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# The Materials Project – A Public Materials Design Platform

Kristin Persson

*Lawrence Berkeley National Laboratory*

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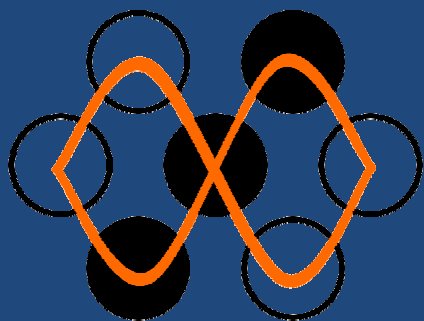
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## Recommended Citation

Kristin Persson, "The Materials Project – A Public Materials Design Platform" in "Harnessing The Materials Genome: Accelerated Materials Development via Computational and Experimental Tools", J.-C. Zhao, The Ohio State Univ.; M. Asta, Univ. of California Berkeley; Peter Gumbsch Institutsleiter Fraunhofer-Institut fuer Werkstoffmechanik IWM; B. Huang, Central South University Eds, ECI Symposium Series, (2013). [http://dc.engconfintl.org/materials\\_genome/11](http://dc.engconfintl.org/materials_genome/11)

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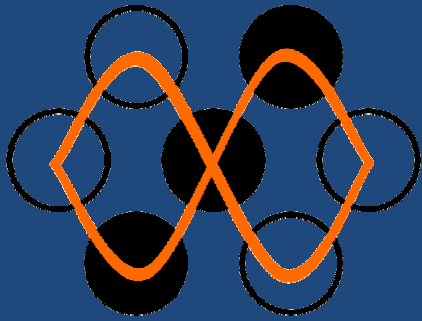
# The Materials Project – A Public Materials Design Platform

Kristin Persson

Lawrence Berkeley National Laboratory

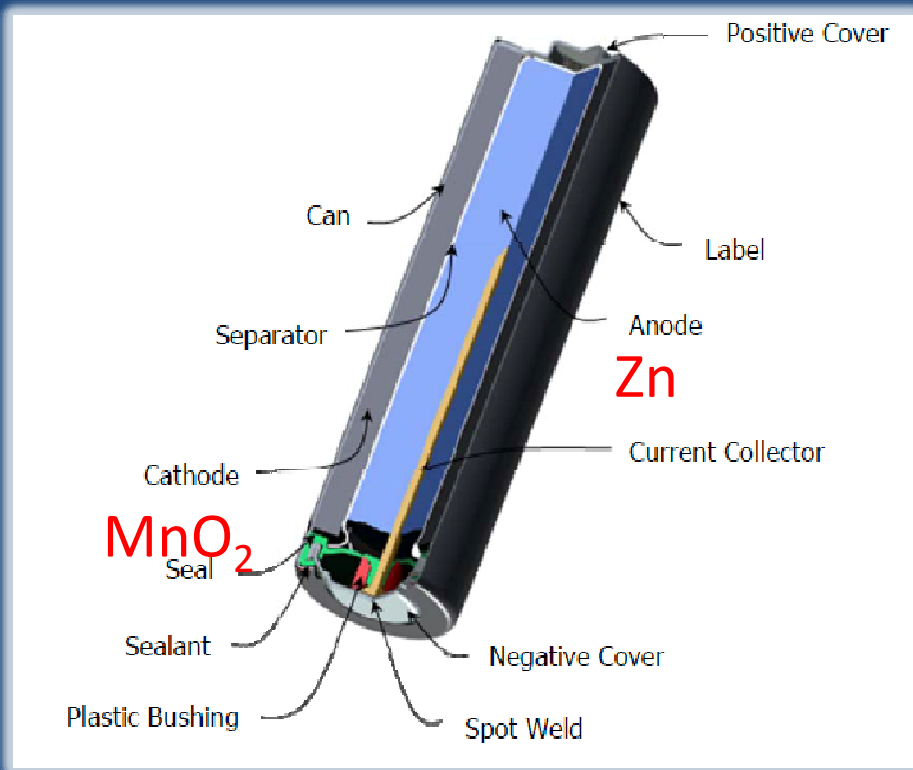
# Outline

- Materials Design for Cathodes
- The Public Platform: [www.materialsproject.org](http://www.materialsproject.org)
  - Pymatgen
  - The Materials API
  - Example Collaborations
- The Vision



# Example: Materials Design for Cathodes

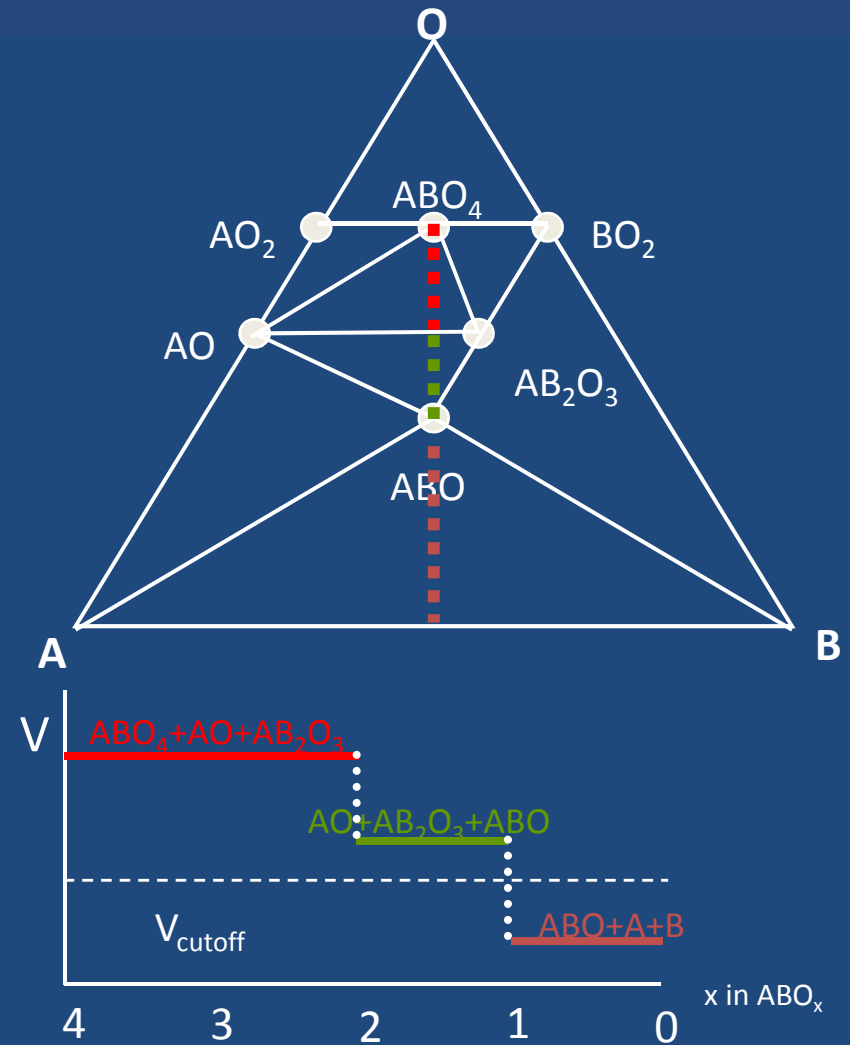
# Finding a better alkaline cathode



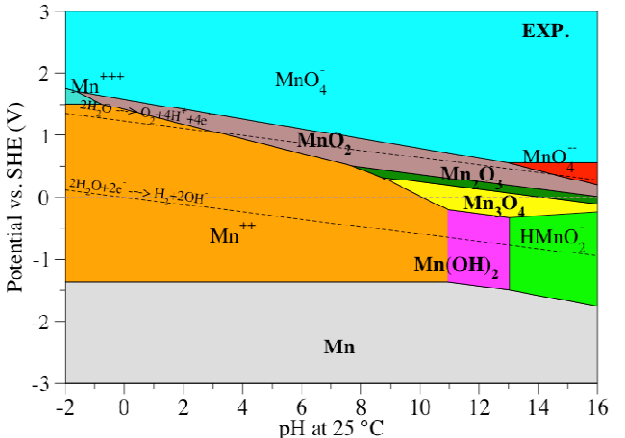
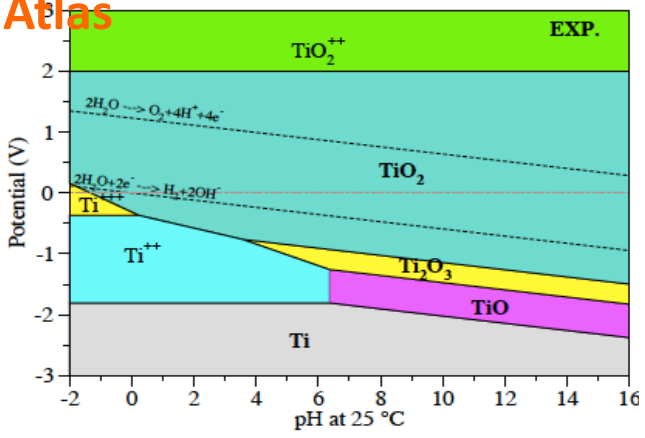
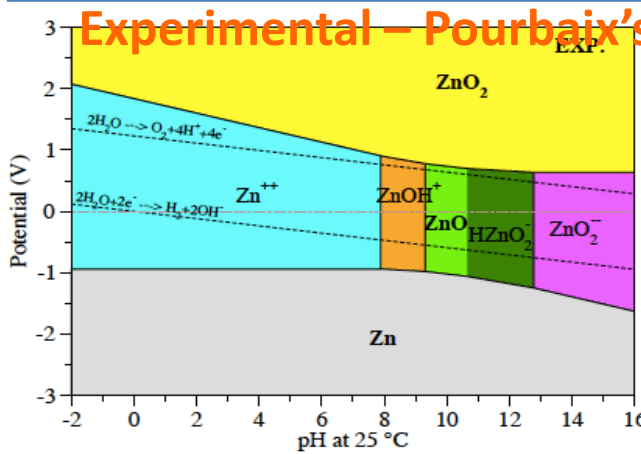
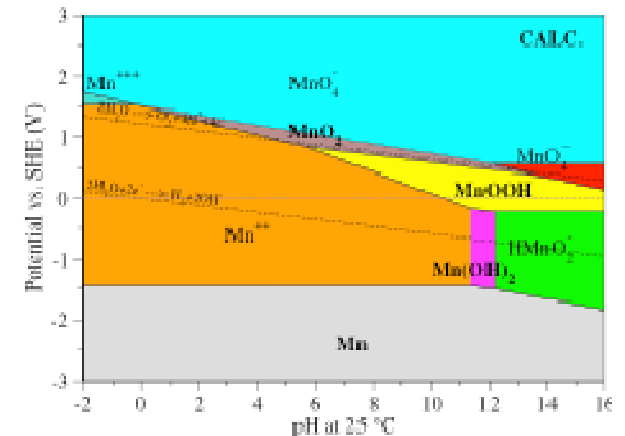
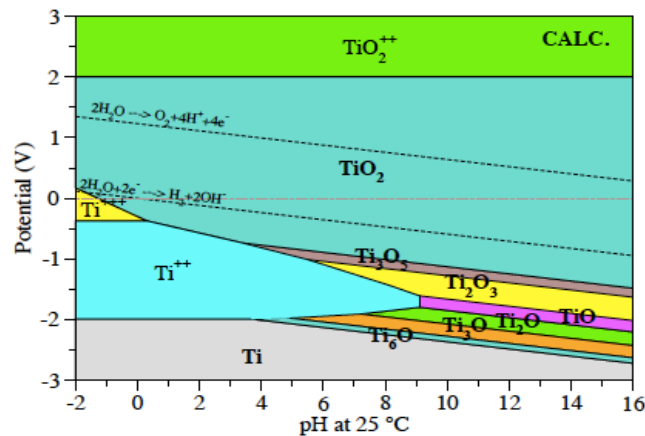
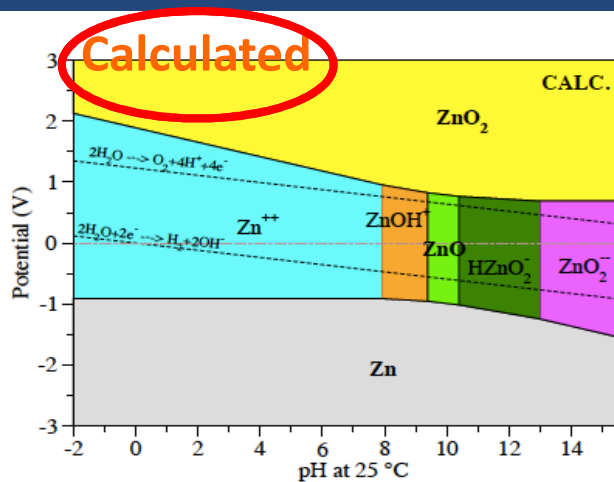
## SPECS:

