MSRI
Mathematical Sciences Research Institute

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NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: Malgorzata Marciniak **Email/Phone:** mmarciniak@lagcc.cuny.edu 5734620411

Speaker's Name: Kristin Persson

Talk Title: The Materials Project – A Google of Materials

Date: 10 / 04 /2018 **Time:** 2 :00 **am / pm (circle one)**

Please summarize the lecture in 5 or fewer sentences:
Modern innovation challenges require fast methods to commercialize materials. In the past it took over 18 years. The Materials Project (www.materialsproject.org) is harnessing the power of supercomputing and quantum mechanical theory to compute the properties of known inorganic materials, design novel materials, and offer the data to public. The current release contains data derived from quantum mechanical calculations for over 80,000 materials and millions of associated properties.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

- ☑ Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.
- ☑ Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.
  - **Computer Presentations**: Obtain a copy of their presentation
  - **Overhead**: Obtain a copy or use the originals and scan them
  - **Blackboard**: Take blackboard notes in black or blue **PEN**. We will **NOT** accept notes in pencil or in colored ink other than black or blue.
  - **Handouts**: Obtain copies of and scan all handouts
- ☑ For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.
- ☑ When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (*YYYY.MM.DD.TIME.SpeakerLastName*)
- ☑ Email the re-named files to notes@msri.org with the workshop name and your name in the subject line.

The Materials Project for Accelerated Materials Design and Discovery

Kristin A. Persson

UC Berkeley/LBNL

Supported by Department of Energy: Basic Energy Sciences

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Materials Innovation Timeline

PV | TCOs | Permanent magnets | Solar Fuel

Thermoelectrics | Energy Storage | …

How to accelerate the innovation and development timeline?

1930 1940 2000

Teflon

Velcro

Titanium

Polycarbonate

GaAs

Amorphous soft magnets

Lithium ion

Diamond-like Thin Films

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We do not have materials data

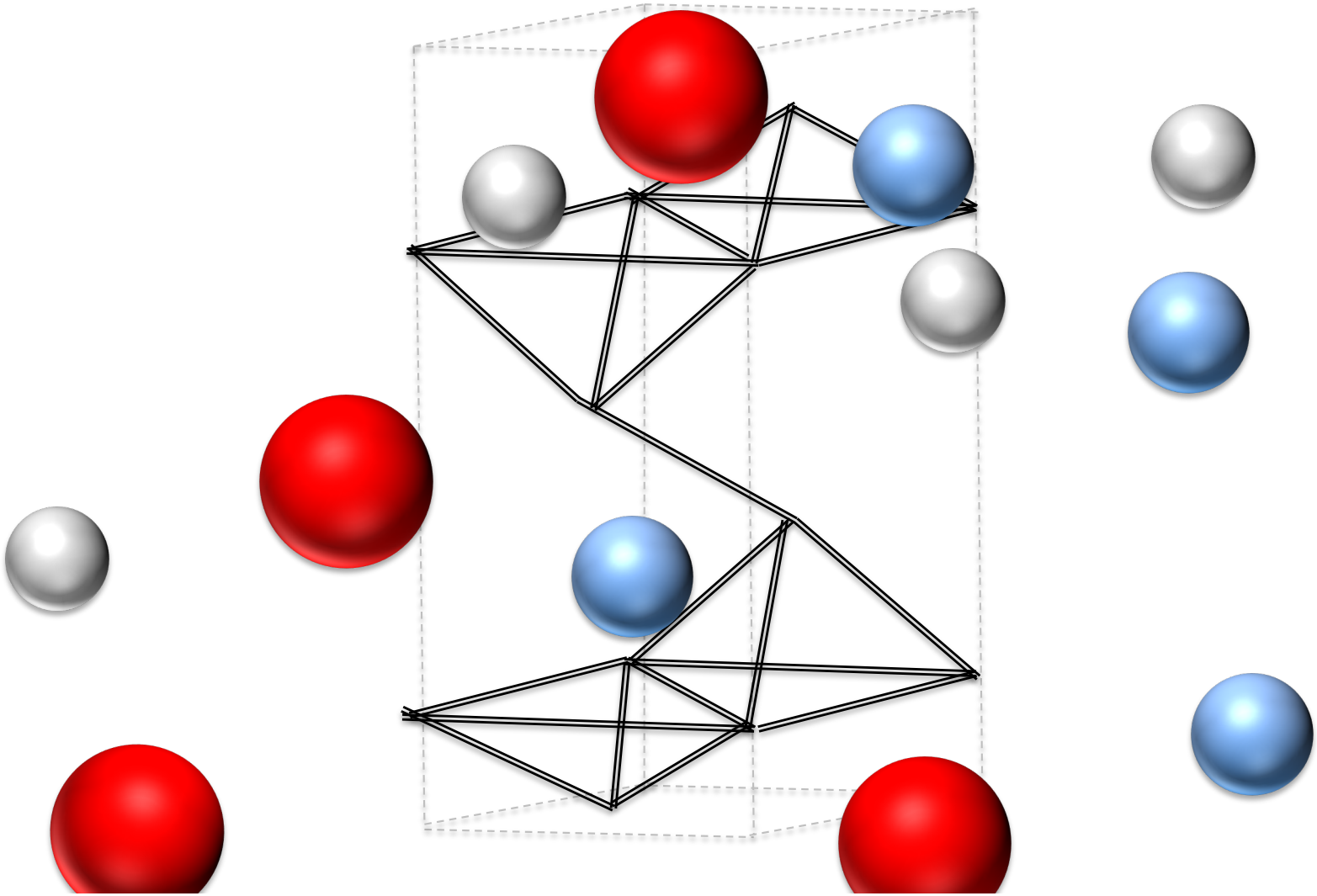
There are about **50,000 to 100,000** known inorganic compounds

Elastic constants: about 200 compounds

Super conductors ≈ 1000

Dielectric constant ≈ 300-400

For almost every property we are below 1% in coverage ….



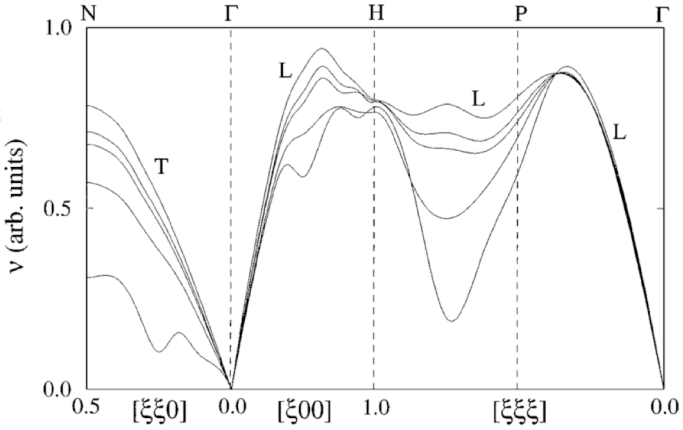
Quantum Mechanics

$$\langle \Psi | \text{better battery} | \Psi^* \rangle$$

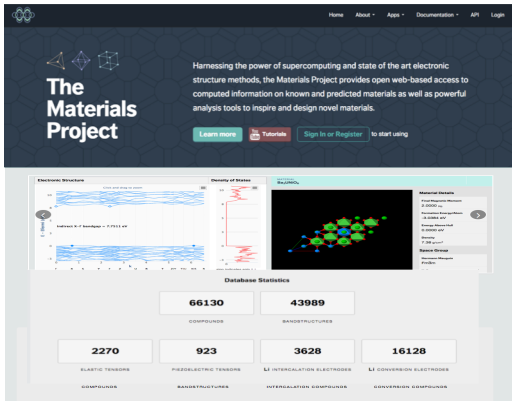
Better materials

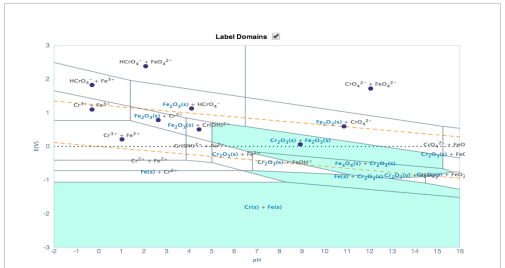
First-Principles Modeling: 1996 - 2018

1996: One year on tungsten



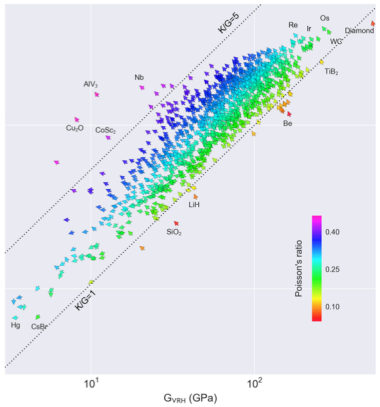
2018: 80,000+ materials on the Materials Project + **millions** of materials properties

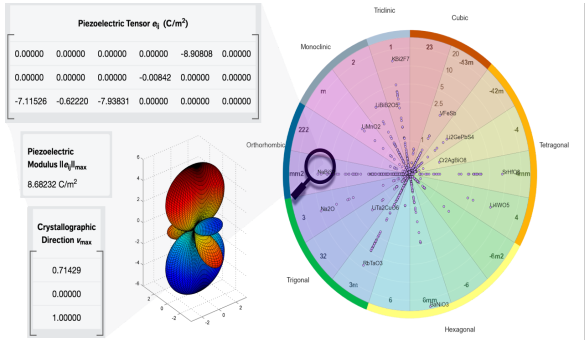




Pourbaix Diagrams on the Materials Project

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





Piezoelectricity Data on the Materials Project

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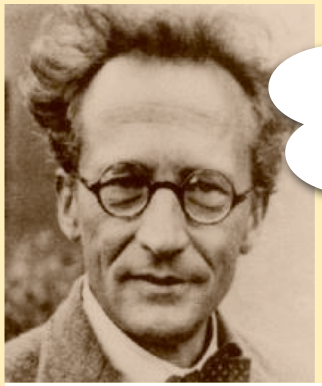
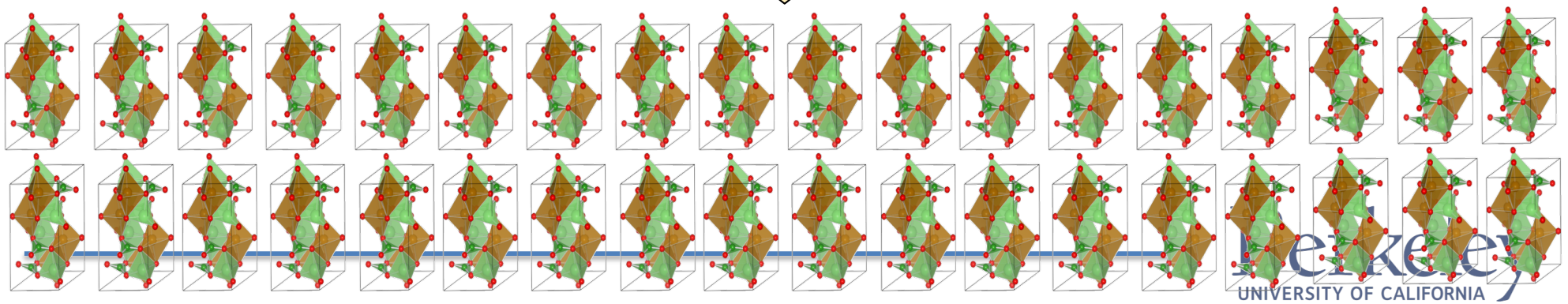
Accelerated Computations



