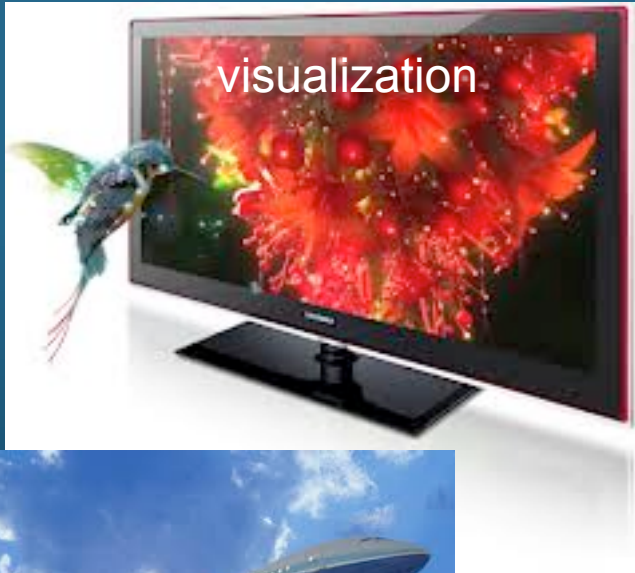


# A Google for Materials?

Kristin Persson

Lawrence Berkeley National Laboratory

# Engineered Materials Enable Society



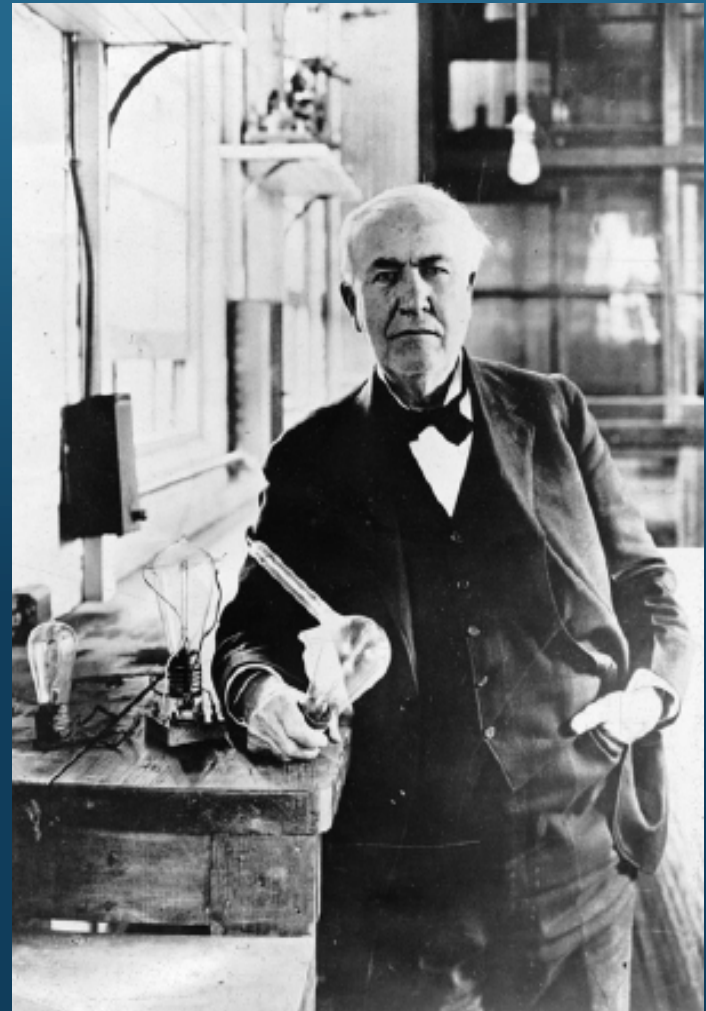
# How are New Materials Invented?