Higher energy density

Both reactants and products stable in high molar KOH

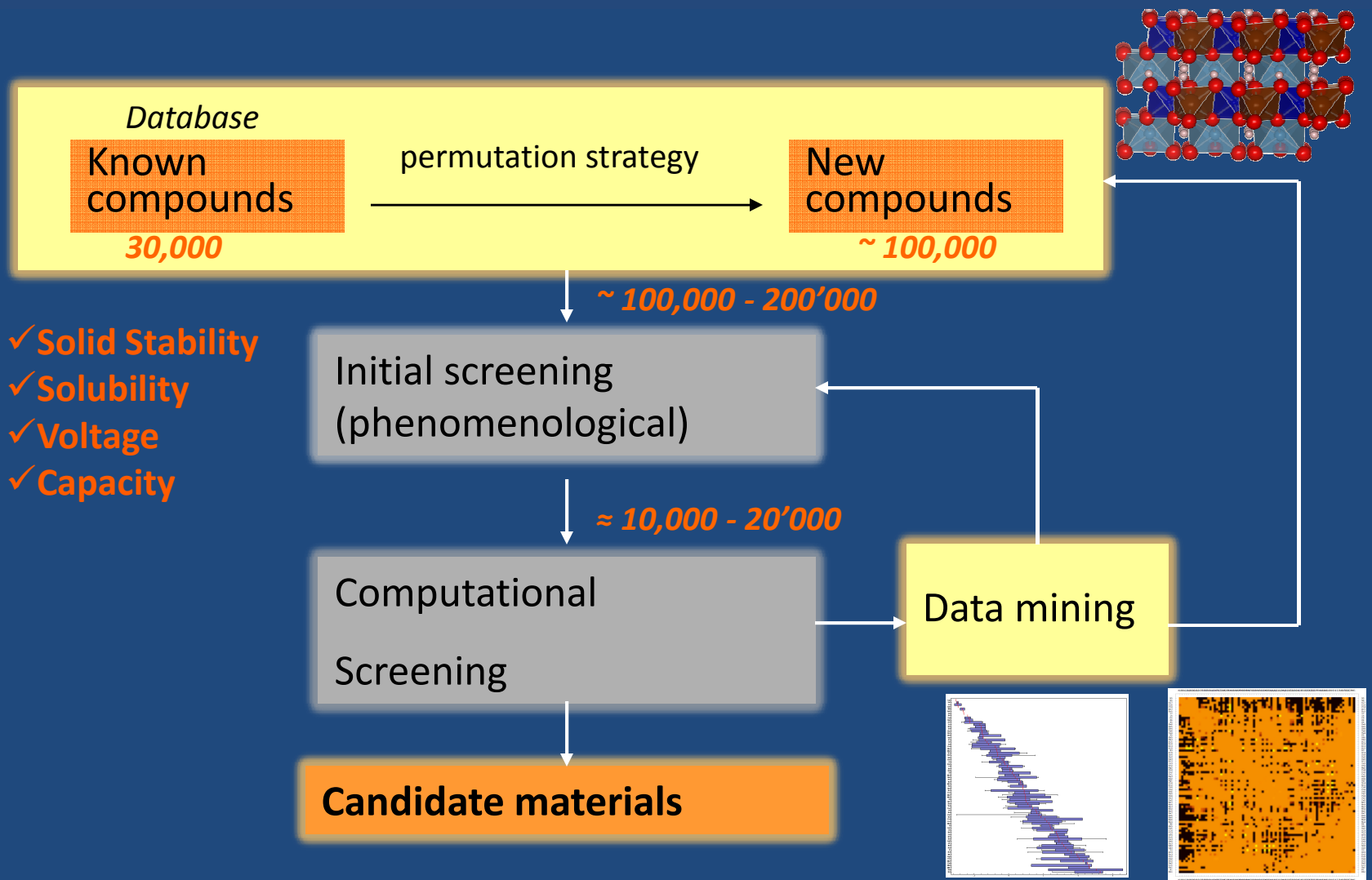


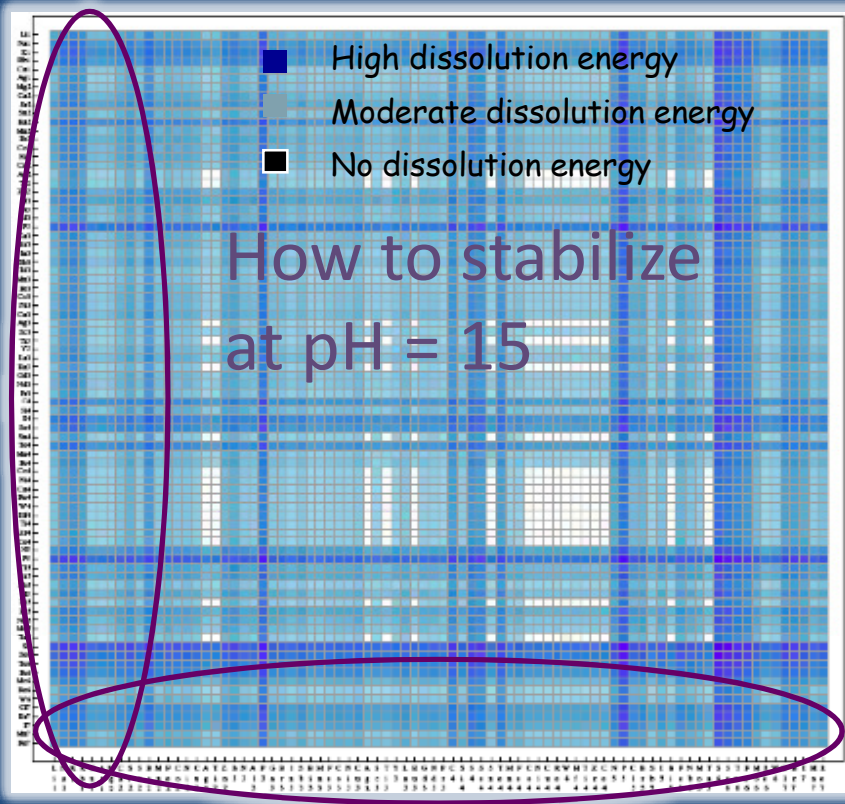
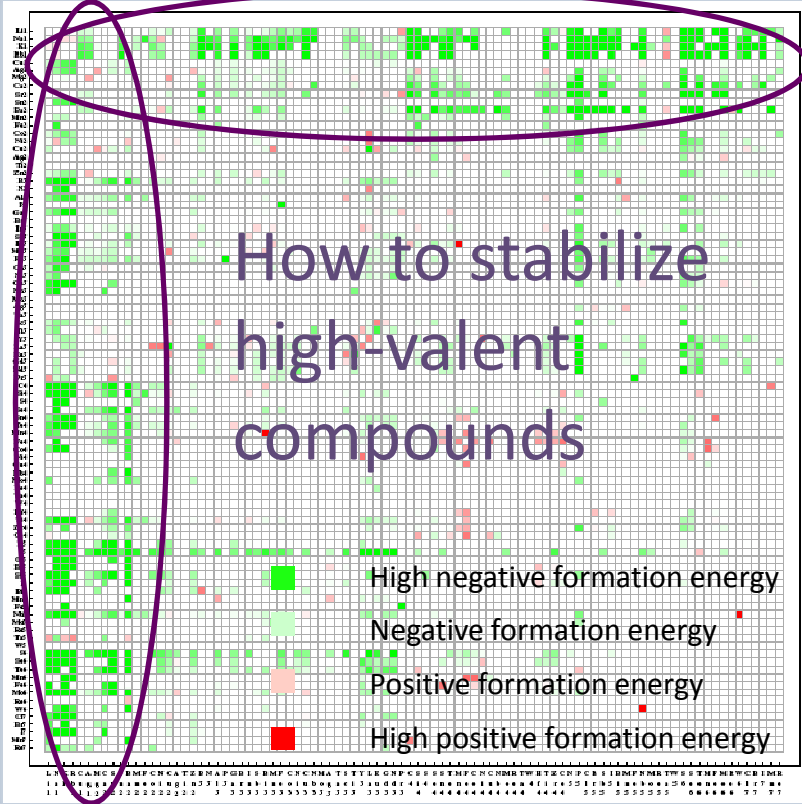
# Calculating solid stability in water



Persson et al, PHYSICAL REVIEW B, 005400 (2012), Prediction of solid-aqueous equilibria: Scheme to combine first-principles calculations of solids with experimental aqueous states

# The Screening Strategy





**Design rules: how to stabilize high energy compounds, which corrosion-resistant elements to add...**



# The winners

> 130,000 compounds considered

- 30,000 known from ICSD
- > 100,000 new generated

Tier 1



> 1500 compounds

- ✓ Capacity > 1 Ah/cc
- ✓ 1.1 V < Ave voltage < 2.2 V
- ✓ Energy density > 1.7Wh/cc

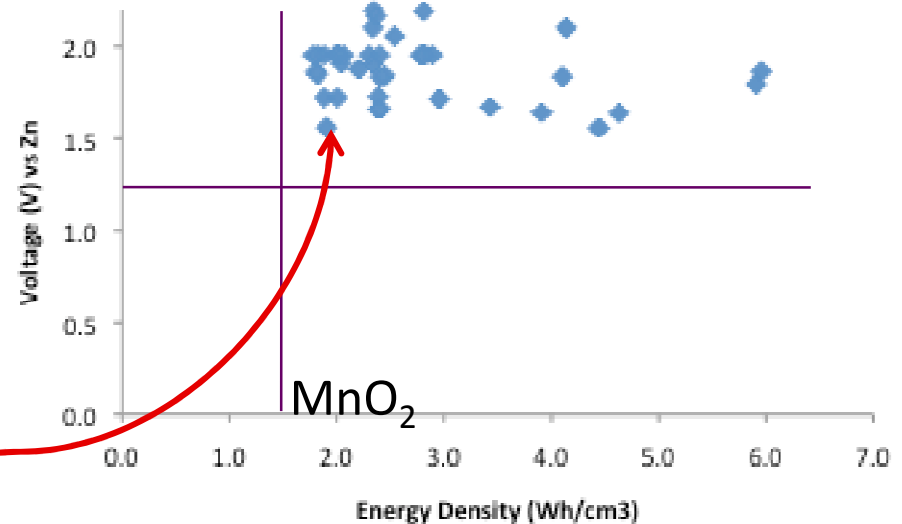
Tier 2



≈ 200 compounds

- ✓ Reactant stable in air
- ✓ Reactant stable in 9N KOH
- ✓ Product stable in 9N KOH

