

The 2017 Materials Project Workshop

*Kristin Persson
UC Berkeley*

*With immense thanks to the team, without
which nothing would have happened and we
wouldn't be here today*

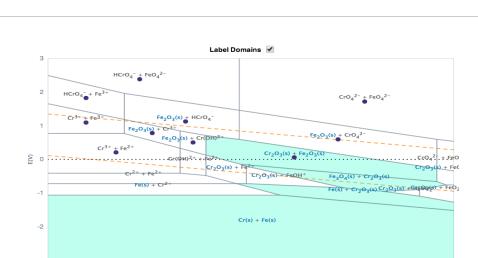
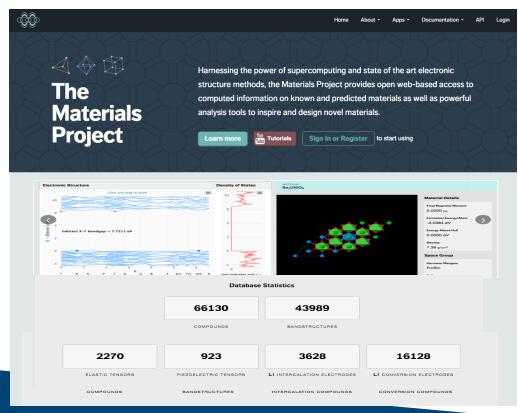


First-Principles Modeling: 1996 - 2017

1996: One year on tungsten

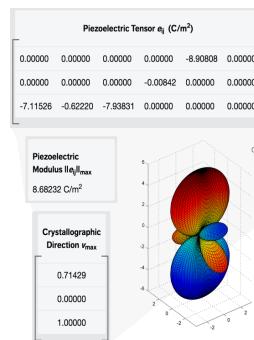
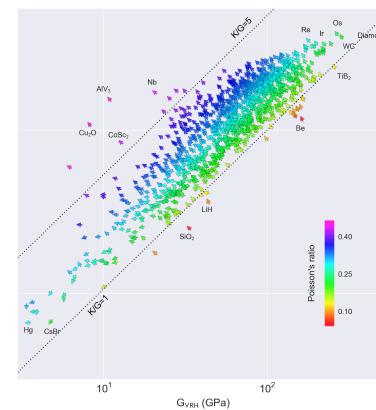


2017: 69,000+ materials on the Materials Project + millions of materials properties

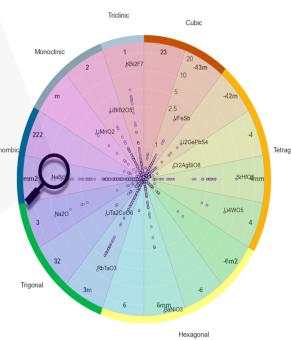


Pourbaix Diagrams on the Materials Project

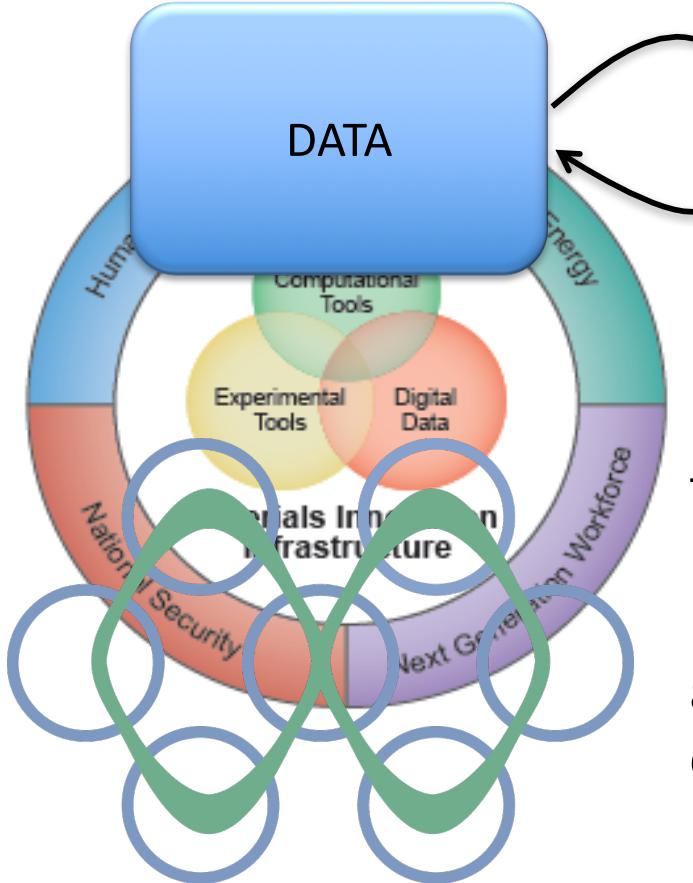
Today, we are excited to announce the release of the Pourbaix diagram app. Pourbaix diagrams are solid-aqueous phase diagrams as a function of pH, standard hydrogen potential and composition that can be used to predict the stability of different species in aqueous environments.