One supercomputer could crunch through ~20,000 structures in 1 day…

$$i\hbar \frac{d\Psi(\{r_i\};t)}{dt} = \hat{H}\Psi(\{r_i\};t)$$

+



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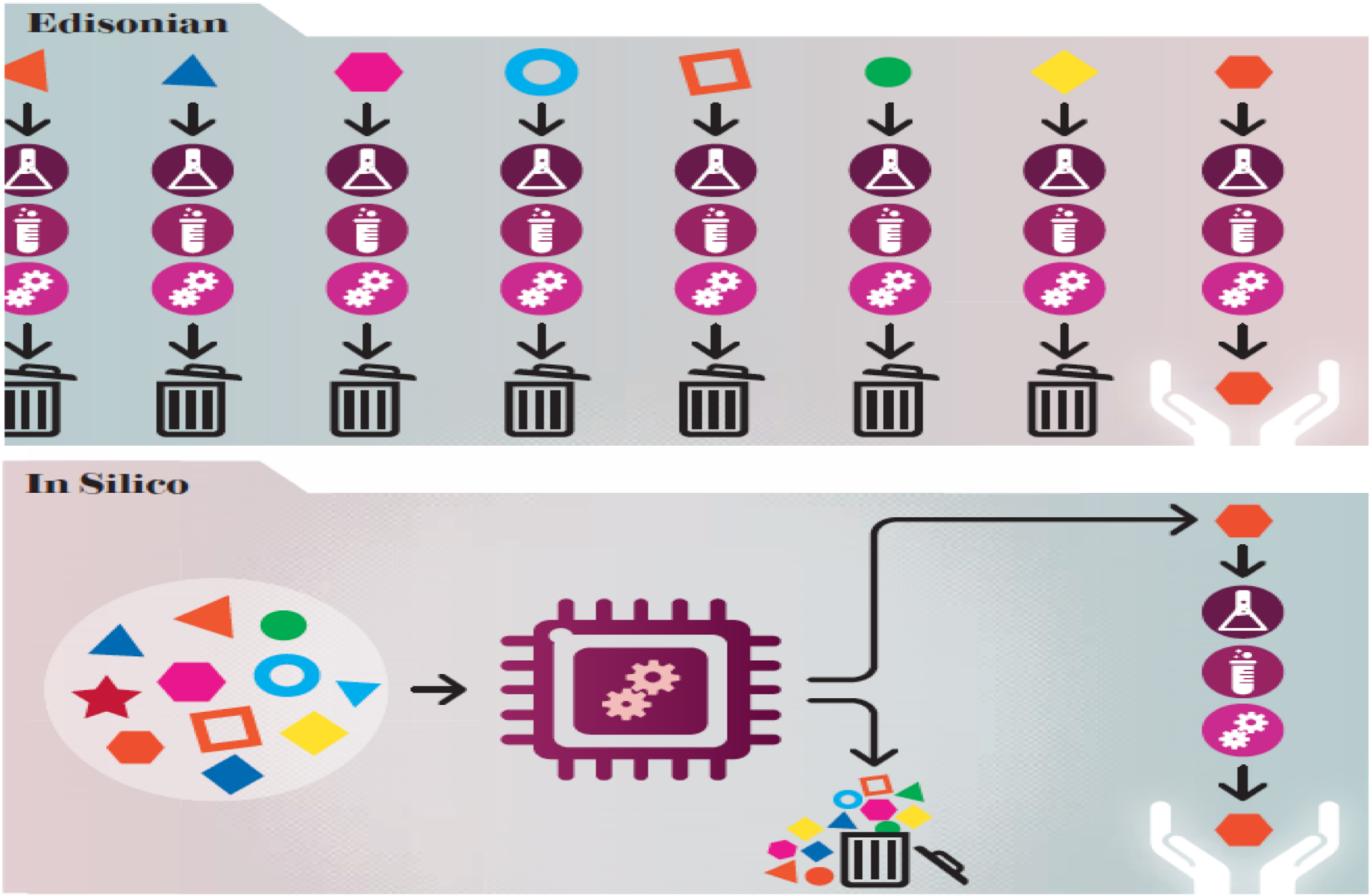
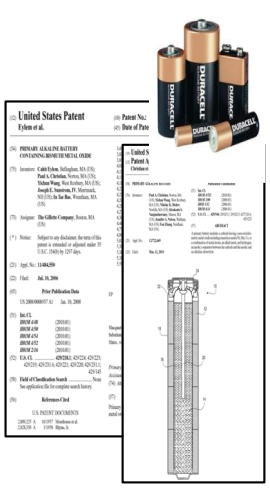
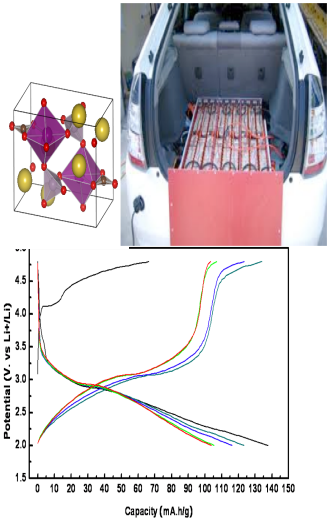

Edisonian
In Silico

New Materials for Sustainable Energy

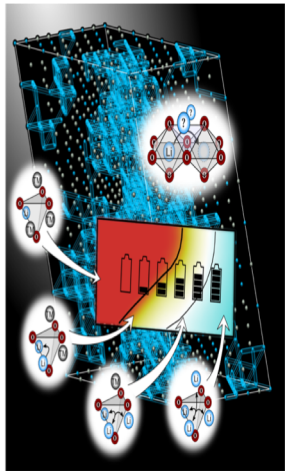
Completely new materials predicted and synthesized based on computational predictions…it is just the beginning



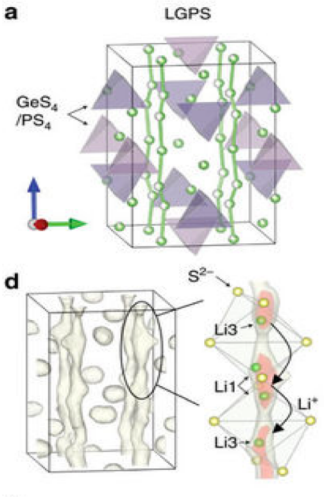
2005:
Novel alkaline batteries



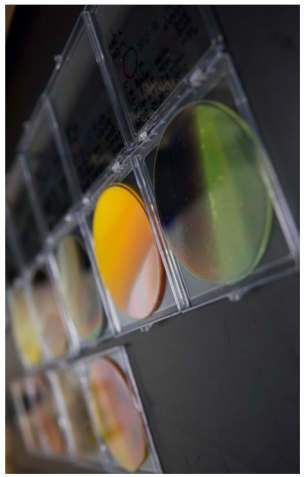
2011:
Li ion electrodes



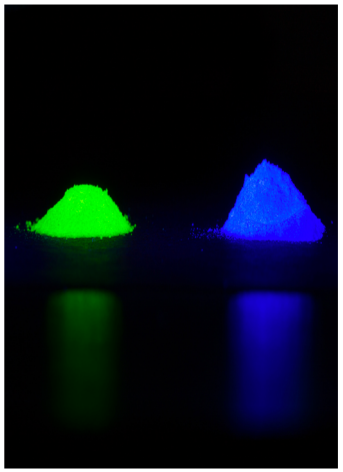
2014:
New class of Li ion cathodes



2015:
Superionic conductors



2016:
Mg cathodes
Photocatalysts
Thermoelectrics



2017:
Piezoelectrics
LEDs
Auxetics
Mg electrolytes
….

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The MGI and the Materials Project

Materials Genome Initiative: A Renaissance of American Manufacturing

Jun… ***utational to…***
me… *…e process of*
dev… ***…nced materia…***
exp… ***…predictable***