Predicted alkaline cathode material performance



Several patents filed by Duracell

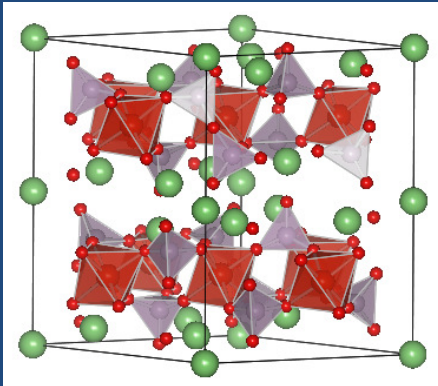
Bit Ni<sup>4+</sup>

(12) United States Patent Eylem et al.	(10) Patent No.: US 7,972,726 B2	(10) Patent No.: US 2011/0223493 A1
(45) Date of Patent: Jul. 5, 2011	(45) Date of Patent: Jul. 5, 2011	(40) Pub. Date: Sep. 15, 2011
(54) PRIMARY ALKALINE BATTERY CONTAINING PENTAVALENT METAL OXIDES	(57) ABSTRACT A primary battery includes a cathode having a non-metallic-oxide metal oxide including pentavalent Ni, Mn, Co, Cr, or a combination thereof, a separator, an anode, and a liquid electrolyte.	(57) ABSTRACT A primary battery includes a cathode having a non-metallic-oxide metal oxide including pentavalent Ni, Mn, Co, Cr, or a combination thereof, a separator, an anode, and a liquid electrolyte.
(75) Inventors: Caiti Eylem, Burlington, MA (US); Paul A. Christian, Norton, MA (US); Yichun Wang, West Roxbury, MA (US); Joseph E. Santostano, IV, Merrimack, NH (US); In Tae Bae, Wrentham, MA (US)	(75) Inventors: Caiti Eylem, Burlington, MA (US); Paul A. Christian, Norton, MA (US); Yichun Wang, West Roxbury, MA (US); Joseph E. Santostano, IV, Merrimack, NH (US); In Tae Bae, Wrentham, MA (US)	(75) Inventors: Caiti Eylem, Burlington, MA (US); Paul A. Christian, Norton, MA (US); Yichun Wang, West Roxbury, MA (US); Joseph E. Santostano, IV, Merrimack, NH (US); In Tae Bae, Wrentham, MA (US)
(73) Assignee: The Gillette Company, Boston, MA (US)	(73) Assignee: The Gillette Company, Boston, MA (US)	(73) Assignee: The Gillette Company, Boston, MA (US)
(*) Notice: Subject to any disclaimer, the term patent is extended or adjusted under 35 U.S.C. 154(b) by 1207 days.	(*) Notice: Subject to any disclaimer, the term patent is extended or adjusted under 35 U.S.C. 154(b) by 1207 days.	(*) Notice: Subject to any disclaimer, the term patent is extended or adjusted under 35 U.S.C. 154(b) by 1207 days.
(21) Appl. No.: 11/484,550	(21) Appl. No.: 11/484,550	(21) Appl. No.: 12/722,649
(22) Filed: Jul. 10, 2006	(22) Filed: Jul. 10, 2006	(22) Filed: Mar. 12, 2010
(51) Int. Cl. H01M 4/48 (2010.01) H01M 4/50 (2010.01) H01M 4/54 (2010.01) H01M 4/52 (2010.01) H01M 2/36 (2010.01)	(51) Int. Cl. H01M 4/48 (2010.01) H01M 4/50 (2010.01) H01M 4/54 (2010.01) H01M 4/52 (2010.01) H01M 2/36 (2010.01)	(51) Int. Cl. H01M 4/48 (2010.01) H01M 4/50 (2010.01) H01M 4/54 (2010.01) H01M 4/52 (2010.01) H01M 2/36 (2010.01)
(52) U.S. Cl. 429/218.1; 429/224; 429/223; 429/219; 429/231.6; 429/221; 429/220; 429/231.E; 429/145	(52) U.S. Cl. 429/218.1; 429/224; 429/223; 429/219; 429/231.6; 429/221; 429/220; 429/231.E; 429/145	(52) U.S. Cl. 429/218.1; 429/224; 429/223; 429/219; 429/231.6; 429/221; 429/220; 429/231.E; 429/145
(58) Field of Classification Search None See application file for complete search history.	(58) Field of Classification Search None See application file for complete search history.	(58) Field of Classification Search None See application file for complete search history.
(56) References Cited U.S. PATENT DOCUMENTS 2,809,253 A 10/1977 Moshore et al. 2,828,350 A 11/1958 Rhyne, Jr.	(56) References Cited U.S. PATENT DOCUMENTS 2,809,253 A 10/1977 Moshore et al. 2,828,350 A 11/1958 Rhyne, Jr.	(56) References Cited U.S. PATENT DOCUMENTS 2,809,253 A 10/1977 Moshore et al. 2,828,350 A 11/1958 Rhyne, Jr.
(59) FOREIGN PATENT DOCUMENTS US 2008/0080937 A1 Jun. 10, 2008	(59) FOREIGN PATENT DOCUMENTS EP 0 127 134 12/1984 (Continued)	(59) FOREIGN PATENT DOCUMENTS EP 0 127 134 12/1984 (Continued)
(59) OTHER PUBLICATIONS Miquant et al., "Synthesis and Structural Studies of the A-Site Substituted Bismuth Oxide Perovskites, Bi <sub>1-x</sub> A <sub>x</sub> O <sub>3</sub> (A = Ca, Sr, Ba), vol. 17, pp. 1905-1909, 2005.	(59) OTHER PUBLICATIONS Miquant et al., "Synthesis and Structural Studies of the A-Site Substituted Bismuth Oxide Perovskites, Bi <sub>1-x</sub> A <sub>x</sub> O <sub>3</sub> (A = Ca, Sr, Ba), vol. 17, pp. 1905-1909, 2005.	(59) OTHER PUBLICATIONS Miquant et al., "Synthesis and Structural Studies of the A-Site Substituted Bismuth Oxide Perovskites, Bi <sub>1-x</sub> A <sub>x</sub> O <sub>3</sub> (A = Ca, Sr, Ba), vol. 17, pp. 1905-1909, 2005.
(59) Primary Examiner: Barbara L. Gilliam Assistant Examiner: Angela J. Martin (74) Attorney, Agent, or Firm: Fish & Richardson P.C.	(59) Primary Examiner: Barbara L. Gilliam Assistant Examiner: Angela J. Martin (74) Attorney, Agent, or Firm: Fish & Richardson P.C.	(59) Primary Examiner: Barbara L. Gilliam Assistant Examiner: Angela J. Martin (74) Attorney, Agent, or Firm: Fish & Richardson P.C.
(57) ABSTRACT Primary alkaline batteries containing pentavalent bismuth metal oxides are disclosed.	(57) ABSTRACT Primary alkaline batteries containing pentavalent bismuth metal oxides are disclosed.	(57) ABSTRACT Primary alkaline batteries containing pentavalent bismuth metal oxides are disclosed.
16 Claims, 11 Drawing Sheets	16 Claims, 11 Drawing Sheets	16 Claims, 11 Drawing Sheets

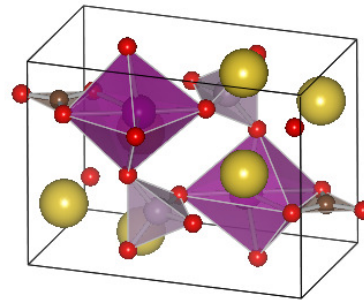
End result – 200 compounds predicted to outperform current cathode AND are predicted stable (through entire reaction) in 9 M KOH

# New Li-ion Cathode Materials Discovered @MIT

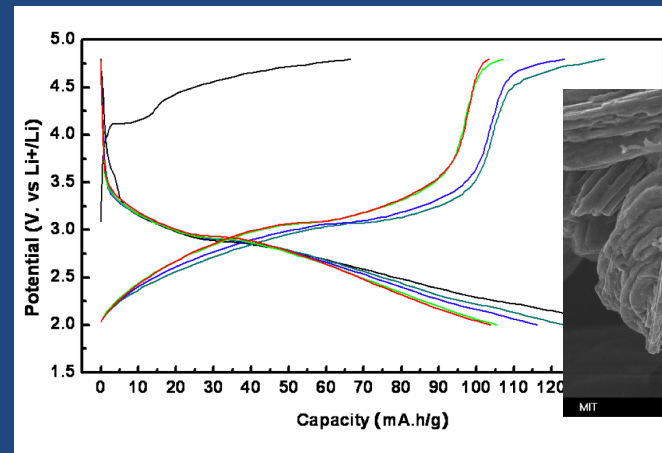
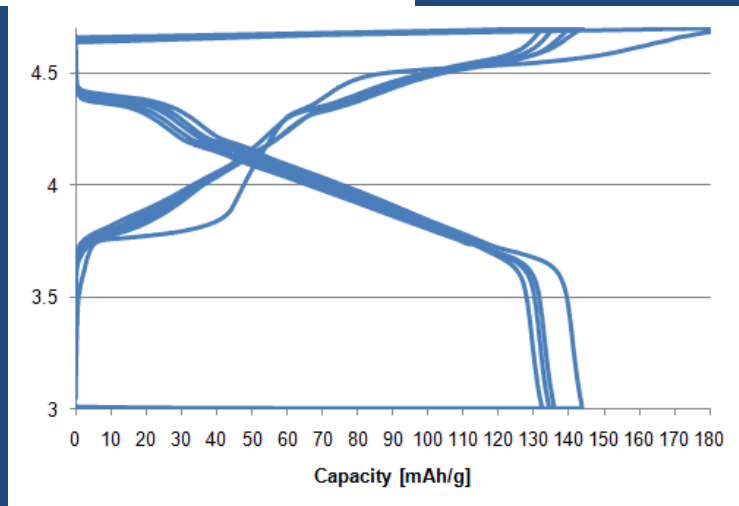
*No Li containing carbon phosphate AT ALL are known in nature !*



New phosphate discovered @MIT through computations



Completely new *class* of materials synthesized based on computational predictions



“Sidorenkites”:  $\text{Li}_3\text{M}(\text{CO}_3)(\text{PO}_4)$  (M = Fe, Mn, Ni, Co)

Courtesy of Ceder et al, MIT



The Public Platform:  
[www.materialsproject.org](http://www.materialsproject.org)

Fill in 'missing' **property data** on inorganic compounds

Assist researchers in **predicting new materials**

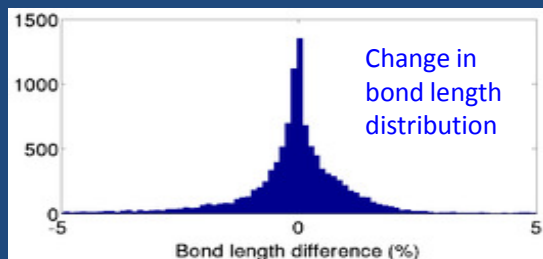
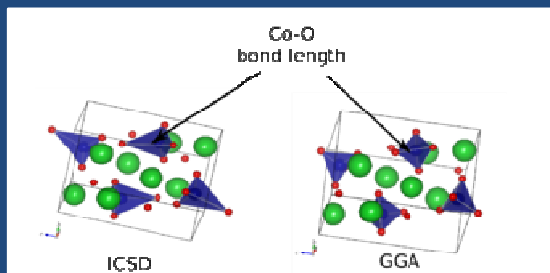
Provide **interactive analysis tools** and codes

Enable rapid screening and **data mining**



# Accuracy

Benchmarking (dV, bond length, enthalpy, ...)  
error checking



<https://materialsproject.org/wiki/>

Home Apps Support About References Profile for kaperrson@lbl.gov :: Log

## SrMg

Warnings: volume change > 20% [?]

