

A Google for Materials?

Kristin Persson

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Engineered Materials Enable Society



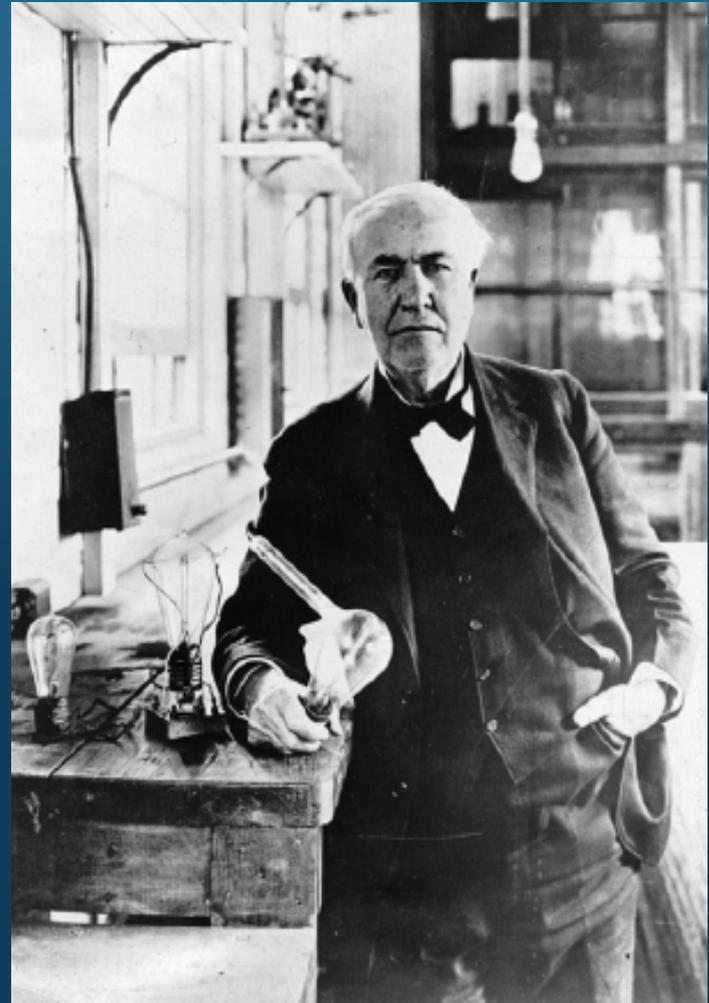
How are New Materials Invented?

“Edison Style”

When looking for a light bulb filament, Edison tried about 3,000 materials

...

And he didn't find the best one ...!



Materials Design: Hollywood Style



Reality Check

18 Years...

From new materials discovery to commercialization!

How to accelerate the innovation and development timeline ?

