The Materials Project
Database

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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
- > 43,000 band structures
- > 2,300 elastic tensors
- > 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)

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

[https://materialsproject.org/](https://materialsproject.org/)  [https://github.com/materialsproject](https://github.com/materialsproject)
Daily Validation

"Raw" MP Simulation Results

Incremental "builders"

REST and Web friendly results

Check and report daily

Validation

Add a new "rule"

Verify and understand the problem

Something is wrong!

Verify and understand the problem
Provenance for every material

ICSD IDs
57958  608370  608371  608372  608375  608376

Submitted by
Michael Kocher  Anubhav Jain  Shyue Ping Ong  Geoffroy Hautier

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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

[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'}

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<td>mp-20379</td>
<td>icsd_id</td>
<td>size = sequence</td>
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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

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
**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
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. First 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)