Edit xtal Mg-Sr PD CIF

Material ID	510407
ICSD ID	642865
Unit cell formula	Sr <sub>1</sub> Mg <sub>1</sub>
Formation energy / atom	-0.0625 eV
Energy above hull	0.0181 eV
Decomposes to	SrMg <sub>2</sub> + Sr
Final magnetic moment	0.0034 $\mu_B$
Final volume	73.87 $\text{Å}^3$
Final density	2.52 g/cm <sup>3</sup>
Run type	GGA [?]
Related tasks	510407 2564

Report issues

### Space Group

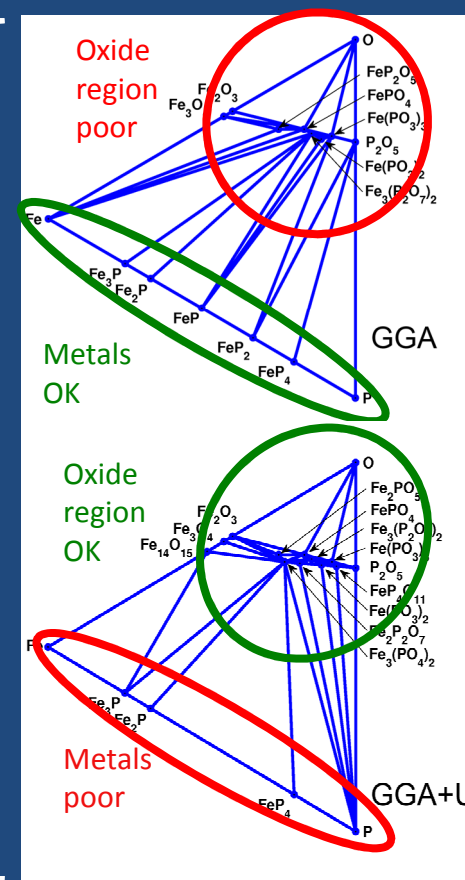
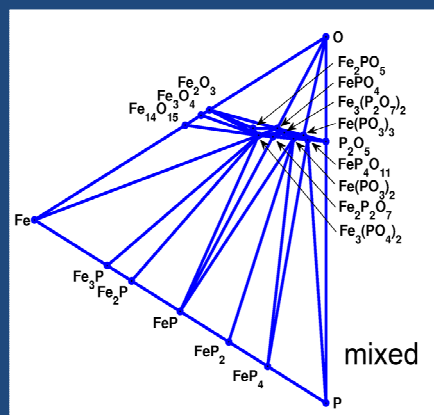
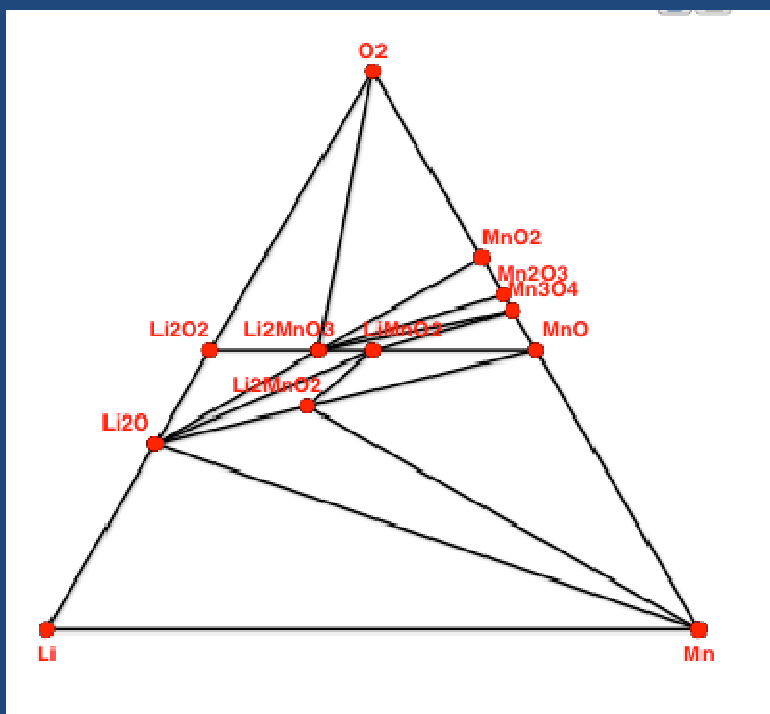
Crystal system	cubic
Number	221
Hermann Mauguin	Pm3m [?]
Hall	-P 4 2 3
Point group	m3m

HM: P 1  
a=4.196Å  
b=4.196Å  
c=4.196Å  
 $\alpha=90.0^\circ$   
 $\beta=90.0^\circ$   
 $\gamma=90.0^\circ$

Space Filling:  off  20%  100%  polyhedra  
Spin:  off  around x axis  around y axis  
Reset to original orientation  
Background color: white

The screenshot shows the Materials Project website interface for the SrMg material. It includes a navigation bar, a warning about volume change, a table of material properties, space group information, and a 3D visualization of the crystal structure with various controls for space filling, spin, and background color.

# Data Compatibility between data sets



Jain et al, *Formation Enthalpies by mixing GGA and GGA+U Calculations*, Physical Review B **84**, 045115 (2011).

# Leveraging the community

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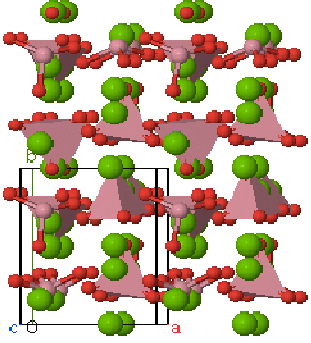
## Ba<sub>2</sub>CoO<sub>4</sub>

Edit xtal Ba-Co-O PD CIF

Material ID	19625
ICSD ID	92321
Unit cell formula	Ba <sub>2</sub> Co <sub>4</sub> O <sub>16</sub>
Formation energy / atom	-2.3808 eV
Energy above hull	0.0000 eV
Decomposes to	Ba <sub>2</sub> CoO <sub>4</sub>
Final magnetic moment	20.0000 μ <sub>B</sub>
Final volume	494.50 Å <sup>3</sup>
Final density	5.34 g/cm <sup>3</sup>
Run type	GGA+U [?]
Related tasks	19625

Report Issues

HM: P 1  
a=6.095Å  
b=7.703Å  
c=10.546Å  
α=90.0°  
β=92.9°  
γ=90.0°



Crystal system: monoclinic  
Number: 14

### 0 comments



★ 0 Stars

Leave a message...

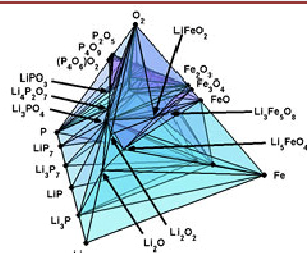
Discussion | Community | My Disqus

TOP DISCUSSIONS ON MATERIALS GENOME

TOP COMMENTERS

-  **Kristin Persson**  
1 comment
-  **Shreyas Cholia**  
1 comment

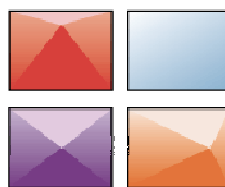
- ❑ Over 26,000 compounds and growing monthly
- ❑ Multiple tools based on computed data



### PhaseDiagramApp

The Phase Diagram App uses density functional database to generate **OK compositional and grand** two to four components. For details of our methodology to the [Phase Diagram App manual](#).

*HTML5-compatible browser recommended, e.g., Chrome, Safari. Non-interactive plots only for IEB.*



### StructurePredictor

Predicting new compounds and their crystal structures is the first step in finding new materials for future technologies. The structure predictor uses data-mined knowledge of experimental crystal data to generate potential new compounds (ionic systems only). **Note:** processing can take several days.



### LithiumBatteryExplorer

The Battery Explorer is a customized tool to search the Materials Project database for lithium battery materials satisfying various critical criteria such as voltage, capacity, stability and energy density. For details and usage tips, please refer to the [Battery Explorer manual](#).

Because of error cancellation, intercalation voltages are expected to be more accurate than conversion voltages.

This app currently contains **214** lithium intercalation compounds and **4158** conversion battery compounds. If you can't find the compound you're looking for, please check back later. We add new ones every week!



### MaterialsExplorer

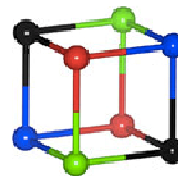
Search for materials information by chemistry, composition, or property.



### ReactionCalculator

The reaction calculator determines energies of solid state reactions using a database of Density Functional Theory calculations. When available, the reaction calculator will also report experimental formation enthalpies for the reaction. For details of our methodology and usage tips, please refer to the [manual](#).

Usage Example: Type "MgO + Al2O3" in the Reactants field and "MgAl2O4" in the Products field and click "Calculate ΔH".



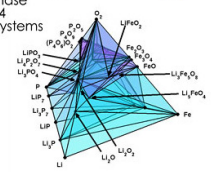
### CrystalToolkit

CrystalToolkit is a structure editor that generates new structures from existing structures in the Materials Project or from an uploaded POSCAR or CIF file. Batch processing of structures is supported.



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**PhaseDiagramApp**  
investigate phase stability for 2-4 component systems



**Phase Diagrams via Density Functional Theory**  
Version 0.3

The Phase Diagram App (PDApp) generates phase diagrams using the Materials Genome database. Compositional and grand potential phase diagrams of up to four compositional components are supported.

Phase diagrams represent the thermodynamic phase equilibria of multicomponent systems and reveal useful insights into fundamental material aspects regarding the processing and reactions of materials.

For the detailed methodology used and usage tips, please refer to the [PDApp manual](#).

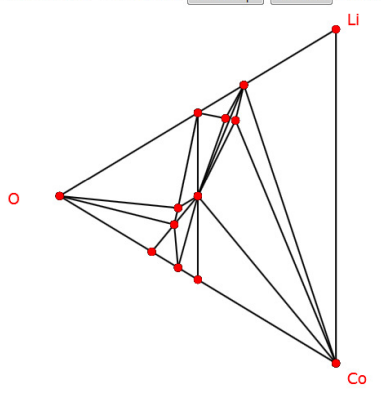
HTML5-compatible browser recommended, e.g., Chrome, Safari, Firefox (3.6 and above) and IE9. Non-interactive plots only for IE8.

Use Examples >

Control Center **Li-Co-O PD**

**Co-Li-O Phase Diagram**

Show Data Table  Show Unstable   [Interpreting PDs](#)



copyright© 2010-11 Materials Genome, db 1.1

Database version 1.1.

Need additional capabilities? E-mail [collaborate\[at\]materialsgenome.org](mailto:collaborate[at]materialsgenome.org)

Questions? E-mail [support\[at\]materialsgenome.org](mailto:support[at]materialsgenome.org)

Phase diagrams  
with available data:

**28,300 SYSTEMS**

Home About Apps Datasets Support Contact

**ReactionCalculator**

The reaction calculator determines energies of solid state reactions using a database of Density Functional Theory calculations. When available, the reaction calculator will also report experimental formation enthalpies for the reaction.