invented

Teflon

Velcro

Titanium

Polycarbonate

GaAs

Diamond-like Thin Films

Amorphous soft magnets

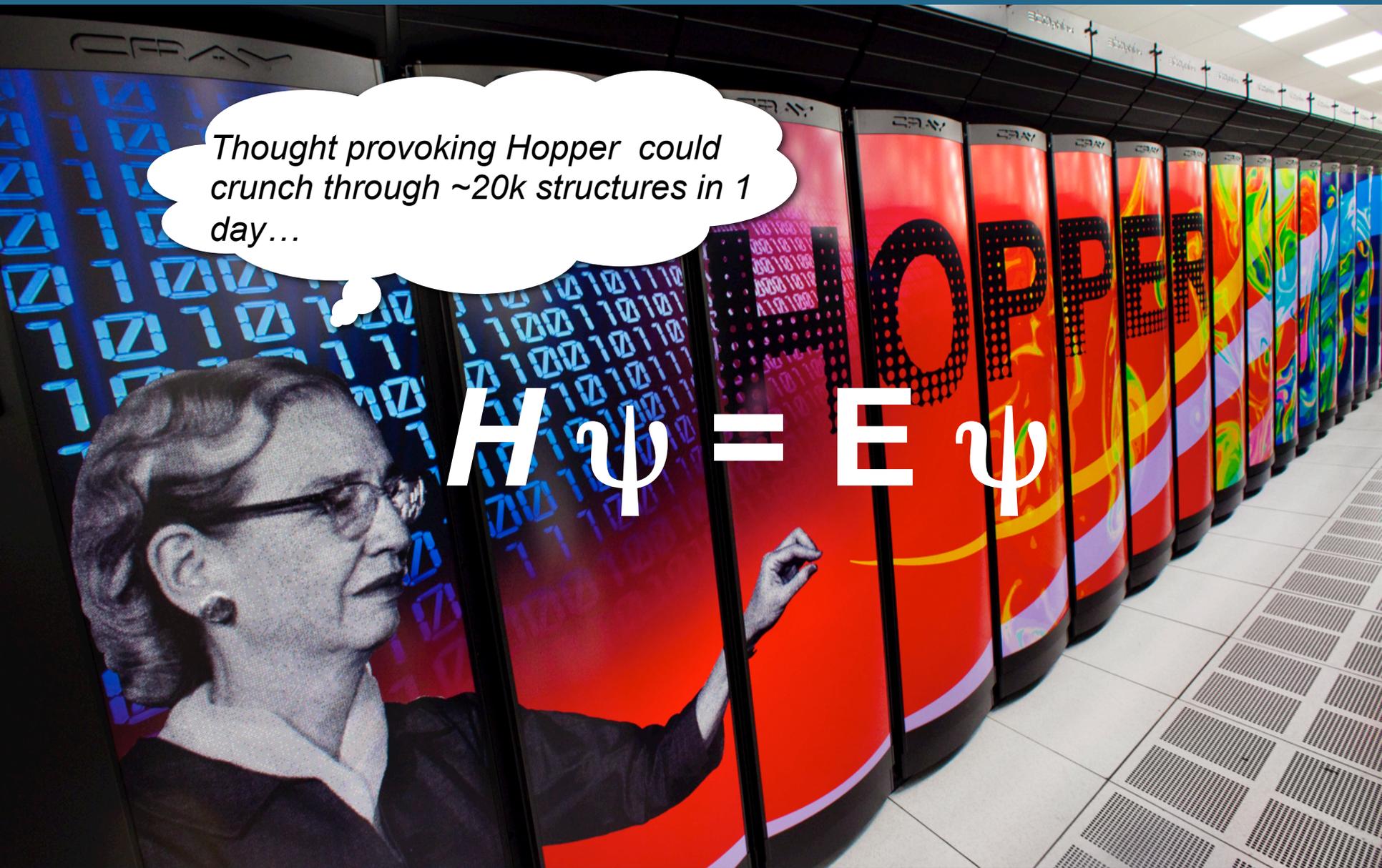
S. Whittingham

Lithium Ion

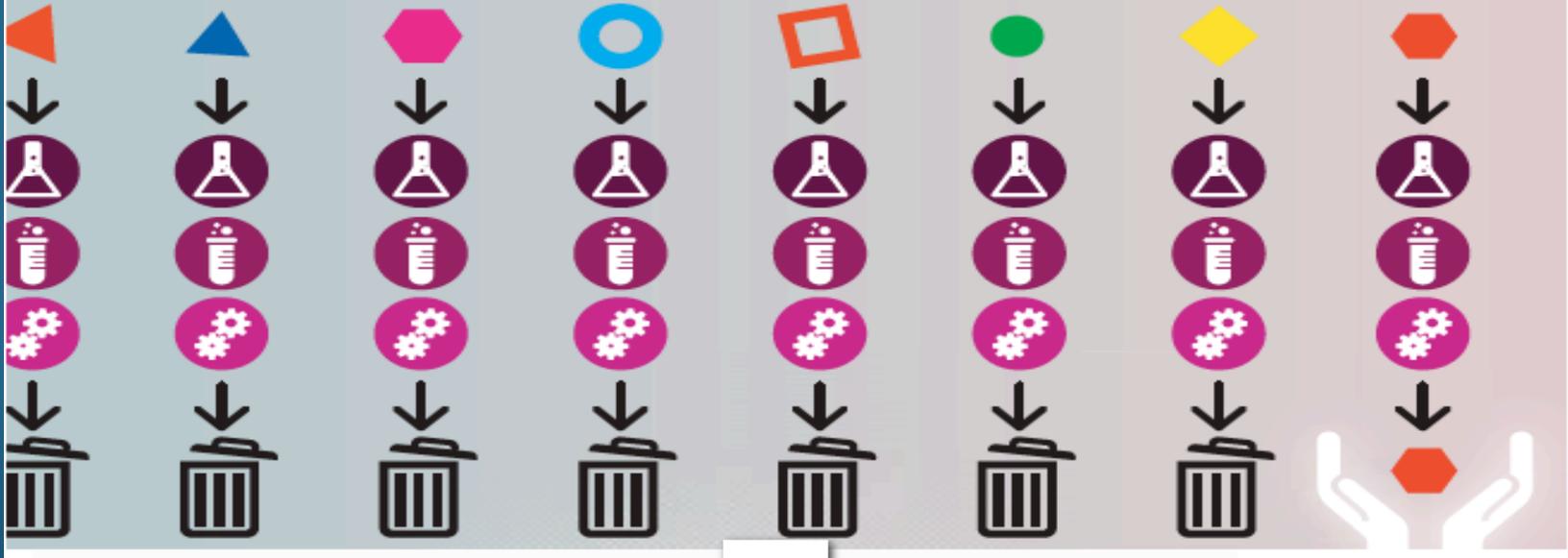
Sony

Thought provoking Hopper could crunch through ~20k structures in 1 day...

$$H \psi = E \psi$$



Edisonian



In Silico



Novel Materials for Alkaline batteries

> 130,000 compounds screened

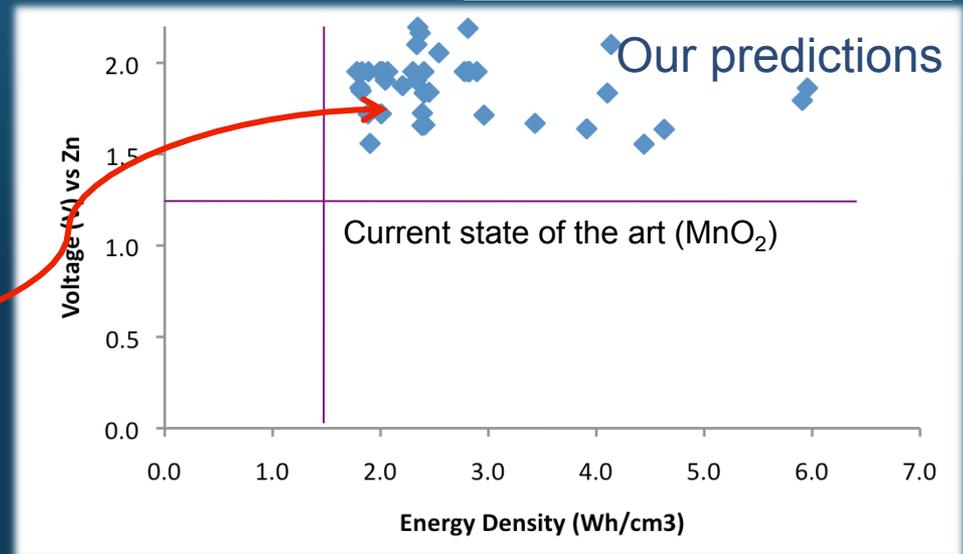
Screening I

> 1500 compounds

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

Screening II

200 compounds
with Electrolyte Stability



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

How to stabilize high-valent compounds

- High negative formation energy
- Negative formation energy
- Positive formation energy
- High positive formation energy

How to stabilize at pH = 15

- High dissolution energy
- Moderate dissolution energy
- No dissolution energy

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

Proof of concept – it's just the beginning...

Completely new materials predicted and synthesized based on computational predictions



(12) **United States Patent**
Eylem et al.

(10) Patent No.:
(45) Date of Pate

(54) **PRIMARY ALKALINE BATTERY**
CONTAINING BISMUTH METAL OXIDE

(75) Inventors: **Cahit Eylem**, Bellingham, MA (US);
Paul A. Christian, Norton, MA (US);
Yichun Wang, West Roxbury, MA (US);
Joseph K. Sauerbrey, IV, Merrimack, NH (US); **In Tae Hae**, Westham, MA (US)

(73) Assignee: **The Gillette Company**, Boston, MA (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 327 days.

(21) Appl. No.: 11/484,551

(22) Filed: Jul. 16, 2006

(65) Prior Art:
US 2008/0080937 A1

(51) Int. Cl. (2006.01)
H01M 4/08 (2006.01) Macroporous
H01M 4/50 (2006.01) Substrate
H01M 4/54 (2006.01) Mater. use
H01M 4/52 (2006.01)
H01M 2/66 (2006.01)

(52) U.S. Cl. (2006.01)
429/218.1; 429/224; 429/223;
429/219; 429/231.6; 429/221; 429/220; 429/231.1; 429/145

(58) Field of Classification Search: None
See application file for complete search history.

