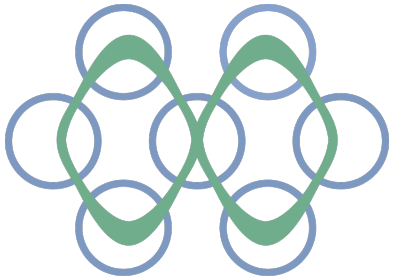


The Materials Project Database

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)

NERSC

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

XSEDE Extreme Science and Engineering Discovery Environment

ICSD Other experimental databases User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)

pymatgen
- Robust materials analysis

S. P. Ong, *et. al.*, Computational Materials Science, 68, 314–319, 2013

Custodian
- Self-healing error recovery

Fireworks
- Smart workflow management

A. Jain, *et. al.*, Concurrency and Computation: Practice and Experience, 1532, 2015

~ 100 Tb

mongoDB

Analysis

Web apps

Materials API

S. P. Ong, *et. al.*, Computational Materials Science, 2015, 97, 209–215.

Workflow Manager

Post-processing and error-checking

Supercomputing Resources

A. Jain*, S.P. Ong*, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K.A. Persson, *"The Materials Project: A materials genome approach to accelerating materials innovation"* APL Materials 1, 011002 (2013)

Progress To Date and Future Data

High-Quality Materials DATA

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

DISSEMINATION

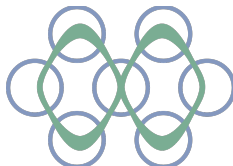
- **Close to 17,000 registered users !**
- **Ten Apps** enabling material searching and design
- **First Materials data API** ; community issues > 1.3M requests/month
- **MPContribs framework:** ALS, NREL EFRC, MAST, for data sharing

DESIGN

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

[1] 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)

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



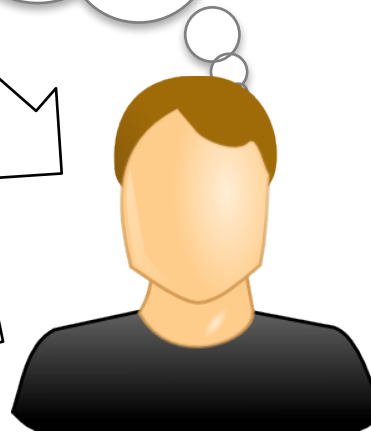
https://materialsproject.org/ https://github.com/materialsproject

Daily Validation

"Raw" MP Simulation Results

Incremental "builders"