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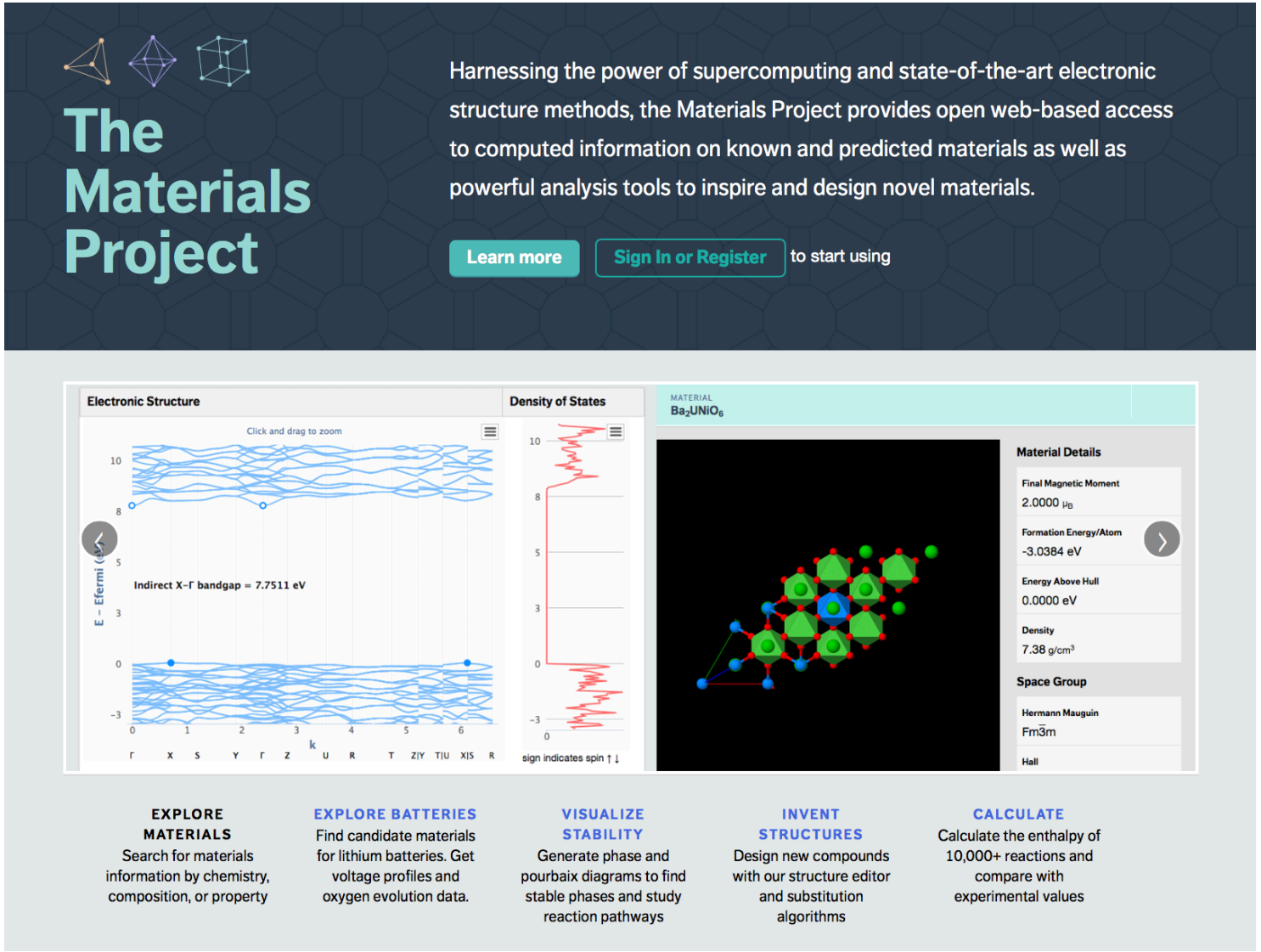
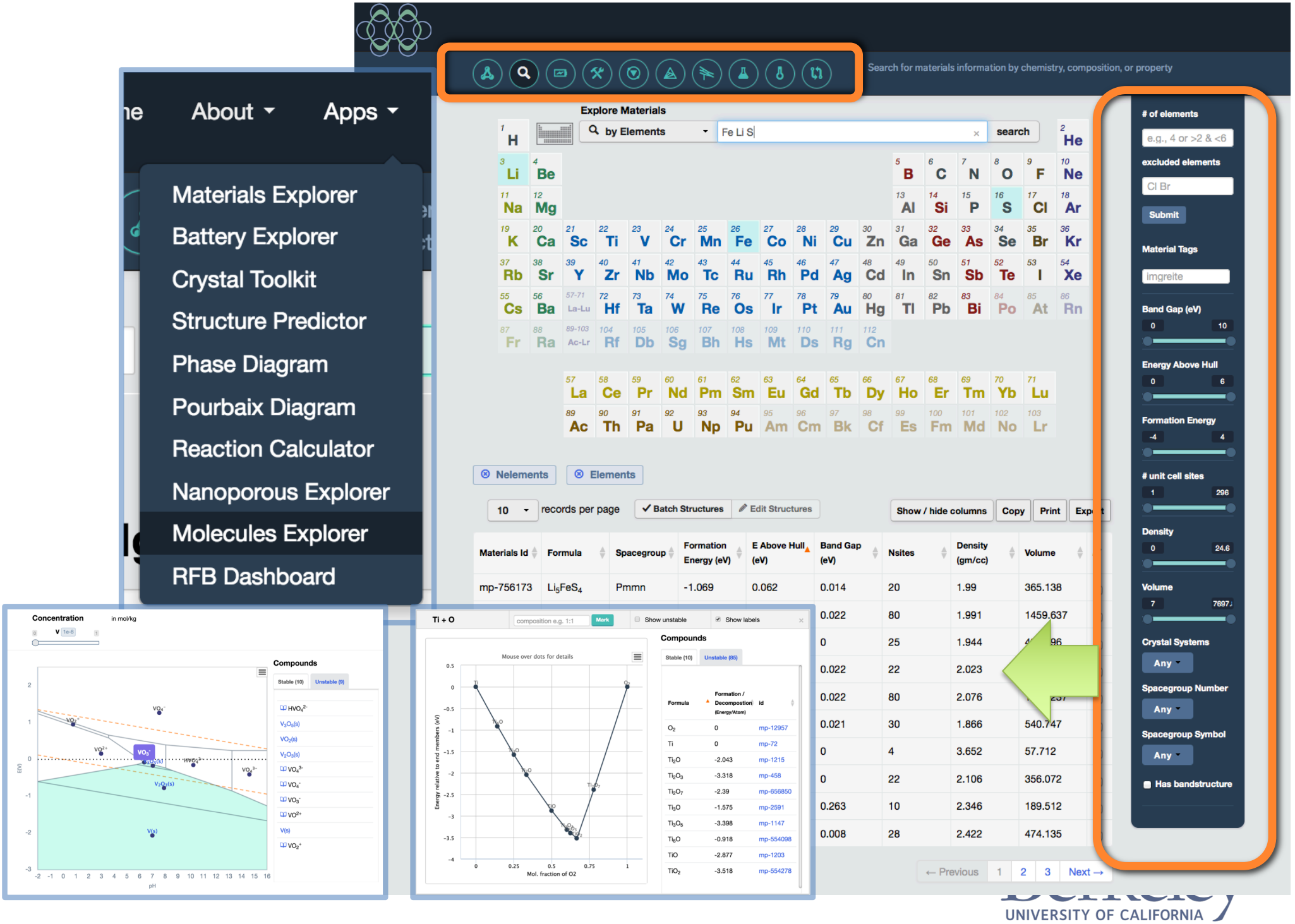
Materials Project web site





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Search for materials information by chemistry, composition, or property

Explore Materials Advanced Search Syntax

by Formula Al2O3

Similar Structures

Explanation of similarity distance measure: Documentation.

material	# of elements	distance

Piezoelectricity

Reference for tensor and properties: Methodology

Piezoelectric Tensor e_{ij} (C/m^2)

0.00000	0.00000	0.00000	0.00000	-0.15142	0.00000
0.00000	0.00000	0.00000	0.57103	0.00000	0.00000
-0.26428	0.79886	0.44492	0.00000	0.00000	0.00000

Piezoelectric Modulus $\|e_{ij}\|_{max}$

0.64163 C/m^2

Crystallographic Direction v_{max}

0.00000
1.00000
1.00000

Elasticity

Reference for tensor and properties:

Stiffne

452	150	10
150	452	10
107	107	45
20	-20	-0
0	0	
0	0	

Equations of State

Reference:

Equations of State
Click and drag to zoom

-6.5

computed

Calculation Summary

Elasticity

Methodology

Structure Optimization

Run Type	Energy Cutoff
GGA	520 eV
# of K-points	U Values
108	--
Pseudopotentials	Final Energy/Atom
VASP PAW: O Al O Al O	-7.4813 eV

Corrected Energy

-79.0267 eV

How do we arrive at this value?

Detailed input parameters and outputs for all calculations

GGA Uniform v2 | GGA band structure v2 | GGA optimize structure (2x) | GGA optimize structure (2x) | GGA optimize structure (2x) | GGA static v2

*Why the **bold** text?*

Show JSON History | Show BibTex Citation | Download BibTex Citation

ICSD IDs

60419 160901 160902 160903 160904 52044 92631 52025 85137 24851 56085 10426 9775 63647 63648 93096 161060 151589 26790 75559 75560 88028 9770 9771 9772 9773 9774 88029 25778 51687 30025 52024 31545 31546 31547 31548 89662 89663 89664 89665 24005 99783 30024 64713 30026 30027 30028 30029 30030 43732 92629 92630 75479 165594 88027 160604 160605 160606 160607 600672 608993 608994 608995 608996 608997 608998 33639 10425 609001 52647 609004 68591 52648 77810 73076 164617 169720 92628 73724 73725

Submitted by

Michael Kocher Anubhav Jain Shyue Ping Ong Geoffroy Hautier

Dielectric Properties

Reference for tensor and properties: Methodology

Dielectric Tensor $\varepsilon_{ij}^{\infty}$ (electronic contribution)

19.00	0.00	0.00
0.00	19.00	0.00
0.00	0.00	20.78

Dielectric Tensor ε_{ij} (total)

31.99	-0.00	0.00
-0.00	31.99	-0.00
0.00	-0.00	38.56

Polycr (electr
19.60

Polycr (total)
34.18

Refrac
4.43

Potent
True

Substrates

Reference for mi

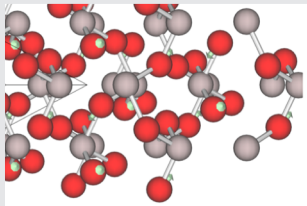
substrate orienta

substrate mate			
GaSe (mp-1943			
LiF (mp-1138)			
GaTe (mp-5428			
SiC (mp-7631)	<1 0 0>	<1 0 1>	0.021
Mg (mp-153)	<1 0 0>	<1 0 0>	0.044
SiO (mp-6930)	<0 0 1>	<1 0 1>	0.045

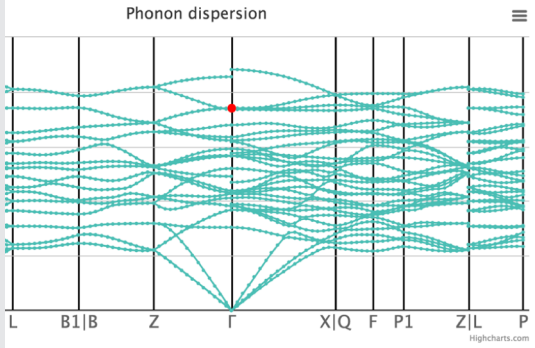
Up to 50 entries displayed.

†minimal coincident interface area.

, ternary, quaternary, etc. structures.



Amplitude: 0.2
Vectors: on
Speed: pause



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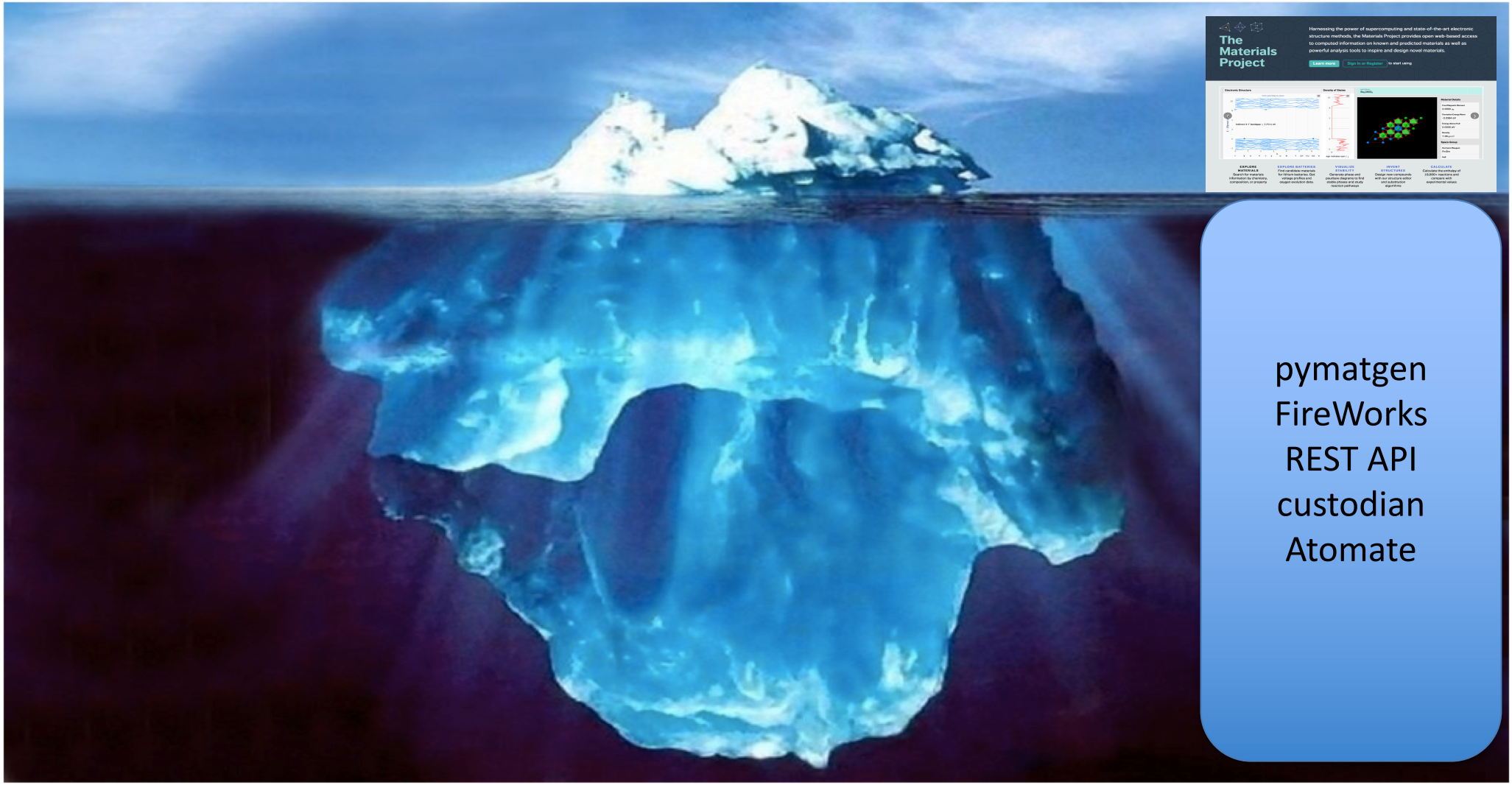
The web site is the tip of the iceberg…