## “Edison Style”

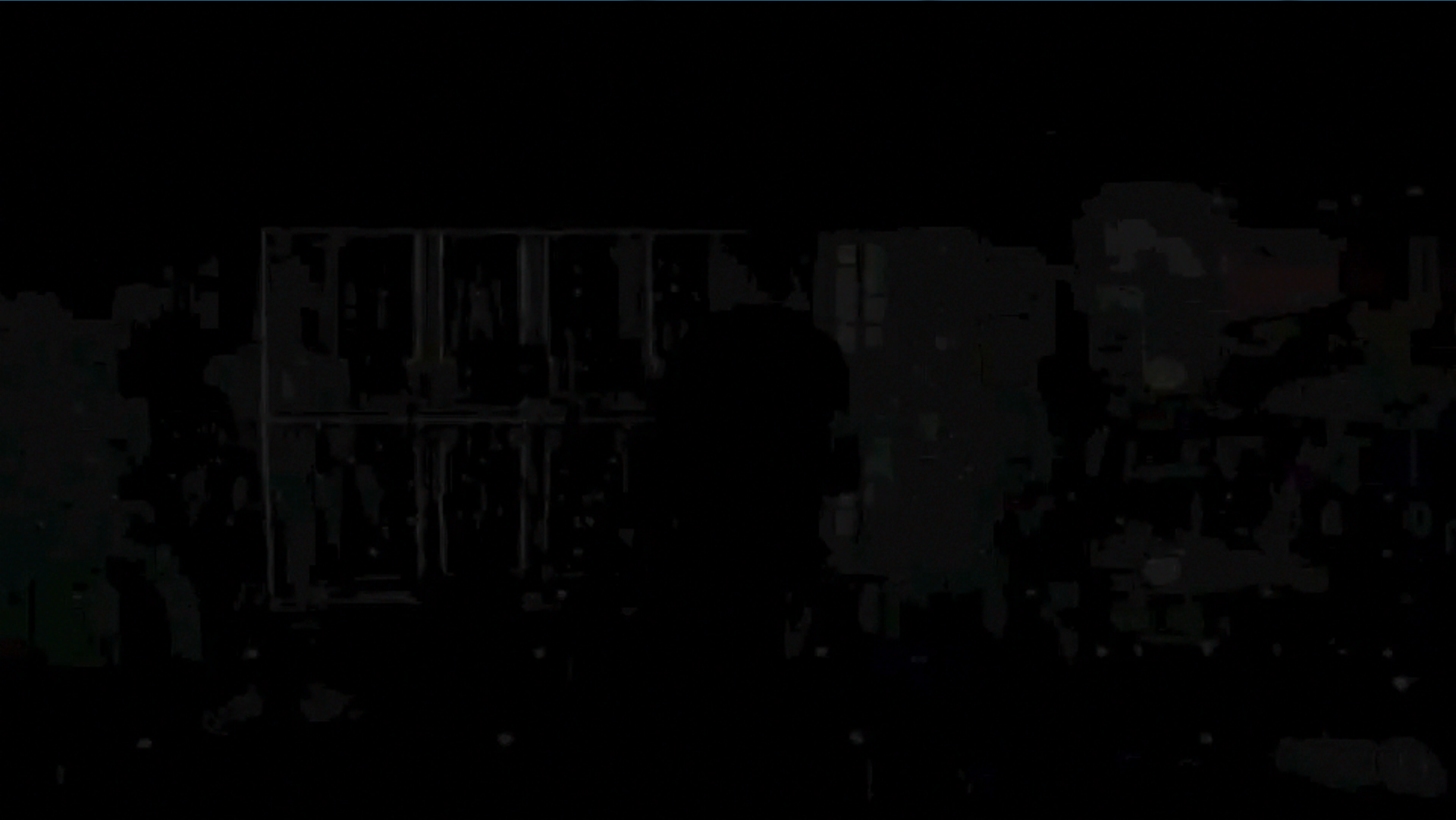
When looking for a light bulb filament, Edison tried about 3,000 materials

...