(56) References Cited:
U.S. PATENT DOCUMENTS
2,806,225 A 10/1977 Mischouse et al.
2,826,350 A 9/1958 Blass, Jr.

(11) United S
(12) Patent A
Christian et

(13) PUBLICATION NO. 2011/0119377

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B01J 23/02 (2006.01)
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B01J 23/08 (2006.01)
B01J 23/10 (2006.01)
B01J 23/12 (2006.01)
B01J 23/14 (2006.01)
B01J 23/16 (2006.01)
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B01J 23/96 (2006.01)
B01J 23/98 (2006.01)
B01J 23/00 (2006.01)

(16) Abstract

A primary battery includes a cathode having a non-transition metal oxide including bismuth metal oxide. The Bi⁵⁺ and Bi⁴⁺ are present in the cathode. The cathode and the anode are electrically connected.

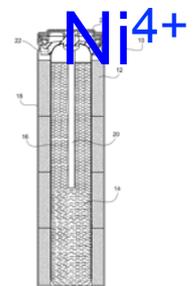
(17) Claims

(18) App. No. 13/721,049

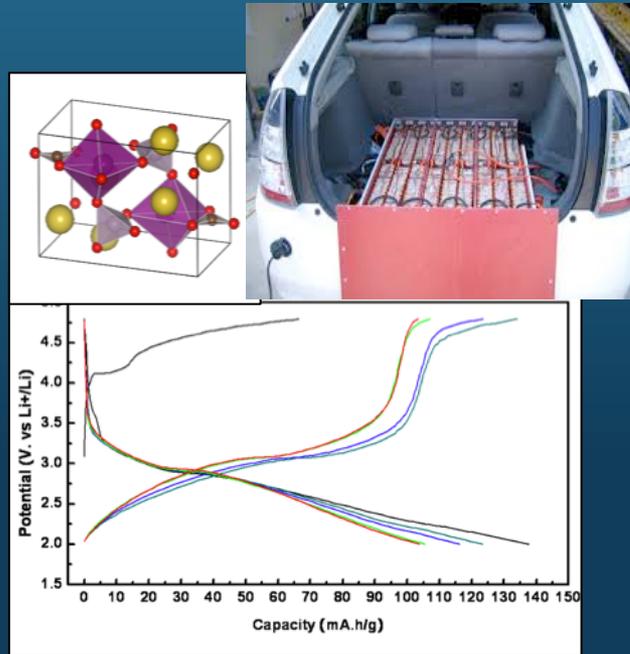
(19) Filed: Mar. 12, 2014

Bi⁵⁺

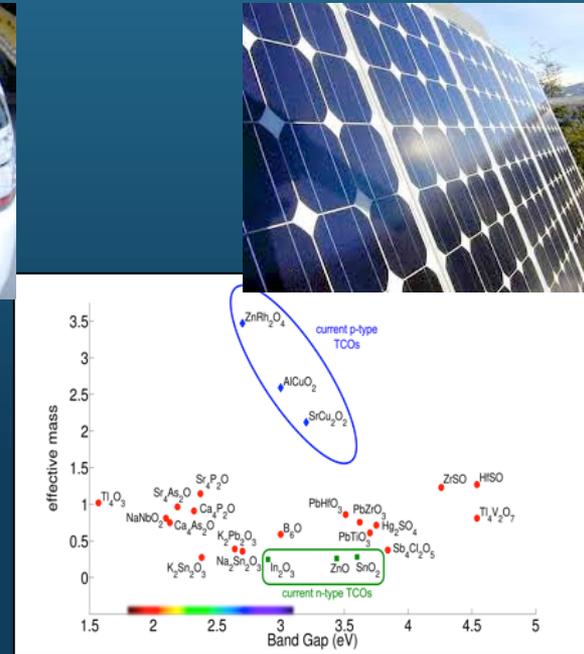
Ni⁴⁺



2005:
Novel stable alkaline
batteries



2011:
Novel class of Li ion
electrodes



2013:
Improved transparent
conductors

Materials Design in the Information Age

The Google logo is centered on a white background. It consists of the word "Google" in its signature multi-colored font: 'G' is blue, 'o' is red, 'o' is yellow, 'g' is blue, 'l' is green, and 'e' is red.

Materials Design in the Information Age

The Google logo is centered on a white background. It consists of the word "Google" in its characteristic multi-colored font: 'G' is blue, 'o' is red, 'o' is yellow, 'g' is blue, 'l' is green, and 'e' is red.

3V < voltage < 4.5V AND good stability AND good Li mobility

Google Search

I'm Feeling Lucky

Today's Status:

- ❑ Over 38,000 compounds and growing monthly
- ❑ Multiple tools based on computed data

The screenshot shows the Materials Project website dashboard. At the top, there is a navigation bar with links for Home, Apps, Resources, About, References, and Electrolyte Genome (which is highlighted). A search bar contains the text "e.g. explore Fe2O3 or Li-Fe-O pd" and is powered by MOOGLE. The main heading is "MATERIALS PROJECT" in large, bold letters, with "PROJECT" in orange. Below this is the tagline "A Materials Genome Approach" and the mission statement: "Accelerating materials discovery through advanced scientific computing and innovative design tools." To the right, "Database Statistics" are listed: 38151 materials, 14618 bandstructures, 610 intercalation batteries, and 16277 conversion batteries. A grid of six tool cards is displayed below, each with an icon and a brief description.

Home Apps Resources About References **Electrolyte Genome** Dashboard :: Logout

MATERIALS PROJECT

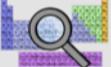
A Materials Genome Approach

Accelerating materials discovery through advanced scientific computing and innovative design tools.

Search e.g. explore Fe₂O₃ or Li-Fe-O pd powered by **MOOGLE**

Database Statistics

38151 materials	14618 bandstructures
610 intercalation batteries	16277 conversion batteries



Materials Explorer

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



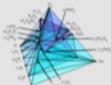
Lithium Battery Explorer

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



Crystal Toolkit

Convert between CIF and VASP input files. Generate new crystals by substituting or removing species.



Phase Diagram App

Computational phase diagrams for closed and open systems. Find stable phases and study reaction pathways.



Reaction Calculator

Calculate the enthalpy of tens of thousands of reactions and compare with experimental values.



Pourbaix Diagrams

Generate Pourbaix Diagrams from experimental ion data

The Materials Genome Initiative



Materials Genome Initiative: A Renaissance of American Manufacturing

June 2011: **Materials Genome Initiative** which aims to *“fund computational tools, software, new methods for material characterization, and the development of open standards and databases that will make the process of discovery and development of advanced materials faster, less expensive, and more predictable”*

The **Materials Project** was recognized by several agencies and publicized at DOE as a ‘First-Of-Its-Kind Search Engine’ for materials research and a groundbreaking project within the recent **Materials Genome Initiative** announcement.