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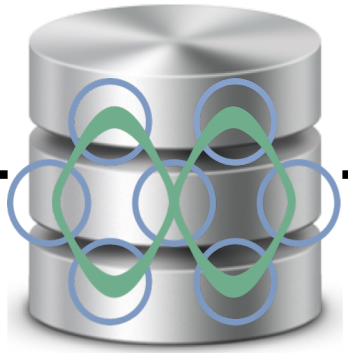
ICSD Other experimental databases User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)



Analysis

Web apps

Materials API

Workflow Manager

Post-processing and error-checking

Supercomputing Resources

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ICSD Other experimental databases User submissions

Input processing & transformations

pymatgen

- Robust materials analysis

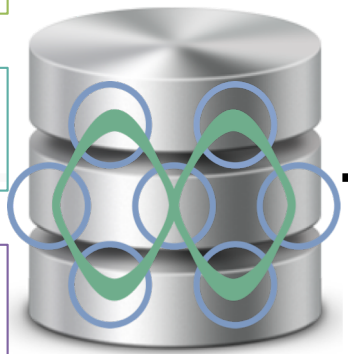
Custodian

- Self-healing error recovery

Fireworks

- Smart workflow management

StructureNotationalLanguage (SNL)



Analysis

Web apps

Materials API

Workflow Manager

Post-processing and error-checking

Supercomputing Resources

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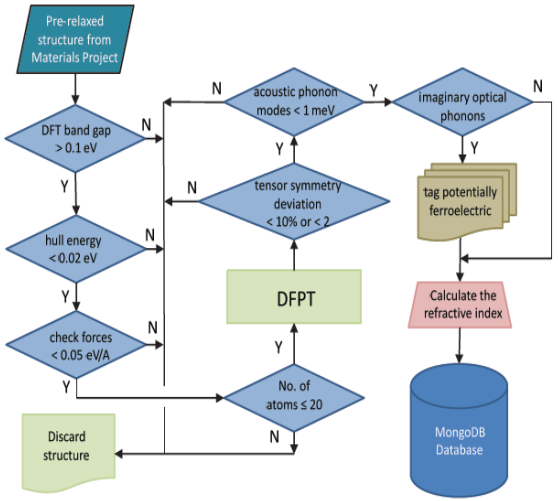
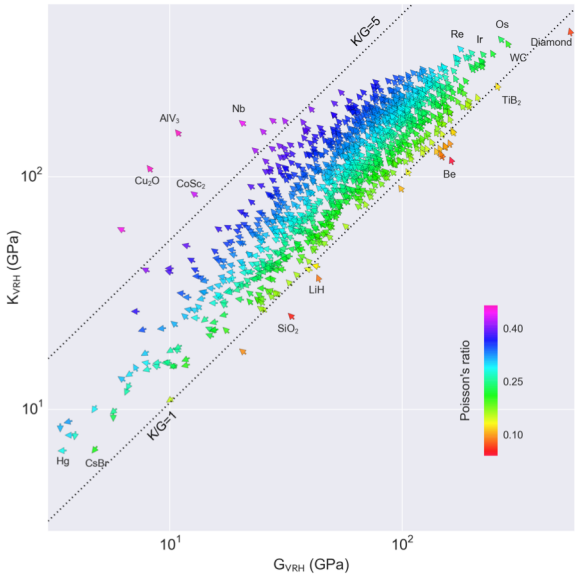
All HT Properties Benchmarked and Automated

Codes/Algorithms → Validation/Benchmarking → Data → Dissemination/Design





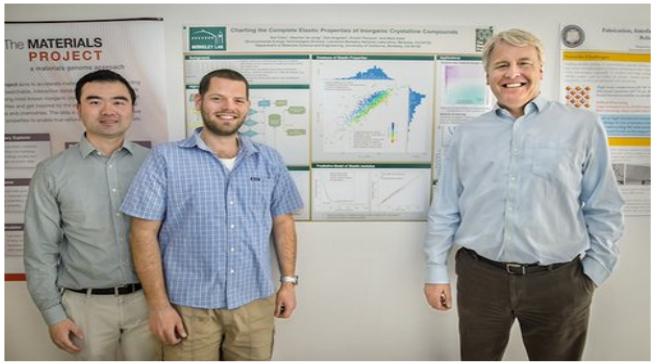
Авраам Хмель @_1134 — Follow

This manuscript is absolutely blowing my mind right now nature.com/articles/sdata… - I'm into extension to third order elastic moduli #compchem

Jordan Lui @jdlui · Apr 7

Largest database of elastic properties: More data online is always good for #research #matsci #science #research bit.ly/1y9P2fO

Phys.org



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....

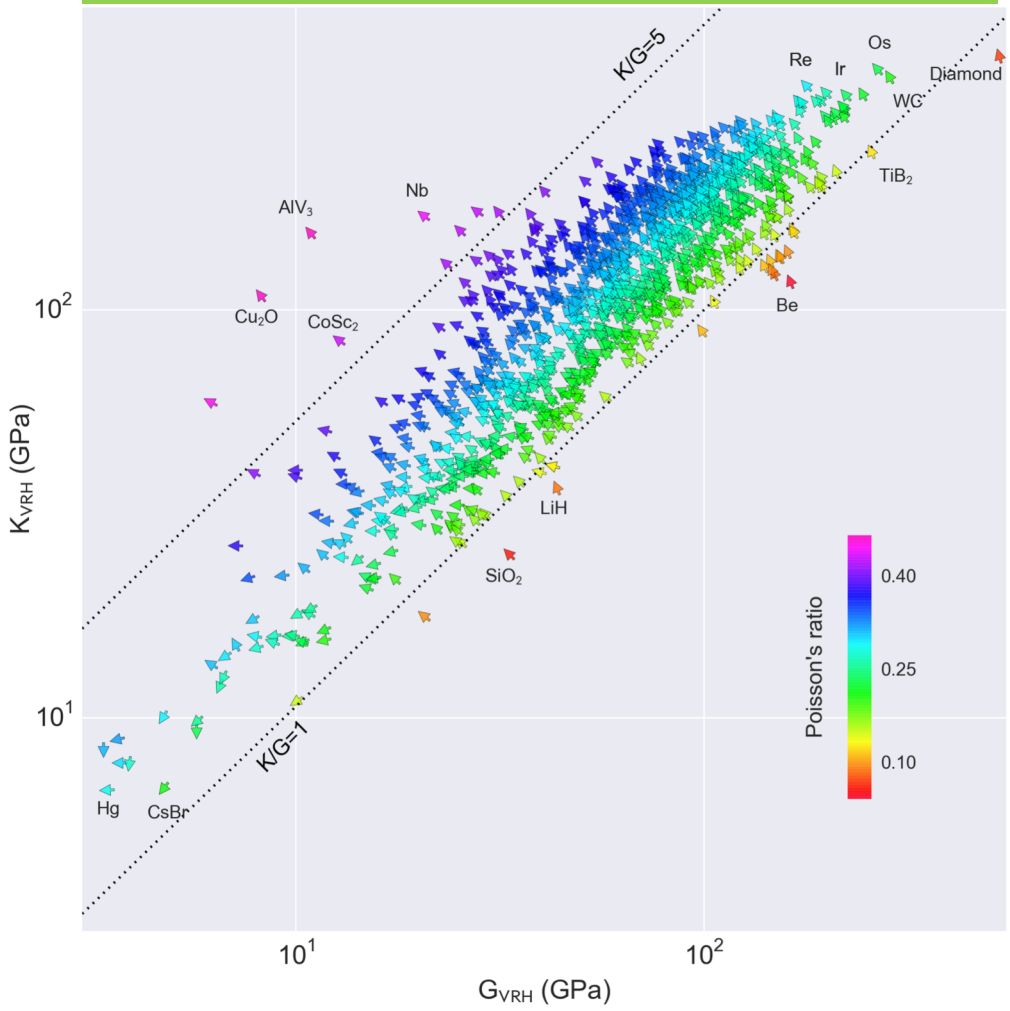
Prof. S.W. Cranford @CranfordLabNEU · Apr 6

An Elastic Tensor-ganza!! "@physorg_com: Accelerating materials discovery of #elasticproperties phy.so/347544689 @BerkeleyLab"

Phys.org

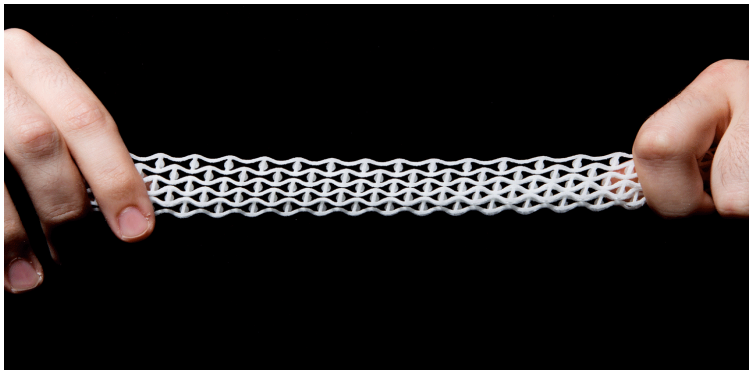
Elastic Data Enables Discovery of Novel Functional Materials

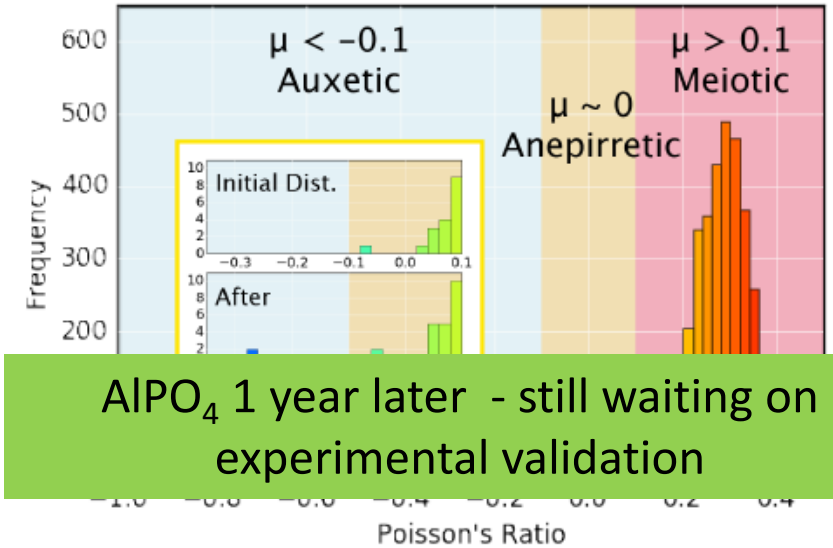
> 6,000 full elastic tensors calculated and counting….