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

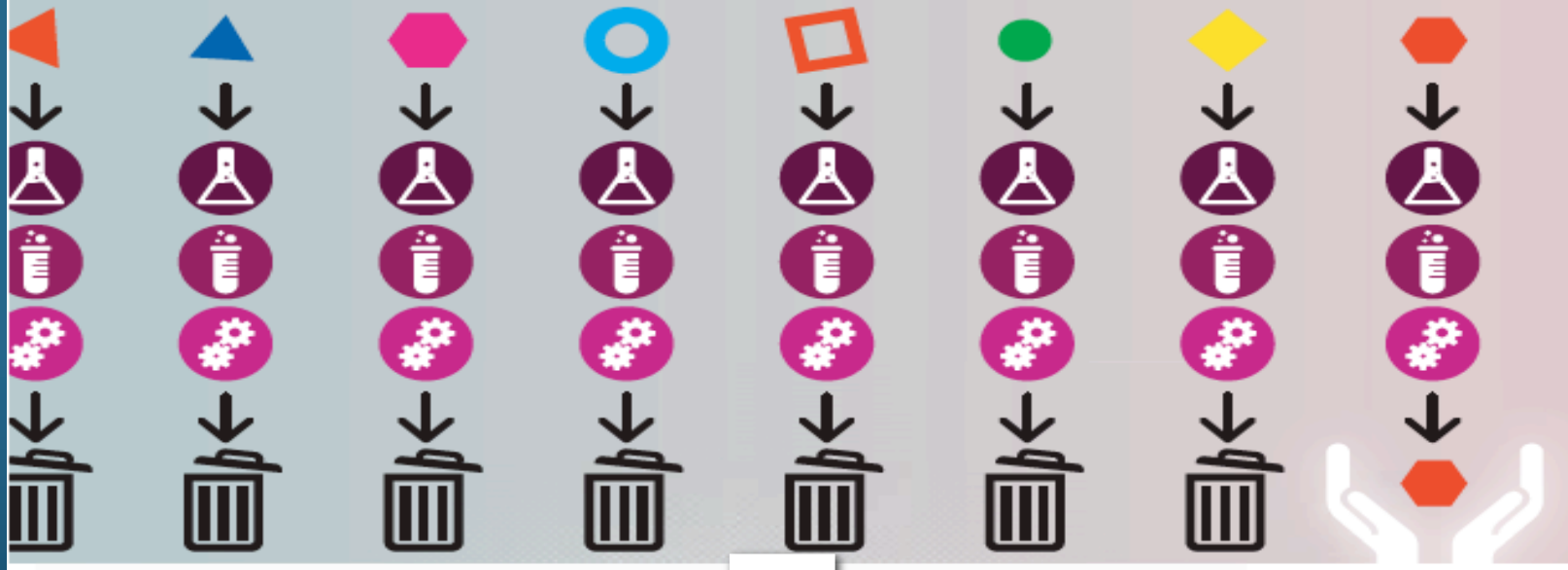
← Sony

*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

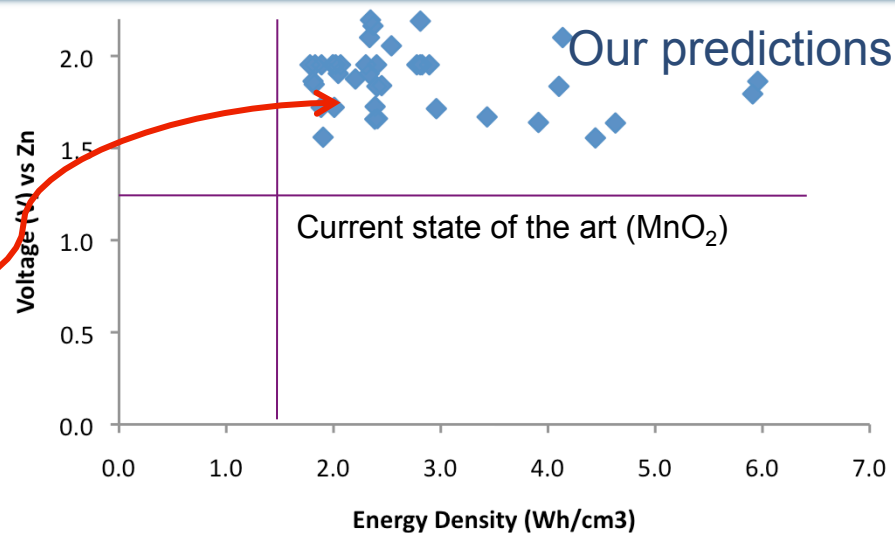
Screening I

> 1500 compounds

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

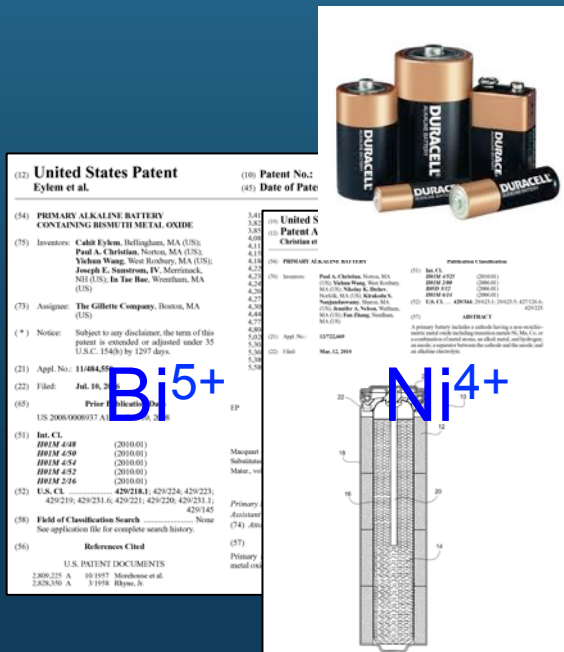
## How to stabilize at pH = 15

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

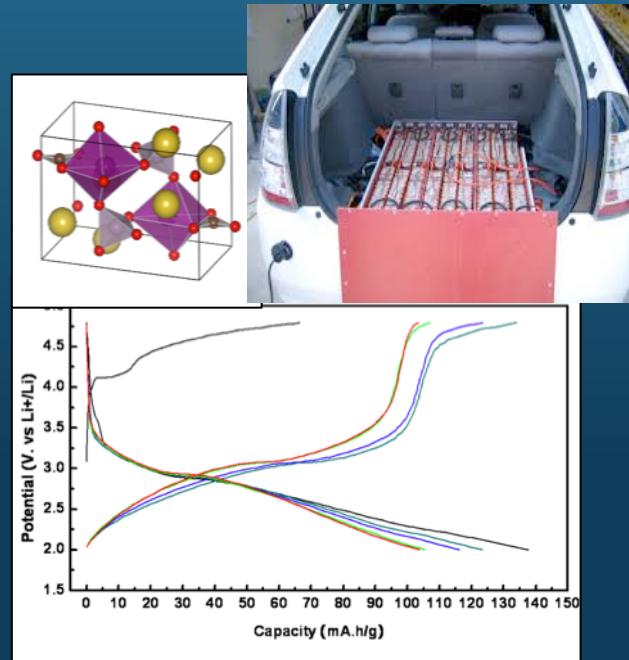
**Design rules:** how to stabilize high energy compounds, which corrosion-resistant elements to add...

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

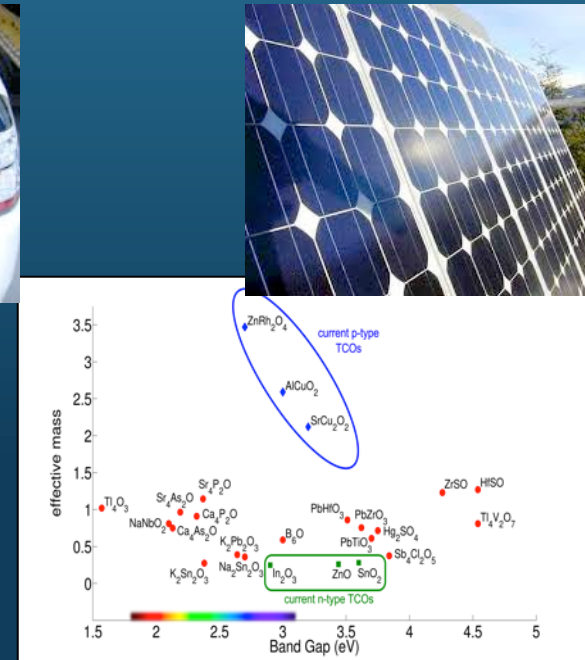
*Completely new materials predicted and synthesized based on computational predictions*



**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 displayed in its characteristic multi-colored font (blue, red, yellow, blue, green, red) on a white background.

Good battery material

Google Search

I'm Feeling Lucky

# Materials Design in the Information Age



$3V < \text{voltage} < 4.5V$  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

[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 powered by **MOOGLE**


## Database Statistics

<b>38151</b> materials	<b>14618</b> bandstructures
<b>610</b> intercalation batteries	<b>16277</b> conversion batteries




### Materials Explorer

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



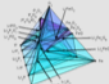
### Lithium Battery Explorer

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. The header is green with the ENERGY.GOV logo and a search bar. Below the header is a navigation bar with links for PUBLIC SERVICES, SCIENCE & INNOVATION, MISSION, News & Blog, and Maps & Data. The main content area has a 'Home' link and a headline: 'First-Of-Its-Kind Search Engine Will Speed Materials Research'. The article is dated November 3, 2011 - 1:05pm. The text of the article describes the launch of the Materials Project, a ground-breaking online tool that 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 from Secretary of Energy Steven Chu is included, stating that this research tool will help the United States compete with other developers of new materials and could potentially create new domestic industries. The article concludes by stating that 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!