The current database contains computations for over 23,000 solid state materials and experimental data for over 1,000 solid state compounds.

The user must specify a set of reactants and products that are comma-separated. There is no need to balance the reaction.

**Usage Example:**  
In 'Reactants Input', put the text: MgO, Al2O3  
In 'Products Input', put the text: MgAl2O4  
(leave 'Advanced Arguments' blank)

Comprehensive details may be found in the reaction calculator [manual](#).

More information

To cite this implementation of the Reaction Calculator, please see: [A High-Throughput Infrastructure for Density Functional Theory Calculations](#)  
Anubhav Jain  
Geoffroy Hautier  
Charles J. Moore  
Shyue Ping Ong  
Christopher Fischer  
Timothy Mueller  
Kristin Persson  
Kristin Persson  
Gerbrand Ceder  
*Computational Materials Science (to be published)*

Accurate Formation Enthalpies by Mixing GGA and GGA+U calculations  
Anubhav Jain  
Geoffroy Hautier  
Shyue Ping Ong  
Charles J. Moore  
Christopher Fischer  
Kristin Persson  
Gerbrand Ceder  
*(to be submitted)*

**Reactants Input**

**Products Input**

**Advanced Arguments**

**Energy Adjustments** [?]  
 (Default: adjust many gases, mix GGA/GGA+U)

MgO + Al<sub>2</sub>O<sub>3</sub> → MgAl<sub>2</sub>O<sub>4</sub>

ΔE of reaction, (comp., 0K): -0.4024 eV (-38.83 kJ)  
MgO - ΔE<sub>f</sub> -6.173 eV (-595.61 kJ)  
Al<sub>2</sub>O<sub>3</sub> - ΔE<sub>f</sub> -17.1476 eV (-1654.51 kJ)  
MgAl<sub>2</sub>O<sub>4</sub> - ΔE<sub>f</sub> -23.723 eV (-2288.94 kJ)

ΔH of reaction (expt., 298K): -0.369 eV (-35.6 kJ)  
MgO - ΔH<sub>f</sub> -6.2351 eV (-601.6 kJ)  
Source: Cox, J.D., Wagman, D.D., Medvedev, V.A., CODATA Key Values for Thermodynamics, Hemisphere Publishing Corp., New York, 1964, 1.  
Al<sub>2</sub>O<sub>3</sub> - ΔH<sub>f</sub> -17.3673 eV (-1675.7 kJ)  
Source: Cox, J.D., Wagman, D.D., Medvedev, V.A., CODATA Key Values for Thermodynamics, Hemisphere Publishing Corp., New York, 1964, 1.  
MgAl<sub>2</sub>O<sub>4</sub> - ΔH<sub>f</sub> -23.9713 eV (-2312.9 kJ)  
Source: O. Kubaschewski, C. Alcock, P. Spencer, Materials Thermochemistry, 6th ed., Oxford, Pergamon Press, 1993.

Database version 1.1.

Need additional capabilities? E-mail [collaborate\[at\]materialsgenome.org](mailto:collaborate[at]materialsgenome.org)

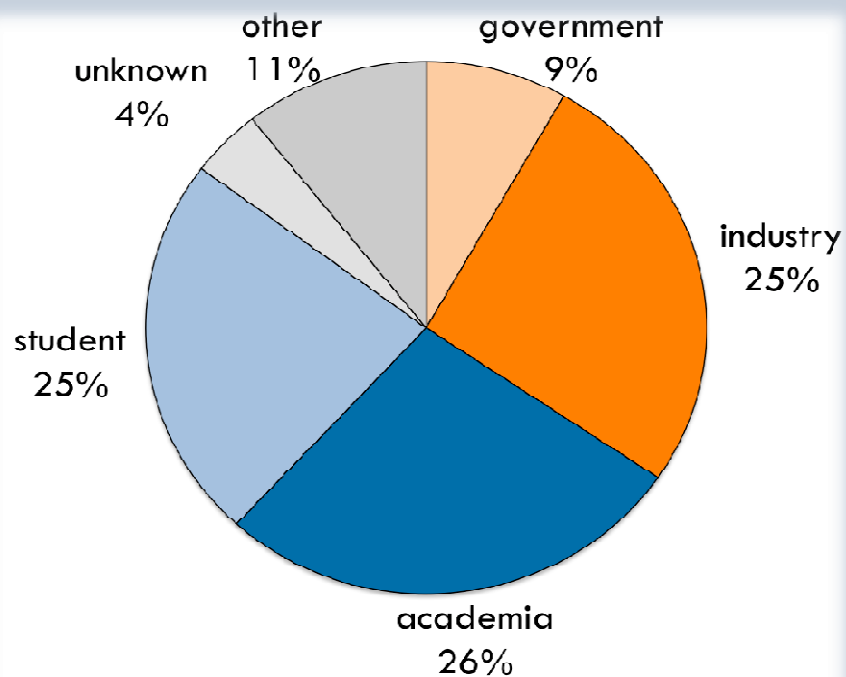
Questions? E-mail [support\[at\]materialsgenome.org](mailto:support[at]materialsgenome.org)

Reaction energies  
already available online:

**>35,000 REACTIONS**

Most measured materials data is of order of 10<sup>2</sup> – elastic constants, band gaps etc...

Launched Oct 2011



- > 7000 phase diagrams generated
- > 1,300 structure prediction requests
- > 2,800 registered users



Lawrence Berkeley National Laboratory

Kristin Persson  
Anubhav Jain  
Daniel Gunter  
Maciej Haranszyk  
Wei Chen



MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Gerbrand Ceder  
Shyue Ping Ong