Full elastic tensor experimentally measured for ~200 systems

Correlations between structure/chemistry features with exotic elastic behavior





$AlPO_4$ 1 year later - still waiting on experimental validation

Dagdelen and Persson, Nat Comm 2017

Full piezoelectric tensor known experimentally for only ~50 systems

Piezoelectric Tensor e_{ij} (C/m^2)

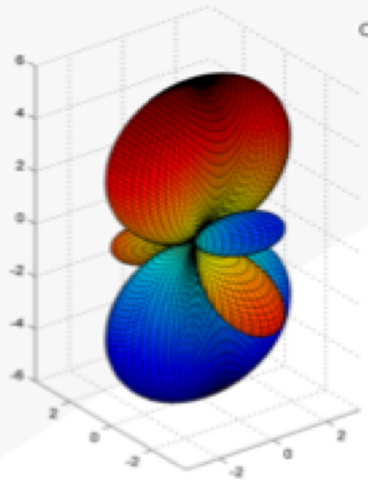
0.00000	0.00000	0.00000	0.00000	-8.90808	0.00000
0.00000	0.00000	0.00000	-0.00842	0.00000	0.00000
-7.11526	-0.62220	-7.93831	0.00000	0.00000	0.00000

Piezoelectric Modulus $\|e_{ij}\|_{max}$

8.68232 C/m^2

Crystallographic Direction v_{max}

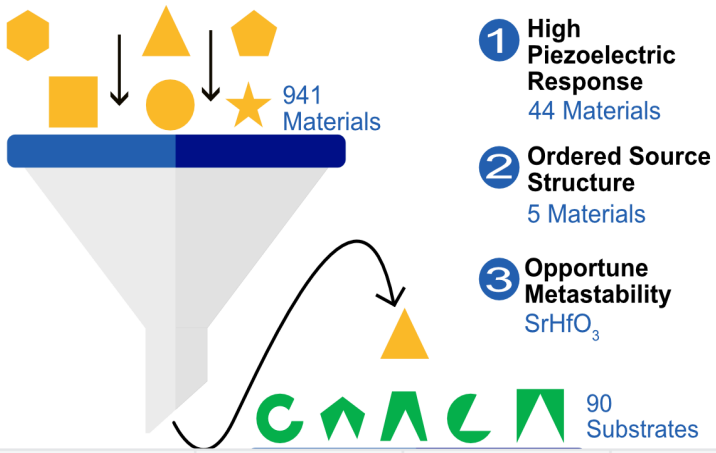
0.71429
0.00000
1.00000

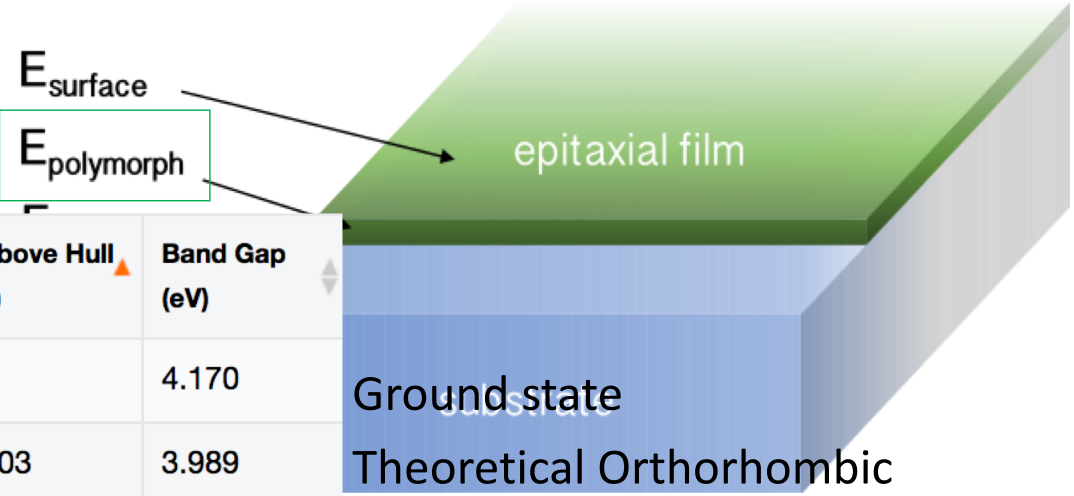


Piezoelectricity Data on the Materials Project

Today, we're proud to officially launch the largest database to-date of calculated piezoelectric properties of inorganic crystalline compounds. The full piezoelectric tensor--and derived properties such as the crystallographic direction of the maximum piezoelectric response and the magnitude of the maximum response--of over 950 piezoelectric materials are now available.

How to target one metastable $SrHfO_3$?





Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	
mp-3378	$SrHfO_3$	Pnma	-3.831	0	4.170	Ground state
mp-13109	$SrHfO_3$	Imma	-3.829	0.003	3.989	Theoretical Orthorhombic
mp-4673	$SrHfO_3$	Cmcm	-3.827	0.004	3.957	Non-Polar Orthorhombic
mp-3721	$SrHfO_3$	I4/mcm	-3.825	0.006	4.058	Non-Polar Tetragonal
mp-550908	$SrHfO_3$	P4/mbm	-3.818	0.013	3.676	Theoretical Tetragonal
mp-13108	$SrHfO_3$	P4mm	-3.798	0.033	3.733	Polar Tetragonal
mp-4551	$SrHfO_3$	$Pm\bar{3}m$	-3.798	0.033	3.729	Cubic nonpolar

Hong, Dwaraknath, Garten, Ndione, Ginley and Persson, The Journal of Physical Chemistry C 120(23), 2016

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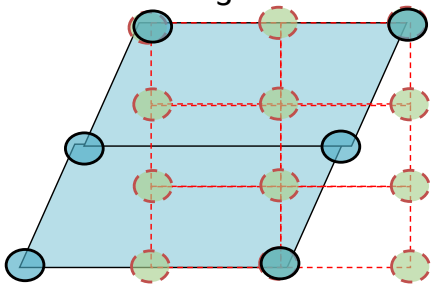
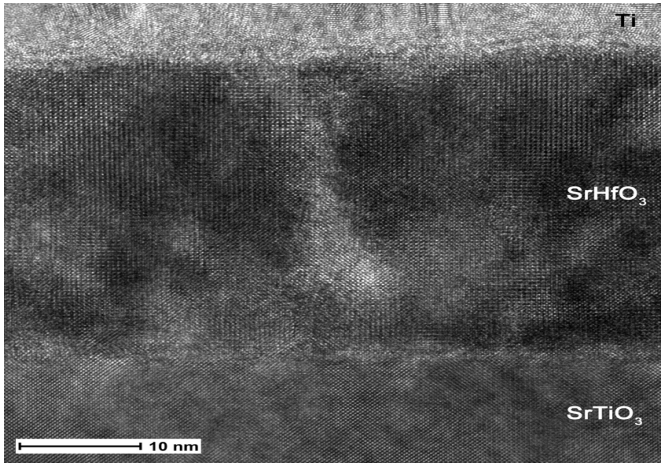
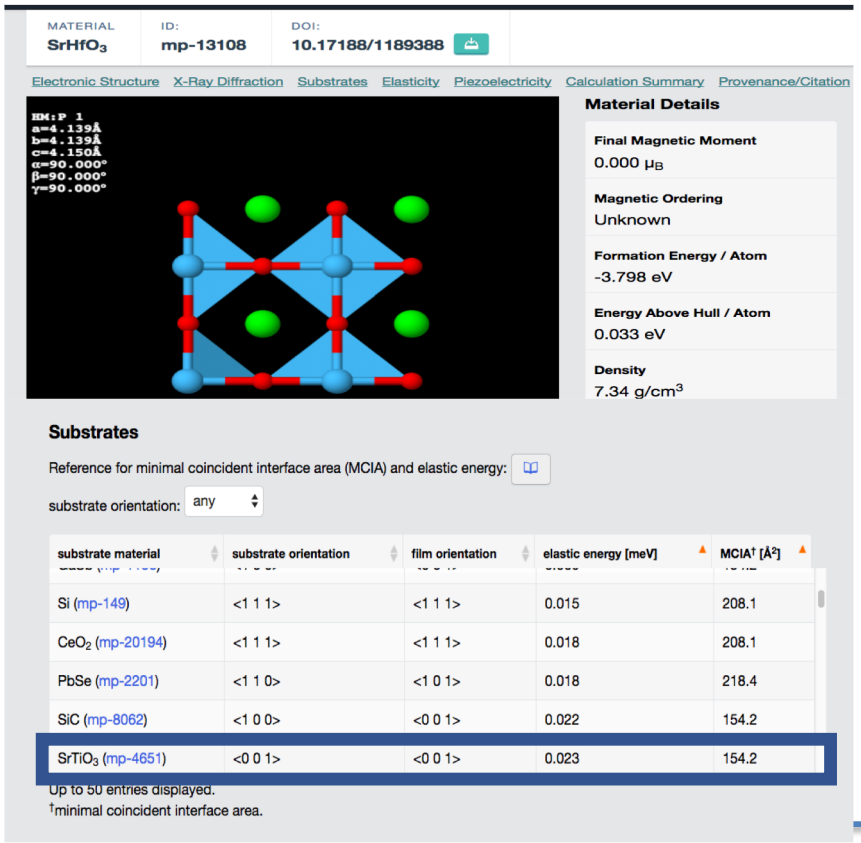
Theory-Guided Thin Film Synthesis

'Substrate Picker' provides good guesses of substrates to grow P4/mm $SrHfO_3$

Algorithm from Zur & Mcgil, 1984; including elastic strain based on Materials Project

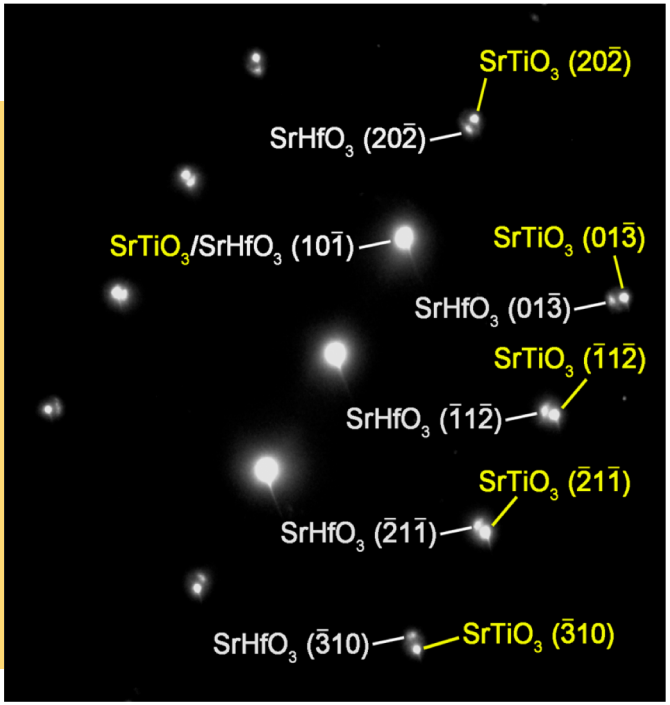






100 mTorr, 700C , → orthorhombic target phase
1mT, 500C, →cubic ground state

The target match the SHO orthorhombic phase and confirmed ferroelectricity as well as piezoelectricity



