical system (Li-Fe-O)

https://www.materialsproject.org/rest/v1/materials/Fe2O3/vasp ENERGY

Preamble

Request type

Data type (vasp, exp, etc.)
GET https://www.materialsproject.org/rest/v1/materials/Fe2O3/vasp/energy

{
    created_at: "2012-09-15T13:12:23.753449",
    valid_response: true,
    version: {
        pymatgen: "2.2.1",
        db: "2012.09.13",
        rest: "1.0"
    },
    response: [
        {
            energy: -132.33005625,
            material_id: 542309
        },
        {
            energy: -66.62512425,
            material_id: 24972
        }
    ],
    copyright: "Copyright 2012, The Materials Project"
}
Launched Oct 11 2011

- >3,000 registered users
- >10,000 phase diagrams generated
- >6,000 structure predictions
“Your product is astounding. I redid work for a recent paper that took weeks in about 15 minutes! ..this is truly “transformative” science in the NSF sense!”

“I am enjoying materialsproject a lot these days - it is wonderful to be able to do research without doing a single calculation!” - Jens Hummelshoj, Stanford

“This is a great database and will be useful for my graduate and my undergraduate students... this will be my one stop location to compare behavior”
- Dunbar Birnie, Rutgers New Brunswick
What’s coming?

More materials (completely new chemistries based on data-mined structure prediction)

More properties (elastic constants, electronic structure, etc.)

More analysis and design apps (Pourbaix diagrams, Materials Design Center, etc.)
Coming soon to Google play

**Materials Explorer**

Material 553090
- Formula: Li₂O
- Unit cell formula: Li₂O₁
- Crystal type: cubic
- Spacegroup: Fm-3m
- Int. Number: 225
- Energy / atom: -4.755 eV
- Form. energy / atom: -2.072 eV
- Energy above hull: 0.000 eV
- Final density: 1.963 g cm⁻³
- Run type: GGA

**Latest News**

Major release of pymatgen (v2.0.0)

A new Li-ion cathode carbonophosphate material synthesized and tested experimentally after identification by high-throughput computing.

Spacegroup determination using Crystal Toolkit

**Battery Explorer**

Battery 540081
- Formula: Li₀.₁FePO₄
- Crystal type: orthorhombic
- Spacegroup: Pnma
- Int. Number: 62
- Average voltage: 3.39 V
- Grav. capacity: 170 mAh g⁻¹
- Vol. capacity: 589 Ah m⁻³
- Specific energy: 576 Wh g⁻¹
- Energy density: 1997 Wh m⁻³
- Voltage profile: Please scroll down

Mooogle beta released!

pymatgen 1.8.0 released

Band Structure and Density of State App Released

**Phase Diagrams**

Choose at least 2 elements
- 8 - O
- 9 - F
- 10 - Ne

**Reaction Calculator**

Calculate Reaction

Li₂O + Al₂O₃ -> 2 LiAlO₂

Calculated:
- Rxn energy (eV): -1.343
- Rxn energy (kJ/mol): -130
- Form. energies:
  - H₂: -17.221
  - Al₂O₃ (kJ/mol): -1662
  - Li₂O (eV): -6.216
The Materials Project is hiring!

Web developers
Materials scientists

Email your CV and a portfolio of your code / web design to support@materialsproject.org.

We also welcome donations of computing time, expertise, software and other resources.