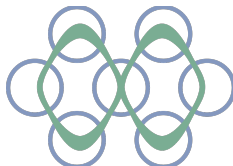
REST and Web friendly results



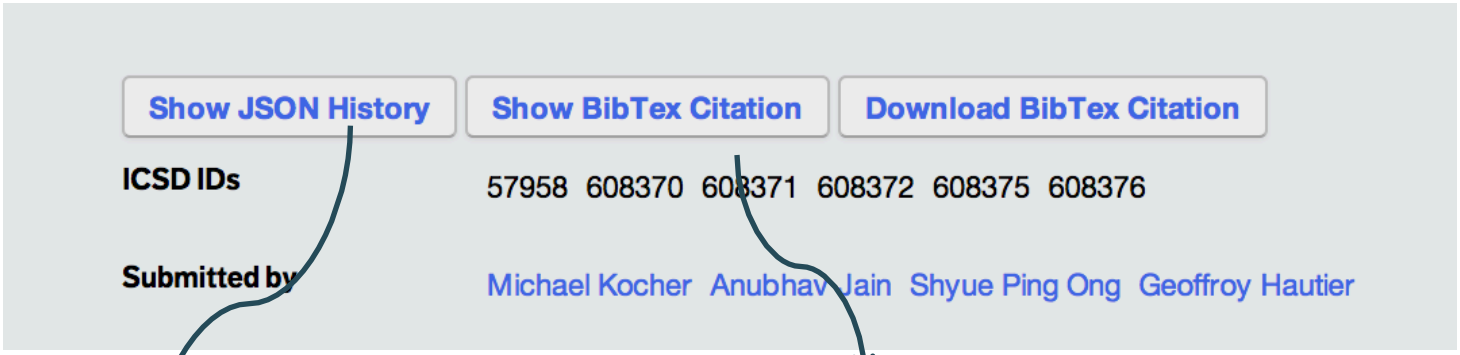
Check and report daily

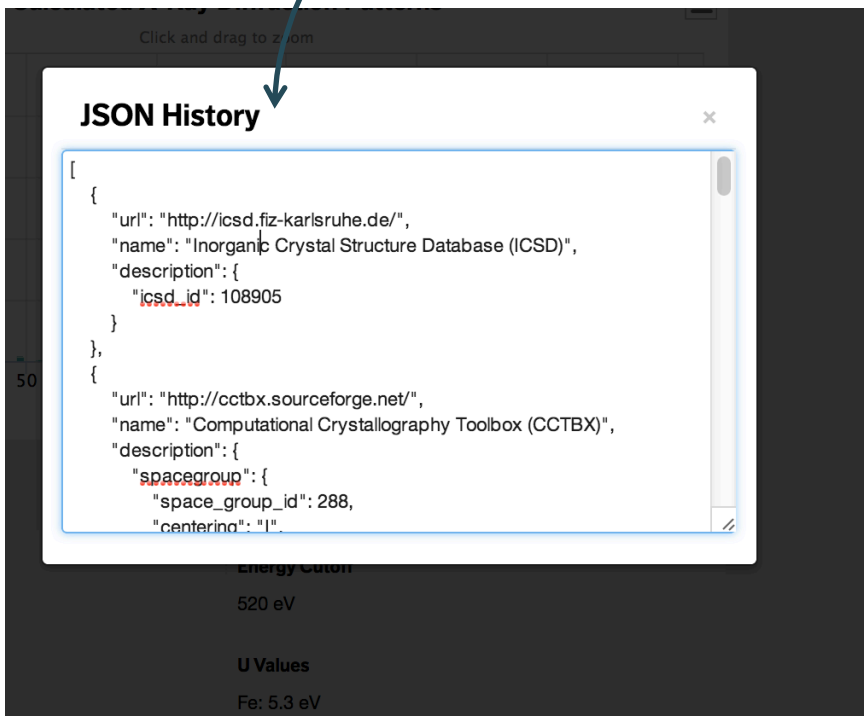
Add a new "rule"