Garten, Dwaraknath, … Persson and Ginley, Submitted 2018

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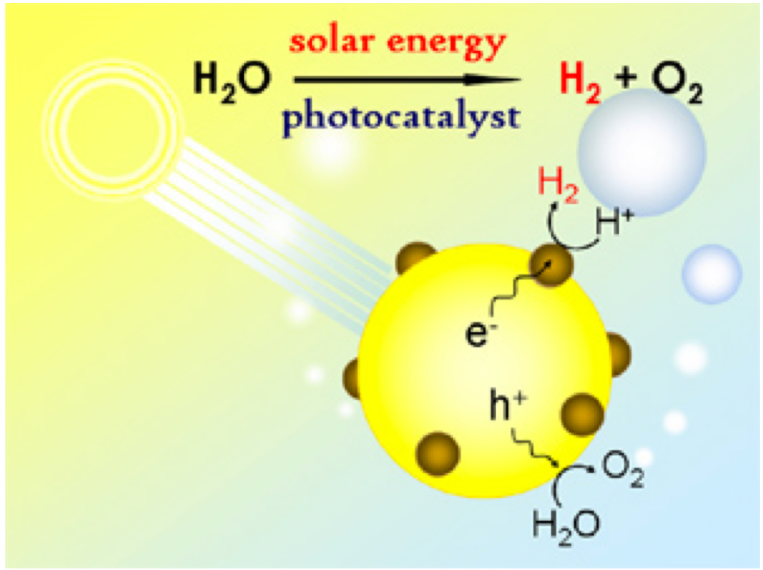
Known Light Absorbers/Photocatalysts



Criteria for a good light absorber

- (i) VBM within 0.1-0.5 eV of OER potential
- (ii) Band gap between 1 and 2 eV
- (iii) Photochemical stability at pH 13

	(i)	(ii)	(iii)
CdSe	Y	N	N
GaP	Y	Y	N
Si	Y	N	N
MoS_2	Y	Y	N
ZnSe	Y	N	N
Ta_3N_5	Y	N	N
Cu_2O	Y	Y	N
CdS	N	N	N
α-Fe_2O_3	N	N	Y
$BiVO_4$	N	N	N
$NaTaO_3$	N	N	Y
$SrTiO_3$	N	N	Y
TiO_2	N	N	Y
WO_3	N	N	N

MP Collaboration with JCAP: First-Principles High-Throughput Approach

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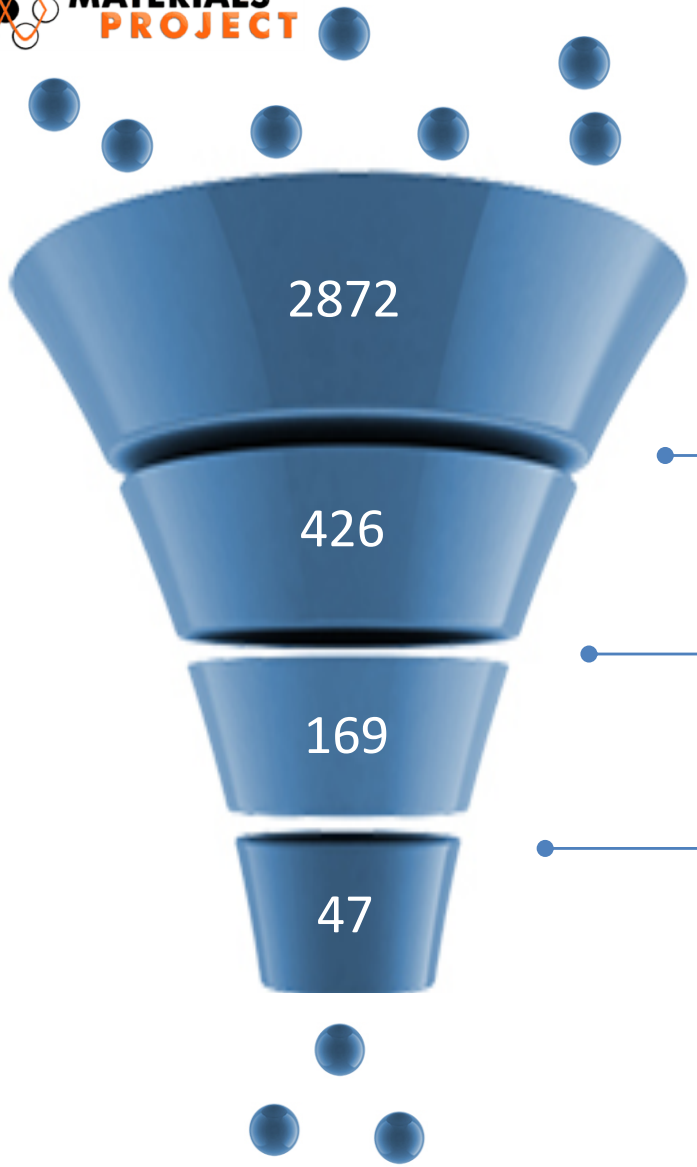
Cr, Mn, and V based ternary oxides



Phase stability

PBE+U band gap

$\Delta H < 50$ 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)

MP database

HSE, bulk

PBE+U, surface

Collaboration with John Gregoire, JCAP; Jeff Neaton and Kristin Persson Materials Project

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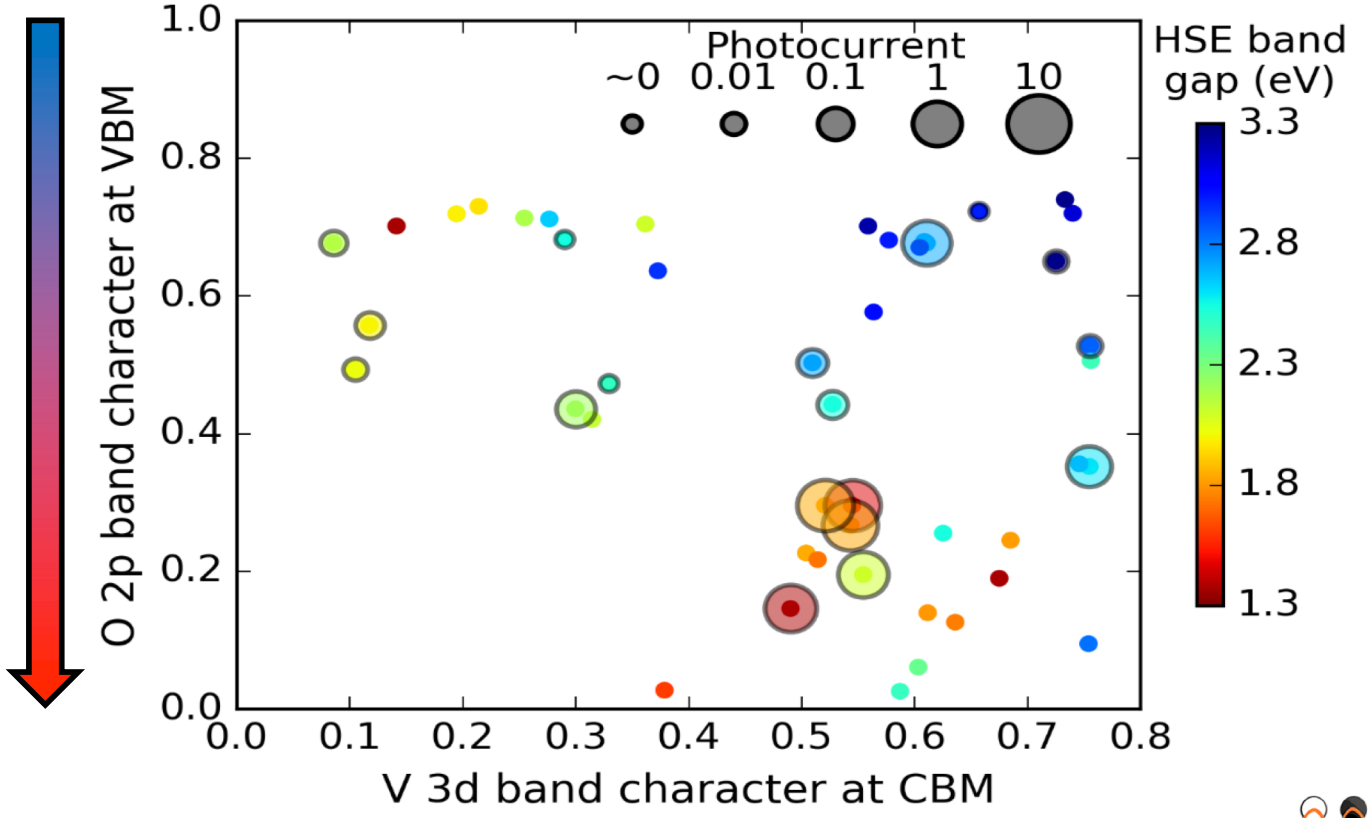
Theory Guided Design and Rapid Synthesis

Courtesy of John Gregoire, Caltech

- 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**

VB with metal (not O 2p) character can provide desired alignment to OER potential



Tuning VB/CB character can yield band gap in desired 1.5-2.8 eV range

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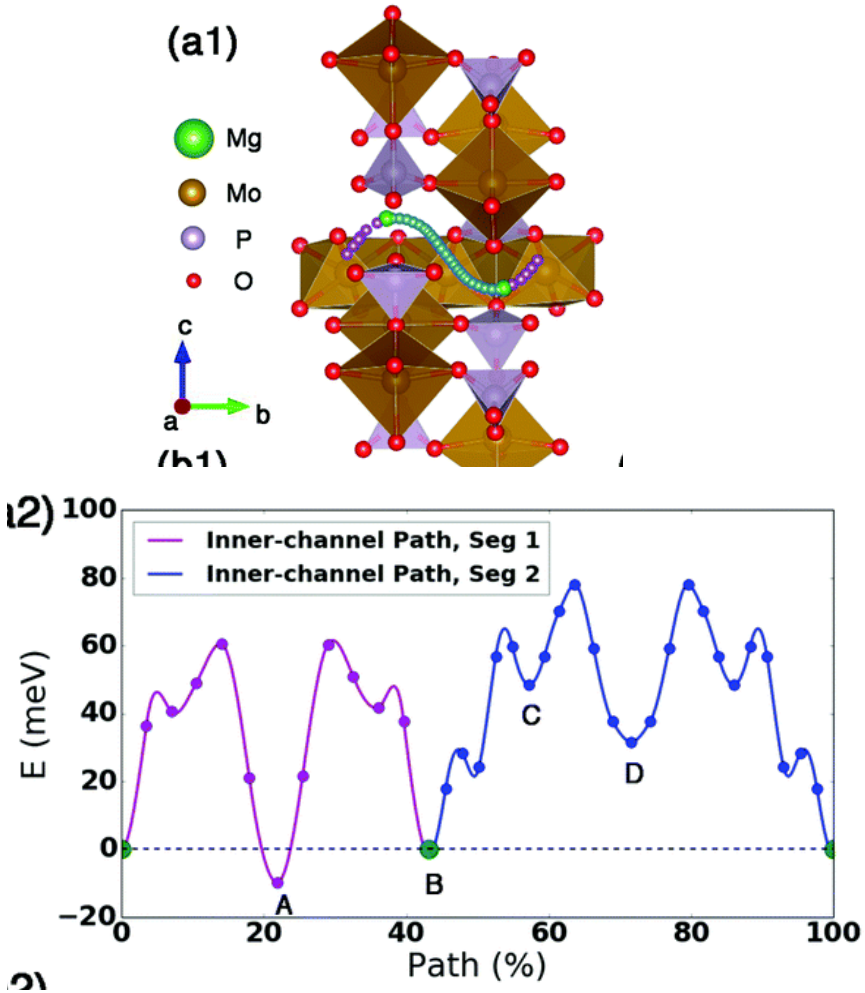
…however mostly: to date unrealized: Mg Cathode: $MgMo_3P_3O_{13}$

https://materialsproject.org/batteries/mvc-1200010538/



Discharged	MgMo3P3O13
mp-id discharged	mvc-10538 ($p2_1/m$)
Charged	Mo3P3O13
mp-id charged	mvc-10615 ($p2_1/m$)
max. Ehull	42 (meV/atom)
Parent compound	CaFe3(PO4)3O
Gravi. Capacity	87 mAh/g
Vol. Capacity	330 mAh/cm^3
Average Voltage	1.90V
Diffusion Barrier	< 100meV

Chem. Commun., 2017, 53, 7998-8001 (Ceder&Persson group)

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How to Accelerate Synthesis of Novel Materials for Energy Applications?

