

# The Materials Project Database

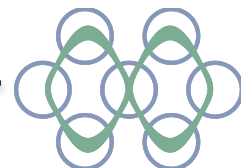
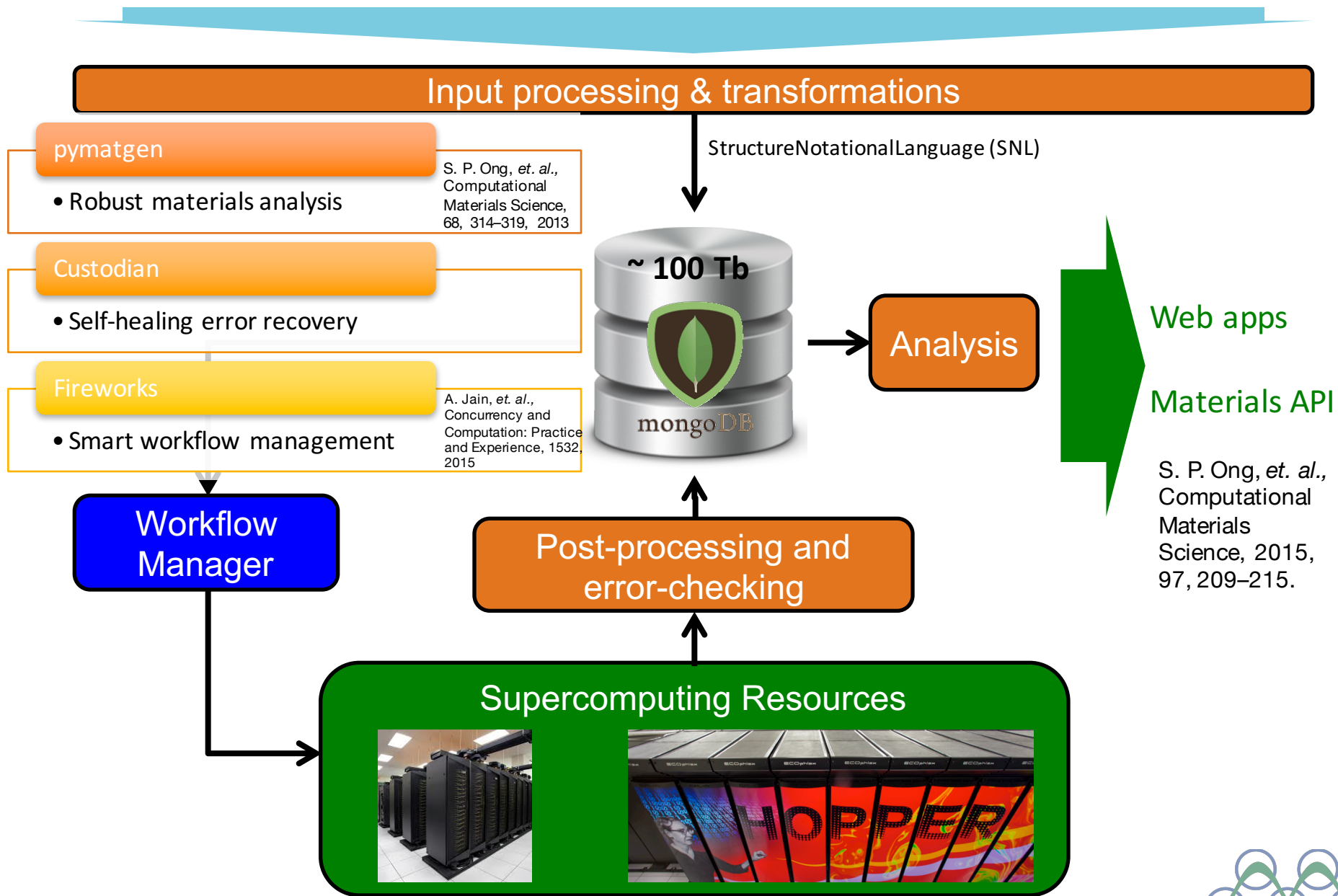
Qimin Yan (LBNL, UC Berkeley)

