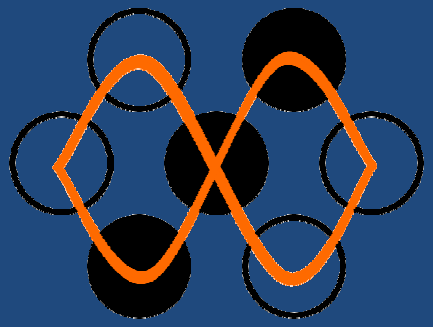
Fall 10-2-2012

The Materials Project – A Public Materials Design Platform

Kristin Persson
Lawrence Berkeley National Laboratory



The Materials Project – A Public Materials Design Platform

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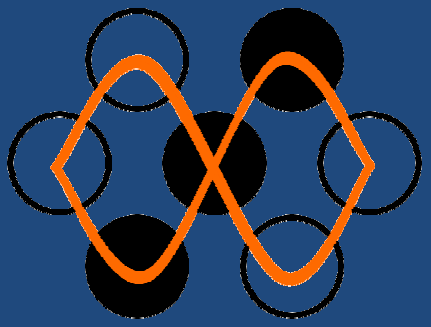
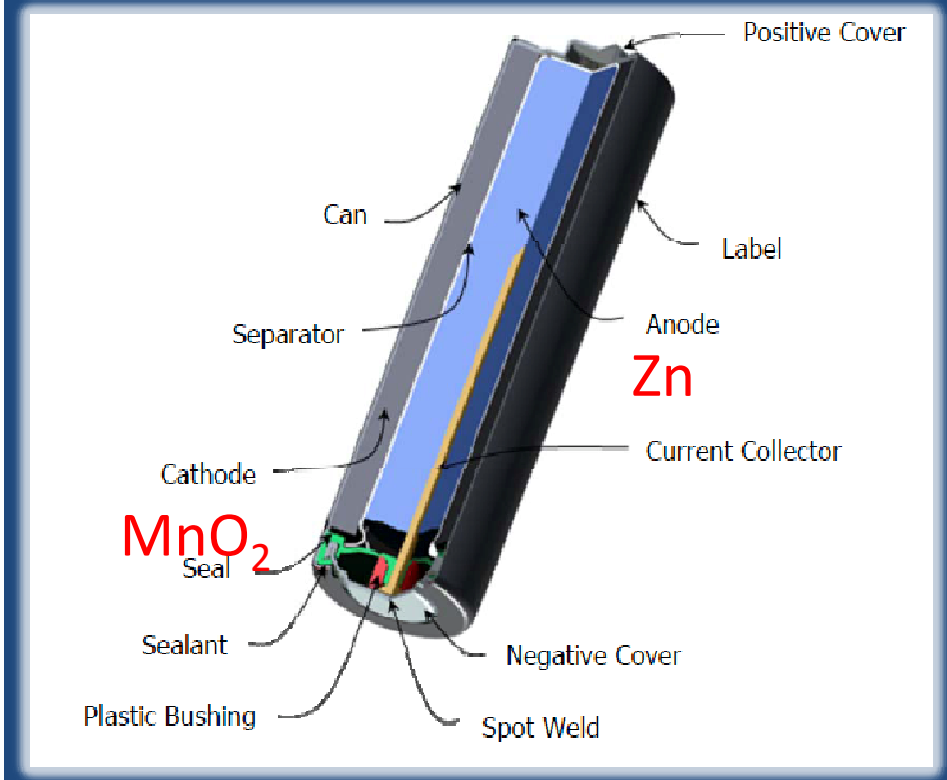
Outline

- Materials Design for Cathodes
- The Public Platform: www.materialsproject.org
  - Pymatgen
  - The Materials API
  - Example Collaborations
- The Vision

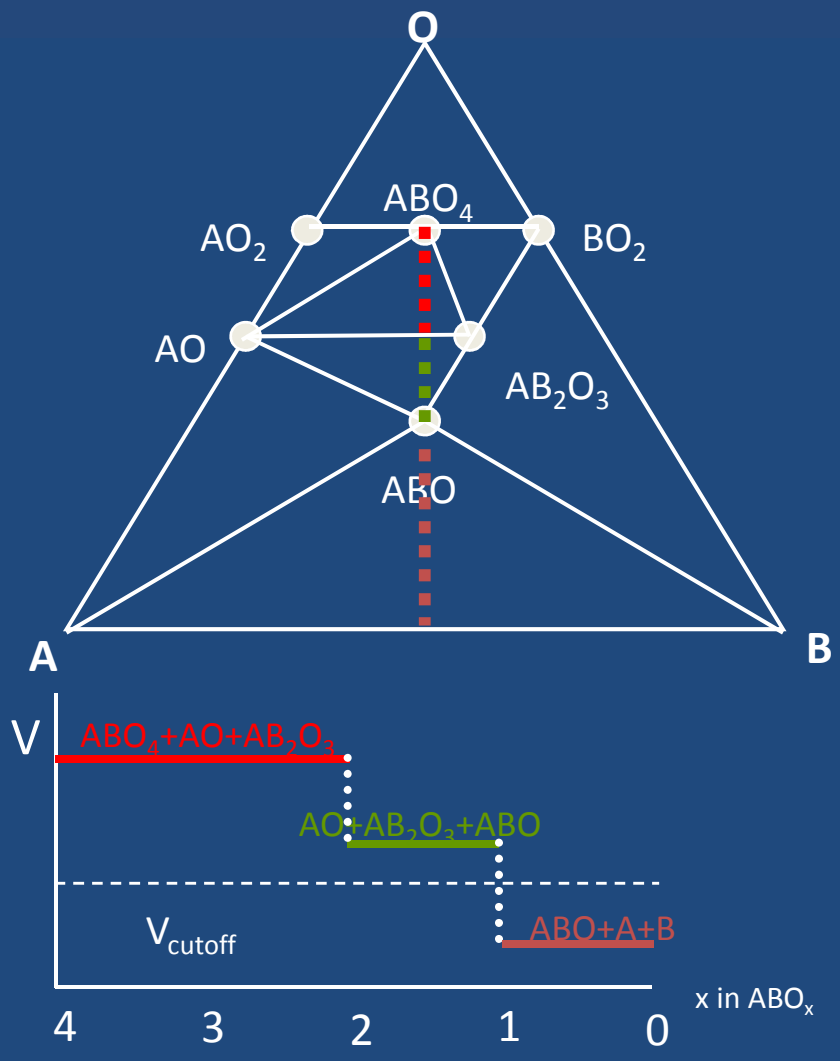


Example: Materials Design for Cathodes

Finding a better alkaline cathode



$MnO_2+H_2O+Zn \rightarrow MnOOH + ZnOH_2$



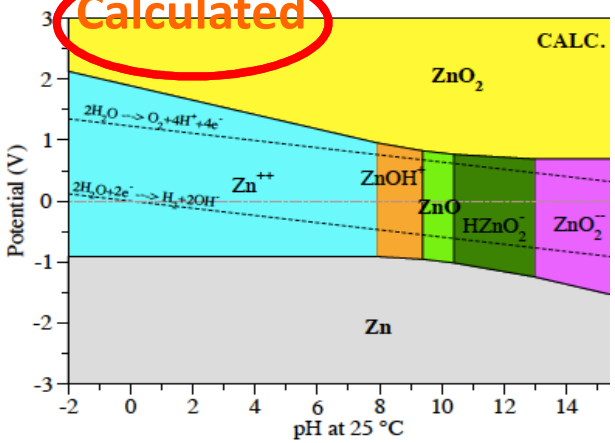
SPECS:

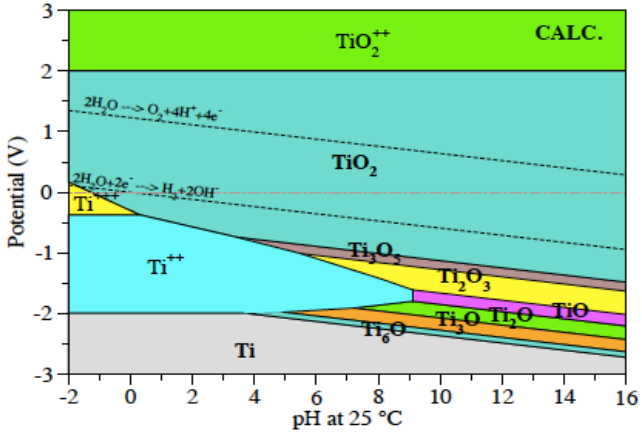
Higher energy density

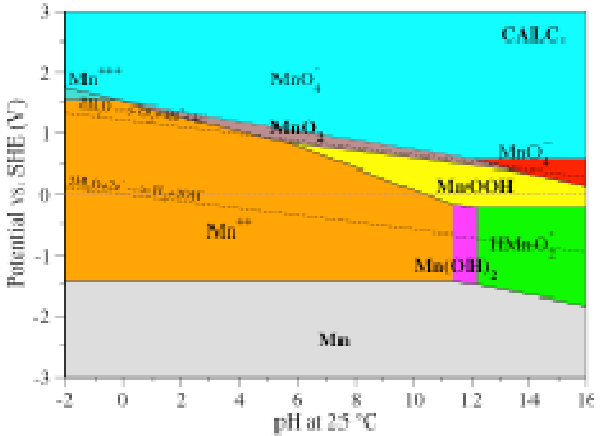
Both reactants and products stable in high molar KOH

Calculating solid stability in water

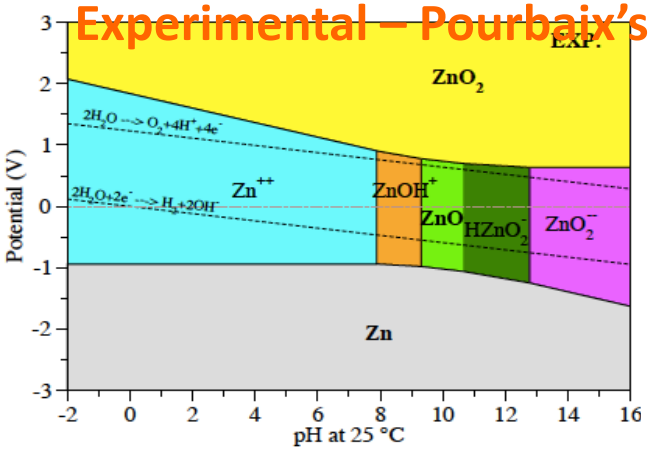
Calculated

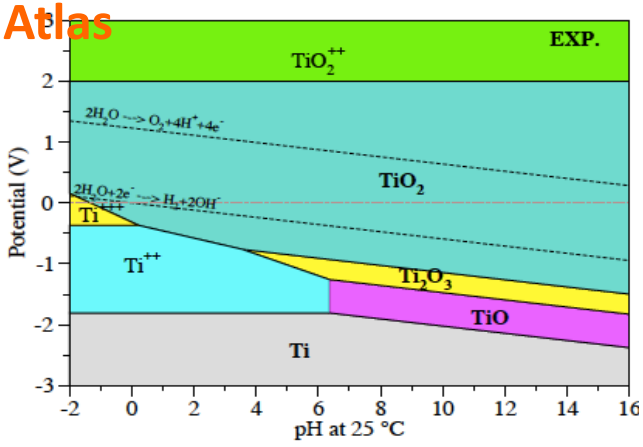


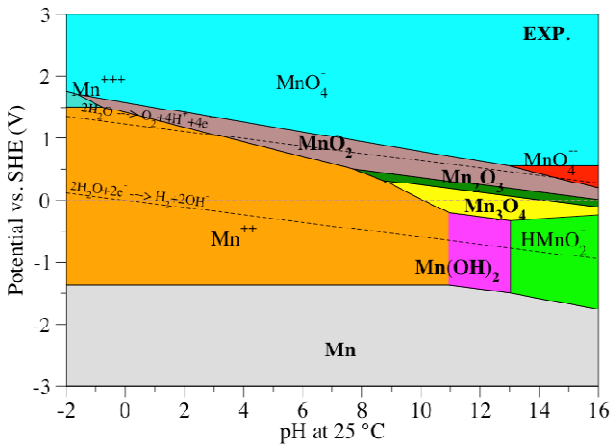




Experimental – Pourbaix's Atlas

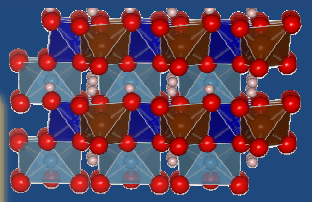






Persson et al, PHYSICAL REVIEW B**, 005400 (2012),** *Prediction of solid-aqueous equilibria: Scheme to combine first-principles calculations of solids with experimental aqueous states*