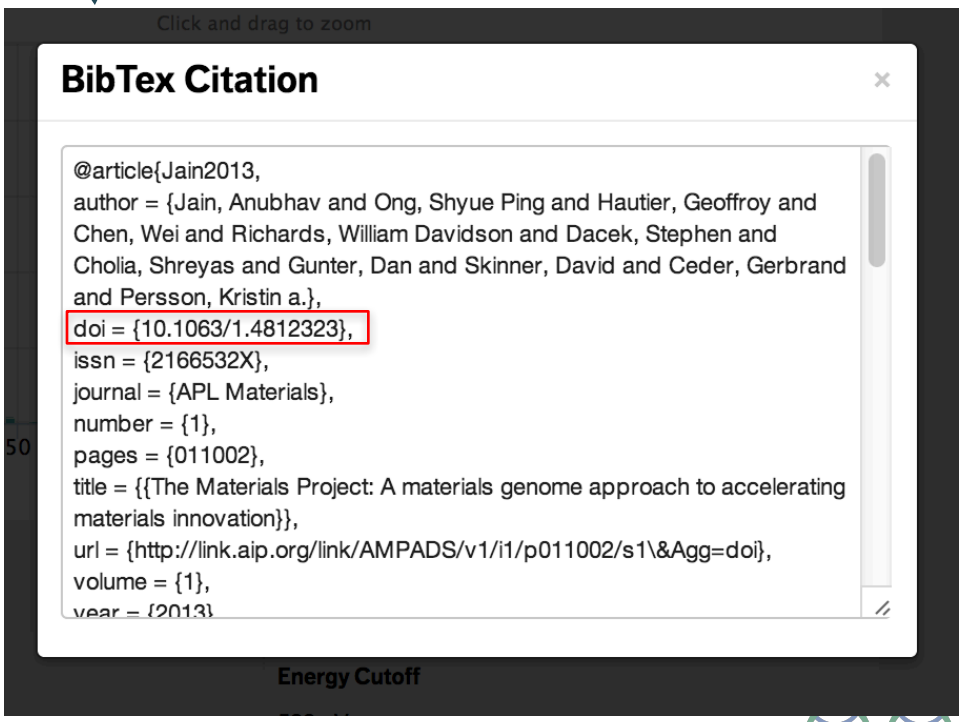
Verify and understand the problem



Provenance for every material







Reports every morning; spanning all db

BERKELEY LAB

Kristin Persson <kapersson@lbl.gov>

[matgen-validate] Validation Report
1 message

dkgunter@lbl.gov <dkgunter@lbl.gov> Sun, Jan 10, 2016 at 1:24 AM
Reply-To: matgen-validate@lists.lbl.gov
To: matgen-validate@lists.lbl.gov

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

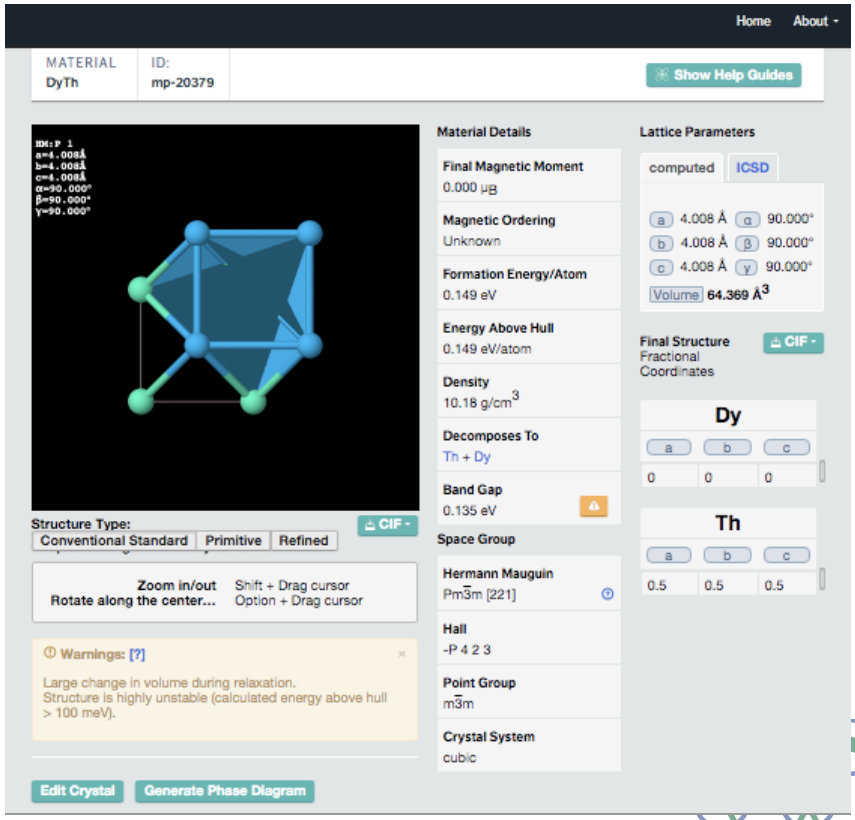
Collection "tasks"

Collection "materials"