Kristin Persson (UCB), Gerd Ceder (UCB), Mark Asta (UCB), Daryl Chrzan (UCB), Jeff Neaton (UCB), Dan Gunter (LBNL), Anubhav Jain (LBNL), Maciej Haranszyk (LBNL), Shyue-Ping Ong (UCSD), Anthony Gamst (UCSD), Stefano Curtarolo (Duke), Jeff Snyder (NW)



Funded by the DOE BES program Grant # EDCBEE  
Additional computational resources by NERSC / XSEDE





# Progress To Date and Future Data

## High-Quality Materials DATA

- > **66,000 relaxed compounds**: validated energy, phase diagrams. etc.
- > **70,000 Pourbaix diagrams**<sup>1</sup>
- > **43,000 band structures**
- > **2,300 elastic tensors**<sup>2</sup>
- > **900 piezoelectric tensors**
- **Dielectric tensor workflow complete. Target release 2016**

## DISSEMINATI ON

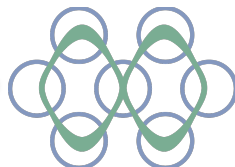
- **Close to 17,000 registered users !**
- **Ten Apps** enabling material searching and design
- **First Materials data API** ; community issues > 1.3M requests/month
- **MPContribs framework**: ALS, NREL EFRC, MAST, for data sharing

## DESIGN

- **MPComplete**; >400 community submissions to date
- Design of **novel functional materials** (photocatalysts, thermoelectrics)

<sup>1</sup> K. A. Persson, *et al.*, " Prediction of solid-aqueous equilibria: Scheme to combine first-principles calculations of solids with experimental aqueous states", *Phys. Rev. B* **85**, 235438 (2012)

<sup>2</sup> M. de Jong, *et al.* "Charting the complete elastic properties of inorganic crystalline compounds" *Scientific Data* **2**, 150009 (2015)



# Daily Validation



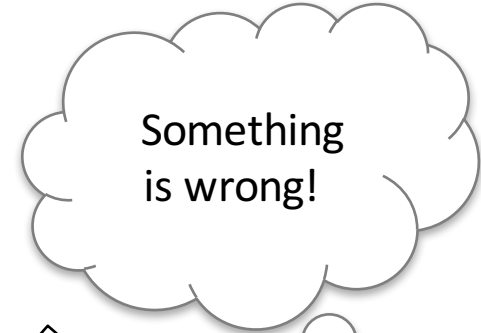
"Raw" MP  
Simulation  
Results



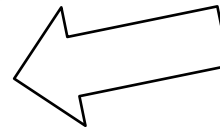
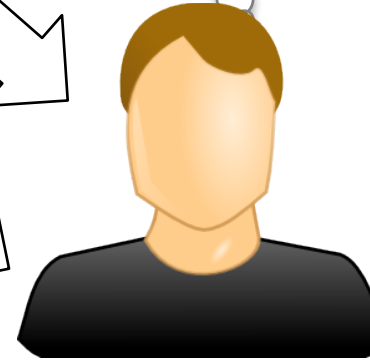
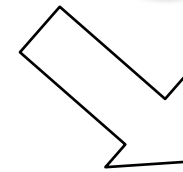
Incremental  
"builders"



REST and Web  
friendly results



Something  
is wrong!



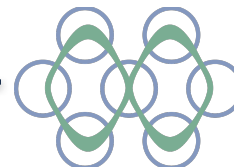
Add a new  
"rule"

Verify and understand  
the problem

Validation



Check and  
report daily



# Provenance for every material

Show JSON History

Show BibTex Citation

Download BibTex Citation

ICSD IDs

57958 608370 608371 608372 608375 608376

Submitted by

Michael Kocher Anubhav Jain Shyue Ping Ong Geoffroy Hautier

## JSON History

```
[
  {
    "url": "http://icsd.fiz-karlsruhe.de/",
    "name": "Inorganic Crystal Structure Database (ICSD)",
    "description": {
      "icsd_id": 108905
    }
  },
  {
    "url": "http://cctbx.sourceforge.net/",
    "name": "Computational Crystallography Toolbox (CCTBX)",
    "description": {
      "spacegroup": {
        "space_group_id": 288,
        "centering": "I"
      }
    }
  }
]
```