The screenshot shows the ENERGY.GOV website interface. At the top, there is a green navigation bar with the text "ENERGY.GOV" and a search prompt "Find information about your town or city." Below this are several menu items: "PUBLIC SERVICES", "SCIENCE & INNOVATION", "MISSION", "News & Blog", and "Maps & Dat". The main content area features a "Home" link and a large blue headline: "First-Of-Its-Kind Search Engine Will Speed Materials Research". Below the headline is the date "November 3, 2011 - 1:05pm" and a paragraph of text: "Washington, D.C. – Researchers from the Department of Energy’s (DOE’s) Lawrence Berkeley National Laboratory (Berkeley Lab) and the Massachusetts Institute of Technology (MIT) jointly launched today a groundbreaking new online tool called the Materials Project, which operates like a ‘Google’ of material properties, enabling scientists and engineers from universities, national laboratories and private industry to accelerate the development of new materials, including critical materials." A quote follows: "By accelerating the development of new materials, we can drive discoveries that not only help power clean energy, but also are used in common consumer products." said Secretary of Energy Steven Chu. "This research tool will help the United States compete with other developers of new materials, and could potentially create new domestic industries." A final paragraph states: "Discovering new materials and strengthening the properties of existing materials are key to improving just about everything humans use – from buildings and highways to modern necessities. For example, advances in a group of materials called ‘critical materials’ are more important to America’s competitiveness than ever before – particularly in the clean energy field. Cell phones,

The Li-ion Battery Explorer



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!



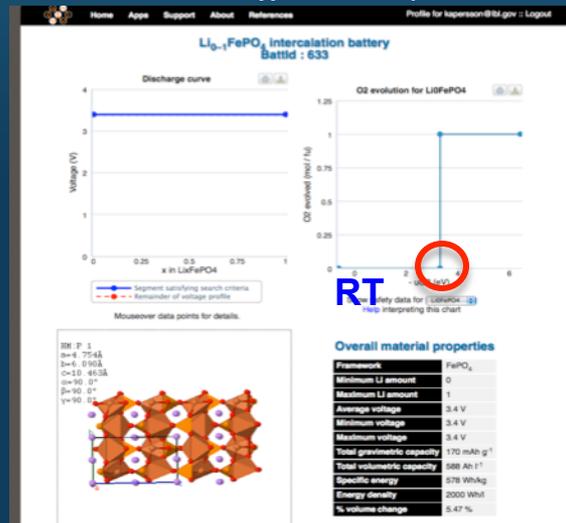
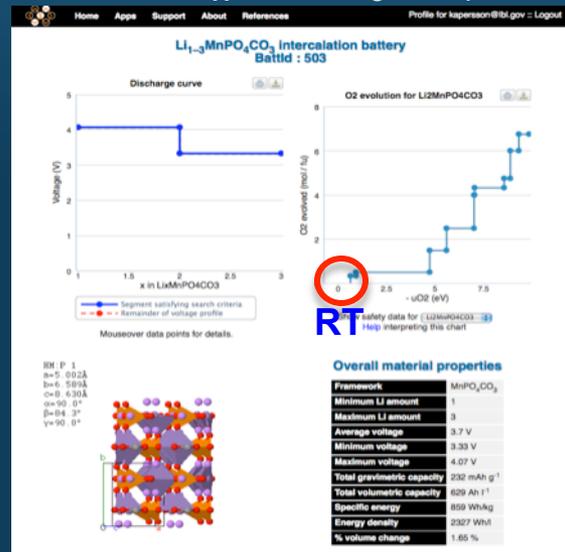
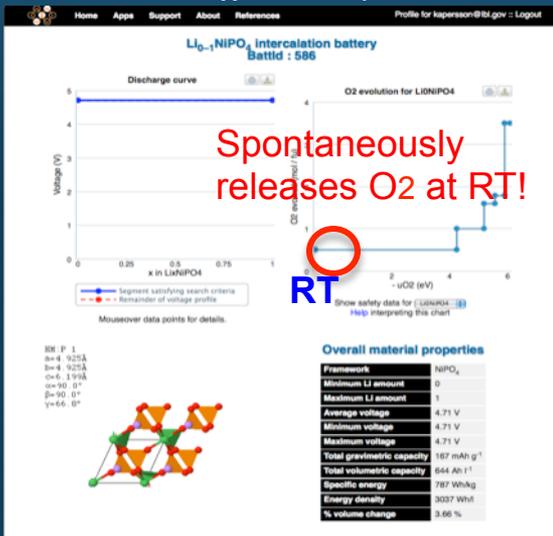
Oxygen release correlates with oxygen chemical potential of cathode



safer



safer



ICSD Other experimental databases User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)



Analysis

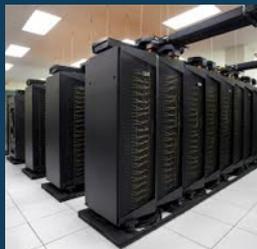
Web apps

Materials API

Workflow Manager

Post-processing and error-checking

Supercomputing Resources



Input processing & transformations

pymatgen

- Robust materials analysis



Custodian

- Self-healing error recovery



Fireworks

- Smart workflow management



StructureNotationalLanguage (SNL)