The Screening Strategy



Database

Known compounds

30,000

permutation strategy

New compounds

~ 100,000

~ 100,000 - 200'000

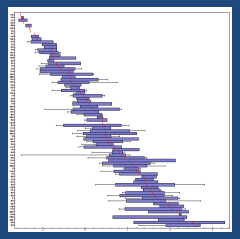
- ✓**Solid Stability**
- ✓**Solubility**
- ✓**Voltage**
- ✓**Capacity**

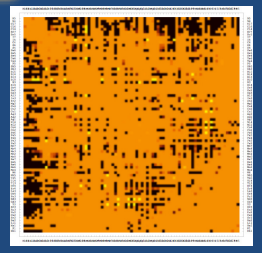
Initial screening (phenomenological)

≈ 10,000 - 20'000

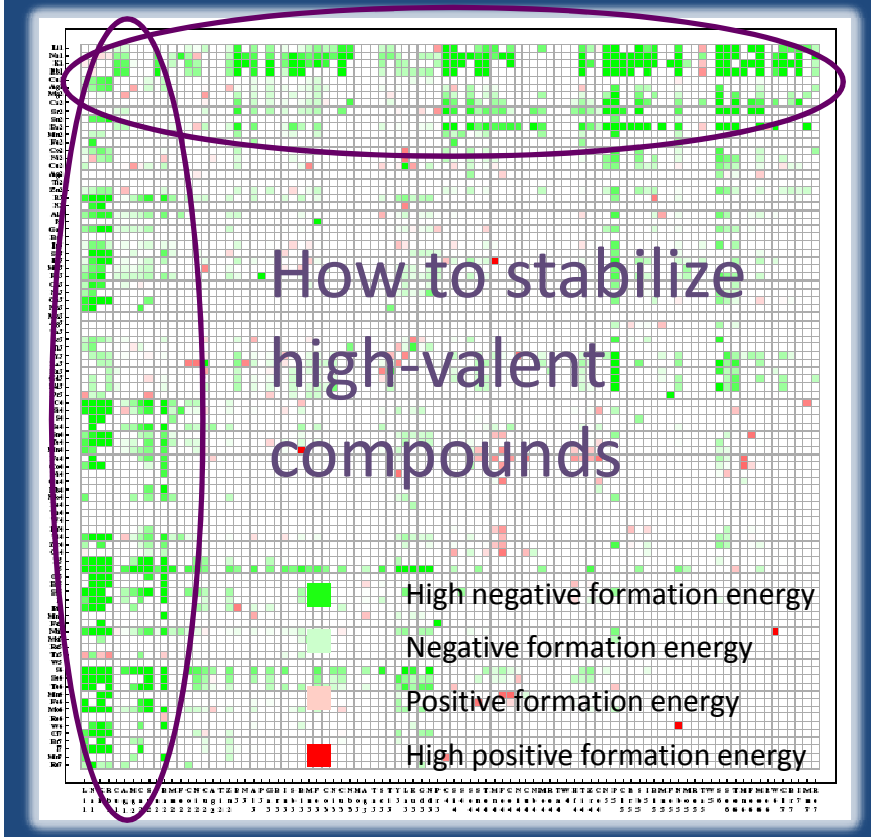
Computational Screening

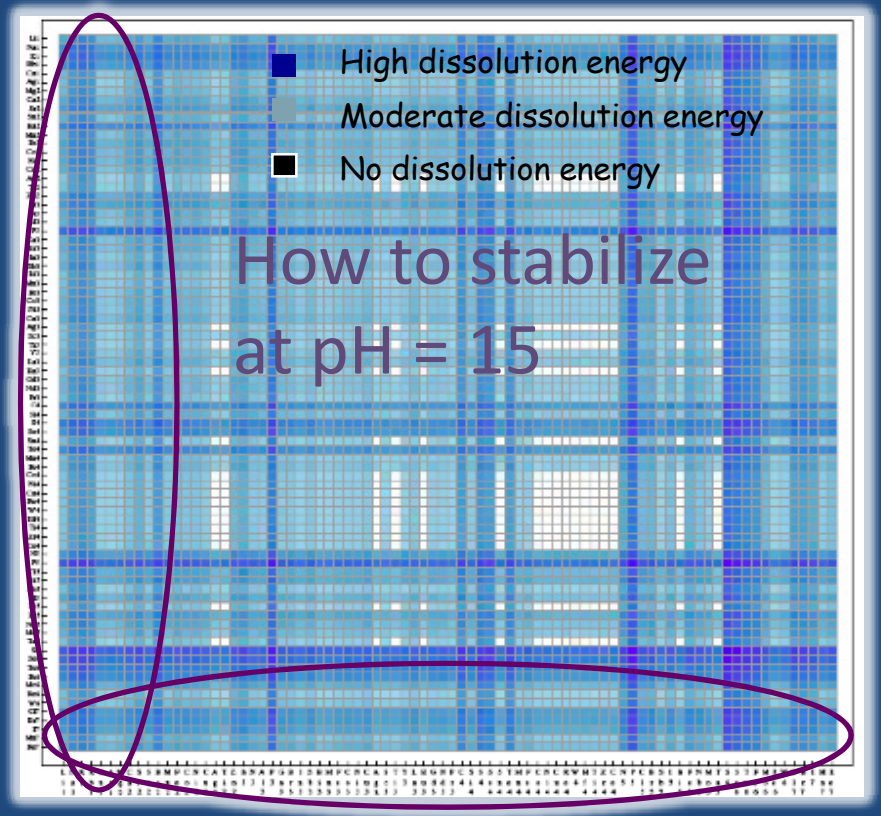
Data mining





Candidate materials





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

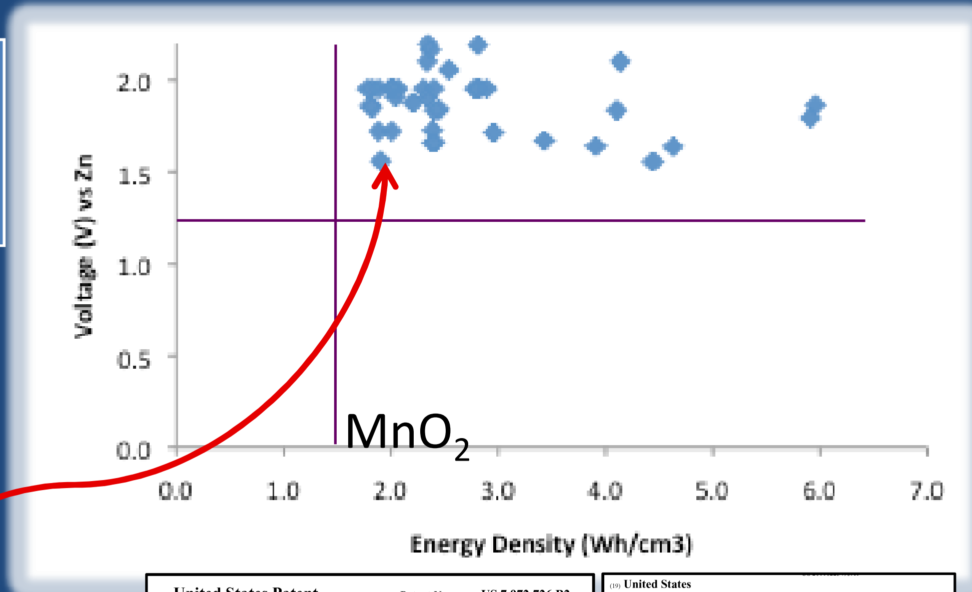
✓ Capacity > 1 Ah/cc
✓ 1.1 V < Ave voltage < 2.2 V
✓ Energy density > 1.7Wh/cc

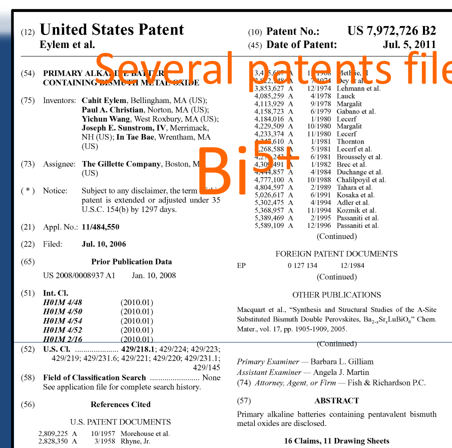
Tier 2

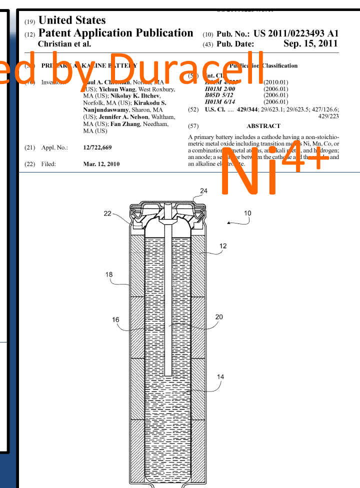
≈ 200 compounds

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

Predicted alkaline cathode material performance







Several patents filed by Duracell

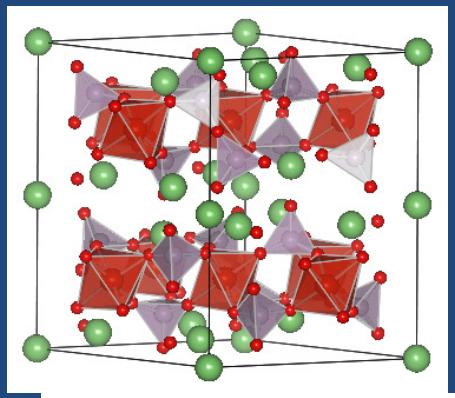
Bi^{5+}

Ni^{4+}

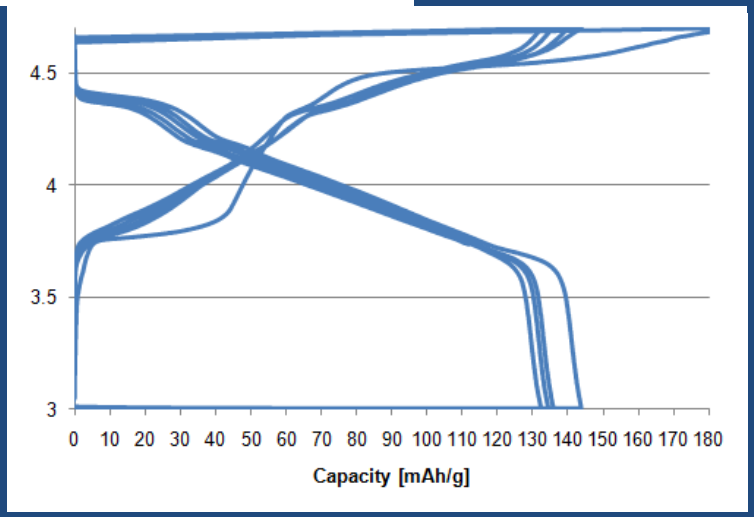
End result – 200 compounds predicted to outperform current cathode AND are predicted stable (through entire reaction) in 9 M KOH

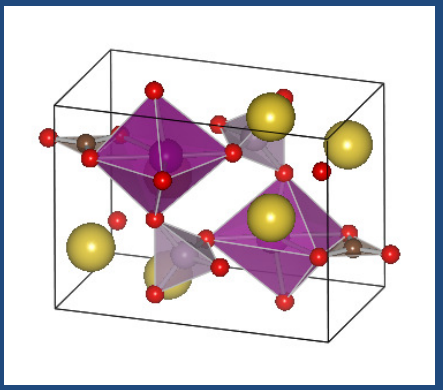
New Li-ion Cathode Materials Discovered @MIT

No Li containing carbono phosphates AT ALL are known in nature !