Piezoelectricity Data on the Materials Project



The MGI and the Materials Project



June 2011 “fund **computational tools, software, new methods ... to make the process of discovery and development of advanced materials faster, less expensive, and more predictable**
Bring unprecedented high quality materials data from first-principles,

Integrate it with state-of-the-art information technology and codes to enable rapid **dissemination**, searching, datamining and enhanced learning

Demonstrate capabilities on **design** of novel functional electronic materials

Materials Project web site

The screenshot shows the Materials Project website's homepage. At the top, there are three small icons representing different crystal structures: a triangular network, a diamond-like shape, and a cube. Below them, the title "The Materials Project" is displayed in large, light blue, sans-serif font. To the right of the title is a descriptive text block: "Harnessing the power of supercomputing and state-of-the-art electronic structure 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." Below this text are two buttons: "Learn more" and "Sign In or Register". A call-to-action text "to start using" follows the buttons. The main content area features two large data visualizations: an "Electronic Structure" plot showing energy bands across a high-symmetry path (Γ-X-S-Y-Γ-Z-U-T-Z'Y-T'U-X'S-R) with an indirect bandgap of 7.7511 eV, and a "Density of States" plot showing states per eV. To the right is a detailed material card for Ba₂UNiO₆, displaying its crystal structure (cubic), material details (Final Magnetic Moment: 2.0000 μ_B , Formation Energy/Atom: -3.0384 eV, etc.), and space group (Hermann Mauguin: Fm $\bar{3}m$, Hall: Hall). Below these are five sections with links: "EXPLORE MATERIALS", "EXPLORE BATTERIES", "VISUALIZE STABILITY", "INVENT STRUCTURES", and "CALCULATE".

Electronic Structure
Click and drag to zoom
Indirect X- Γ bandgap = 7.7511 eV

Density of States

MATERIAL
Ba₂UNiO₆

Material Details

- Final Magnetic Moment
2.0000 μ_B
- Formation Energy/Atom
-3.0384 eV
- Energy Above Hull
0.0000 eV
- Density
7.38 g/cm³
- Space Group
Hermann Mauguin
Fm $\bar{3}m$
Hall

EXPLORE MATERIALS
Search for materials information by chemistry, composition, or property