Analysis

Web apps
Materials API

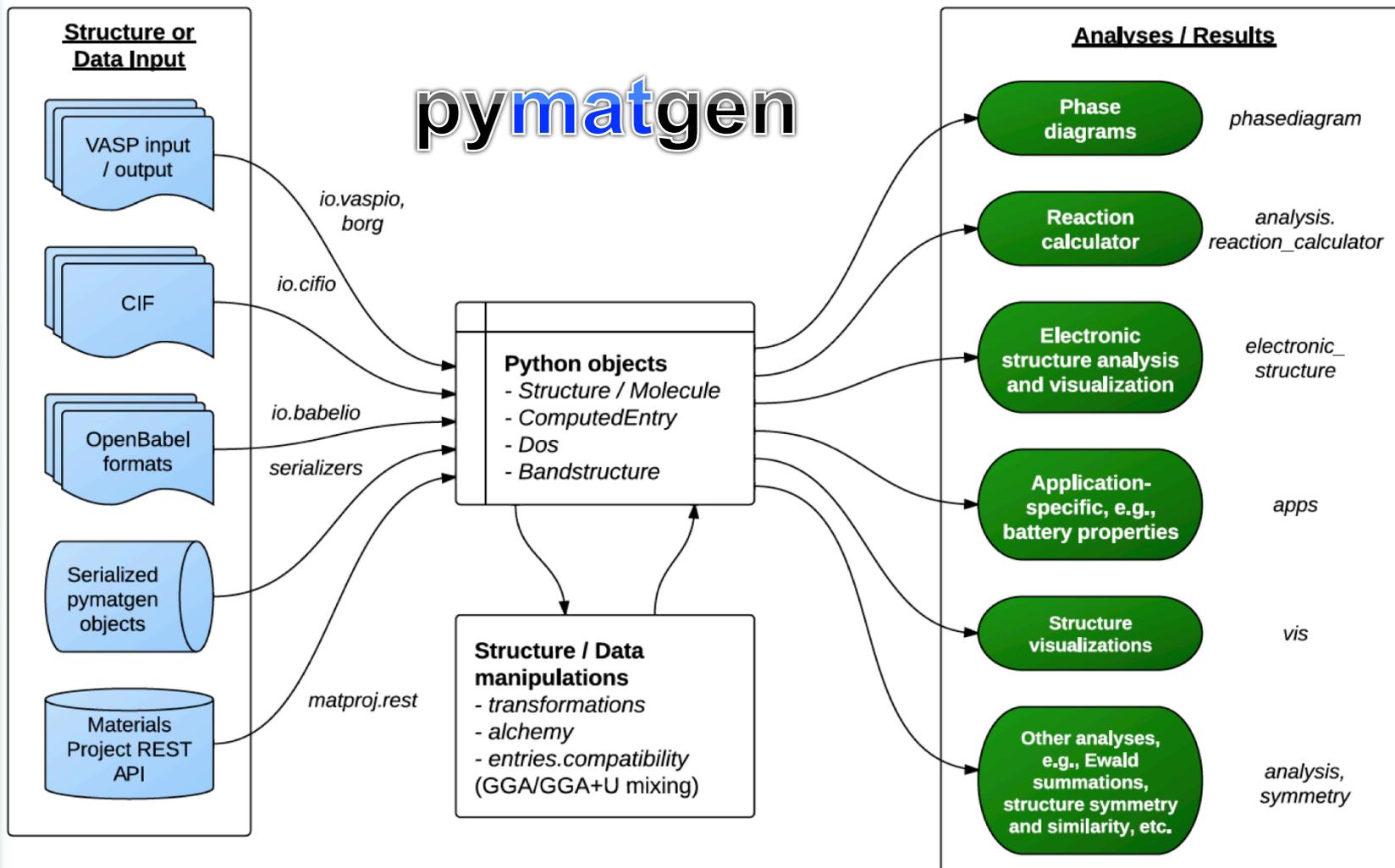
Workflow Manager

Post-processing and error-checking

Supercomputing Resources



Open Source Codes



Building robust software that lasts... :

All pymatgen classes and methods come with **unit tests**

All code have proper **documentation**

pymatgen 2.2.1 documentation > next | modules | index

pymatgen

Introduction

Pymatgen (Python Materials Genomics) is a robust, open-source Python library for materials analysis. It currently powers the public Materials Project (<http://www.materialsproject.org>), an initiative to make calculated properties on a large number of materials available to materials researchers and designers. These are some of the main features:

1. Highly flexible classes for the representation of Element, Site, Molecule, Structure objects.
2. Extensive io capabilities to manipulate many VASP input and output files (<http://cms.mpi.univie.ac.at/vasp/>) and the crystallographic information file format. This includes generating Structure objects from vasp input and output. There is also support for Gaussian input files and XYZ file for molecules.
3. Comprehensive tool to generate and view compositional and grand canonical phase diagrams.
4. Electronic structure analyses (DOS and Bandstructure).
5. Integration with the Materials Project REST API.

The pymatgen library is free (as in free beer) to download and to use. However, we would also like you to help us improve this library by making your own contributions as well. These contributions can be in the form of additional tools or modules you develop, or even simple things such as bug reports. Please read the [Contributing](#) section or contact the maintainer of this library (shyue@mit.edu) to find out how to include your contributions via github or for bug reports.

Note that pymatgen, like all scientific research, will always be a work in progress. While the development team will always strive to avoid backward incompatible changes, they are sometimes unavoidable, and tough decisions have to be made for the long term health of the code.

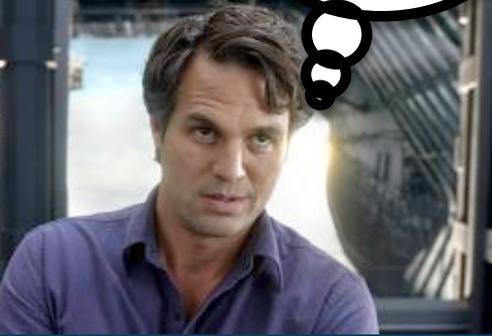
The most up-to-date documentation is available at our github page (<http://materialsproject.github.com/pymatgen/>), where you can also report any bugs/issues. If you wish to be notified via email of pymatgen releases, you may become a member of [pymatgen's Google](#)

any analysis scripts.
MetricData.
ion classes.
with v1 release of the Materials API.
ous bug fixes and speed improvements.

- Older versions
 - Version 2.2.0
 - Version 2.1.2
 - Version 2.0.0
 - Version 1.9.0

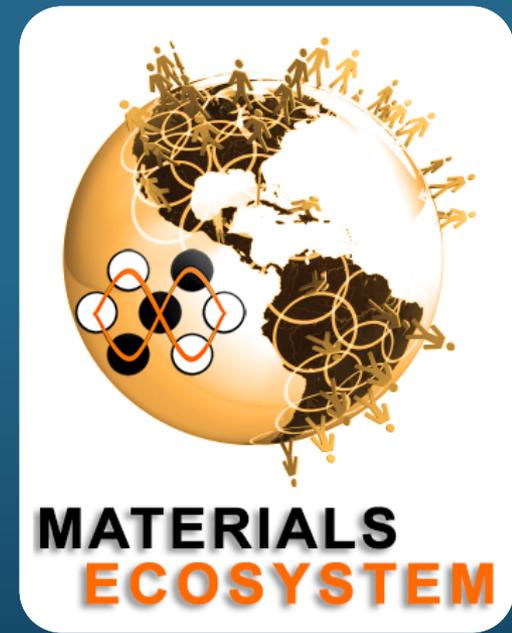
Does anyone remember how to run 'GoBabyMonte.c' ???

Nah – Bob left in 2004....