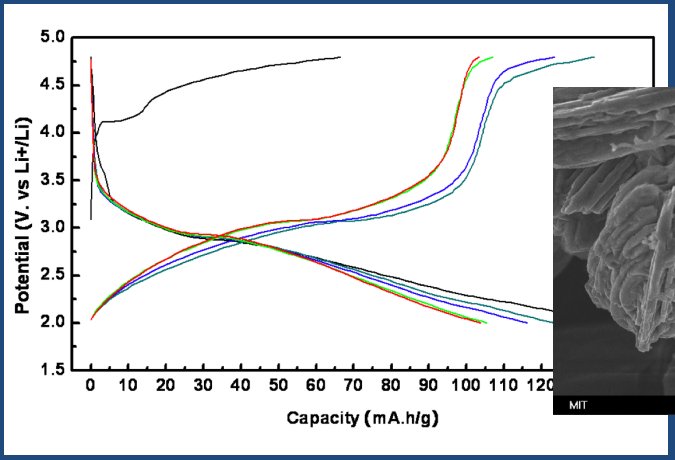


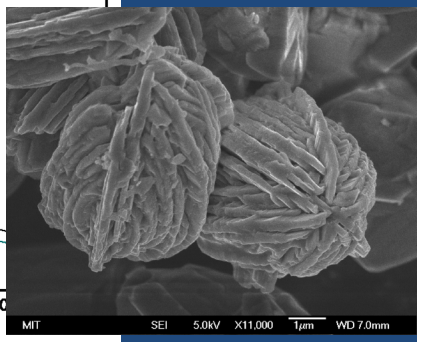
New phosphate discovered @MIT through computations





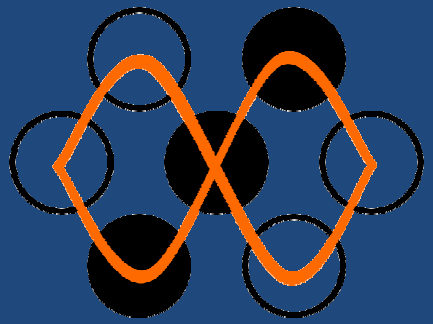
Completely new *class* of materials synthesized based on computational predictions





"Sidorenkites": $Li_3M(CO_3)(PO_4)$ (M = Fe, Mn, Ni, Co)

Courtesy of Ceder at al, MIT



The Public Platform: www.materialsproject.org

Fill in ‘missing’ property data on inorganic compounds

Assist researchers in predicting new materials

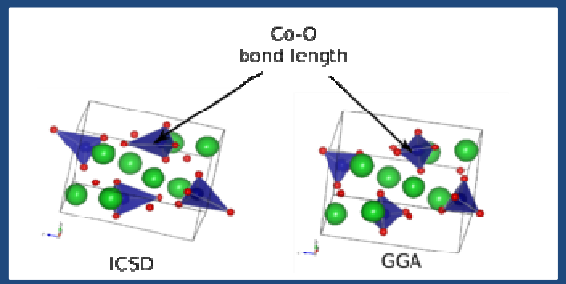
Provide interactive analysis tools and codes

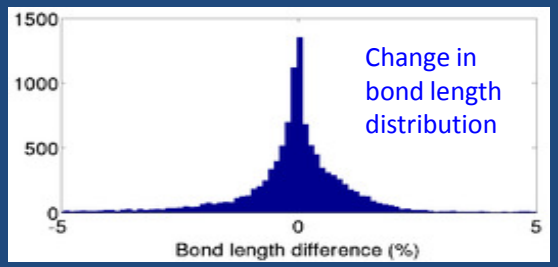
Enable rapid screening and data mining

Accuracy

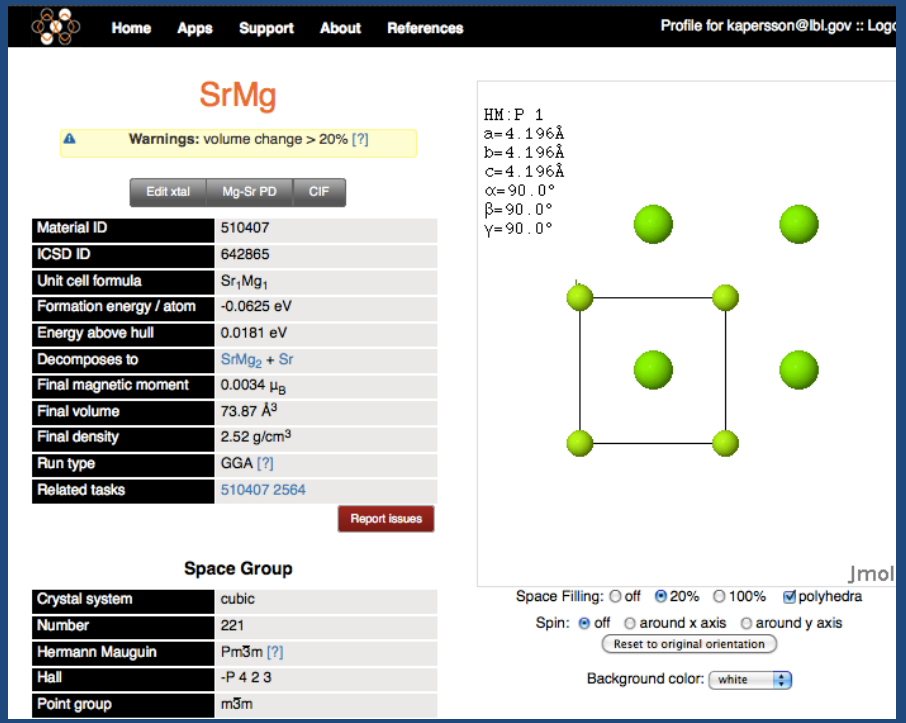
Benchmarking (dV, bond length, enthalpy, …)