## BibTex Citation

```
@article{Jain2013,
author = {Jain, Anubhav and Ong, Shyue Ping and Hautier, Geoffroy and
Chen, Wei and Richards, William Davidson and Dacek, Stephen and
Cholia, Shreyas and Gunter, Dan and Skinner, David and Ceder, Gerbrand
and Persson, Kristin a.},
doi = {10.1063/1.4812323},
issn = {2166532X},
journal = {APL Materials},
number = {1},
pages = {011002},
title = {{The Materials Project: A materials genome approach to accelerating
materials innovation}},
url = {http://link.aip.org/link/AMPADS/v1/i1/p011002/s1\&Agg=doi},
volume = {1},
year = {2013}}
```



# Reports every morning; spanning all db



Kristin Persson <kapersson@lbl.gov>

## [matgen-validate] Validation Report

1 message

dkgunter@lbl.gov <dkgunter@lbl.gov>  
Reply-To: matgen-validate@lists.lbl.gov  
To: matgen-validate@lists.lbl.gov

Sun, Jan 10, 2016 at 1:24 AM

## Materials Project Validation Report

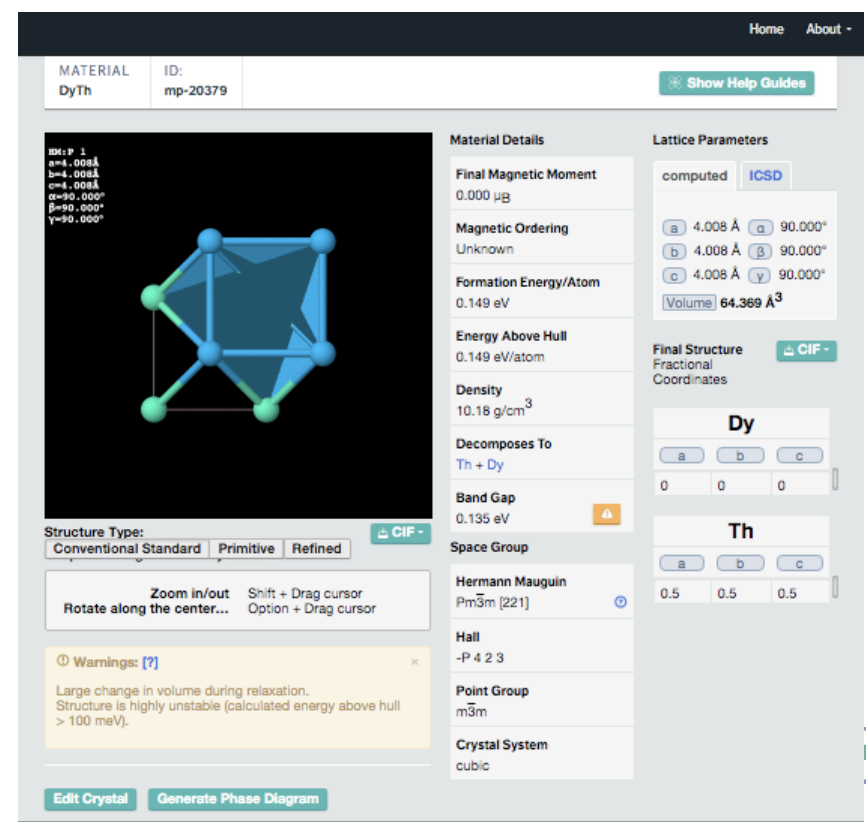
Report time  
2016-01-10 08:00:02  
Report user  
dang  
Report host  
matgen1  
Database  
mg\_core\_dev  
Limit  
0  
Elapsed time  
5085.58s

### Collection "tasks"

### Collection "materials"

### Constraint Violations A

Condition					
{'task_id': 'mp-20379'}					
	<b>Id</b>	<b>TaskId</b>	<b>Field</b>	<b>Constraint</b>	<b>Value</b>
	53be0ae9e051814d8fe721b3	mp-20379	icsd_id	size =	sequence

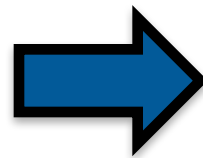
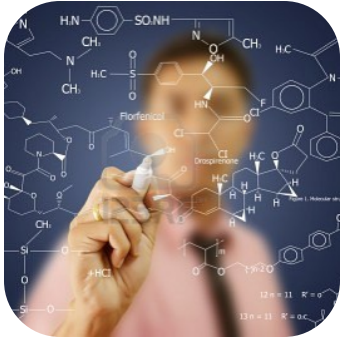