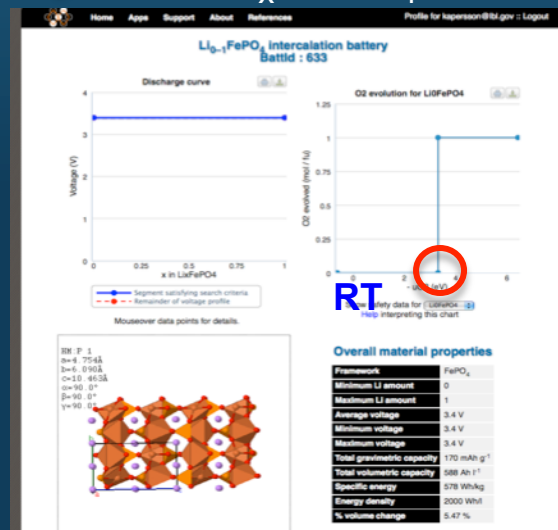
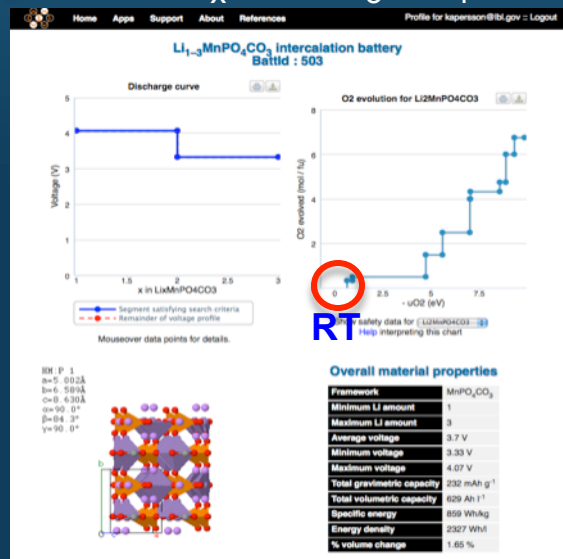
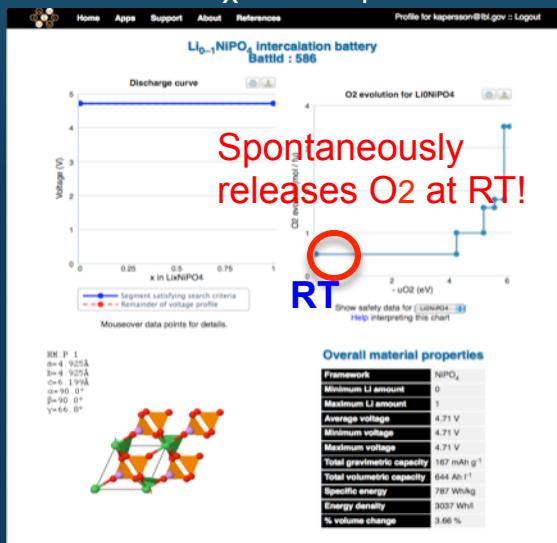
Oxygen release correlates with oxygen chemical potential of cathode



safer



safer



ICSD    Other experimental databases    User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)