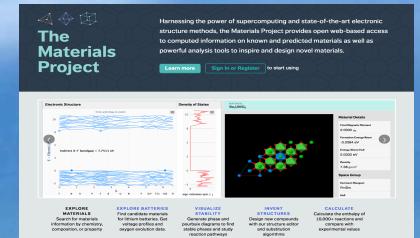
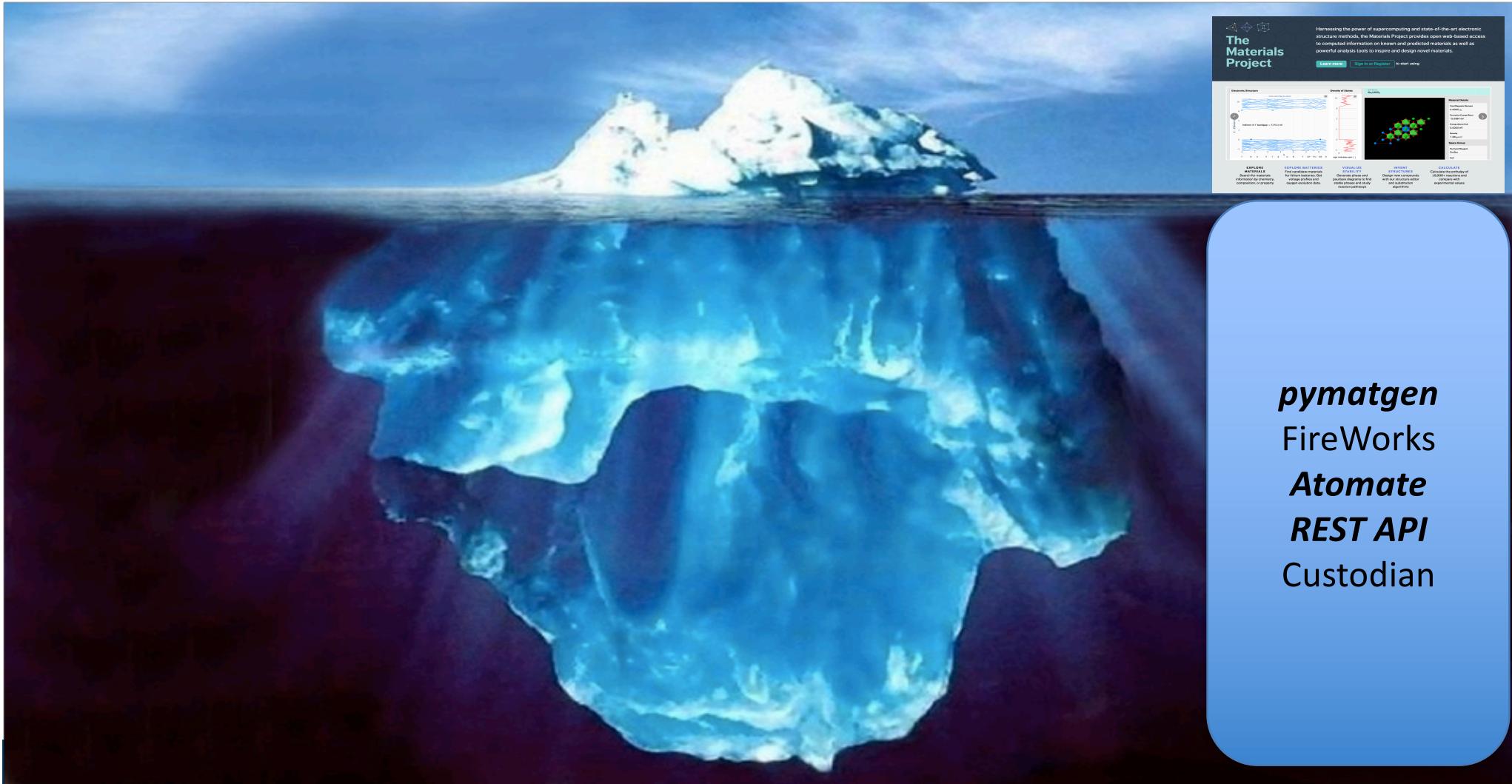
EXPLORE BATTERIES
Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

VISUALIZE STABILITY
Generate phase and pourbaix diagrams to find stable phases and study reaction pathways

INVENT STRUCTURES
Design new compounds with our structure editor and substitution algorithms

CALCULATE
Calculate the enthalpy of 10,000+ reactions and compare with experimental values

The web site is the tip of the iceberg...



pymatgen
FireWorks
Atomate
REST API
Custodian

ICSD

Other experimental databases

User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)