The screenshot shows the Materials Project web interface for material mp-20379. The interface includes a navigation bar with 'Home' and 'About' links, and a 'Show Help Guides' button. The main content area is divided into several sections:

- MATERIAL:** DyTh, ID: mp-20379
- Material Details:**
  - Final Magnetic Moment: 0.000  $\mu_B$
  - Magnetic Ordering: Unknown
  - Formation Energy/Atom: 0.149 eV
  - Energy Above Hull: 0.149 eV/atom
  - Density: 10.18 g/cm<sup>3</sup>
  - Band Gap: 0.135 eV
  - Space Group: Hermann Mauguin Pm $\bar{3}m$  [221]
  - Hall: -P 4 2 3
  - Point Group: m $\bar{3}m$
  - Crystal System: cubic
- Lattice Parameters:**
  - computed ICSD
  - a: 4.008 Å, b: 4.008 Å, c: 4.008 Å
  - $\alpha$ : 90.000°,  $\beta$ : 90.000°,  $\gamma$ : 90.000°
  - Volume: 64.369 Å<sup>3</sup>
- Final Structure:** Fractional Coordinates (Dy, Th + Dy, Th)

A 3D ball-and-stick model of the crystal structure is shown in the center. A warning box at the bottom of the structure view states: "Warnings: [?] Large change in volume during relaxation. Structure is highly unstable (calculated energy above hull > 100 meV)."

# MPContribs: Collaborative platform/template for user data

A screenshot of the MPContribs materials data interface for  $Cr_2O_3$ . The interface shows a 3D ball-and-stick model of the crystal structure, a list of material details, and a table of fractional coordinates for the Cr atoms.

**MATERIAL**  
 $Cr_2O_3$  mp-19399

**Material Details**

Final Magnetic Moment: 12.000  $\mu_B$

Formation Energy/Atom: -2.340 eV

Energy Above Hull: 0.000 eV/atom

Density: 4.89  $g/cm^3$

Decomposes To: Stable

Band Gap: 0.788 eV

Magnetic Ordering: Non-magnetic

Space Group: Hermann Mauguin  $R\bar{3}c$  [167]

Hall:  $-P 3^+ 2n$

Point Group:  $\bar{3}m$

Crystal System: trigonal

**Lattice Parameters**

computed ICSD

a	b	c
5.453 Å	5.453 Å	55.673 Å
5.453 Å	5.453 Å	55.673 Å

Volume: 103.163 Å<sup>3</sup>

**Final Structure**  
Fractional Coordinates CIF

O		
a	b	c
0.0509	0.75	0.4491
0.25	0.5509	0.9491
0.4491	0.0509	0.75
0.5509	0.9491	0.25
0.75	0.4491	0.0509
0.9491	0.25	0.5509

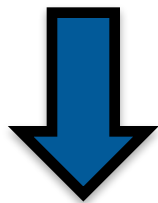
Cr		
a	b	c
0.1503	0.1503	0.1503
0.3497	0.3497	0.3497
0.6503	0.6503	0.6503
0.8497	0.8497	0.8497

Structure Type: Conventional Standard Primitive Refined CIF

Tags: Chromium sesquioxide | Dichromium trioxide | Eskolaite  
Chromium oxide - mesoporous | Eskolaite, mesoporous  
Chromium oxide

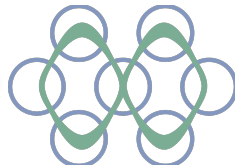
Edit Crystal Generate Phase Diagram

“I have this great dataset, but need help sharing it with the world”