World Wide Usage





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

Improved
accessibility of
data

More
developers of
analyses and
apps

Increased
data value

Separate databases



User not in group,
sees only core data



User in group, sees a
unified view of both
sandbox and core data

MATERIALS PROJECT
A Materials Genome Approach
Accelerating materials discovery through advanced scientific computing and innovative design tools.

Database Statistics

34598 materials	14387 bandstructures
445 intercalation batteries	16016 conversion batteries

Tools: Materials Explorer, Lithium Battery Explorer, Crystal Toolkit, Phase Diagram App, Reaction Calculator, Structure Predictor.

Latest News: pymatgen v2.5.2 by Shyue Ping Ong - Feb 19, 2013

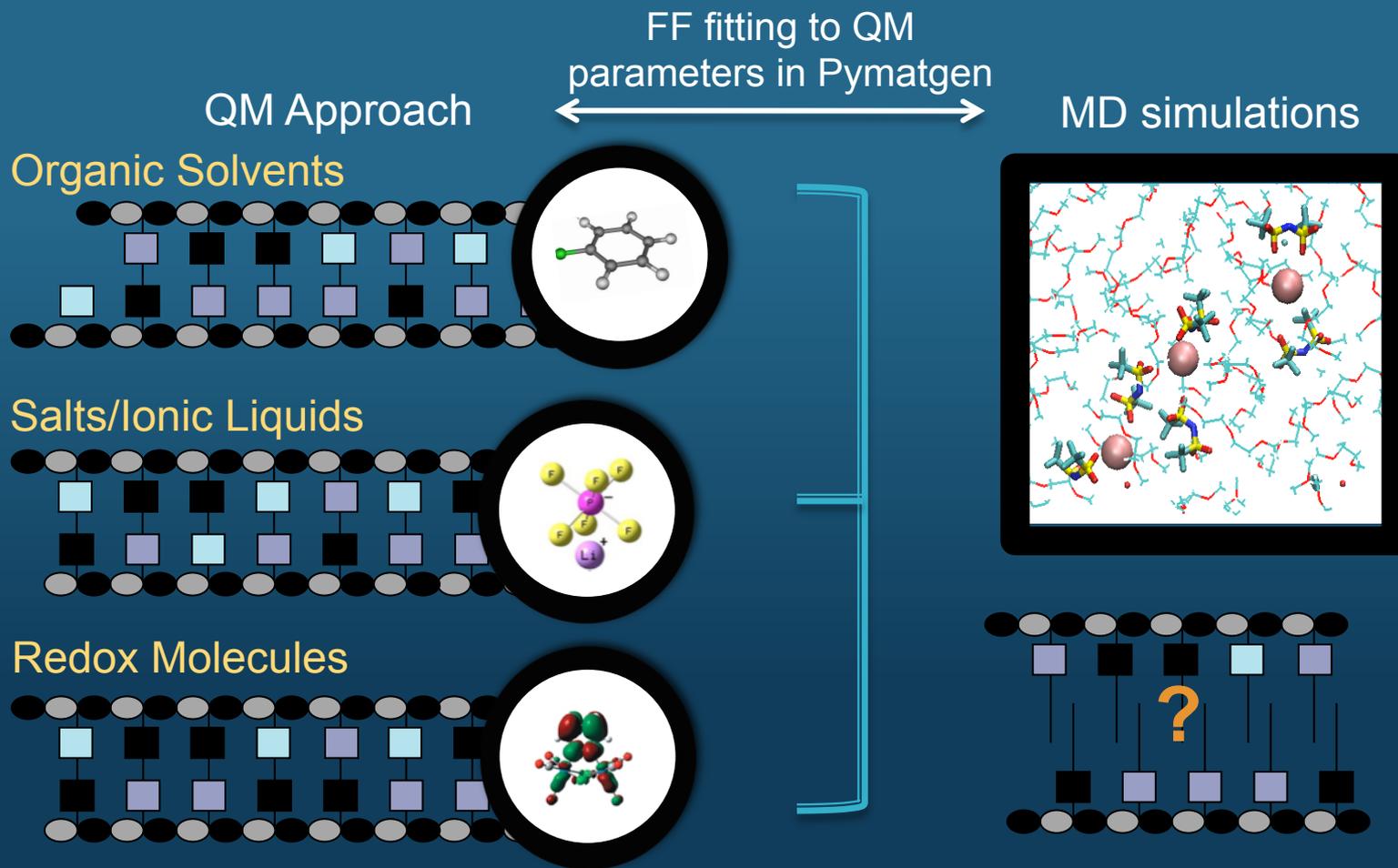
Core data



Unified View

Sandbox can be
shared by a
group of users

A 'Genomic' Approach to Electrolytes



Substitution, mutation and selection to arrive at optimal electrolytes and redox molecules

JCESR Sandbox: The Electrolyte Genome

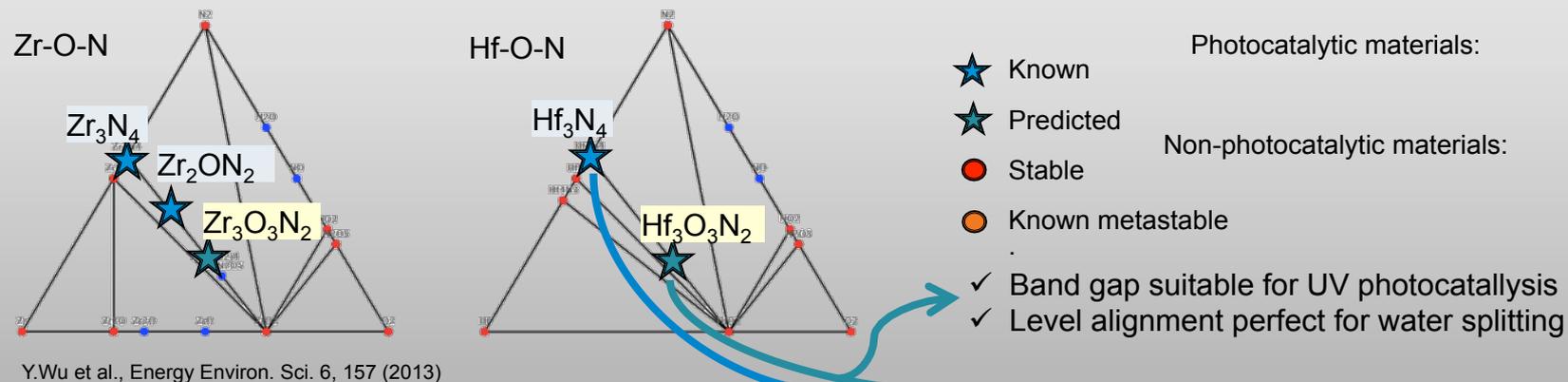
The screenshot displays the Materials Project website interface. The top navigation bar includes links for Home, Apps, Resources, About, References, and **Electrolyte Genome** (highlighted with an orange box), along with a Dashboard and Logout option. A search bar contains the text "e.g. explore Fe2O3 or Li-Fe-O pd" and is powered by MOOGL. The main content area features the "MATERIALS PROJECT" logo and a search for "H8C9N2". A sidebar on the left offers filters for Charge, EA, IE, and Point Group. A central plot titled "IE/EA vs. Molecule" shows data points for the search query. Below the plot is a table of results.