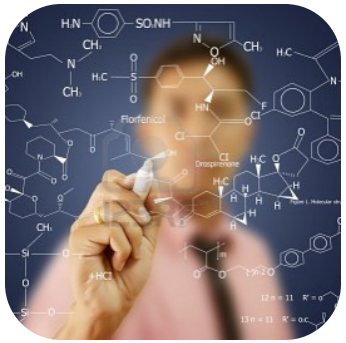
Constraint Violations A

Condition
{'task_id': 'mp-20379'}

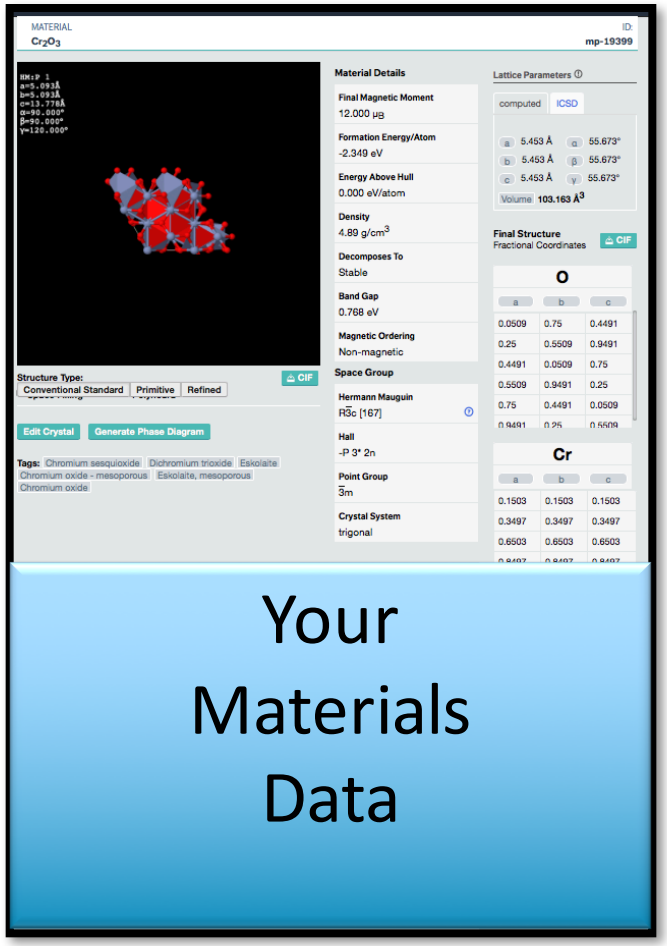
Id	TaskId	Field	Constraint	Value
53be0ae9e051814d8fe721b3	mp-20379	icsd_id	size = sequence	