Analysis

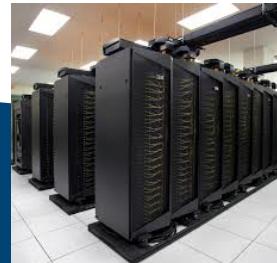
Web apps

Materials API

Workflow Manager

Post-processing and
error-checking

Supercomputing Resources



ICSD

Other experimental databases

User submissions

Input processing & transformations

pymatgen

- Robust materials analysis



Custodian

- Self-healing error recovery



Fireworks

- Smart workflow management



StructureNotationalLanguage (SNL)



Analysis

Workflow Manager

Post-processing and error-checking

Web apps

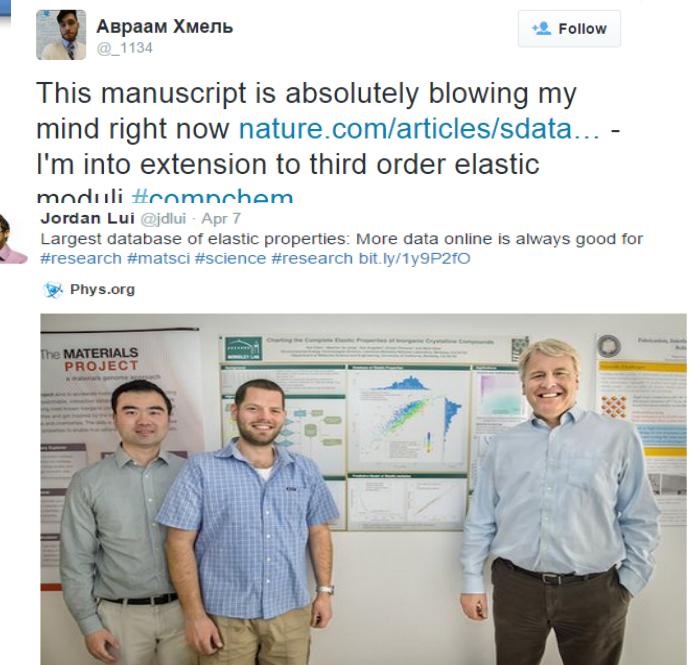
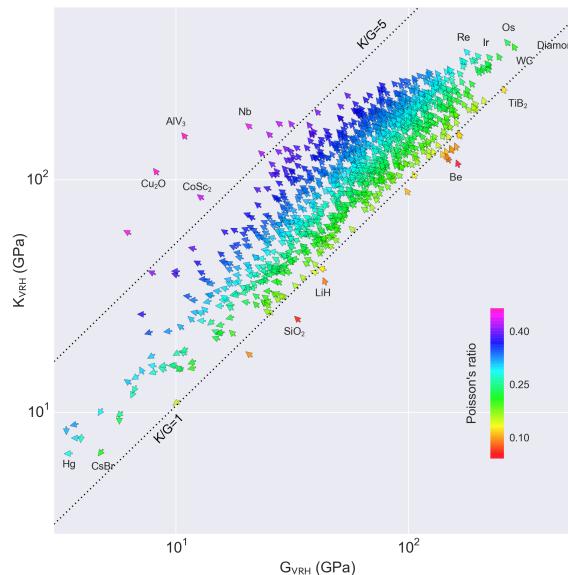
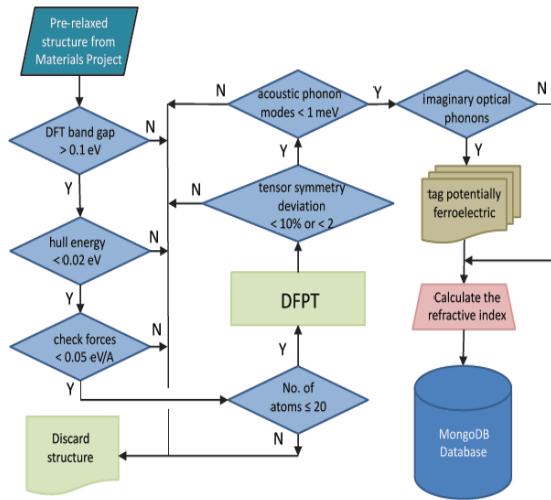
Materials API

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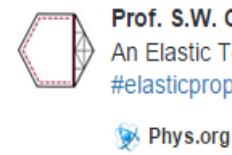


Supercomputing Resources

All HT Properties Benchmarked and Automated



Accelerating materials discovery with world's largest database of...
Scientists at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) have published the world's largest set of data on the complete elastic properties of inorganic compounds....