National Energy Research Scientific Computing Center

David Skinner  
Shreyas Cholia  
Jack Deslippe



University of California, Berkeley

Mark Asta



Stefan Adams



THE UNIVERSITY OF WISCONSIN MADISON

Dane Morgan



Stefano Curtarolo

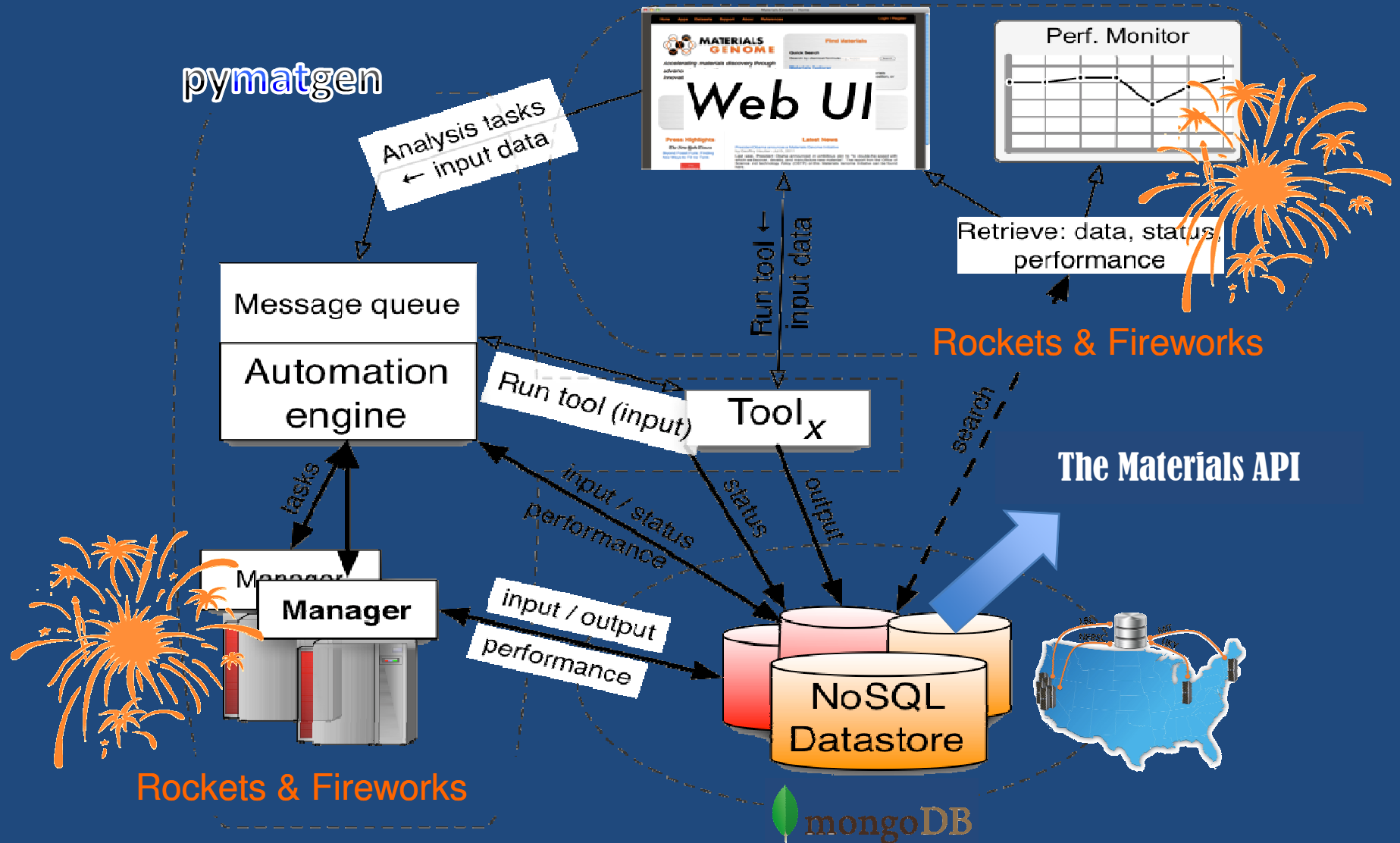


Alan Dozier  
Raphael Fink

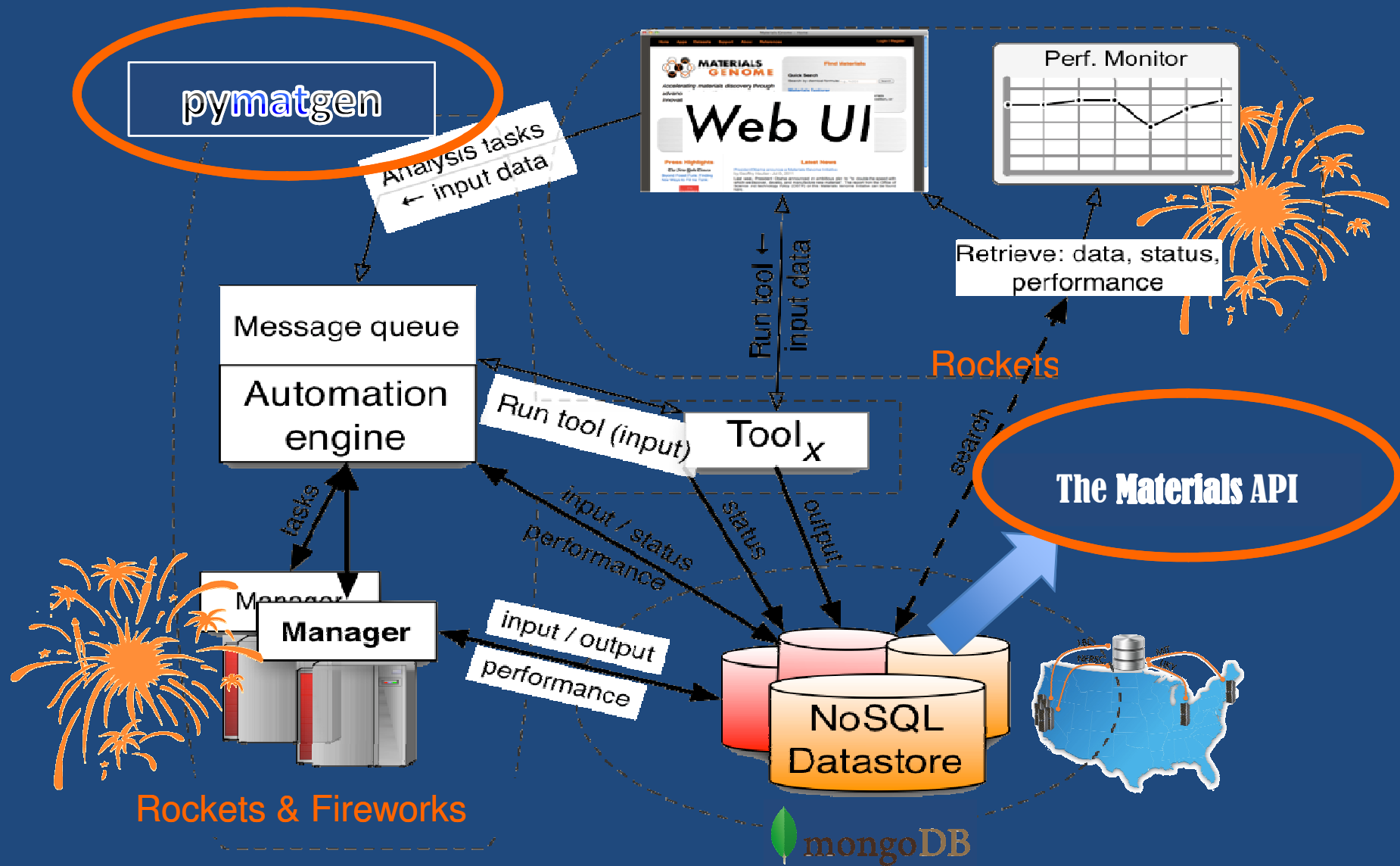
UCL  
Université Catholique de Louvain, Belgium

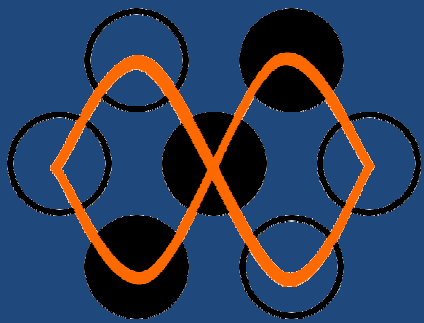
Geoffroy Hautier

# Large Software Infrastructure Structure



# Large Software Infrastructure Structure



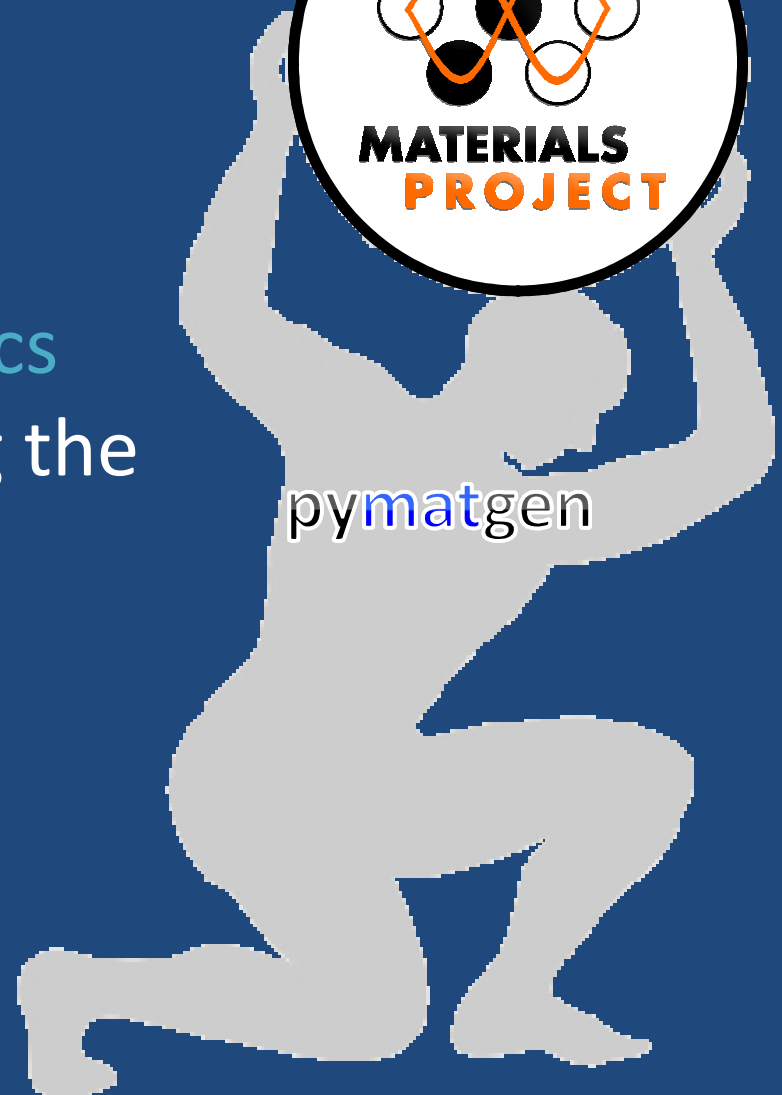


Pymatgen

python materials genomics  
is the codebase powering the  
Materials Project.

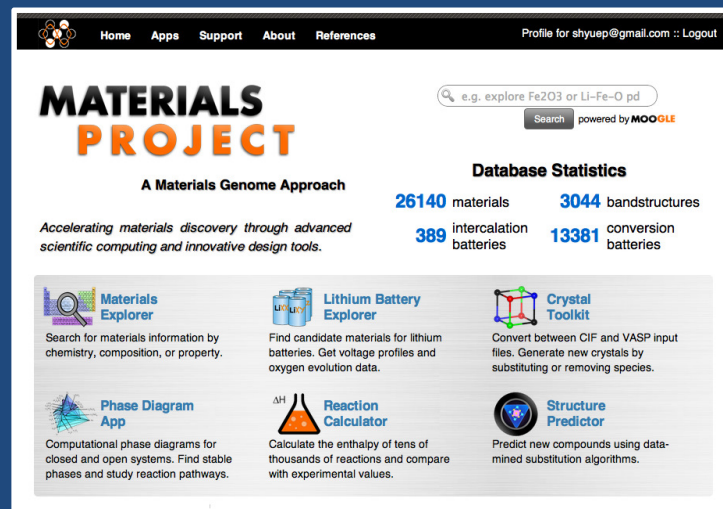


py**mat**gen





Or sql ☺



django

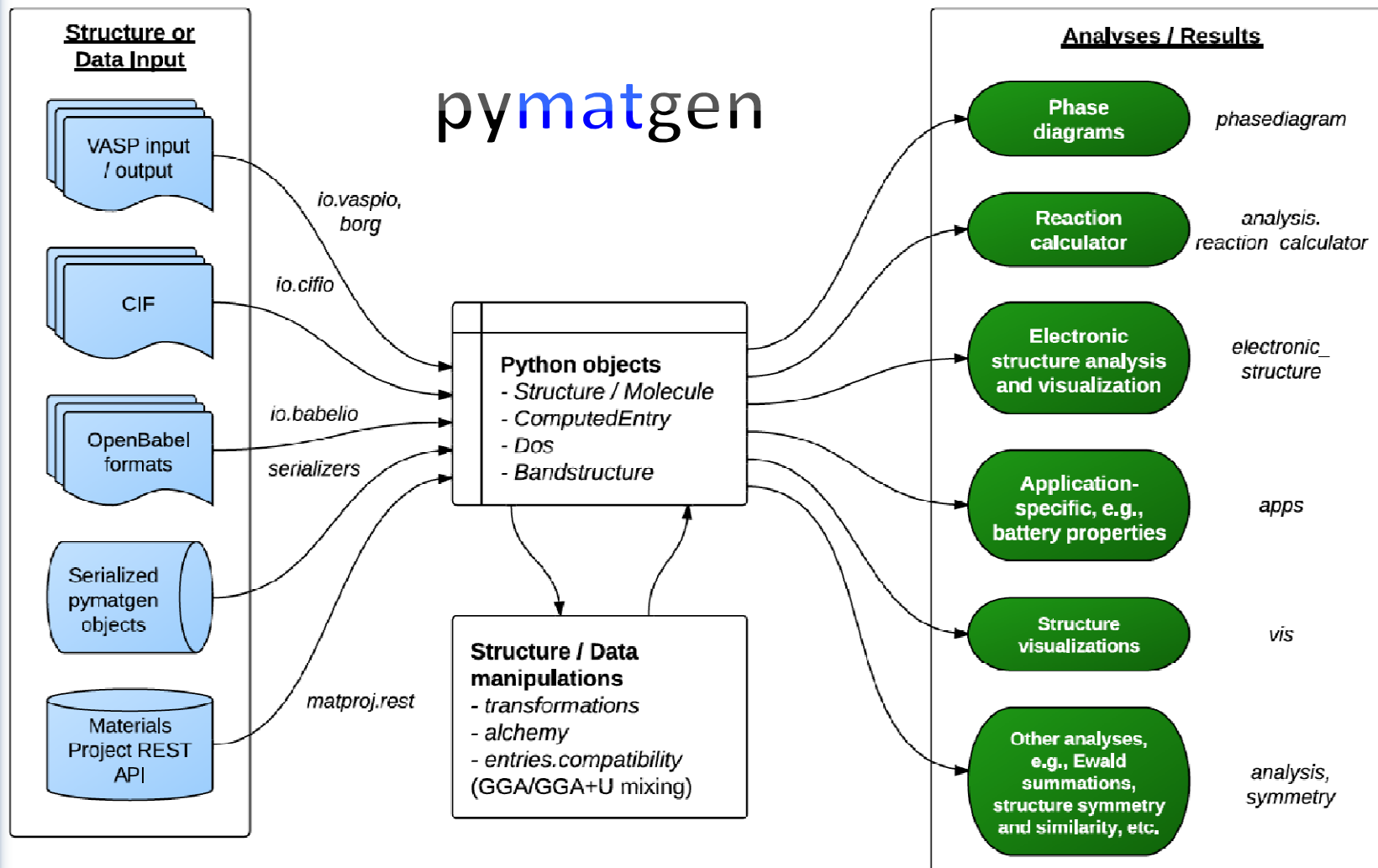
pymatpro

- Database interface
- Run management (fireworks)

pymatgen

Defines core **extensible** Python objects for materials data representation.