error checking



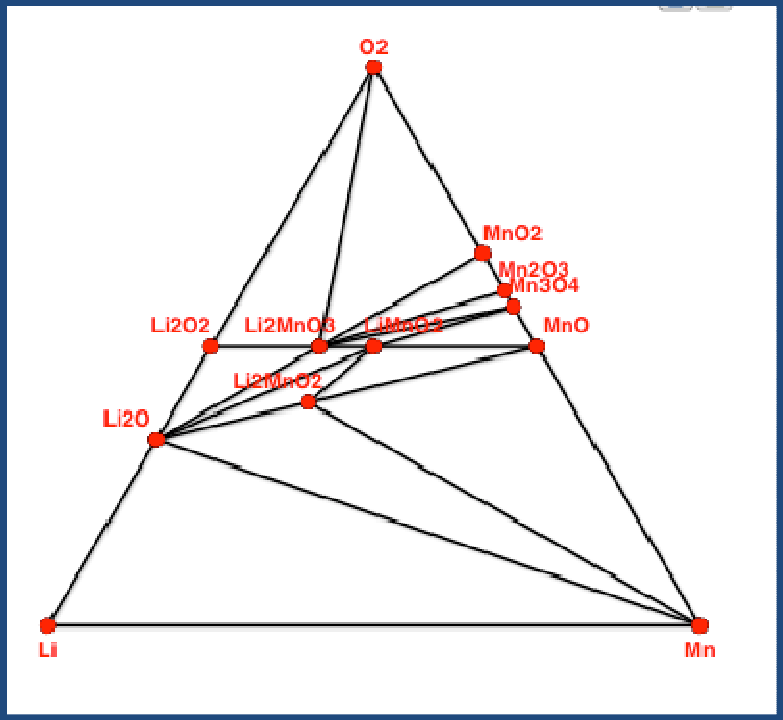


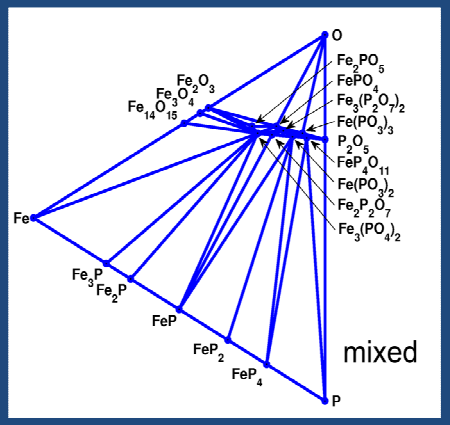
https://materialsproject.org/wiki/

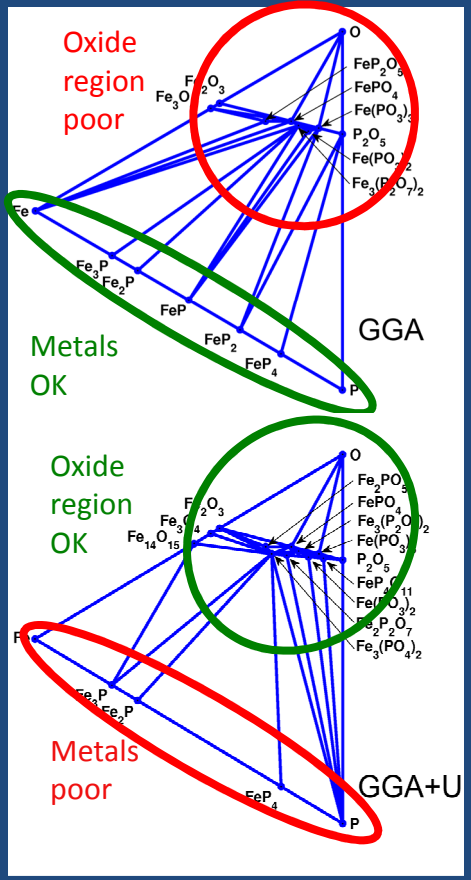


Data Compatibility

between data sets

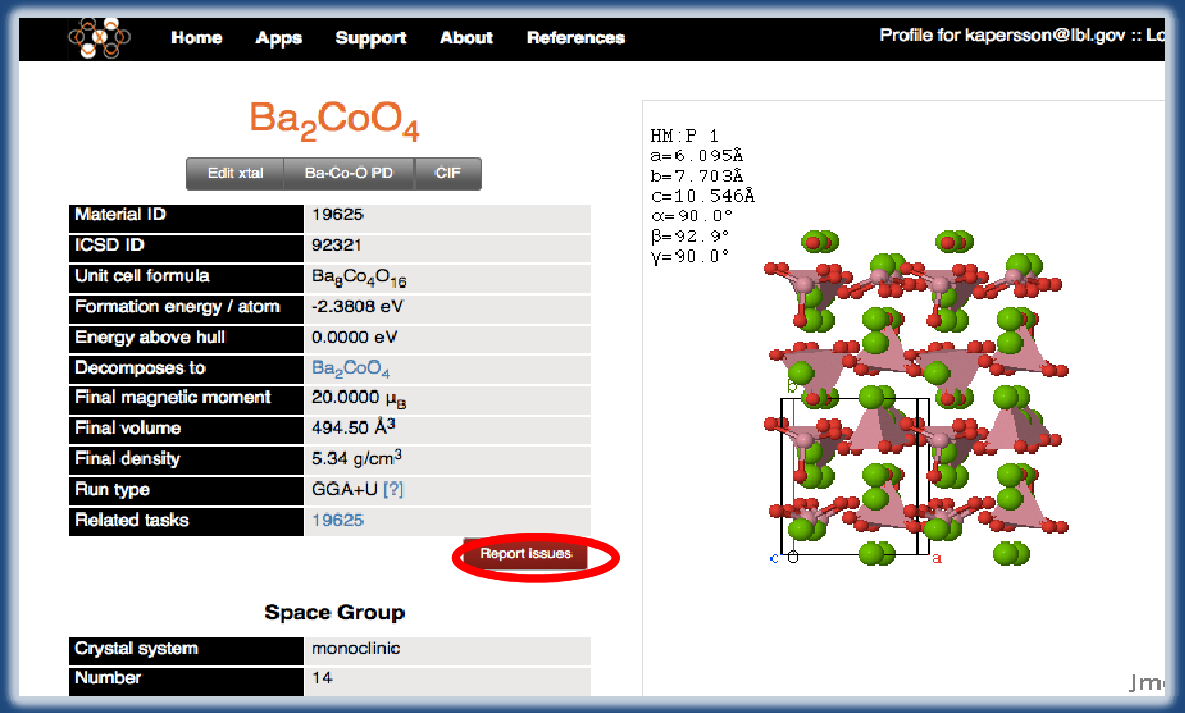


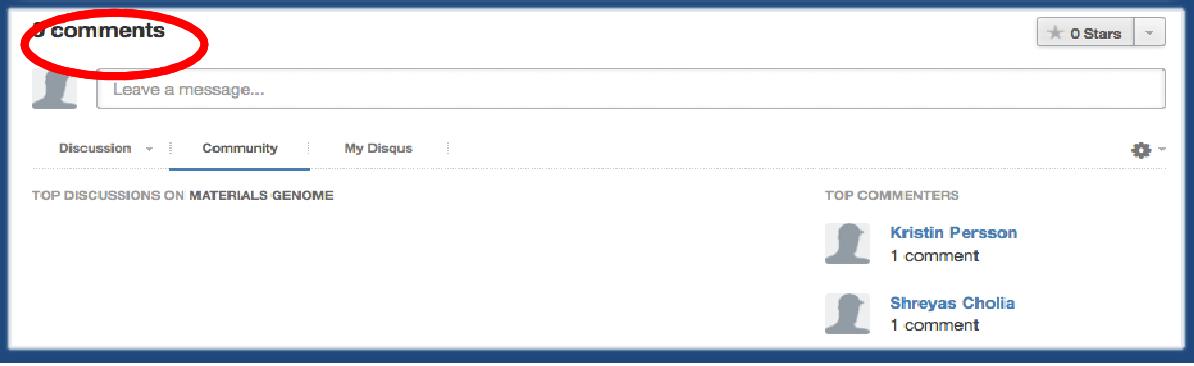




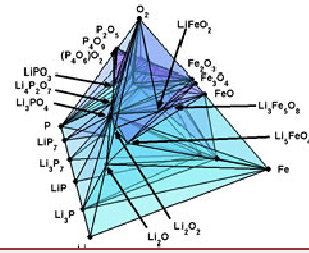
Jain et al, *Formation Enthalpies by mixing GGA and GGA+U Calculations,* Physical Review B **84, 045115 (2011).**

Leveraging the community





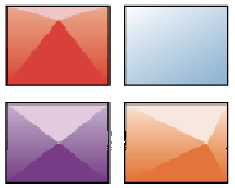
- Over 26,000 compounds and growingmonthly
- Multiple tools based on computed data



PhaseDiagramApp

The Phase Diagram App uses density functional
database to generate **0K compositional and grand**
two to four components. For details of our methodolog
to the Phase Diagram App manual.

HTML5-compatible browser recommended, e.g., Chrome, Safar
Non-interactive plots only for IE8.



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!

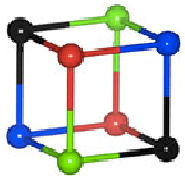
MaterialsExplorer

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

ReactionCalculator

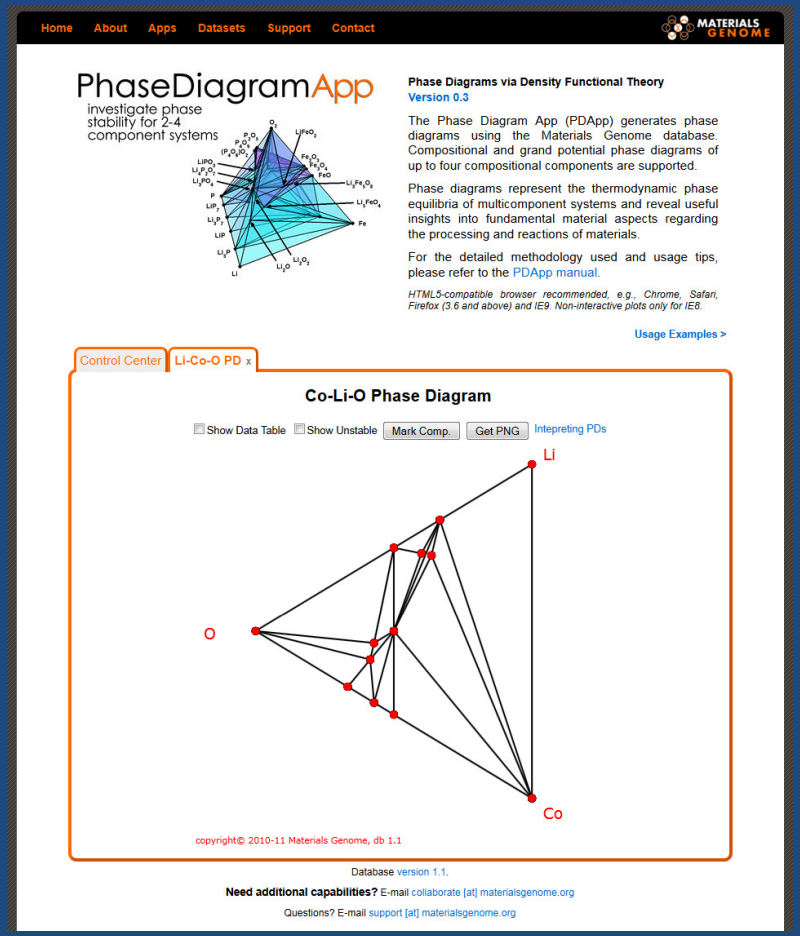
The reaction calculator determines energies of solid state reactions using a database of Density Functional Theory calculations. When available, the reaction calculator will also report experimental formation enthalpies for the reaction. For details of our methodology and usage tips, please refer to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

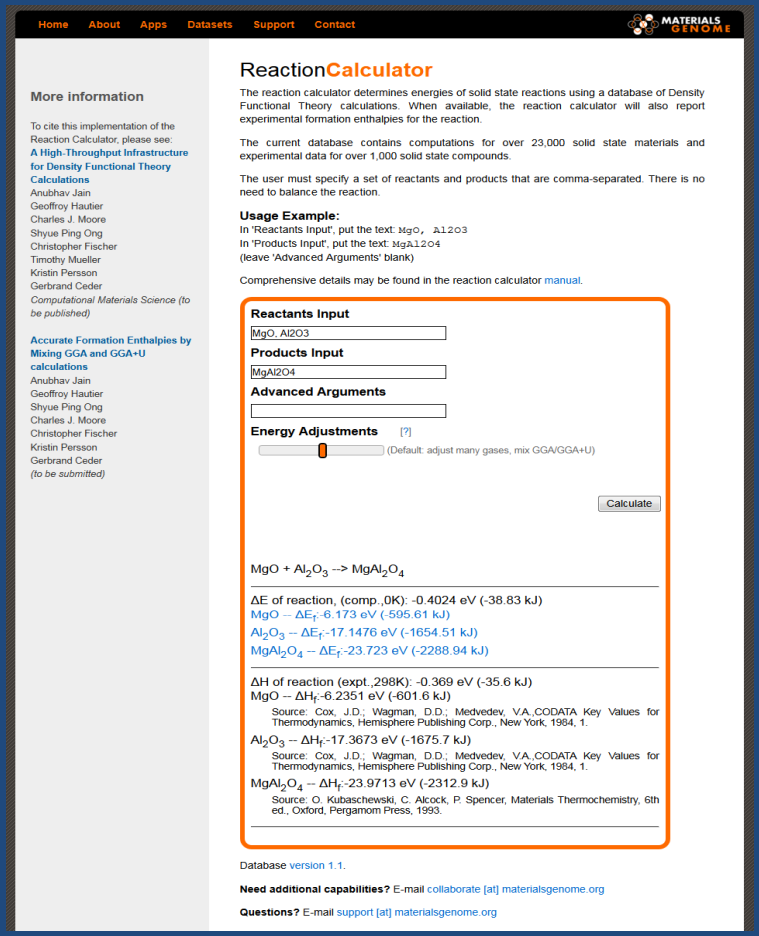
Usage Example: Type "MgO + Al2O3" in the Reactants field and "MgAl2O4" in the Products field and click "Calculate ΔH".



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.





Phase diagrams
with available data:

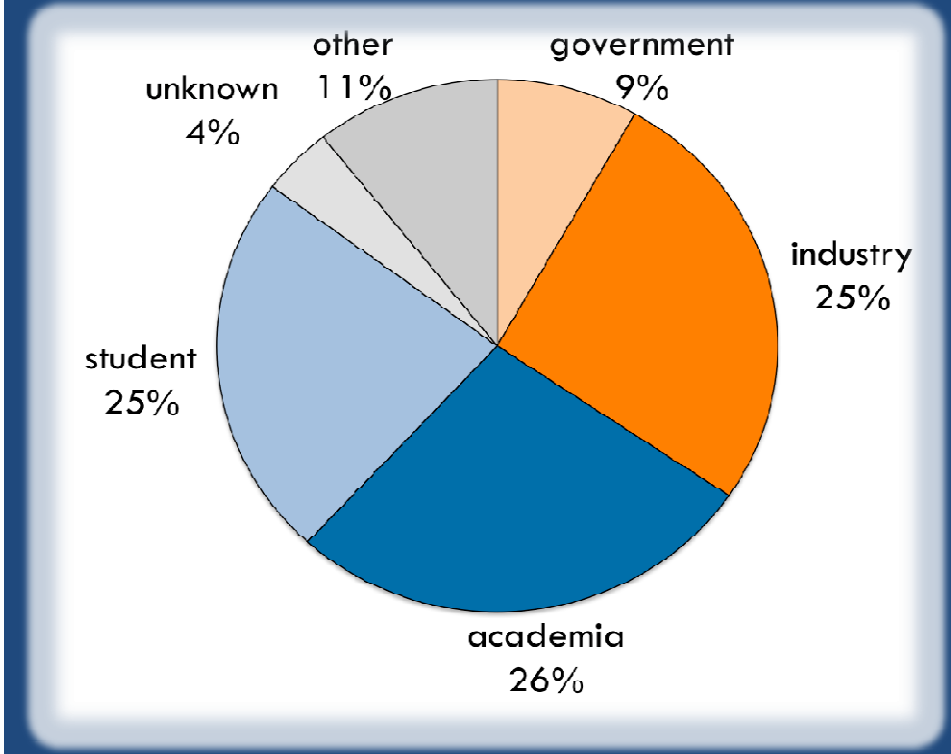
28,300 SYSTEMS

Reaction energies
already available online:

>35,000 REACTIONS

Most measured materials data is of order of 10^2 – elastic constants, band gaps etc…

Launched Oct 2011



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

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Dane Morgan

Duke University
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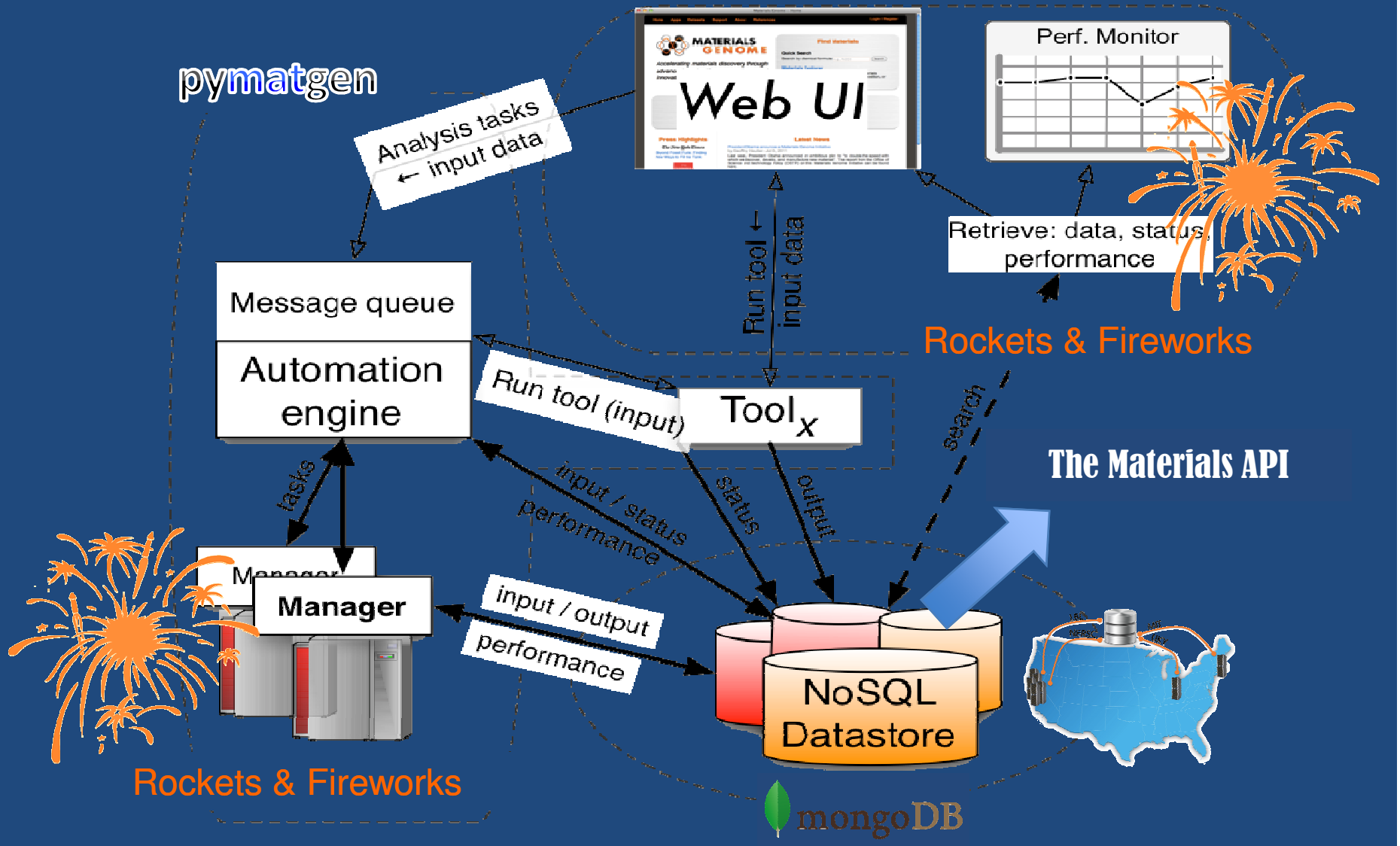
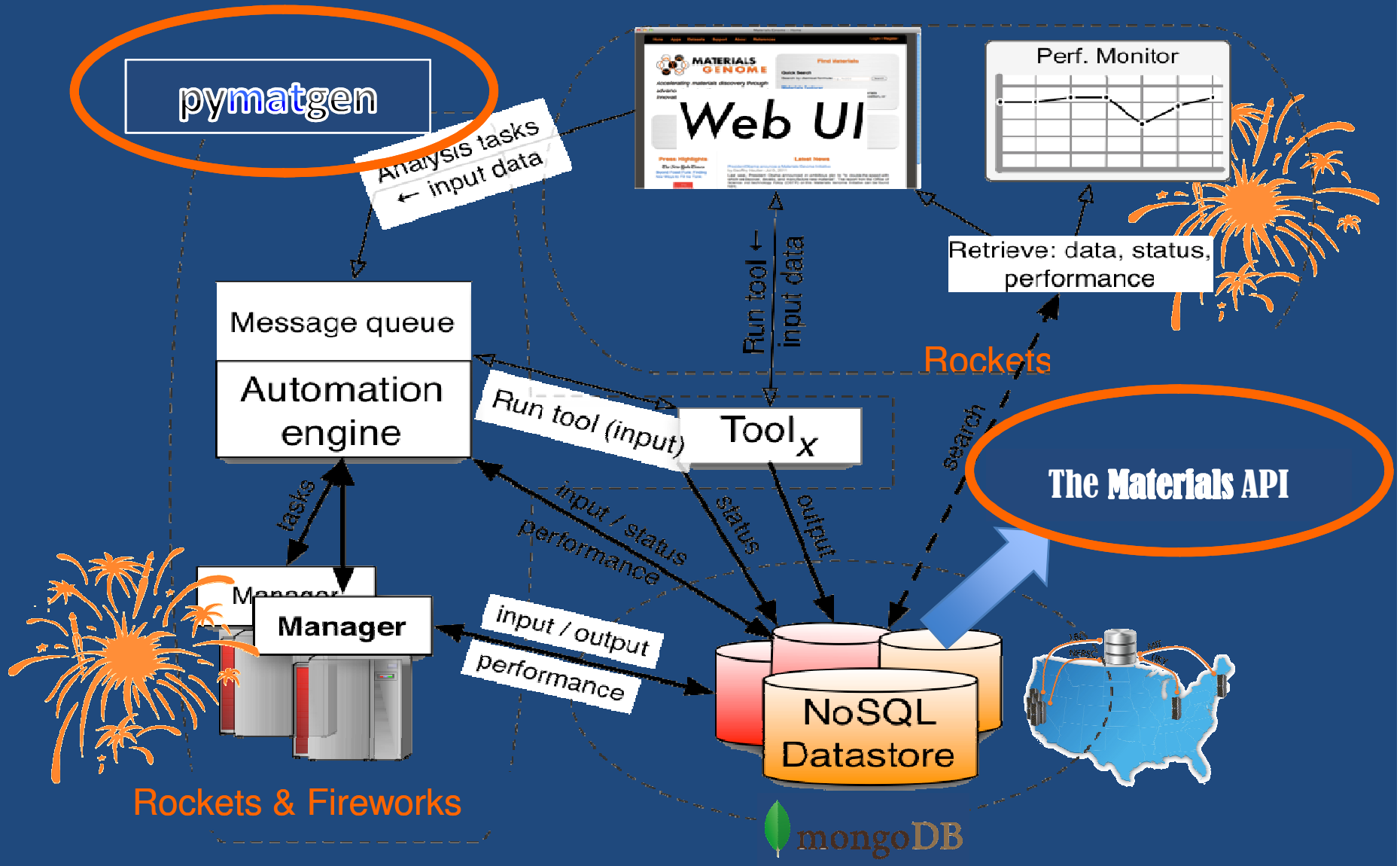
University of Kentucky
Alan Dozier
Raphael Fink

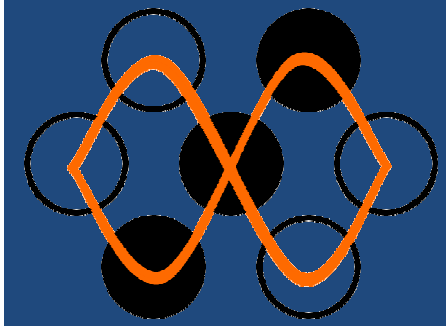
UCL Université Catholique de Louvain, Belgium
Geoffroy Hautier

Large Software Infrastructure Structure



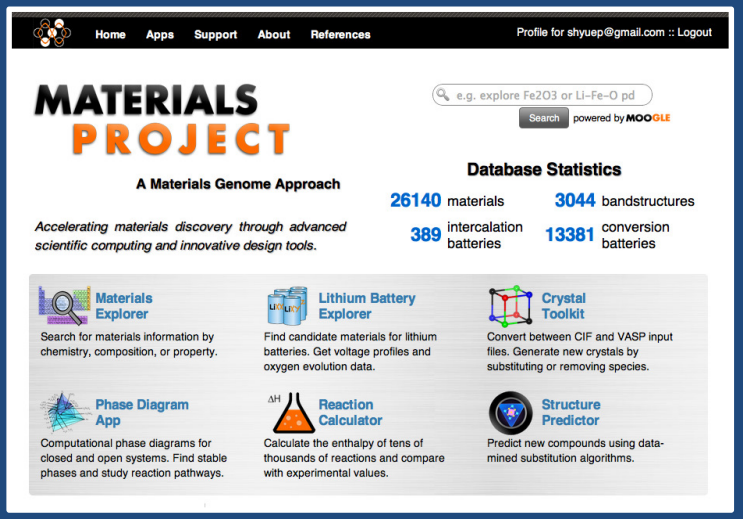
Large Software Infrastructure Structure





Pymatgen

python materials genomics
is the codebase powering the Materials Project.