Prof. S.W. Cranford @CranfordLabNEU · Apr 6
An Elastic Tensor-ganza!! "@physorg_com: Accelerating materials discovery of #elasticproperties phy.so/347544689 @BerkeleyLab"

Materials Explorer

Battery Explorer

Crystal Toolkit

Structure Predictor

Phase Diagram

Pourbaix Diagram

Reaction Calculator

Nanoporous Explorer

Molecules Explorer

RFB Dashboard

Explore Materials

Search for materials information by chemistry, composition, or property

of elements
e.g., 4 or >2 & <6

excluded elements
Cl Br

Submit

Material Tags
imgreite

Band Gap (eV)
0 10

Energy Above Hull
0 6

Formation Energy
-4 4

unit cell sites
1 296

Density
0 24.6

Volume
7 7897

Crystal Systems
Any

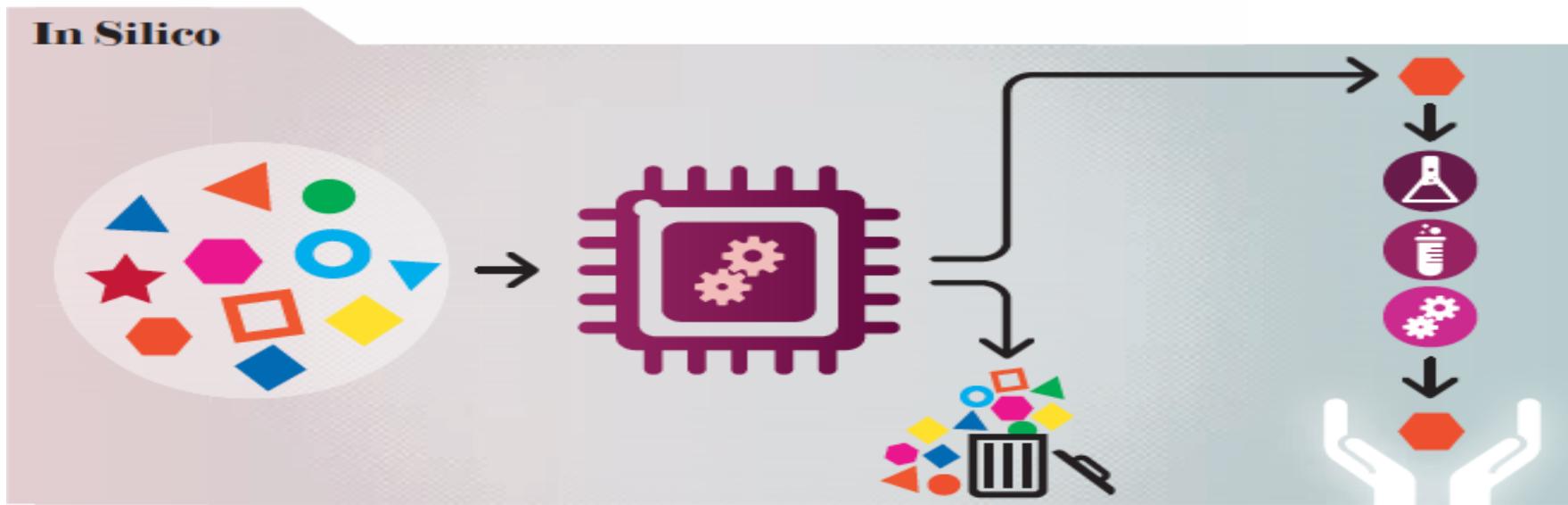
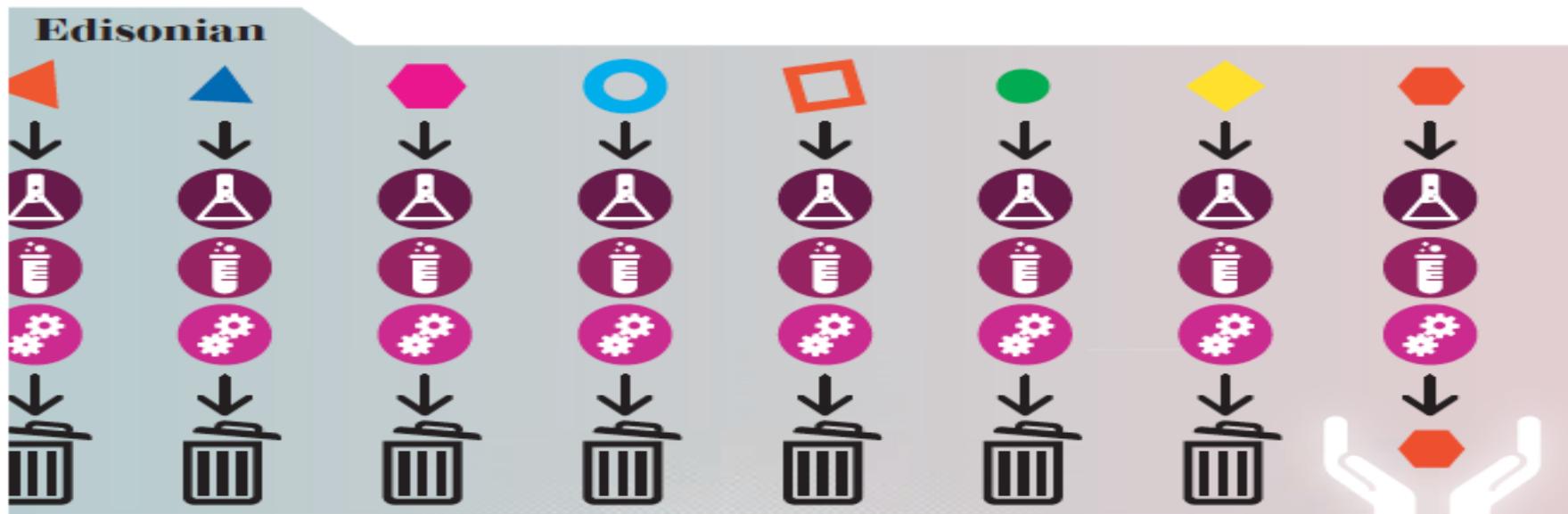
Spacegroup Number
Any