smiles	svg	EA	point group	charge	formula	IE
c1(cc2c(cc1)nccn2)C		0.409	Cs	0	H ₈ C ₉ N ₂	8.663
c1c(c2c(cc1)nccn2)C		0.451	Cs	0	H ₈ C ₉ N ₂	8.503
c1cc2c(cc1)nccn2)C		0.428	Cs	0	H ₈ C ₉ N ₂	8.686

Find out more about our [open Materials API](#) and [pymatgen library](#) for querying large amounts of data.

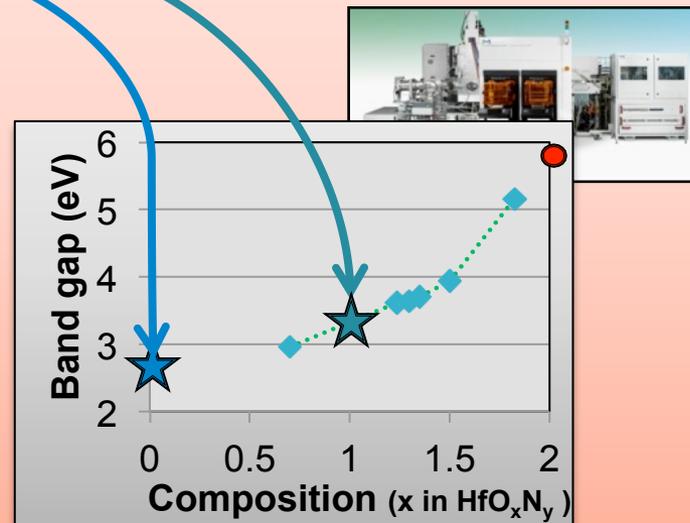
Intermolecular : New Materials for Photocatalysis

Superior new materials for water-splitting photocatalysis predicted theoretically by the members of Materials Project



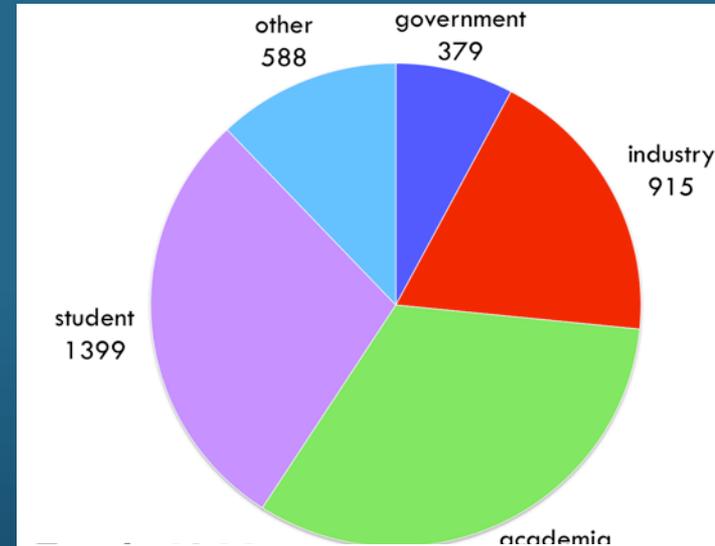
Materials developed by Intermolecular show properties matching these predictions

- ✓ Focus on materials with multiple applications
- ✓ Synthesis methods developed
- ✓ Range of O:N compositions scanned
- ✓ Optical characterization data match the predicted band gap
- ✓ Future workflow could focus on optimizing the water splitting capabilities

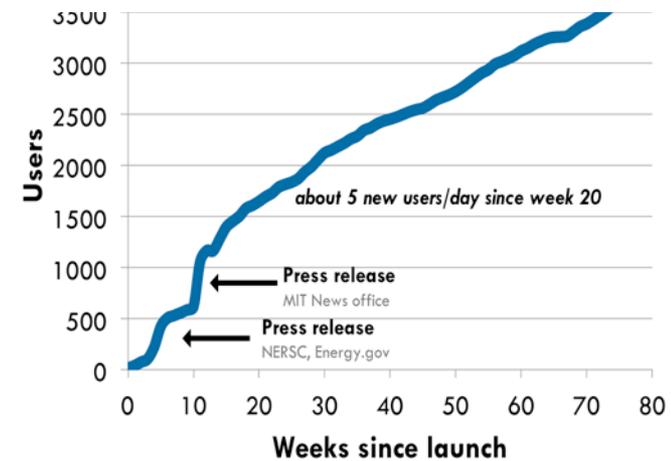


A Rapidly Growing Resource

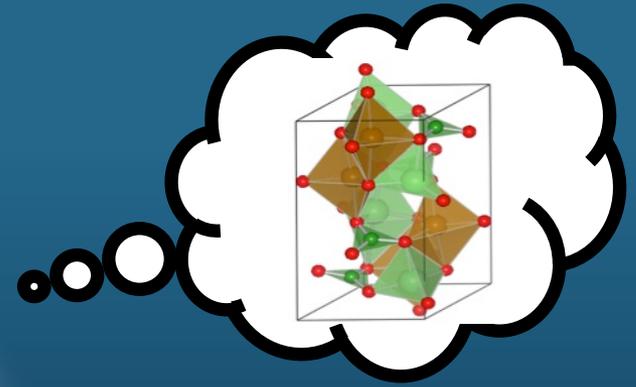
- ❑ **Launched** online Oct 2011
- ❑ **Grants:** 2012 DOE Center, JCESR, U Madison NSF Center, JCAP
- ❑ **Users:** > 5600 and counting...
- ❑ **Course-ware :** UC San Diego, UC Davis, UC Irvine, U Michigan, John-Hopkins, Cornell, ...
- ❑ **Partner institutions:** UC Berkeley, UC San Diego, MIT, Duke, U Wisconsin, U Kentucky, U Louvain Belgium, Cambridge UK, Caltech, ...
- ❑ **Companies:** Toyota, Sony, Bosch, 3M, Honda, Samsung, LG Chem, Dow Chemicals, GE Global Research, Intermolecular, Applied Materials, Energizer, Advanced Materials, General Motors, Corning, DuPont, Nippon Steel, L'Oreal USA, Caterpillar, HP, Unilever, Lockheed Martin, Texas Instruments, Ford, Bose, Sigma-Aldrich, Siemens, Raytheon, Umicore, Seagate, ...