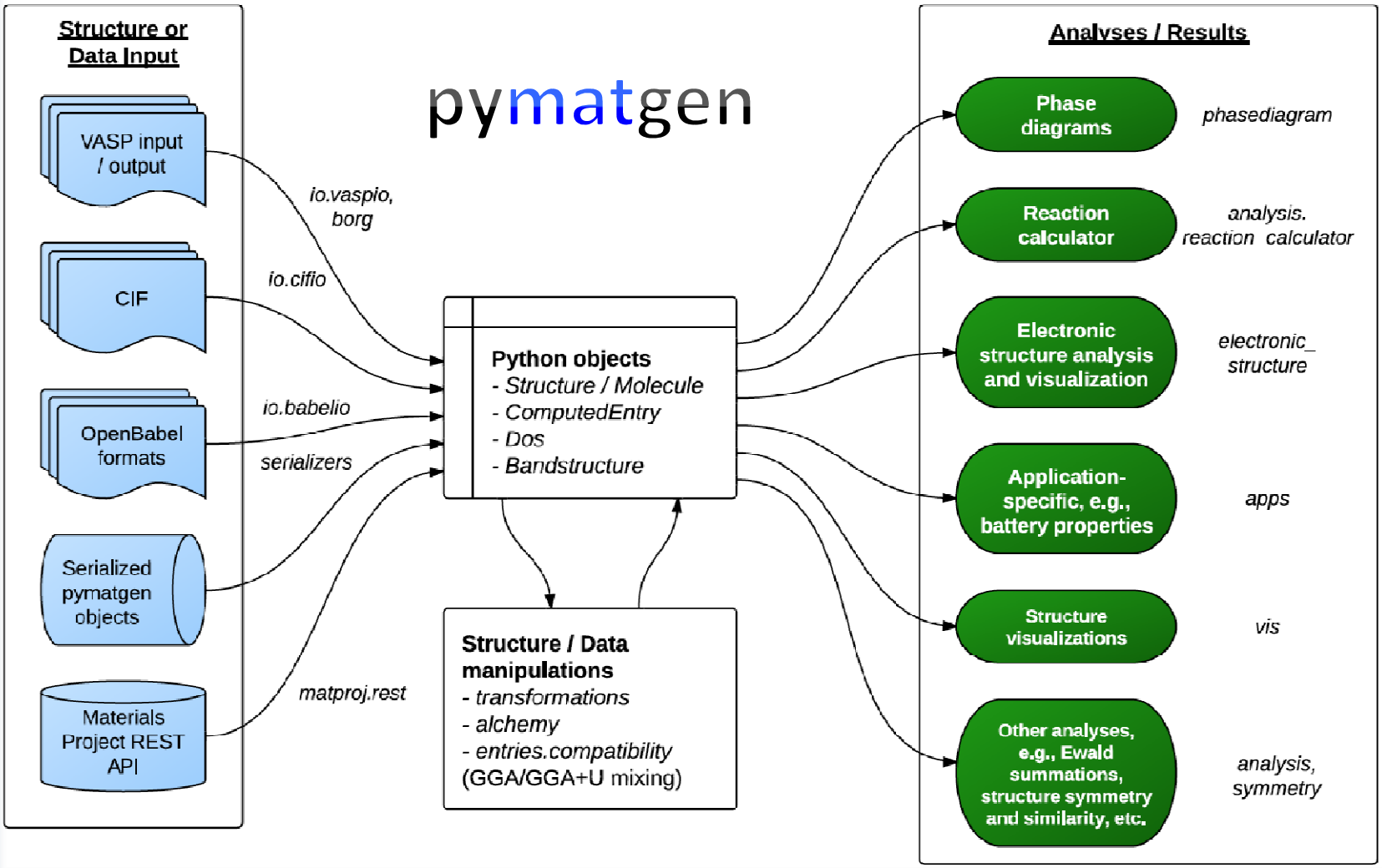


pymatpro

- Database interface
- Run management (fireworks)

pymatgen

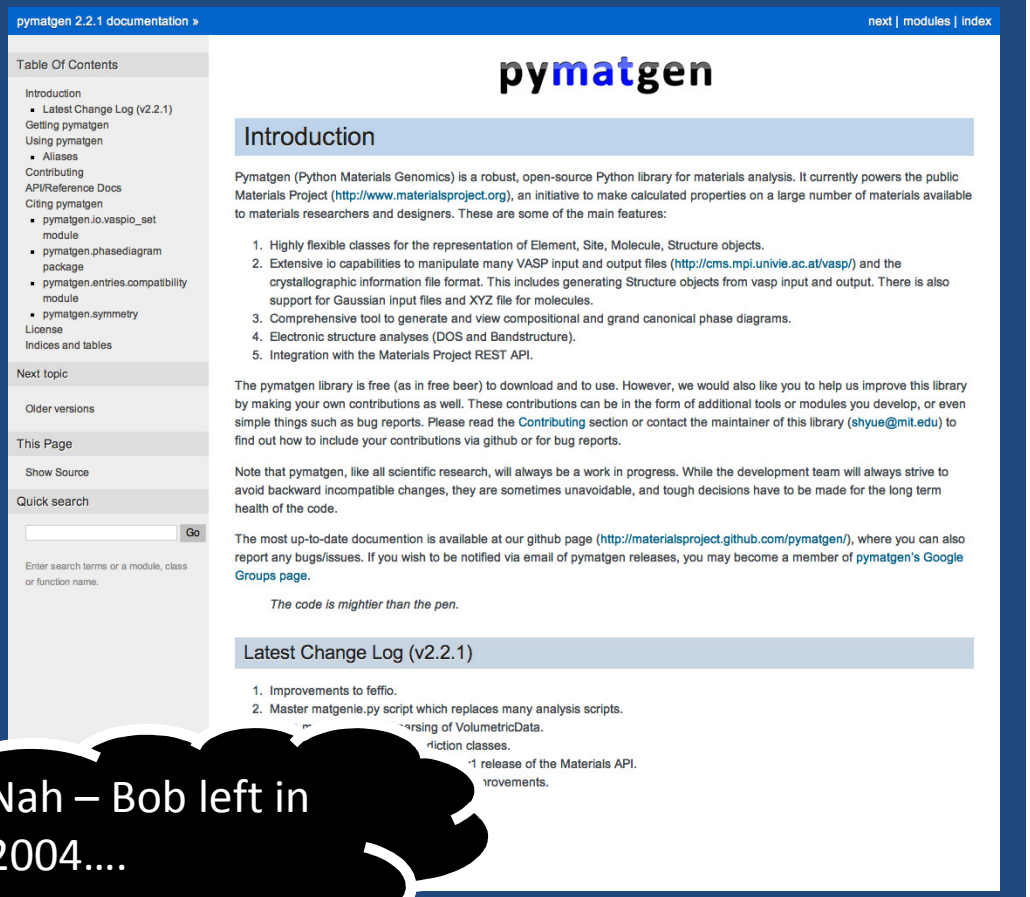
Defines core extensible Python objects for materials data representation.


Structure or Data Input
VASP input / output
CIF
OpenBabel formats
Serialized pymatgen objects
Materials Project REST API
io.vaspio, borg
io.cifio
io.babelio
serializers
matproj.rest
pymatgen
Python objects
- Structure / Molecule
- ComputedEntry
- Dos
- Bandstructure
Structure / Data manipulations
- transformations
- alchemy
- entries.compatibility
(GGA/GGA+U mixing)
Analyses / Results
Phase diagrams
phasediagram
Reaction calculator
analysis. reaction calculator
Electronic structure analysis and visualization
electronic_ structure
Application-specific, e.g., battery properties
apps
Structure visualizations
vis
Other analyses, e.g., Ewald summations, structure symmetry and similarity, etc.
analysis, symmetry

Building robust software that lasts… :

All pymatgen classes and methods come withunit tests

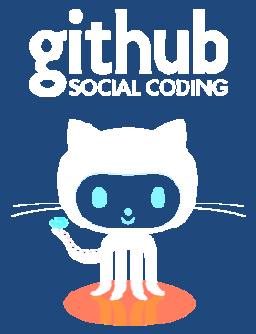
All code have proper documentation



Does anyone remember how to run ‘GoBabyMonte.c’ ?????

Nah – Bob left in 2004….

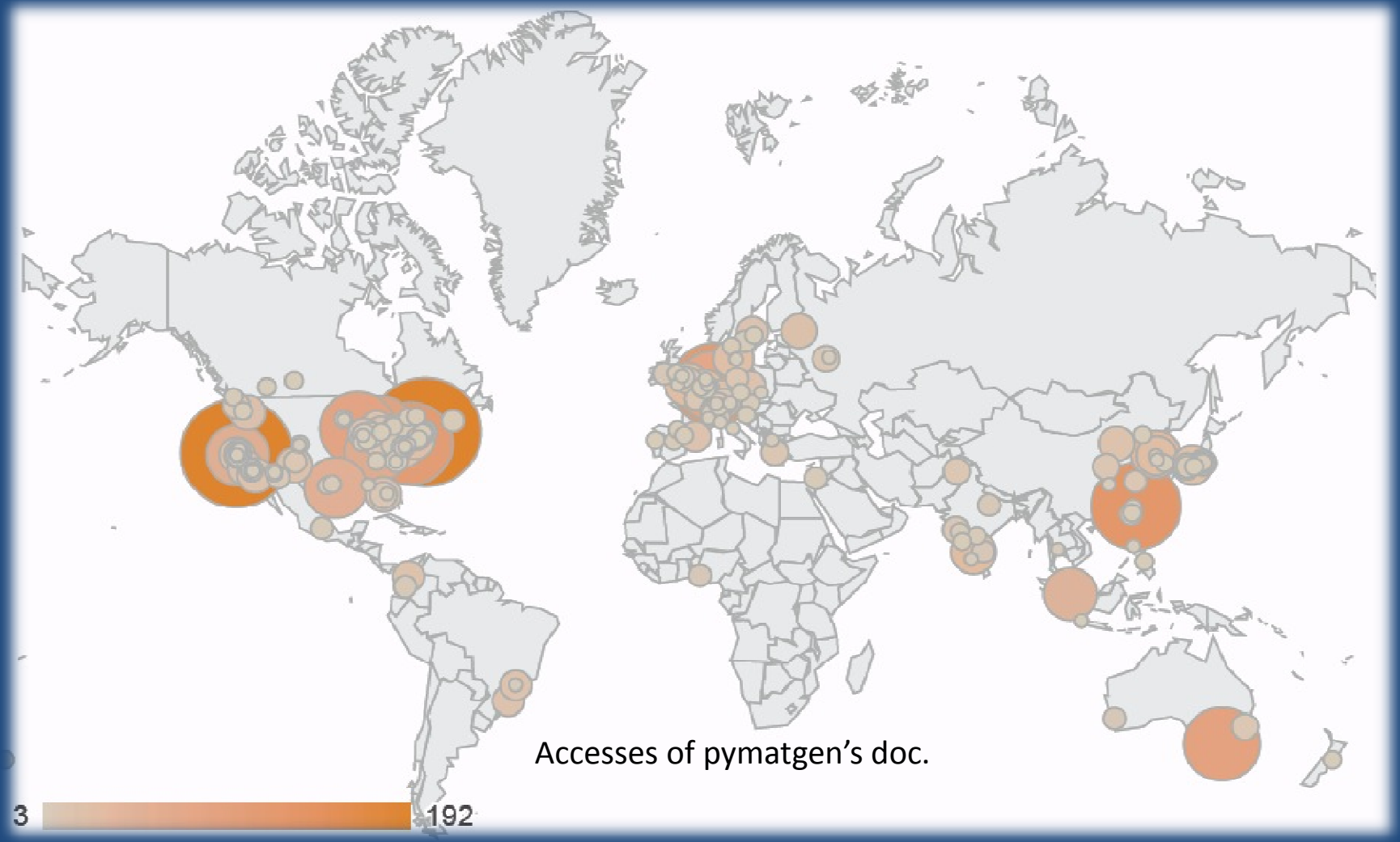
pymatgen is managed via

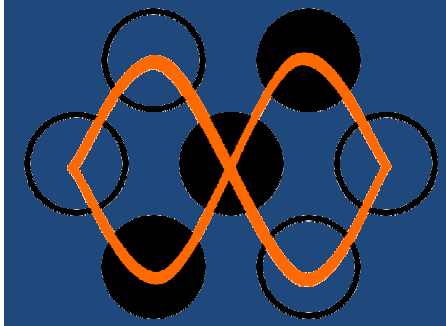


Licensed under the MIT license

Stable versions are available on the popular Python Package Index (PyPI) at http://pypi.python.org/pypi/pymatgen