Spacegroup Symbol
Any

Has bandstructure

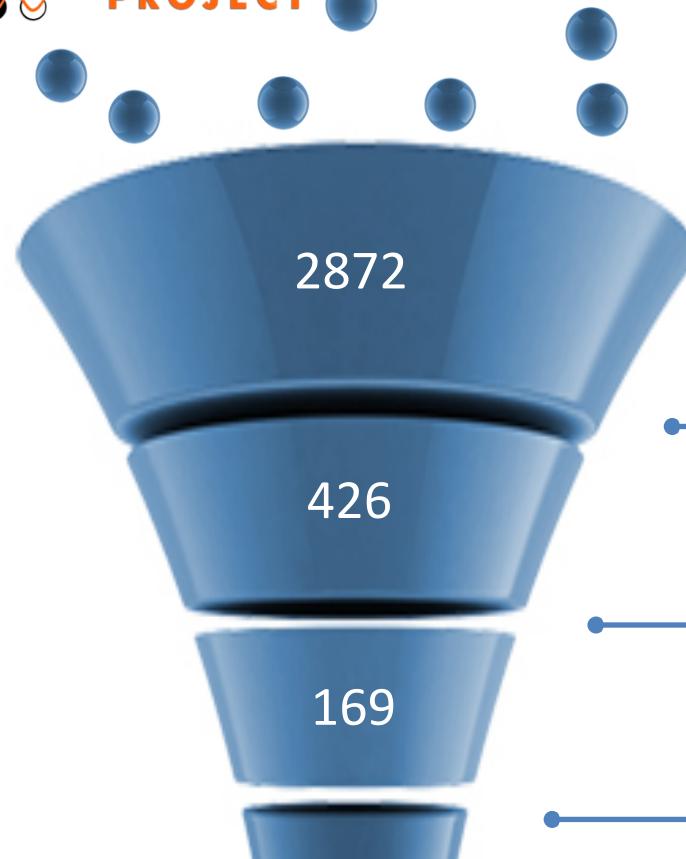
Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	Nsites	Density (gm/cc)	Volume
mp-756173	Li ₅ FeS ₄	Pmmn	-1.069	0.062	0.014	20	1.99	365.138
			0.022	1.991	1459.637	80		
			0.022	2.023	4.96	25	1.944	
			0.022	2.076	257	80	1.866	540.747
			0.021	3.652	57.712	30	2.021	
			0	3.652	356.072	4	2.021	
			0.263	2.346	189.512	10	2.026	
			0.008	2.422	474.135	28	2.008	