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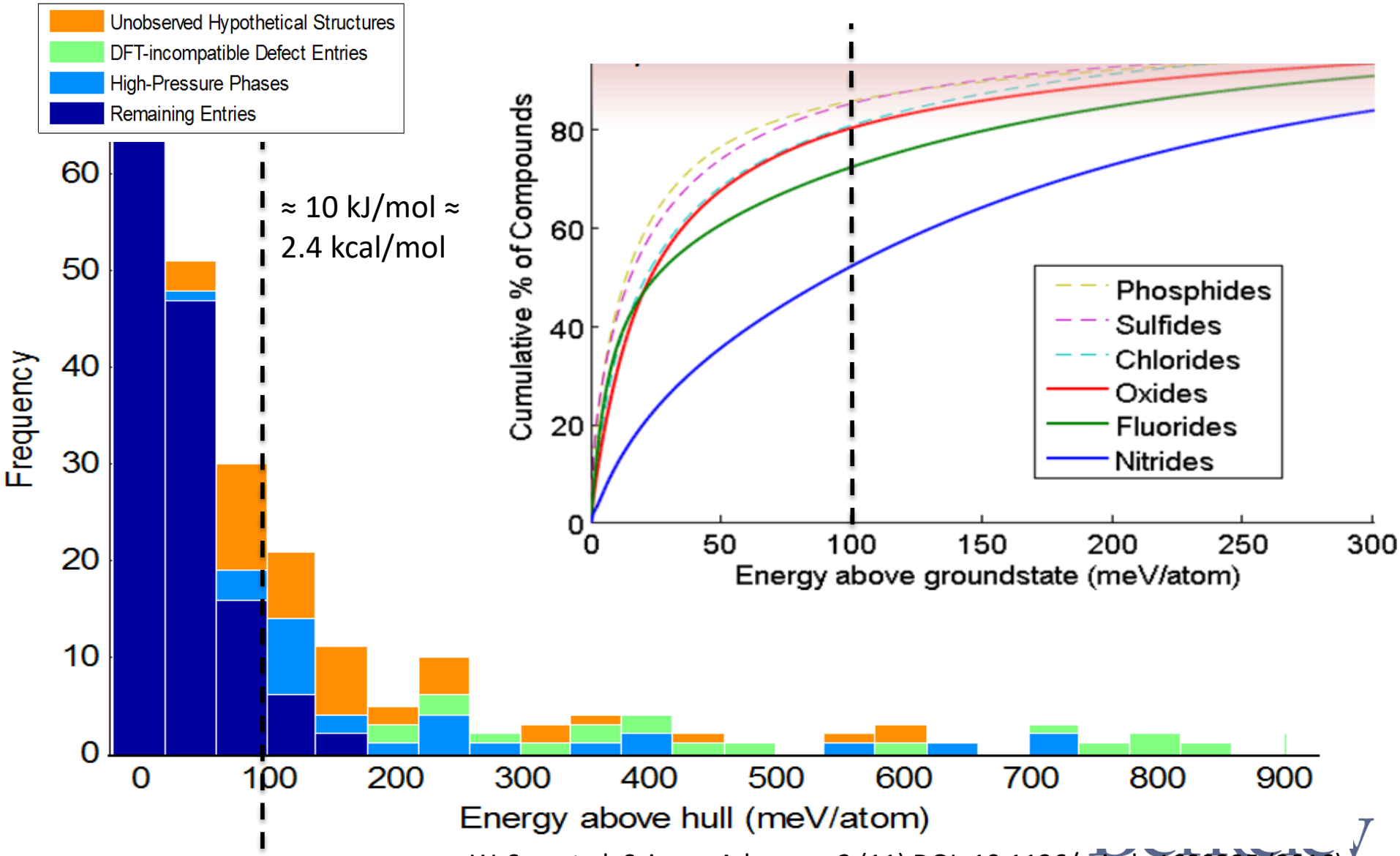
Statistics on the ICSD covering most known inorganic materials



W. Sun et al. Science Advances 2 (11) DOI: 10.1126/sciadv.1600225 (2016)

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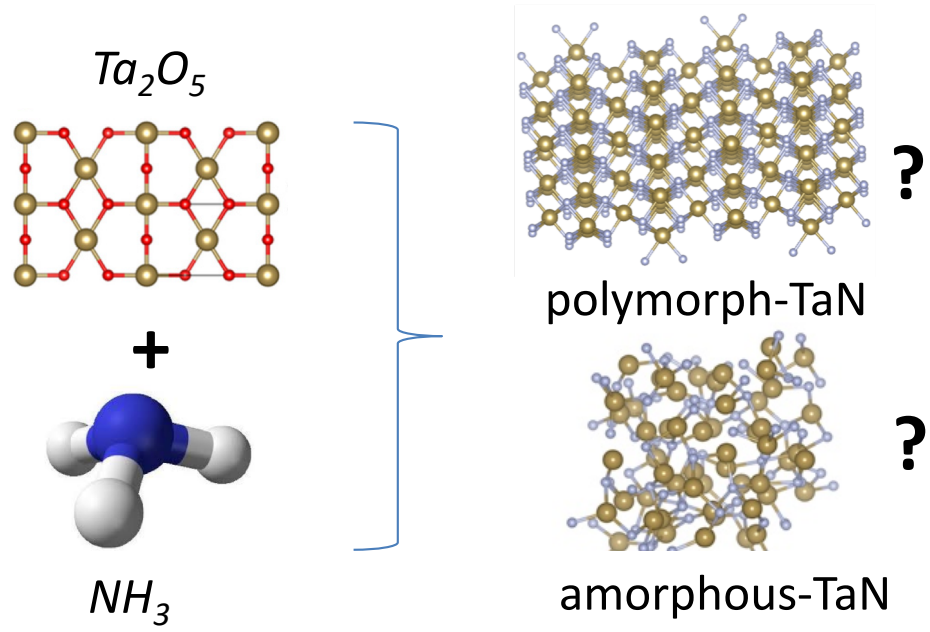
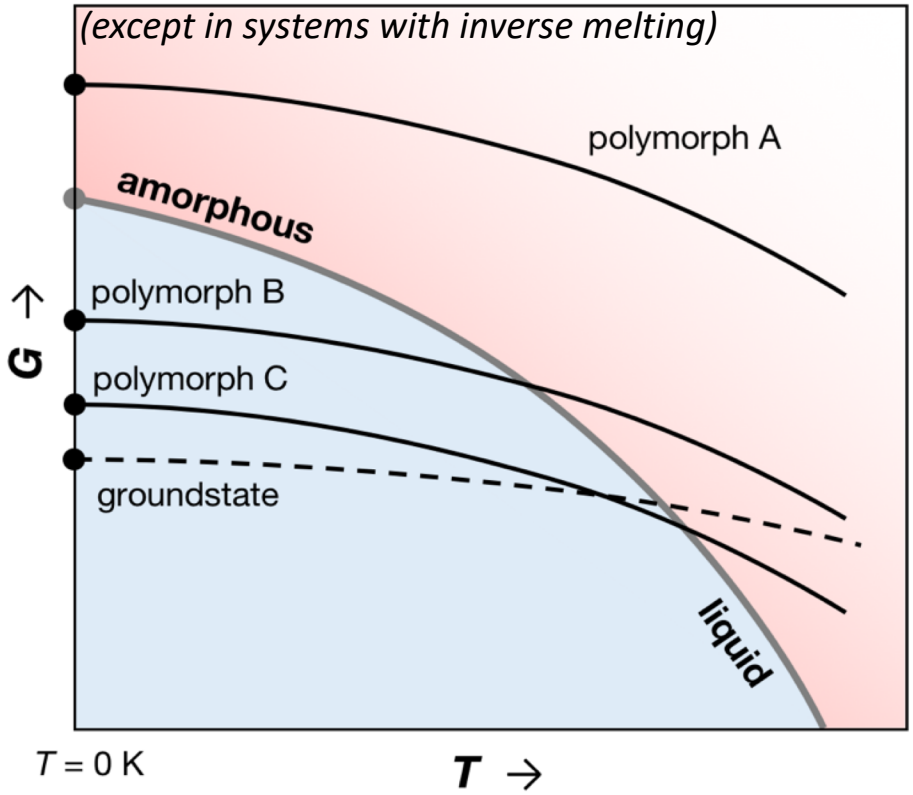
Hypothesis: the amorphous phase is always kinetically possible to form

… Ta_2O_5 nanosized powder was placed in a quartz tube furnace and subjected to nitridation in flowing NH_3 gas at a flow rate o 1 L/min at 8001C for 6 h. J. Am. Ceram. Soc., 88 [12] 3519–3521 (2005)



The liquid-like amorphous state samples largest structural phase space within same stoichiometry (except in systems with inverse melting)



Aykol, Dwaraknath, Sun and Persson, Sci Adv 2018

Hence, an energy limit of polymorph synthesizability at any T is set by the *enthalpy* of the analogous amorphous state

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The synthesizability "skyline"

Chemical sensitivity | Compositional sensitivity | No arbitrary limits | Efficient screening

Aykol, Dwaraknath, Sun and Persson, Sci Adv 2018

Build it and They will Come ?