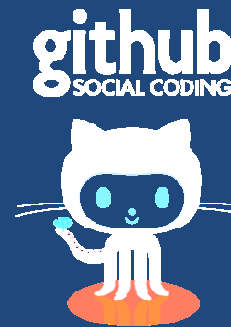
# pymatgen







pymatgen is managed via

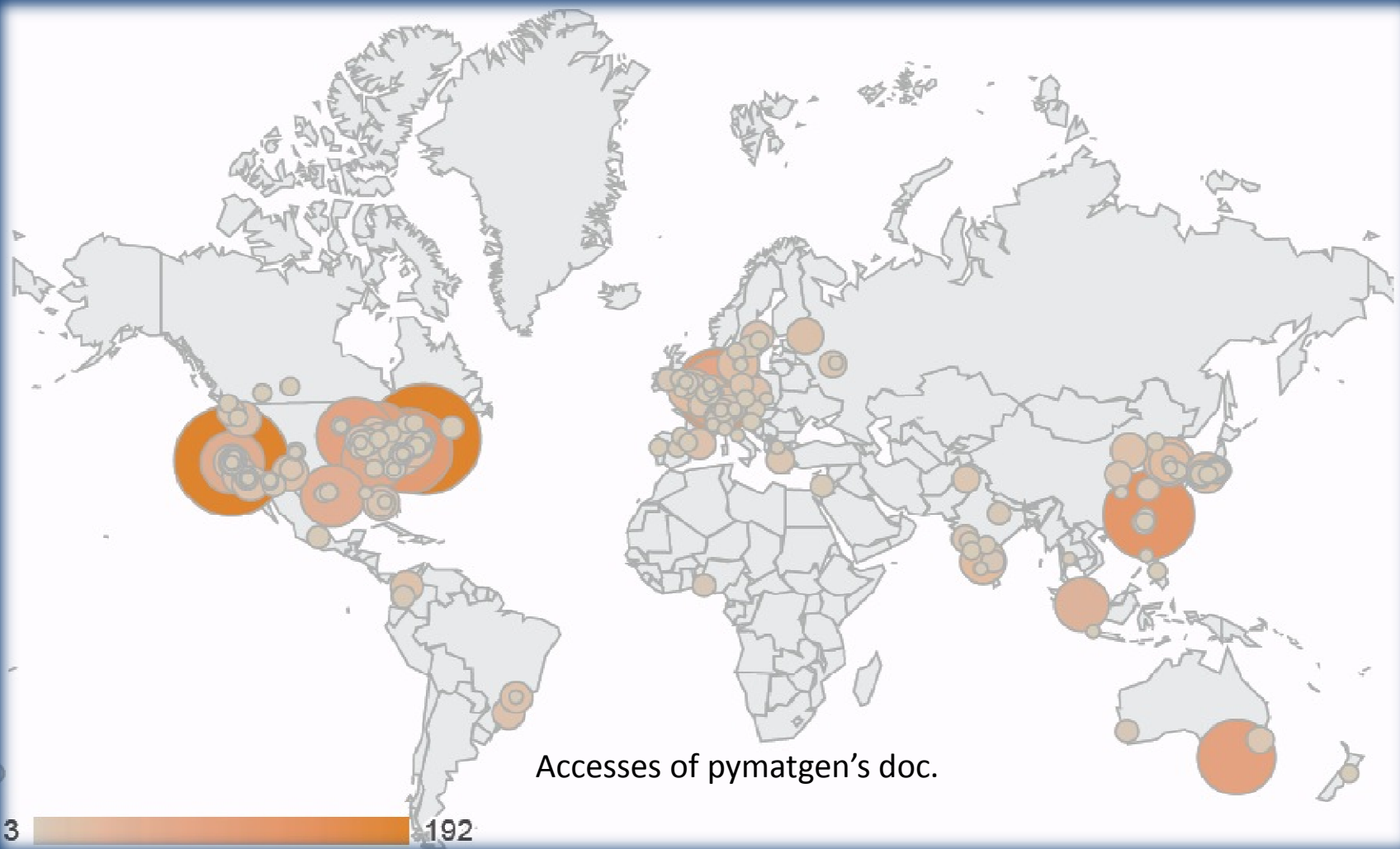


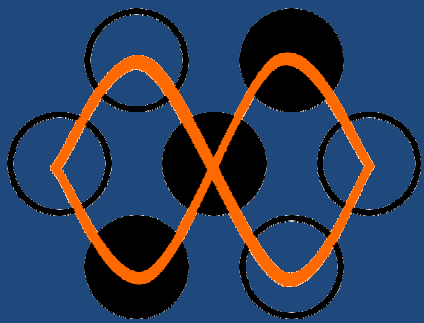
Licensed under the MIT license

Stable versions are available on the popular Python Package Index (PyPI) at

<http://pypi.python.org/pypi/pymatgen>

# pymatgen global





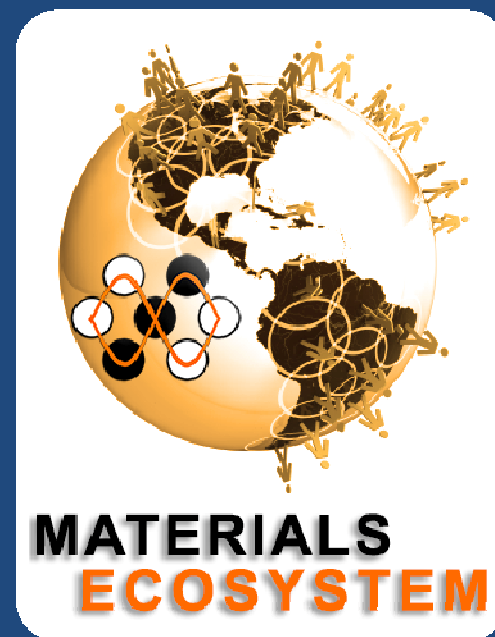
# The Materials API

# The Materials API

An **open** platform for accessing Materials Project data based on REpresentational State Transfer (REST) principles

**Flexible and scalable** to cater to large number of users, with different access privileges

Simple to use and **code agnostic**



Improved  
accessibility of  
data

More  
developers of  
analyses and  
apps

Increased data  
value

Identifier, typically a formula (Fe2O3), id (1234) or chemical system (Li-Fe-O)

Preamble

Property

<https://www.materialsproject.org/rest/v1/materials/Fe2O3/vasp/energy>

Request  
type

Data type  
(vasp, exp,  
etc.)

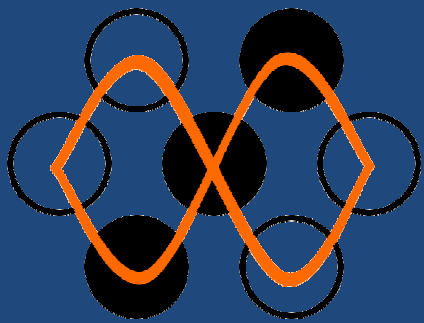
# Secure access

An individual **API key** provides secure access with **defined privileges**

API keys available at

<https://www.materialsproject.org/profile>



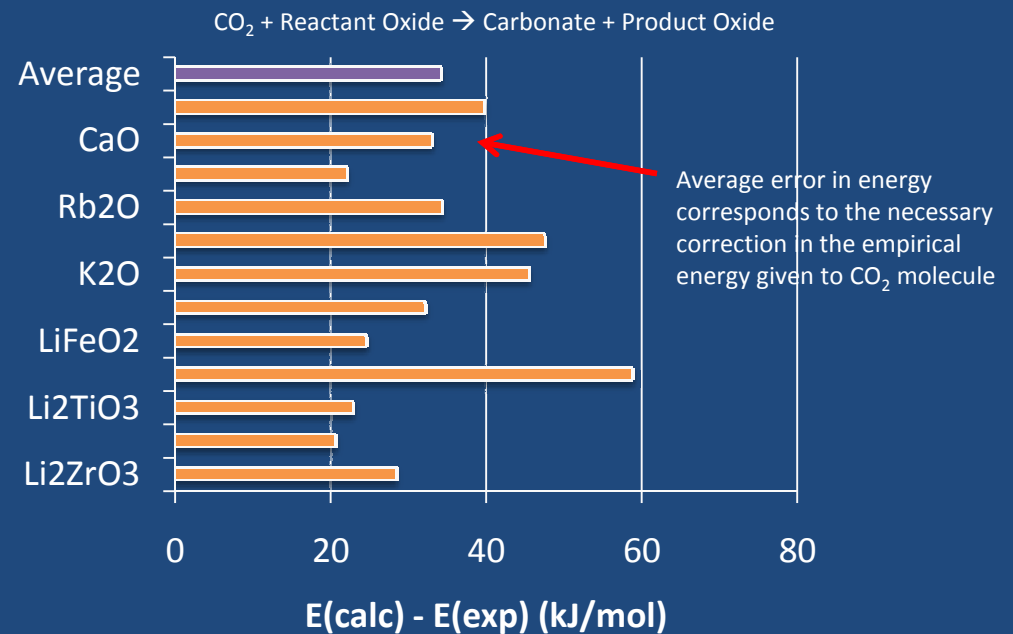
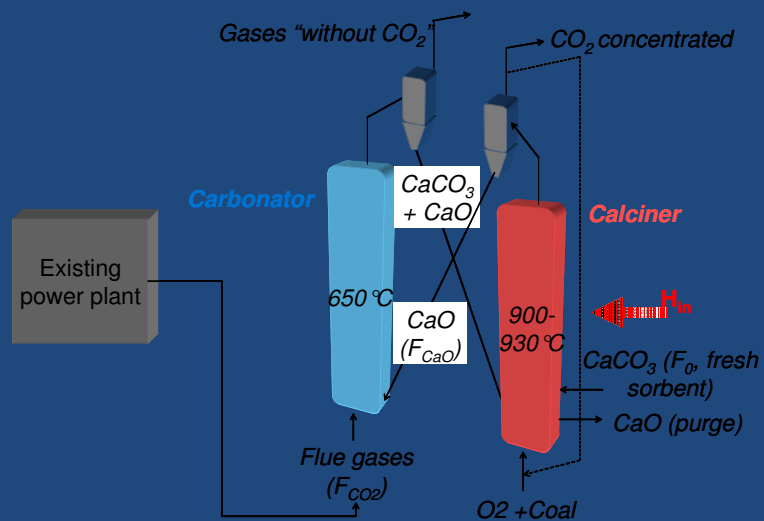


## Example collaborations

# Screening for CO<sub>2</sub> sorbents (Grey et al)

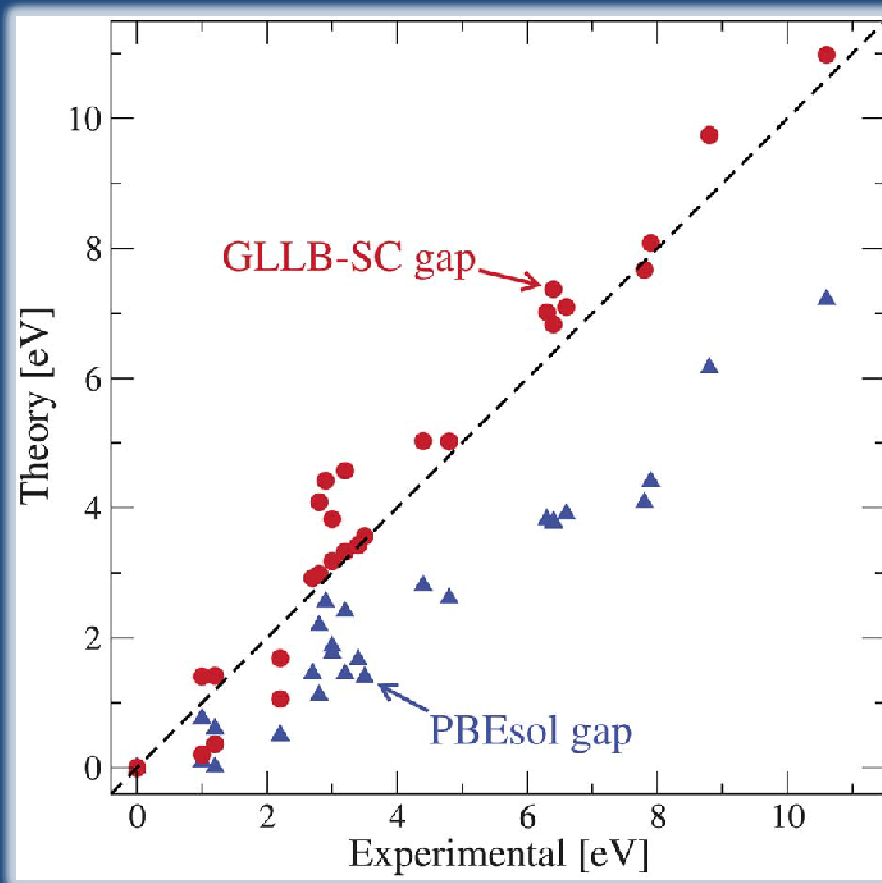
Calculating reaction energies of thousands of oxides with CO<sub>2</sub>