← Previous 1 2 3 Next →



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One example of Leveraging MP: Photocatalyst Design



Cr, Mn, and V based ternary oxides

Phase stability

PBE+U band gap

$\Delta H < 50 \text{ meV/atom}$

$0.2 \text{ eV} < E_g < 3.5 \text{ eV}$

Semi-empirical U's

Wang et al,
Phys. Rev. B **73**, 195107 (2006)

HSE band gap

$1.2 \text{ eV} < E_g < 3.2 \text{ eV}$

Band edge energies

Stability in water

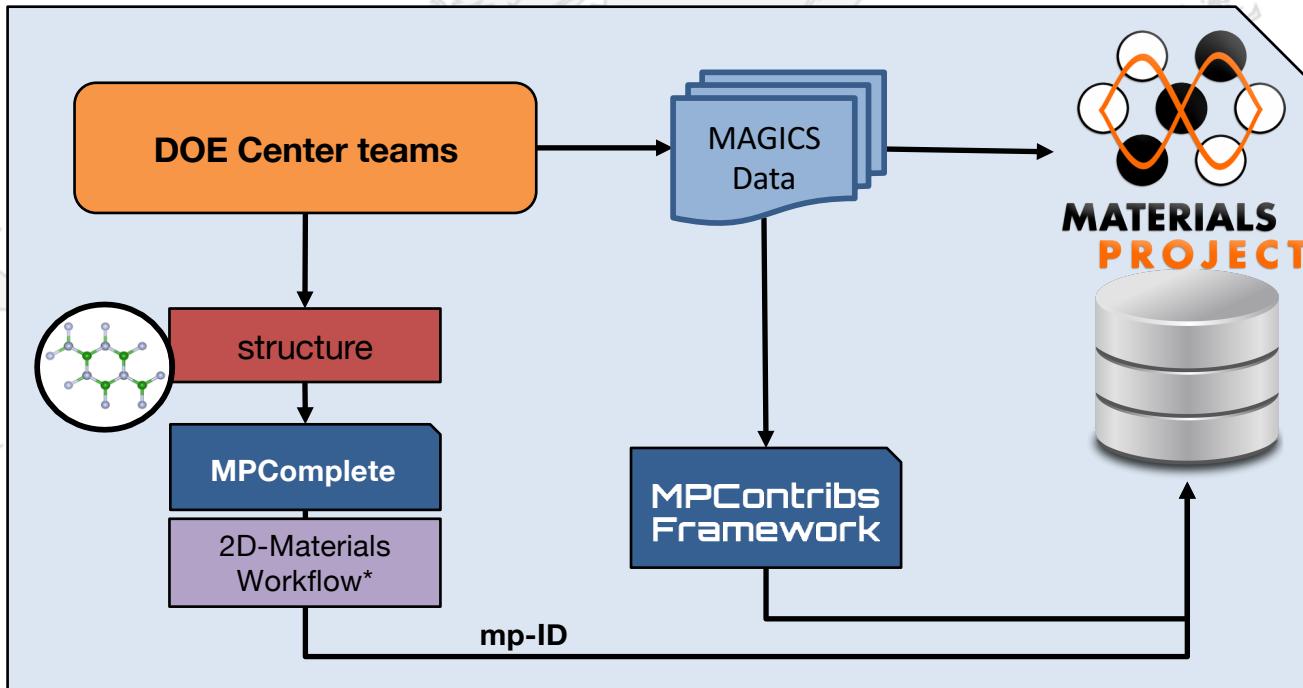
Pourbaix diagrams

Persson et al,
Phys. Rev. B **85**, 235438 (2012)

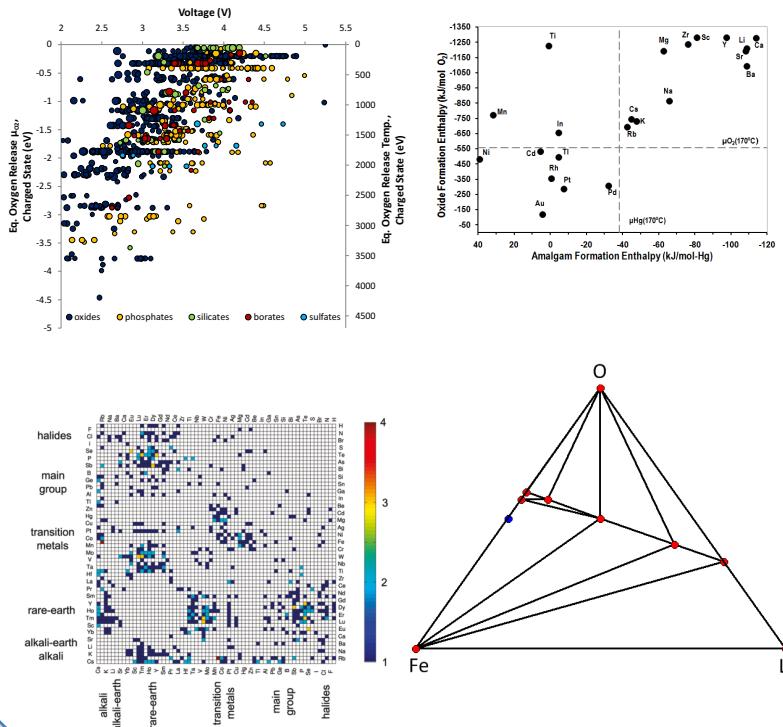
- 47 phases passed computation criteria
- **17 of the 47 phases synthesized through combinatorial synthesis experiments**