Analysis

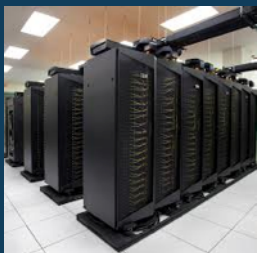
Web apps

Materials API

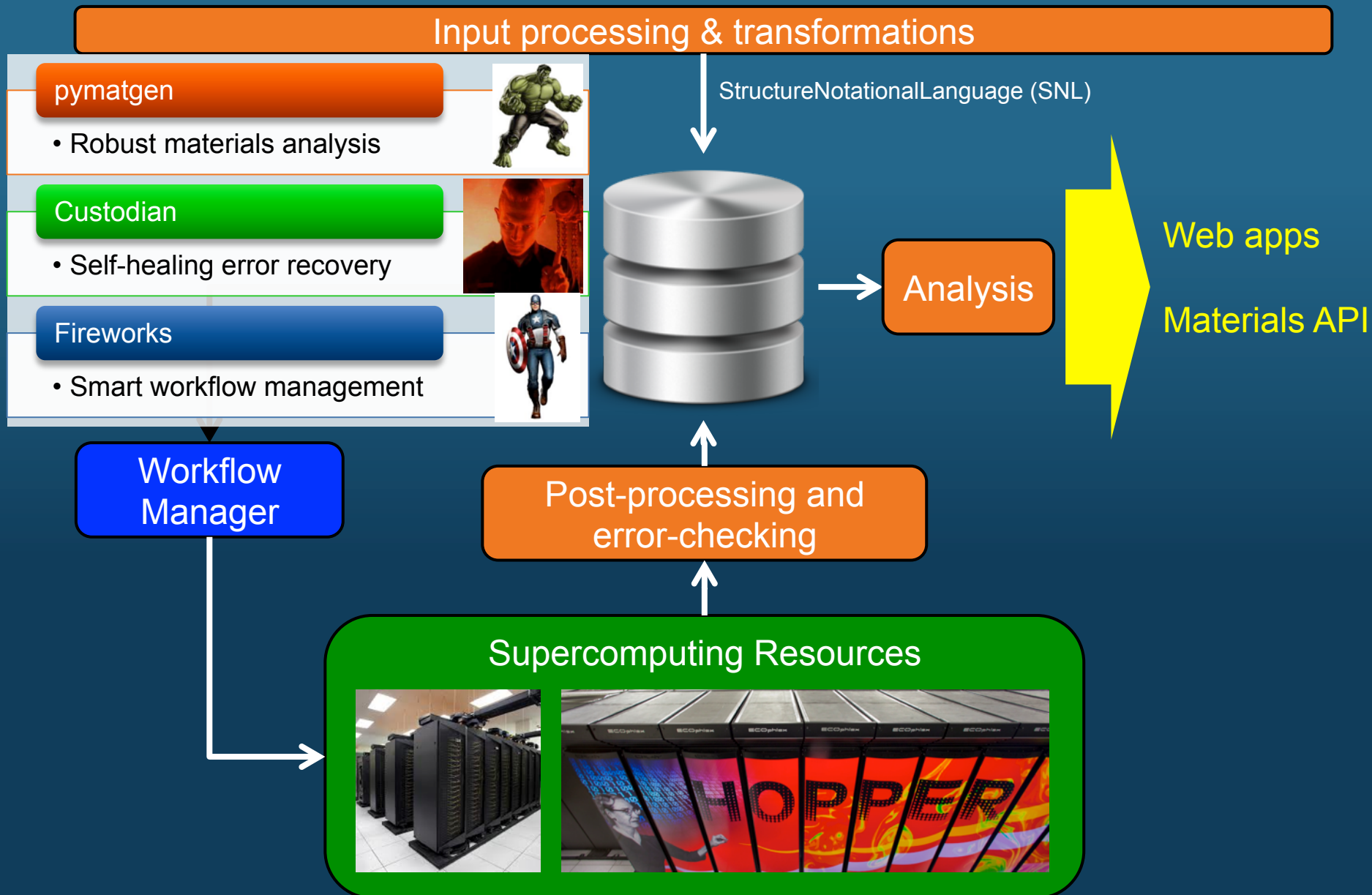
Workflow  
Manager

Post-processing and  
error-checking

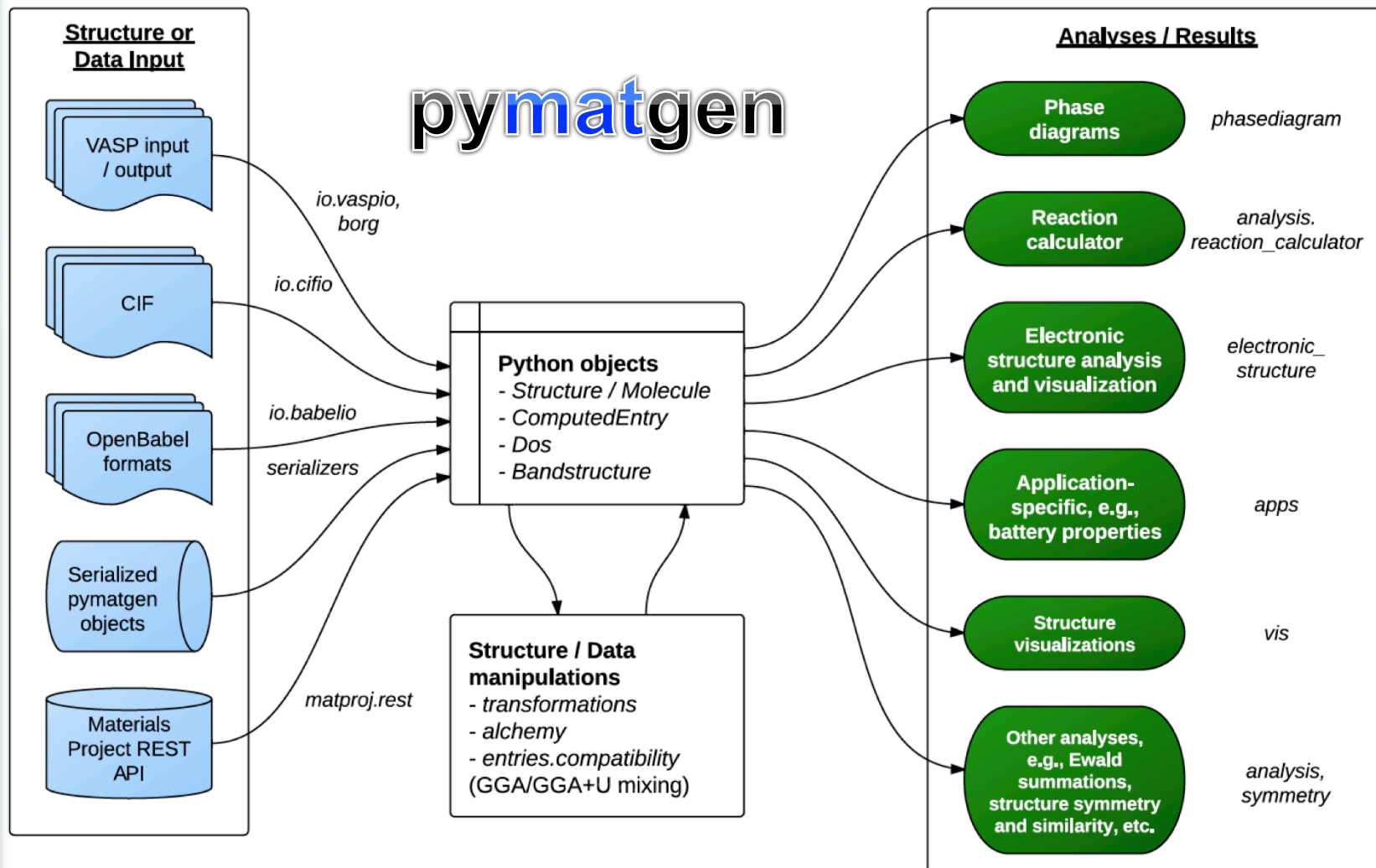
Supercomputing Resources







# Open Source Codes



# Building robust software that lasts... :

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

## All code have proper **documentation**

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

Nah – Bob left in 2004....

pymatgen 2.2.1 documentation » next | modules | index

### Table Of Contents

- Introduction
  - Latest Change Log (v2.2.1)
- Getting pymatgen
  - Aliases
- Contributing
- API Reference Docs
- Citing pymatgen
  - pymatgen.io.vaspio\_set module
  - pymatgen.phasediagram package
  - pymatgen.entries.compatibility module
  - pymatgen.symmetry
- License
- Indices and tables

### Next topic

Older versions

### This Page

Show Source

Quick search

Enter search terms or a module name

Go

## 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](mailto: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](#)