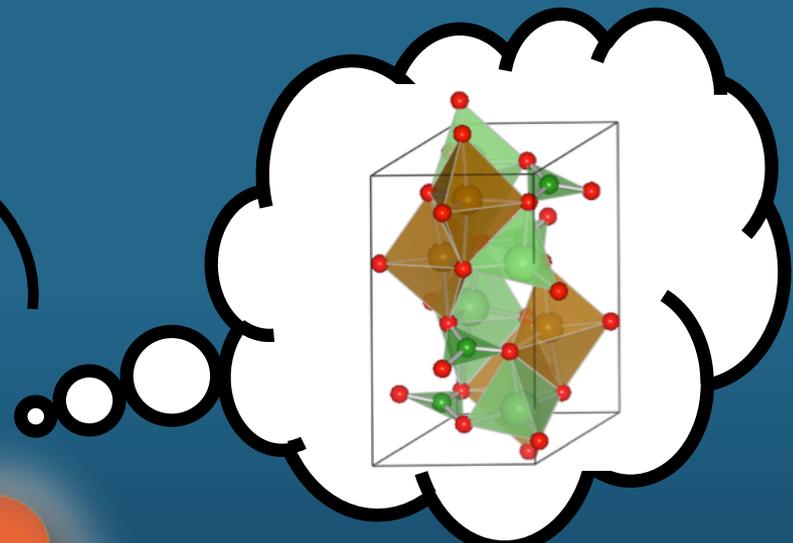
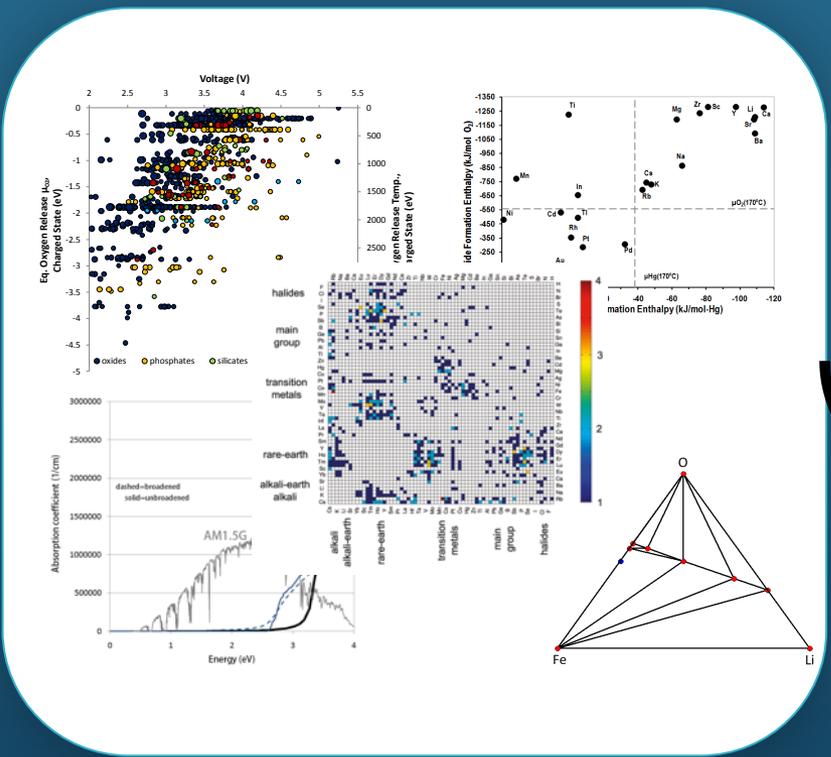


As of today: 5622 users

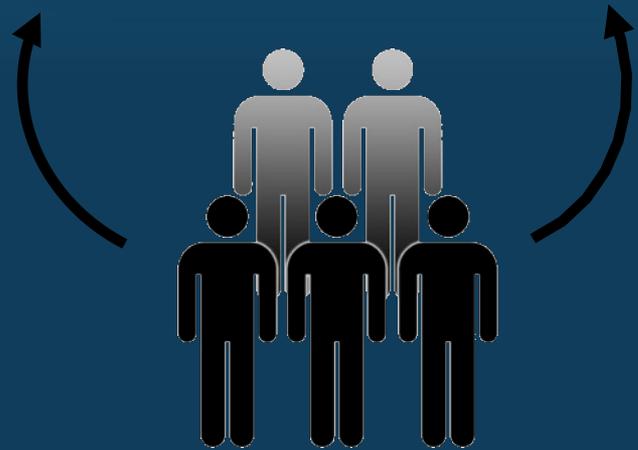


From single entities...





... towards a materials genome



“Con
fi

Thank you for your attention!

Thanks to sponsors:

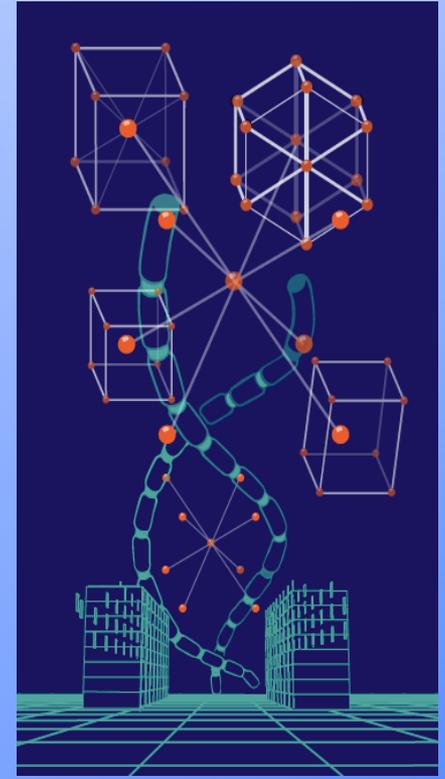


U.S. DEPARTMENT OF
ENERGY



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 Mark Asta Anthony Gamst Wei Chen Qimin Yan Bharat Mehdsani Geoffroy Hautier
Shreyas Cholia Maciej Haranszyk Will Richards Jeff Neaton Maarten De Jong Sai Jayaram Wenhao Sun William Richards



rese

*“I am so incredibly happy an effort like this exists now... I have been lamenting for years that despite the importance of materials we have remained relatively unaided by the information age. **Please please don't stop growing!**”* Cymbet