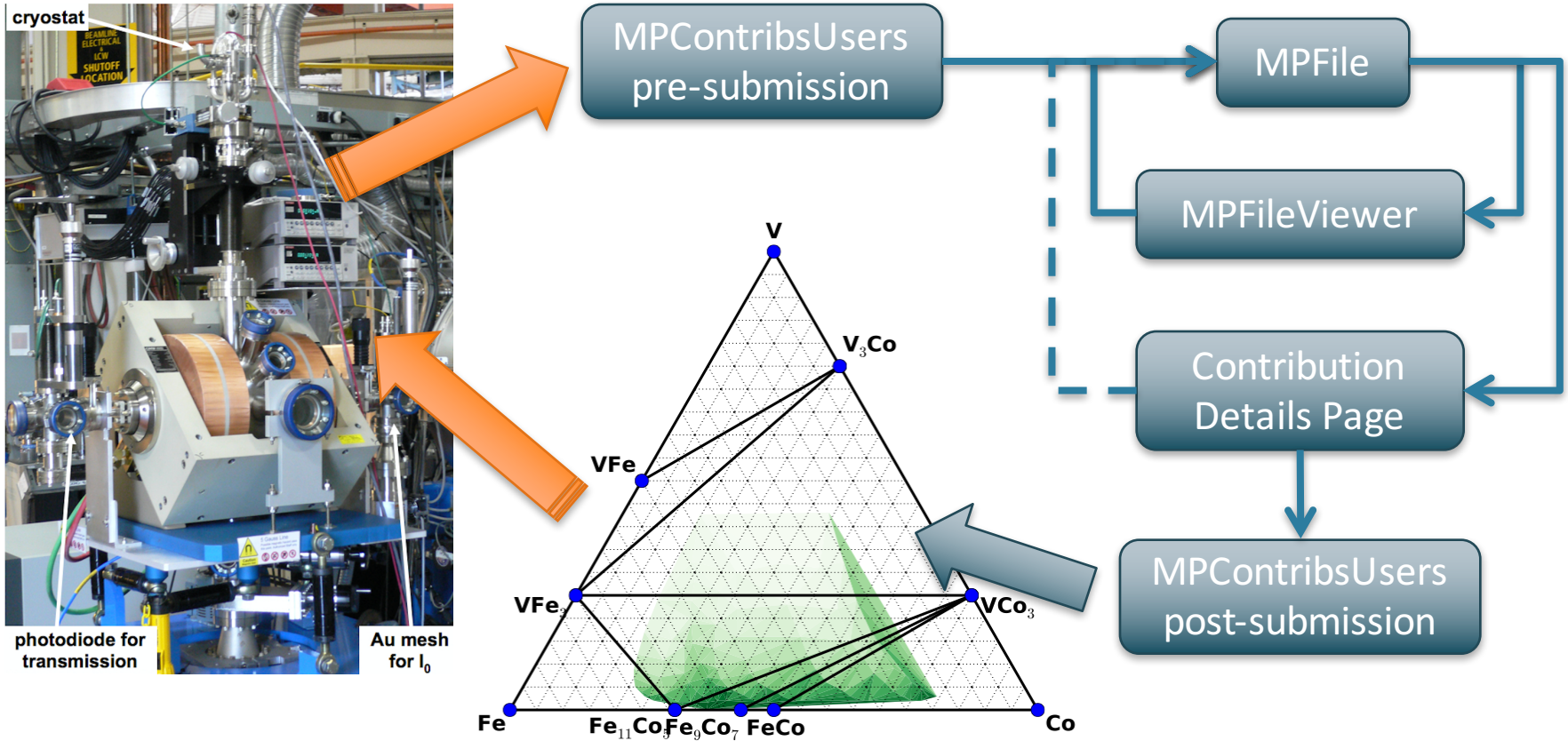


Your Own App

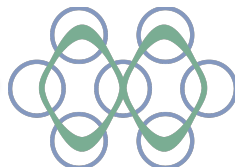
Your Materials Data



# MPCONTRIBS Process



- pre-processing of user output data and conversion into MPFile
- visual and iterative checking of MPFile by user (“get data in shape”)
- MPFile submission via command line or web portal (through REST)
- contributed data can be easily displayed on MP