pymatgenis global





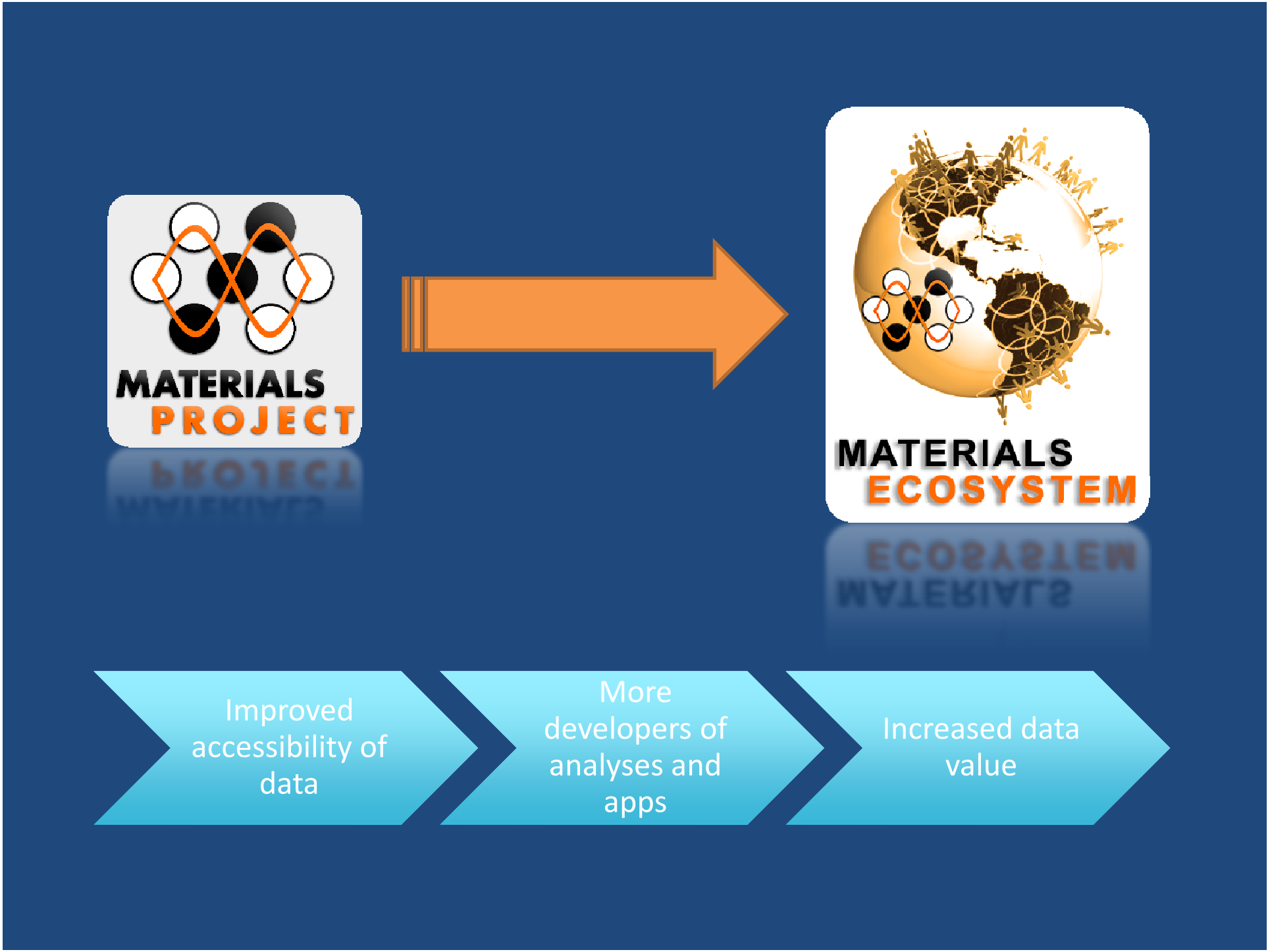
The Materials API

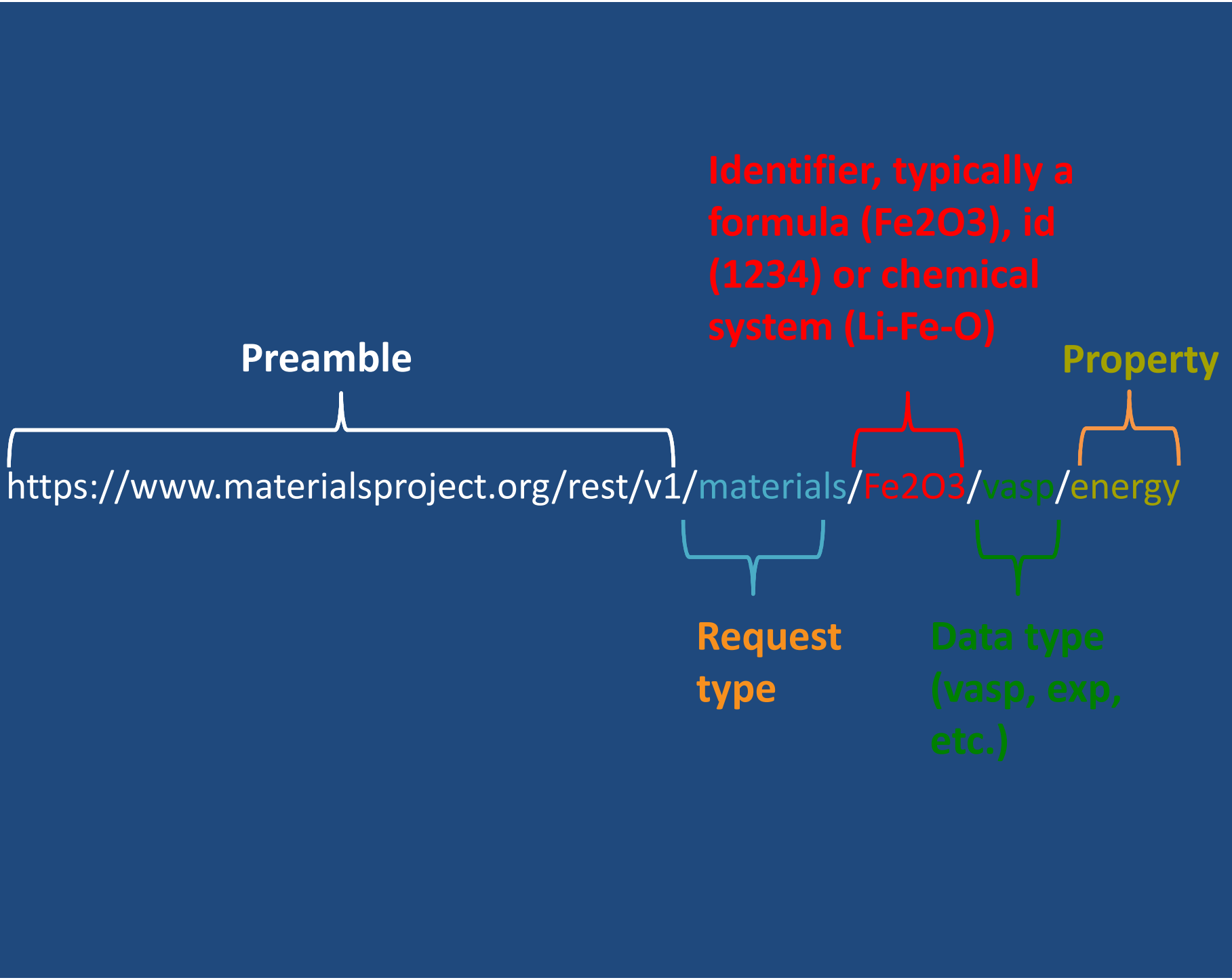
The Materials API

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

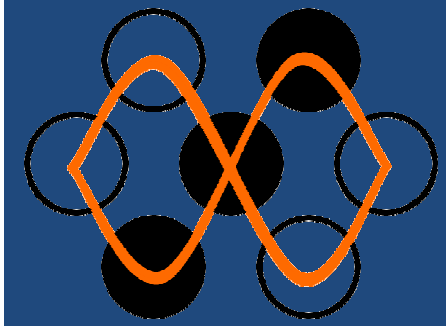

MATERIALS
PROJECT
MATERIALS
ECOSYSTEM
Improved accessibility of data
More developers of analyses and apps
Increased data value


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

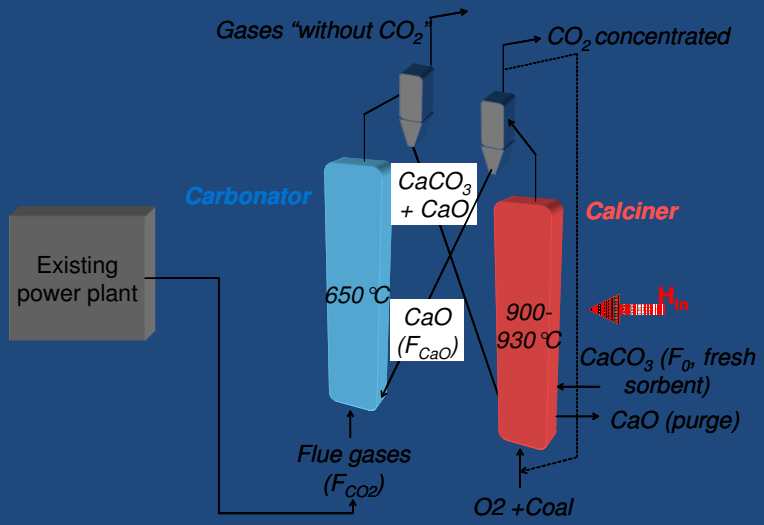


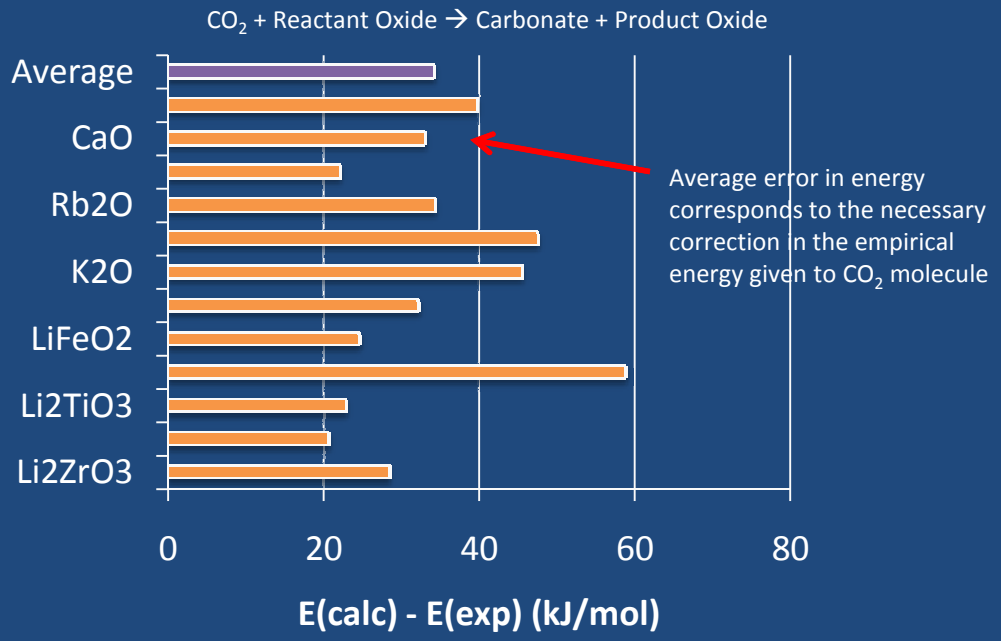
Example collaborations

Screening for CO_2 sorbents (Grey et al)