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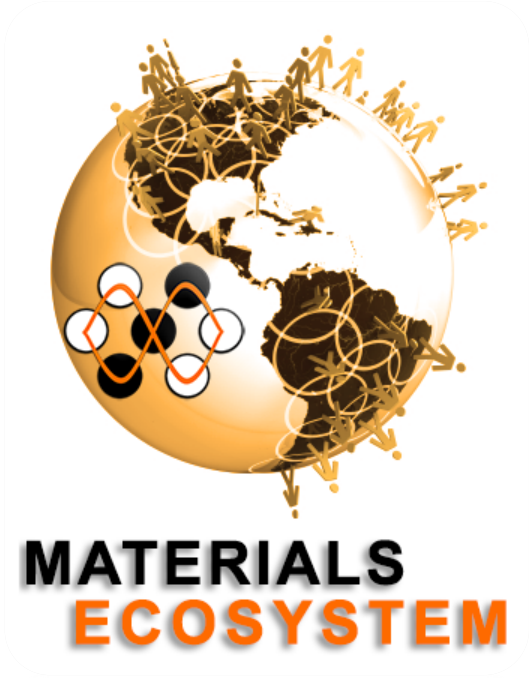
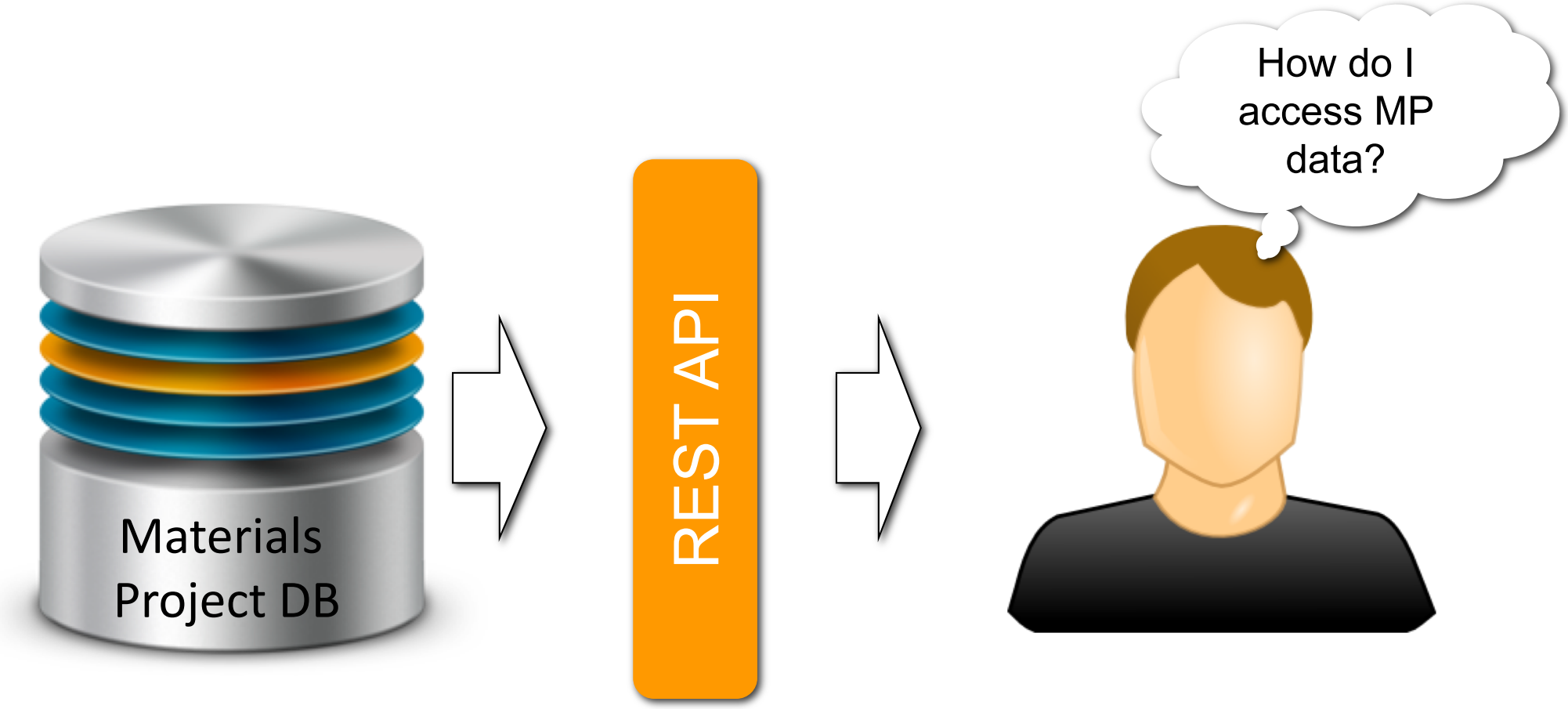


Improved accessibility of data

More developers of analyses and apps

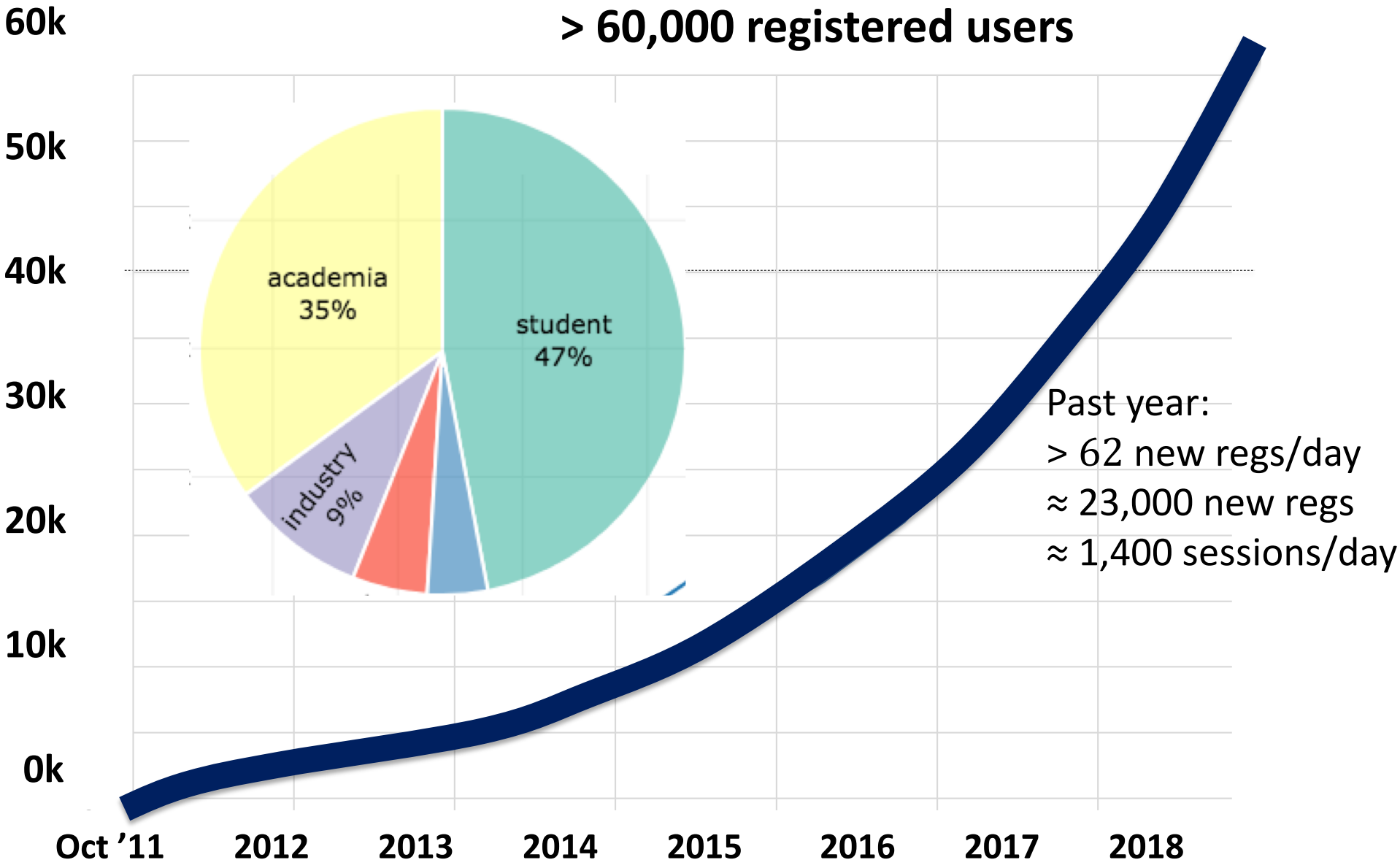
Increased data value

Materials Project REST API

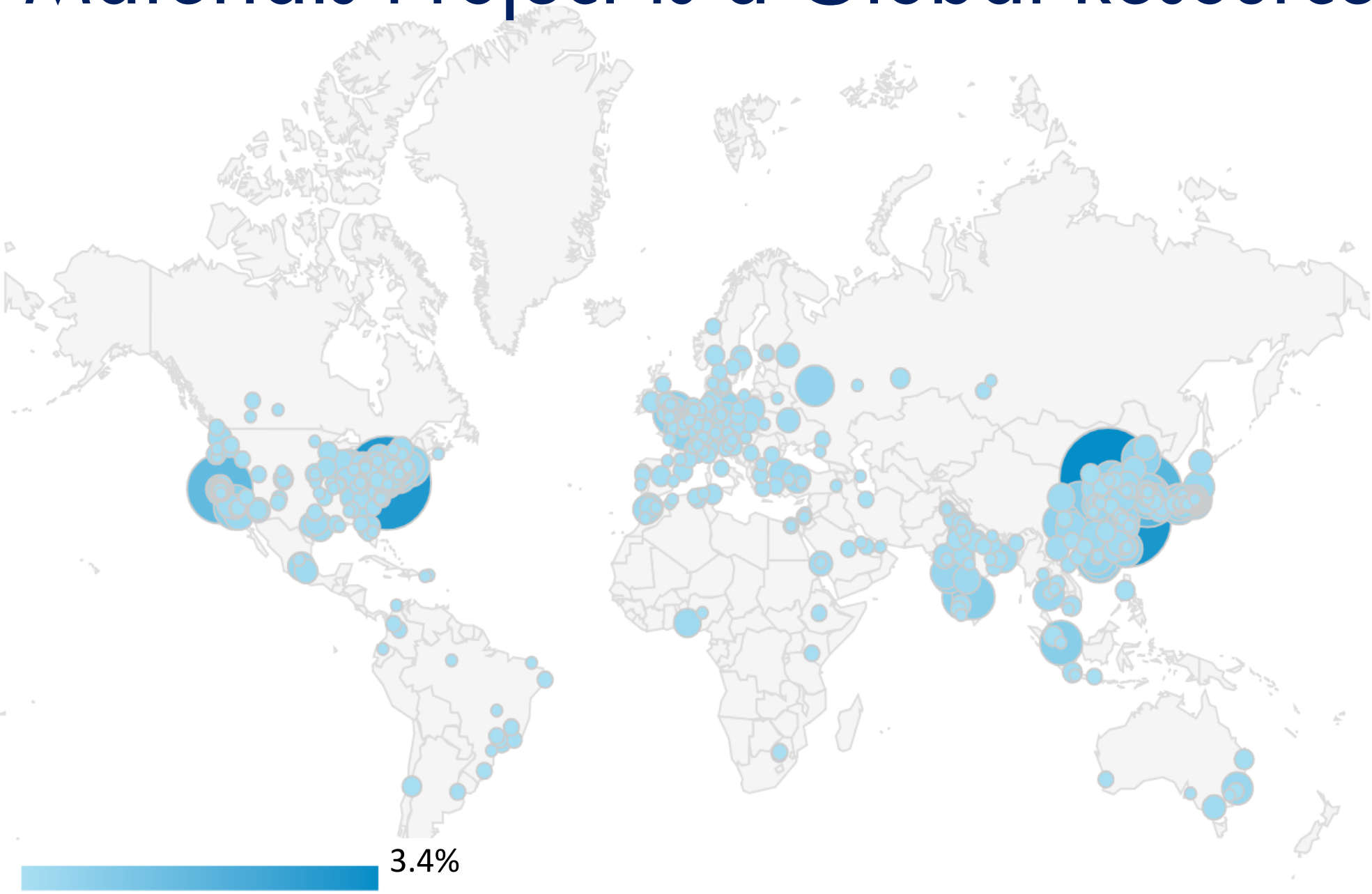


> 160M requests served in last year

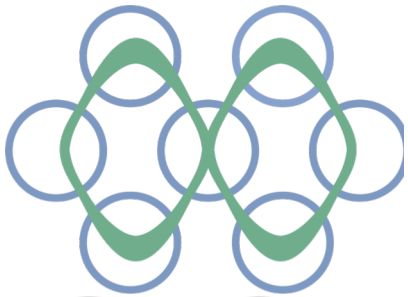
Rapidly Increasing Users



Materials Project is a Global Resource



- *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 !

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)