- **16 of these 17 phases exhibit photocurrent at OER potential**

MP Going Interactive: MPComplete and MPContribs

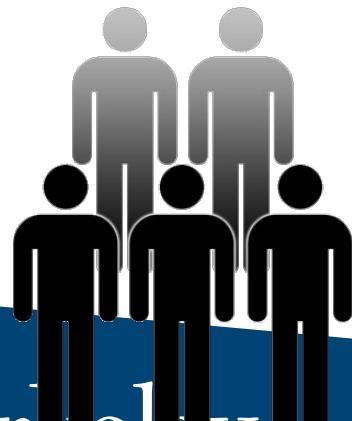
User geolocation over year of June 2016 – May 2017



US Professor: “I was wondering if you ever considered **a way for the community to contribute to the Materials Project?** ... I really like the approach and I think that this is exactly where (especially computational) materials science has to go. ”



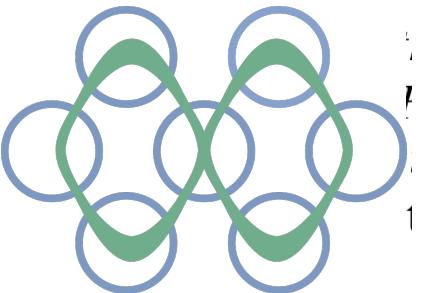
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... towards the materials genome



- 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 DOE/NSF
for funding!



U.S. DEPARTMENT OF
ENERGY

Office of
Science

- 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)