Calculating reaction energies of thousands of oxides with CO_2

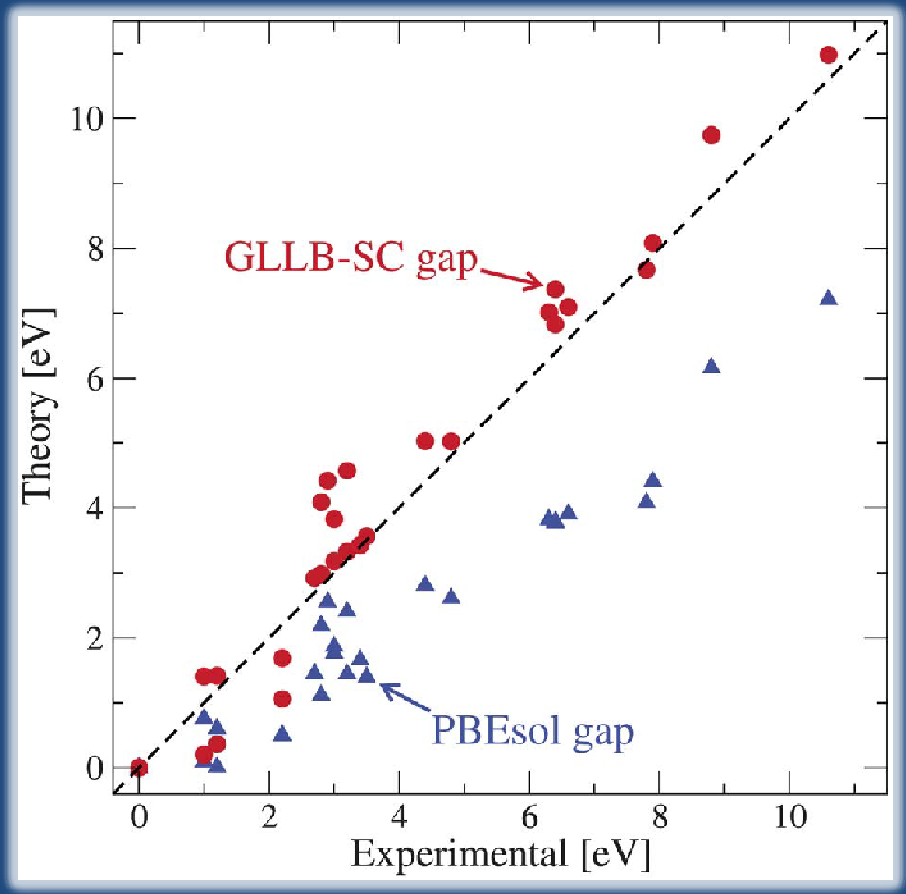
- High selectivity and absorption capacity for CO2 at elevated temperatures (400-900°C)
- Good absorption/desorption kinetics - preferably under a wide range of p(CO_2)
- Good cyclability for absorption/desorption processes
- Good hydrothermal and mechanical properties





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

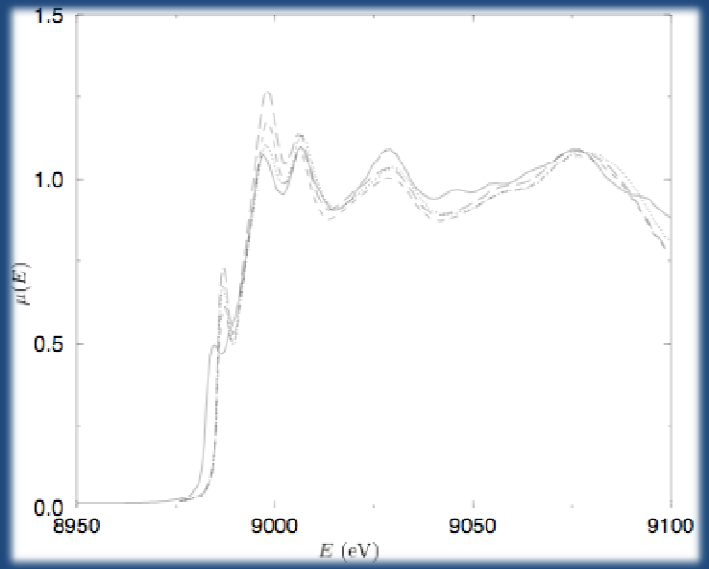


I.E. Castelli, T. Olsen, S. Datta, D.D. Landis, S. Dahl, K.S. Thygesen, and K.W. Jacobsen, Energy & Environmental Science 1–6 (2012).

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).

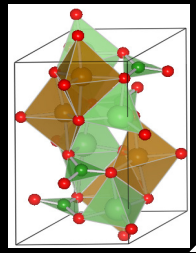
via pymatgen and Rockets/ Fireworks

Disseminate data via Materials Project Source (MPS)

MPS

about

crystal



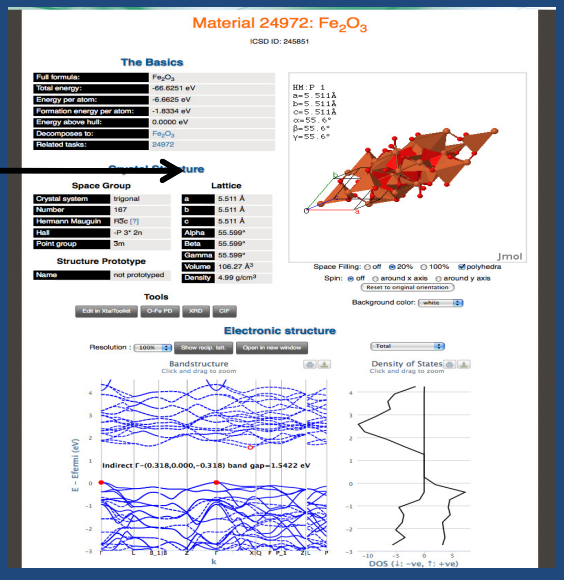
about

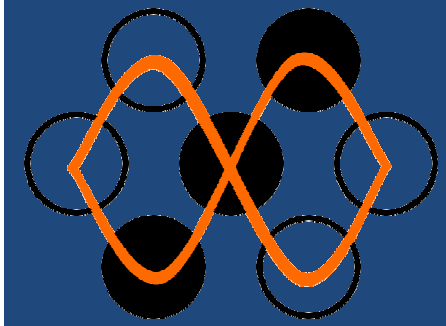
- *Who authored the xtal?*
- *What papers to cite?*
- *Is the xtal linked to any known databases?*
- *What codes operated on the xtal?*
- *What metadata is associated with the xtal?*

Send to Materials Project

200+ relaxed structures from that last CE

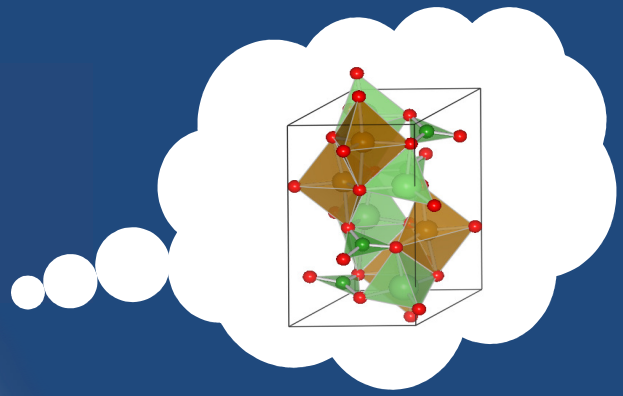
author, publication reference and link…

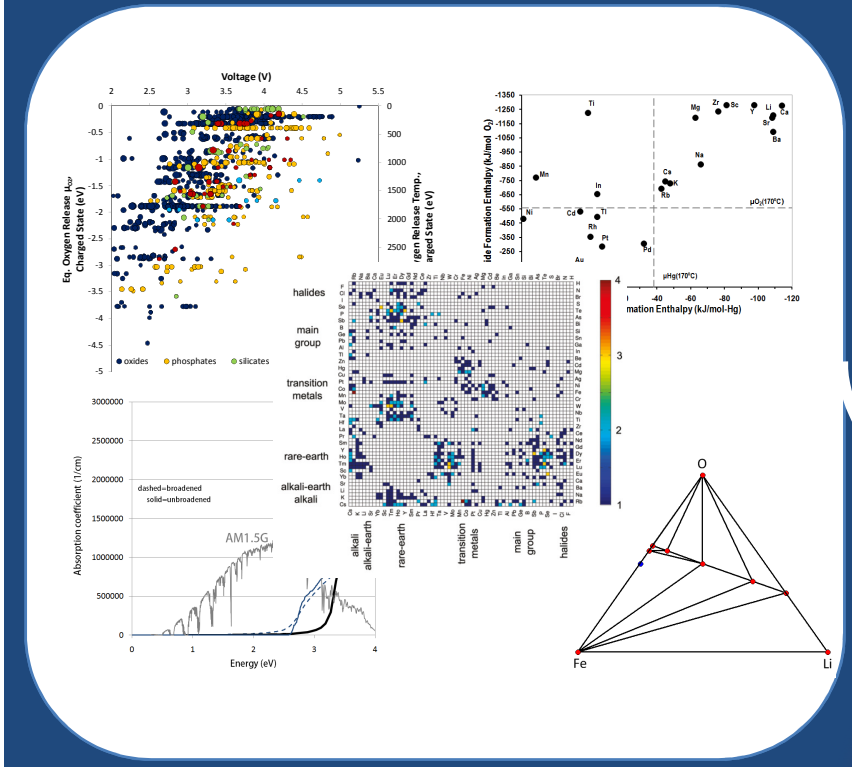


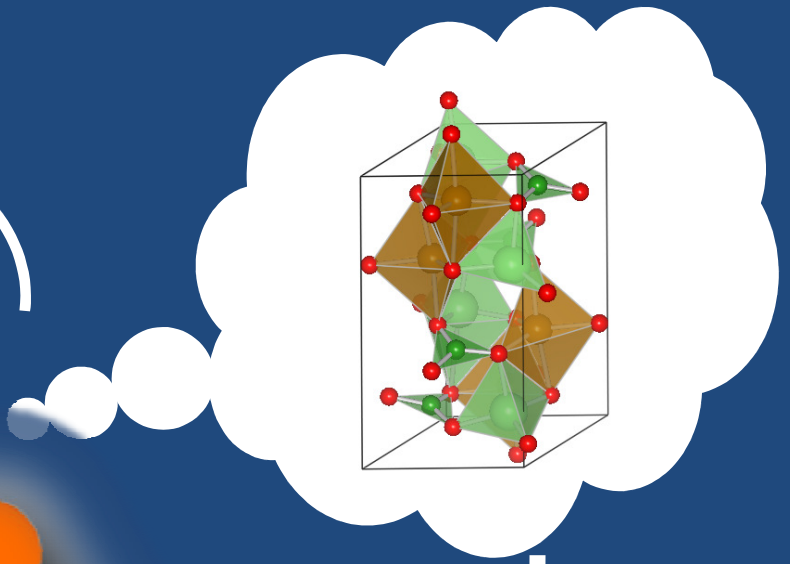


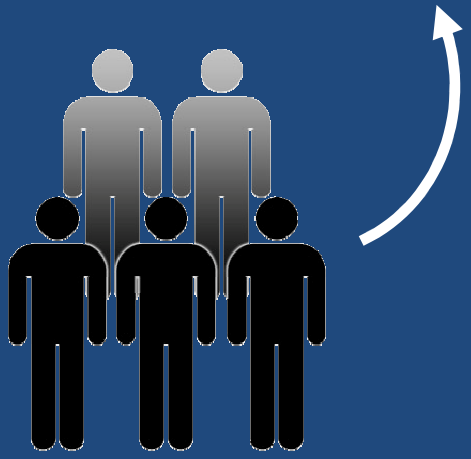
The Vision

From single entities…









… towards amaterials genome

Thank you for your attention

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U.S. DEPARTMENT OF ENERGY

National Science Foundation
WHERE DISCOVERIES BEGIN

And thanks to the team:

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