- High selectivity and absorption capacity for CO<sub>2</sub> at elevated temperatures (400-900°C)
- Good absorption/desorption kinetics - preferably under a wide range of p(CO<sub>2</sub>)
- Good cyclability for absorption/desorption processes
- Good hydrothermal and mechanical properties



# Testing new functional (Jacobsen et al)

- Developed a new functional: GLLB-SC
- GLLB-SC improves performance on band gaps
- GLLB-SC requires much more testing
- **Optimized structures from the Materials Project** allow for testing GLLB-SC over tens of thousands of compounds

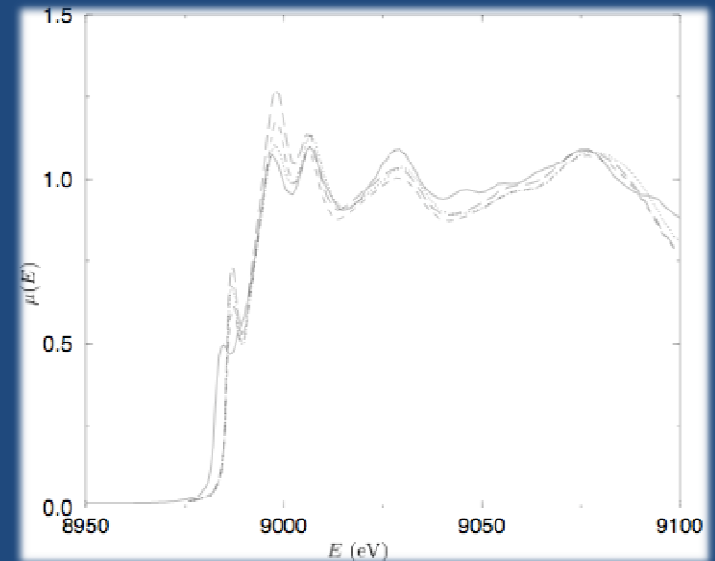


I.E. Castelli, T. Olsen, S. Datta, D.D. Landis, S. Dahl, K.S. Thygesen, and K.W. Jacobsen, *Energy & Environmental Science* 1–6 (2012).

# FEFF (Dozier and Rehr)

## Adding

- computed K-edge cross sections
- L-edge in future...
- XANES, EXAFS, EELS, ...
- cluster of atoms – not periodic solid



Cu XANES spectrum from exp and FEFF;  
*Inelastic Losses in X-ray Absorption Theory*,  
Thesis, Luke Campbell (2002).

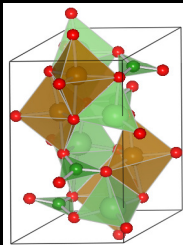
via `pymatgen` and `Rockets/ Fireworks`

# Disseminate data via Materials Project Source (MPS)

MPS

about

crystal



about

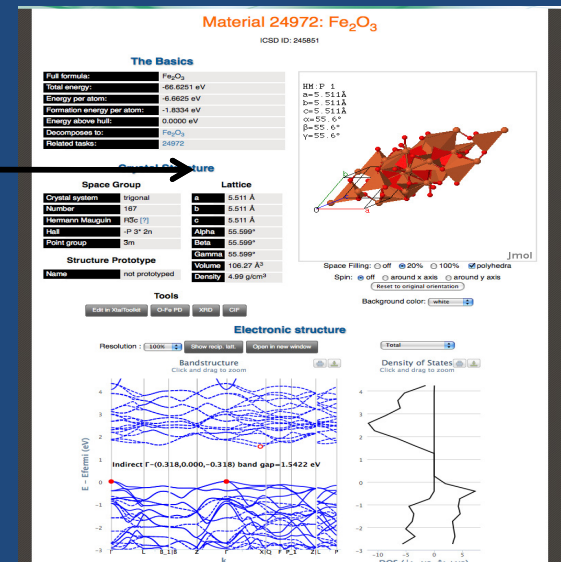
- Who authored the xtal?
- What papers to cite?
- Is the xtal linked to any known databases?
- What codes operated on the xtal?
- What metadata is associated with the xtal?

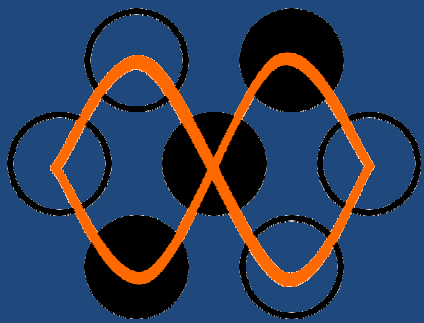
Send to  
Materials  
Project

author, publication  
reference and link...



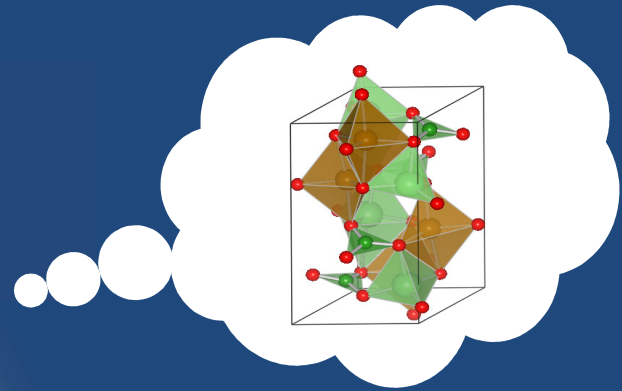
200+ relaxed  
structures from  
that last CE

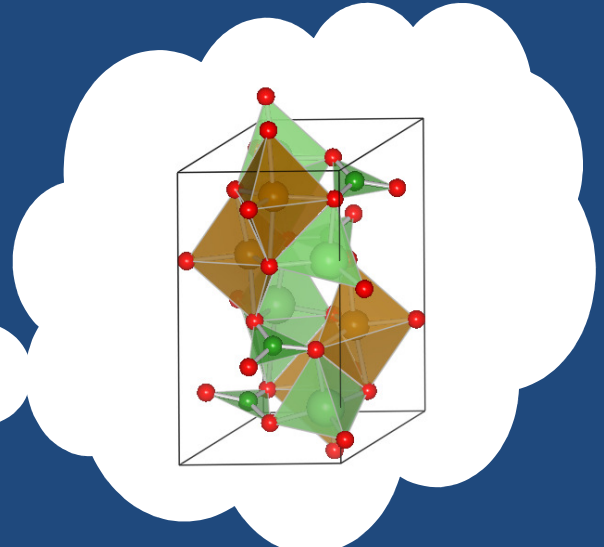
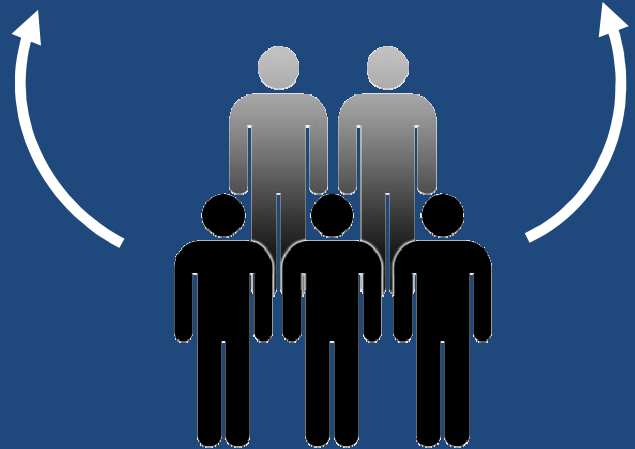
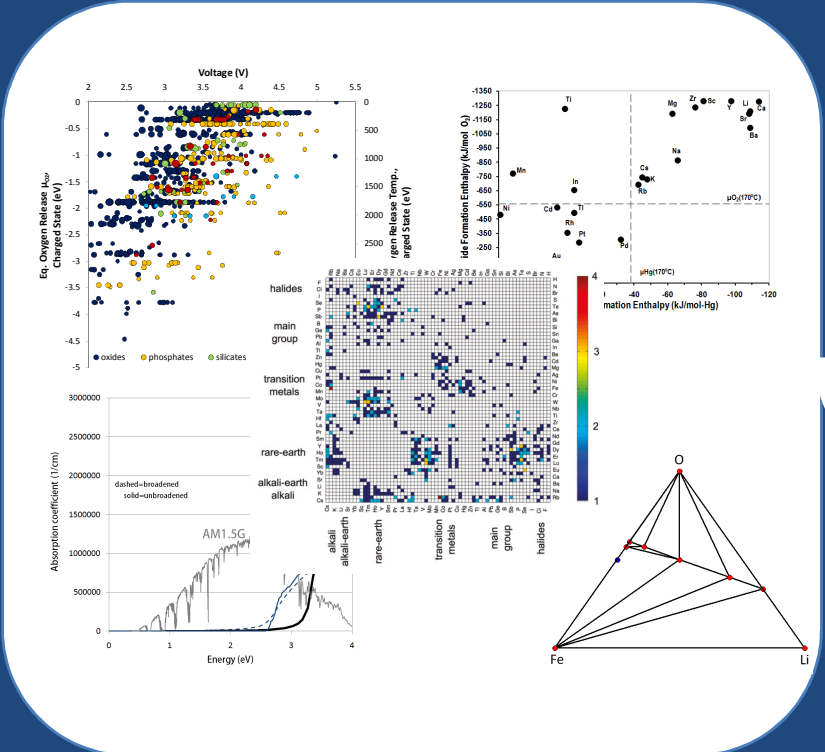




# The Vision

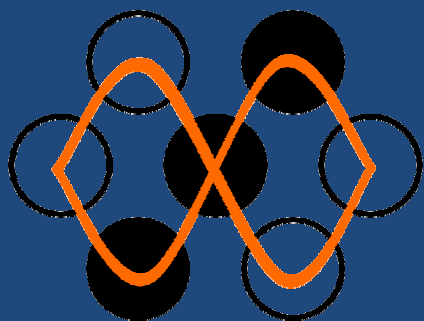
From single entities...





... towards a materials genome





# Thank you for your attention

## Thanks to sponsors:



U.S. DEPARTMENT OF  
**ENERGY**



National Science Foundation  
WHERE DISCOVERIES BEGIN

## And thanks to the team:

Anubhav Jain   Alan Dozier   Gerbrand Ceder   Stefano Curtarolo   Daniel Gunter   Jeff Grossman   Dane Morgan   Rafael Fink  
Shyue Ping Ong   David Skinner   Stefan Adams   Mark Asta   Jack Deslippe   Anthony Gamst   Wei Chen  
Geoffroy Hautier   Shreyas Cholia   Michael Kocher   Maciej Haranszyk   Will Richards   Jeff Neaton