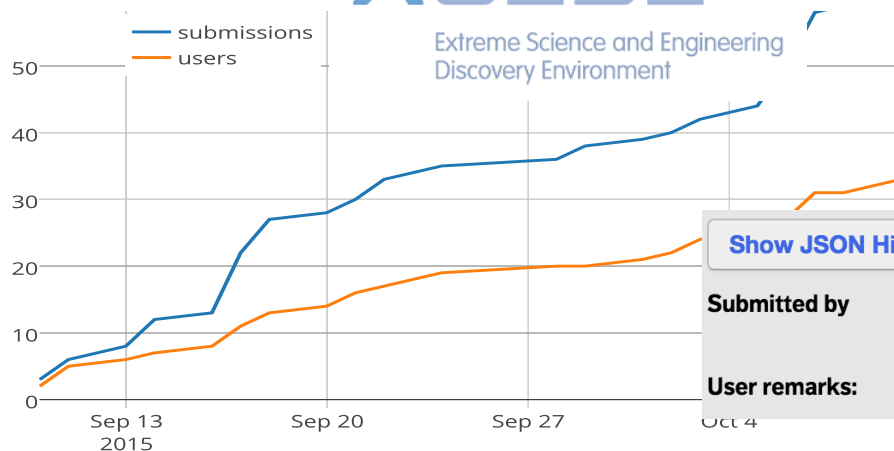
# MPComplete: Crowd-sourcing MP

*Launched Sept 2015*

- **Motivation:** new compounds supplied directly by community
- Users suggest structures; MP checks for uniqueness and runs full suite of calculations.
- Ensures user-relevant materials with *consistent provenance*

Powered by **XSEDE**

Extreme Science and Engineering  
Discovery Environment



Convert between CIF, MP-JSON, and VASP input files. Generate new crystals by substituting or removing species.

$K_2Nb_2O_7$

Supercell Dimensions  
Insert as scaling matrix

1	0	0
0	1	0
0	0	1

generate

Substitute Remove

K

Nb

O

Remove by fraction

Space Filling  Polyhedra

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

Download Submit Structure

**beta** **MP-Complete:**  
Crowd-sourcing MP Compounds

We are proud to announce the public beta release of MP-Complete, a new initiative for users to recommend new crystals for calculation.

Show JSON History

Show BibTex Citation

Submitted by

Bin Xu

User remarks:

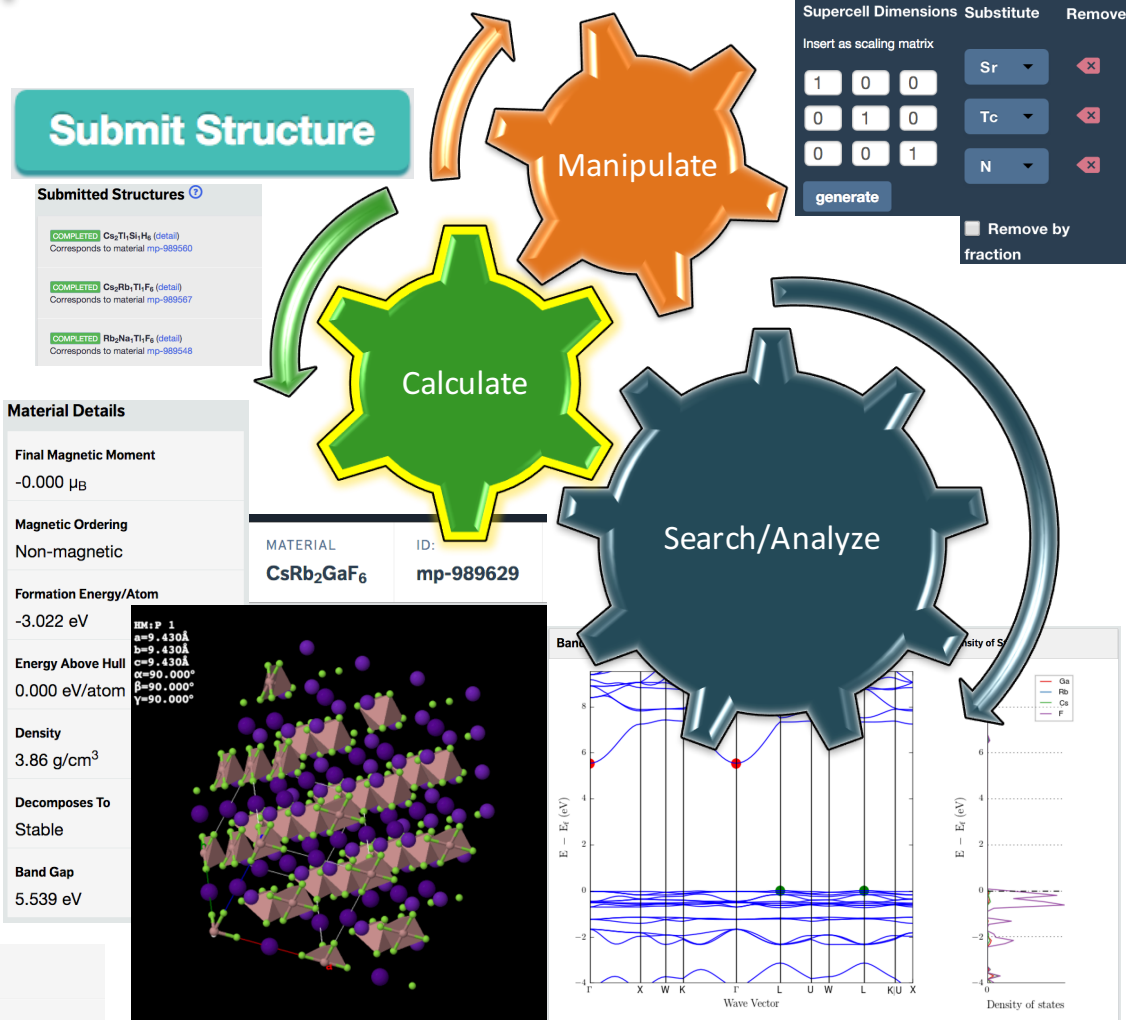
MP user submission

Materials Project performed nearly 100,000 calculations. Included many new compounds and significantly expanded available. We have also received many valuable like yourselves on new structures to include in our at such user feedback is critical to ensuring that the s up-to-date and relevant, and MP-Complete is our process.



# MPComplete Use Cases

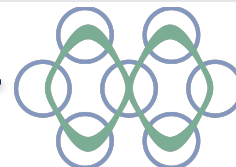
- One-at-a-time, or in bulk:
  - One user contributed **four new lead halide PV compounds**, one at a time. (design)
  - One user submitted 64 ABN<sub>3</sub> perovskites, **associating with publication**. (data sharing)
  - Another user submitted 131 structures to **check for stability** against all MP compounds (validation and data sharing)
- User dashboard links to workflow details → can monitor progress



112 completed Workflows for submission\_group\_id=88359

RUNNING ARCHIVED WAITING FIZZLED READY RESERVED COMPLETED DEFUSED

ID	Name	Created On
1443523	Cl6 Na1 Rb2 Ti1	2015-12-10 02:00:53.609000
1443520	Cs2 F6 In1 Ti1	2015-12-10 02:00:53.449000
1444366	Cs2 F6 Rb1 Ti1	2015-12-10 02:00:52.500000

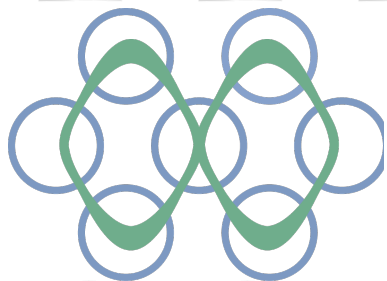


- *First I would like to thank you a lot for this project, it is incredibly useful. I work in the field of materials design of multiphase and anisotropic materials. (US Student)*
  - *I have registered with the Materials Project and expect to try the software. Do, or can, users contribute to the library(s)? (US Professor)*

- *In this framework, I would like to ask if it would be possible to organize a short training course on materials modelling using the Materials Project capabilities. (Professor in Greece)*
  - *Thank you very much and thank you for offering this fantastic data base! (US Student)*

- *I'm currently writing a website to host a database of EELS spectra (the redevelopment of EELS database if you're familiar with it). The site is similar to the Materials Project Explorer in a number of ways - browsing by formula and so on - it would be great if we could link out to you guys from spectra pages if possible. (UK scientist)*

- *I noticed the change already. Very fast response, you guys are awesome! (US student)*



# Thanks to the community and for your attention !

- *I am a brazilian research in materials science. Firt of all I would like to congratulation for the app's they are very usefull. (Brazilian student)*
- *I am enjoying materialsproject.org a lot these days - it is wonderful to be able to do research without doing a single calculation. (US researcher)*