MPContribs: Collaborative platform/template for user data



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

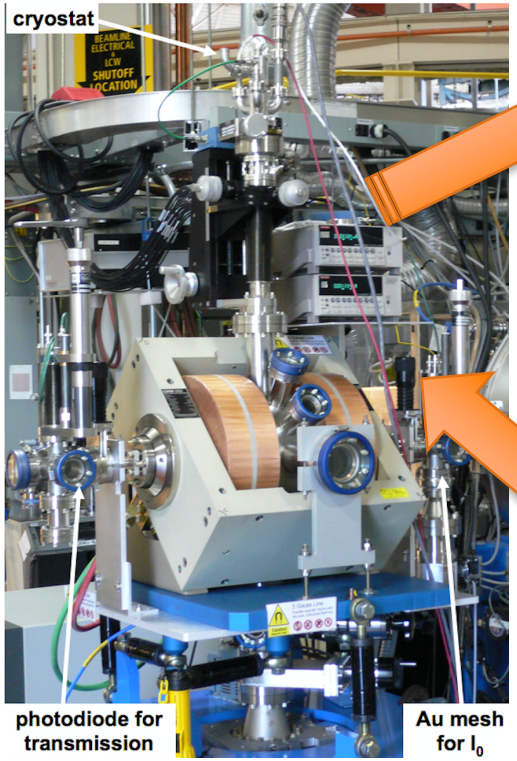


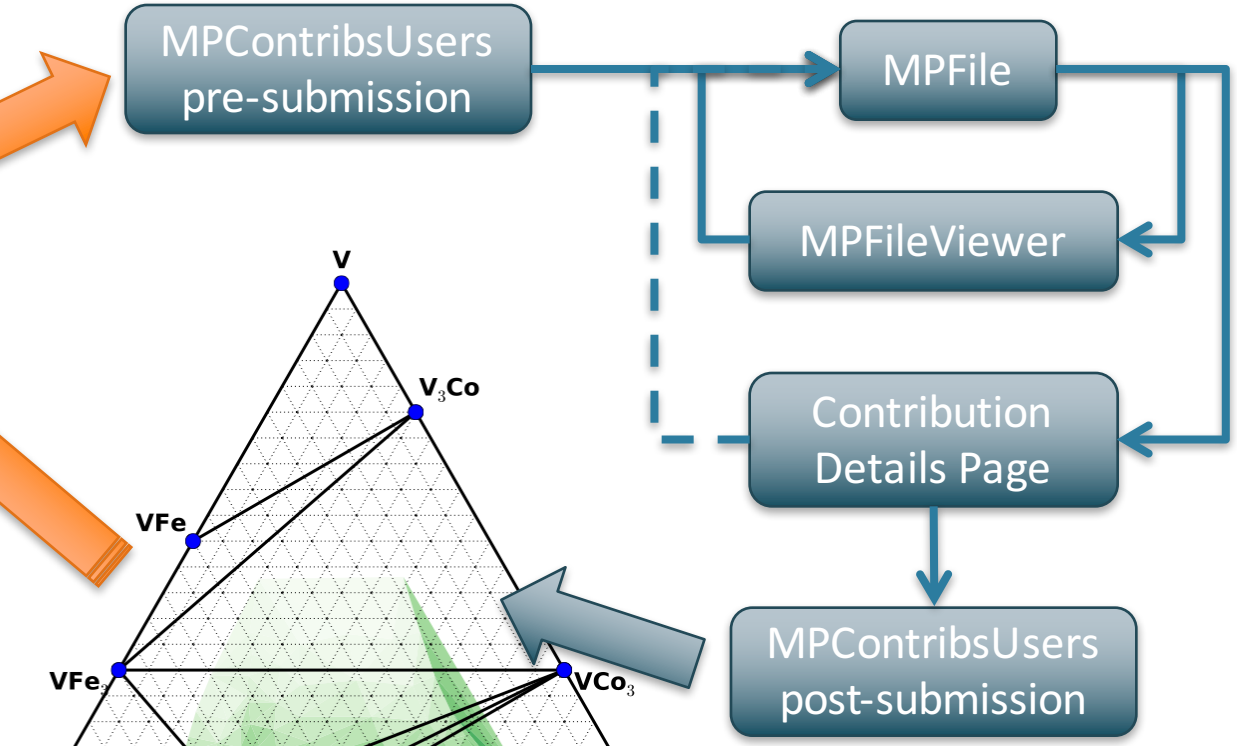
Your Materials Data

Your Own App

Huck, P.; Cholia, S.; Gunter, D.; Winston, D.; N'Diaye, A. T.; Persson K.; "User Applications Driven by the Community Contribution Framework MPContribs in the Materials Project" Proceedings of 10th Gateway Computing Environments Workshop (2015), Concurrency in Computation: Practice and Experience, arXiv:1510.05727

MPContribs Process



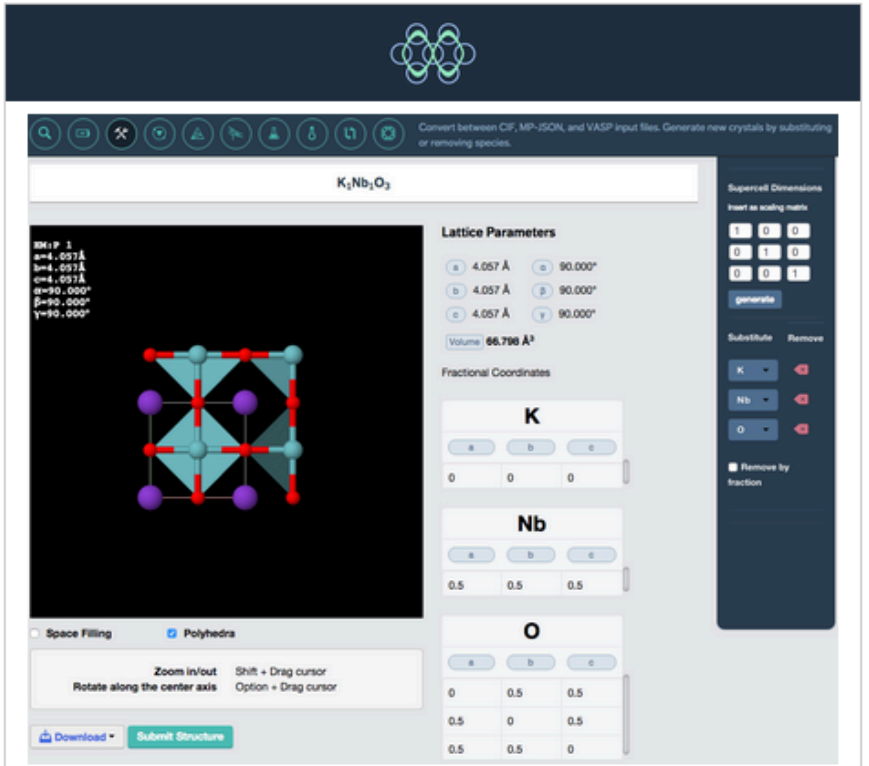


- pre-processing of user output data and conversion into MPFile
- visual and iterative checking of MPFile by user ("get data in shape")
- MPFile submission via command line or web portal (through REST)
- contributed data can be easily displayed on MP

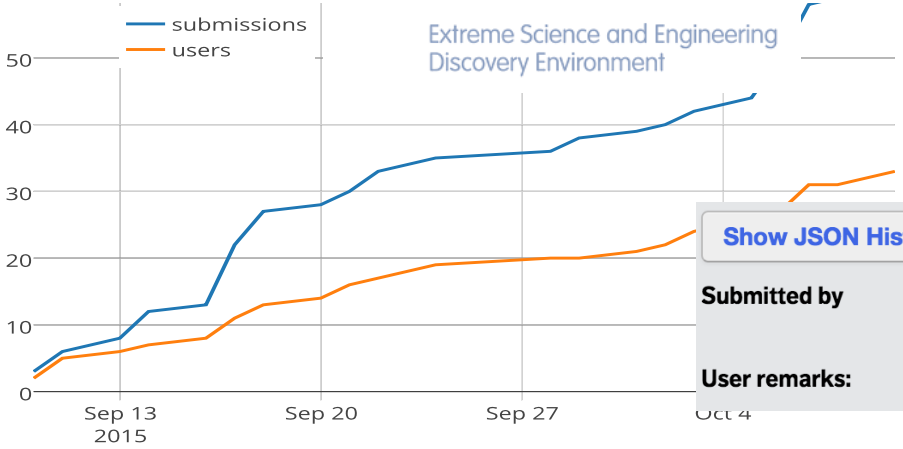
MPComplete: Crowd-sourcing MP

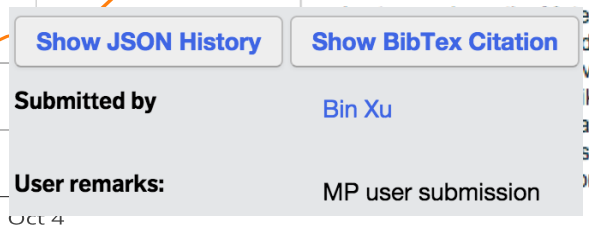
Launched Sept 2015

- **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*



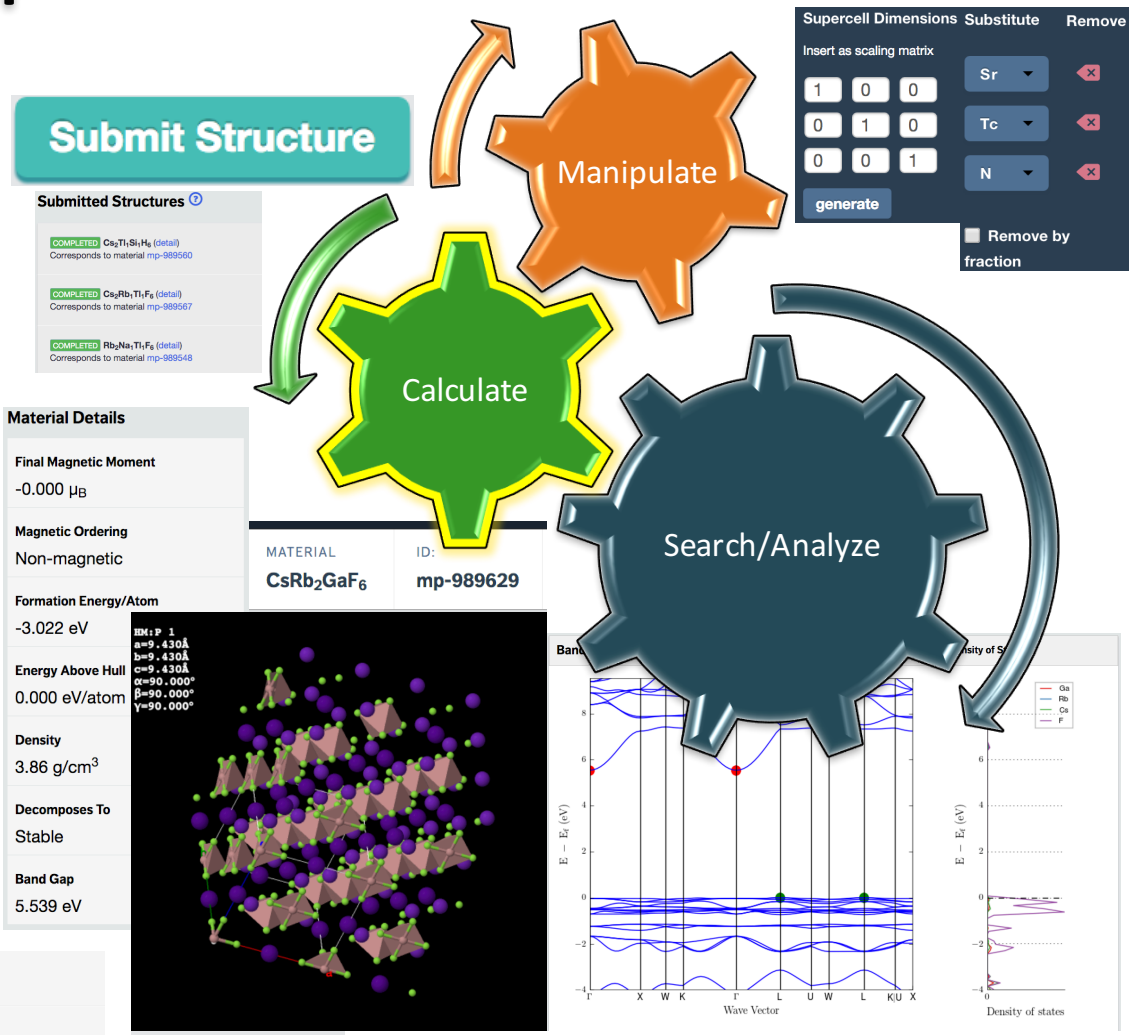
Powered by XSEDE
Extreme Science and Engineering Discovery Environment





MPComplete Use Cases

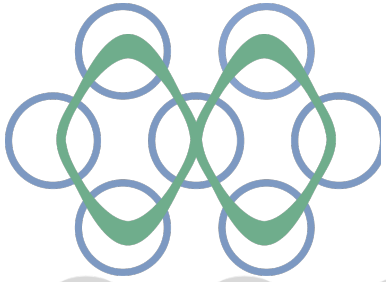
- One-at-a-time, or in bulk:
  - One user contributed **four new lead halide PV compounds**, one at a time. (design)
  - One user submitted 64 ABN_3 perovskites, **associating with publication**. (data sharing)
  - Another user submitted 131 structures to **check for stability** against all MP compounds (validation and data sharing)
- User dashboard links to workflow details ➔ can monitor progress



Submitted by

Felix Faber Alexander Lindmaa O. Anatole von Lilienfeld Rickard Armiento

- *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)