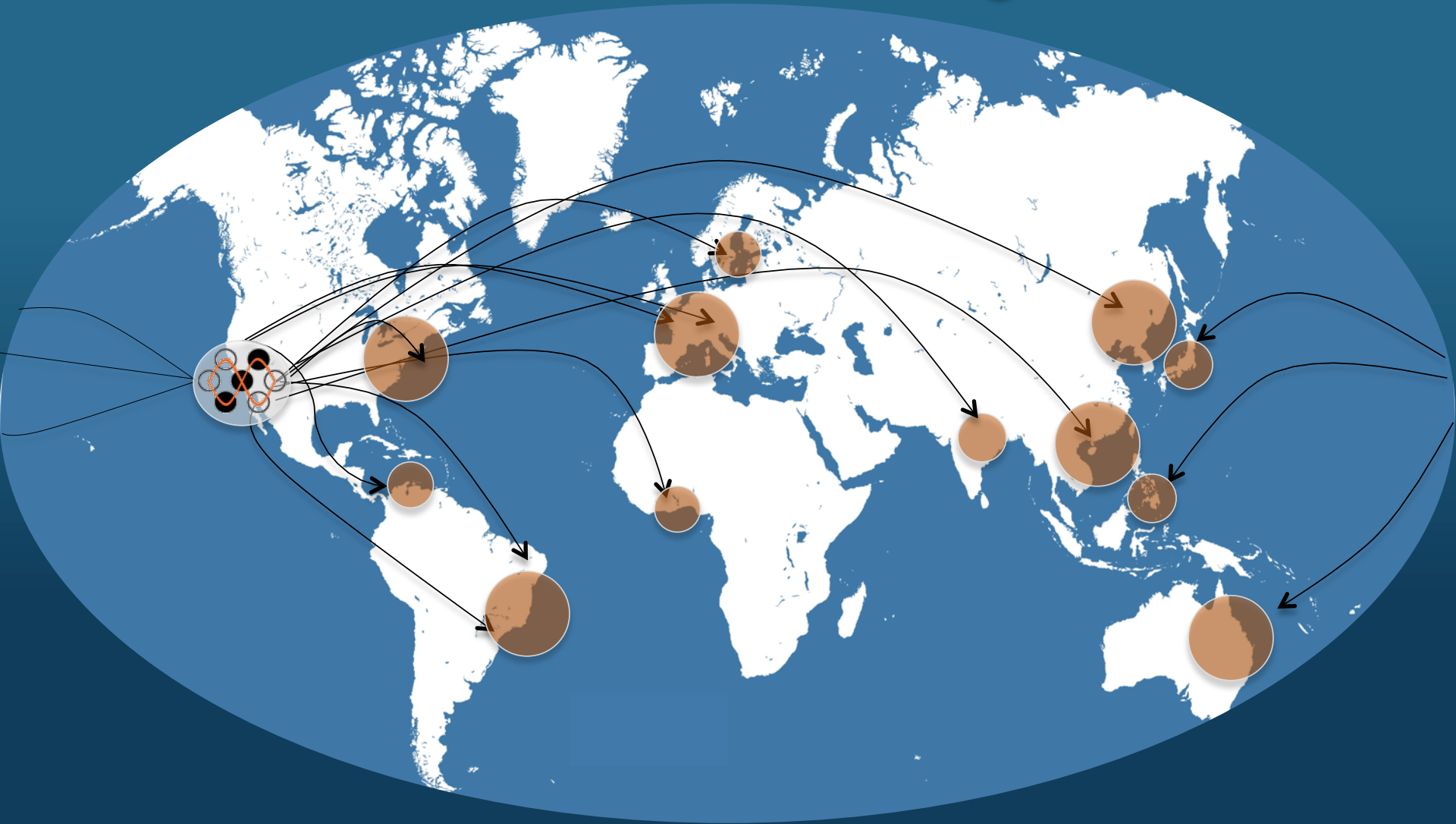
### Older versions

- Version 2.2.0
- Version 2.1.2
- Version 2.0.0
- Version 1.9.0

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



# 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.

Register now for free, full access.

- Unlimited access
- Up to 500 search results
- History of your searches and analyses

Or try the apps in demo mode

- 10 minute usage limit
- Search results limited to 10 best matches
- Just click an app to start

**Database Statistics**

34598 materials	14387 bandstructures
445 intercalation batteries	16016 conversion batteries

**Tools:**

- 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.
- Structure Predictor**: Predict new compounds using data-mined substitution algorithms.

Find out more about our open Materials API and pymatgen library for querying large amounts of data.

**Tutorials**

**MATERIALS PROJECT Tube**

**Press Highlights**

The New York Times

Beyond Fossil Fuels: Finding New Ways to Fill the Tank

**Latest News**

pymatgen v2.5.2  
by Shiyue Ping Ong - Feb 19, 2013  
Version 2.5.2 of pymatgen has been released! Check out the change log at <https://pypi.python.org/pypi/pymatgen> for information on the latest changes.

pymatgen v2.5.2  
The Materials Project is hiring!  
A new year, a new pymatgen  
Journal article on the Python Materials Genomics library

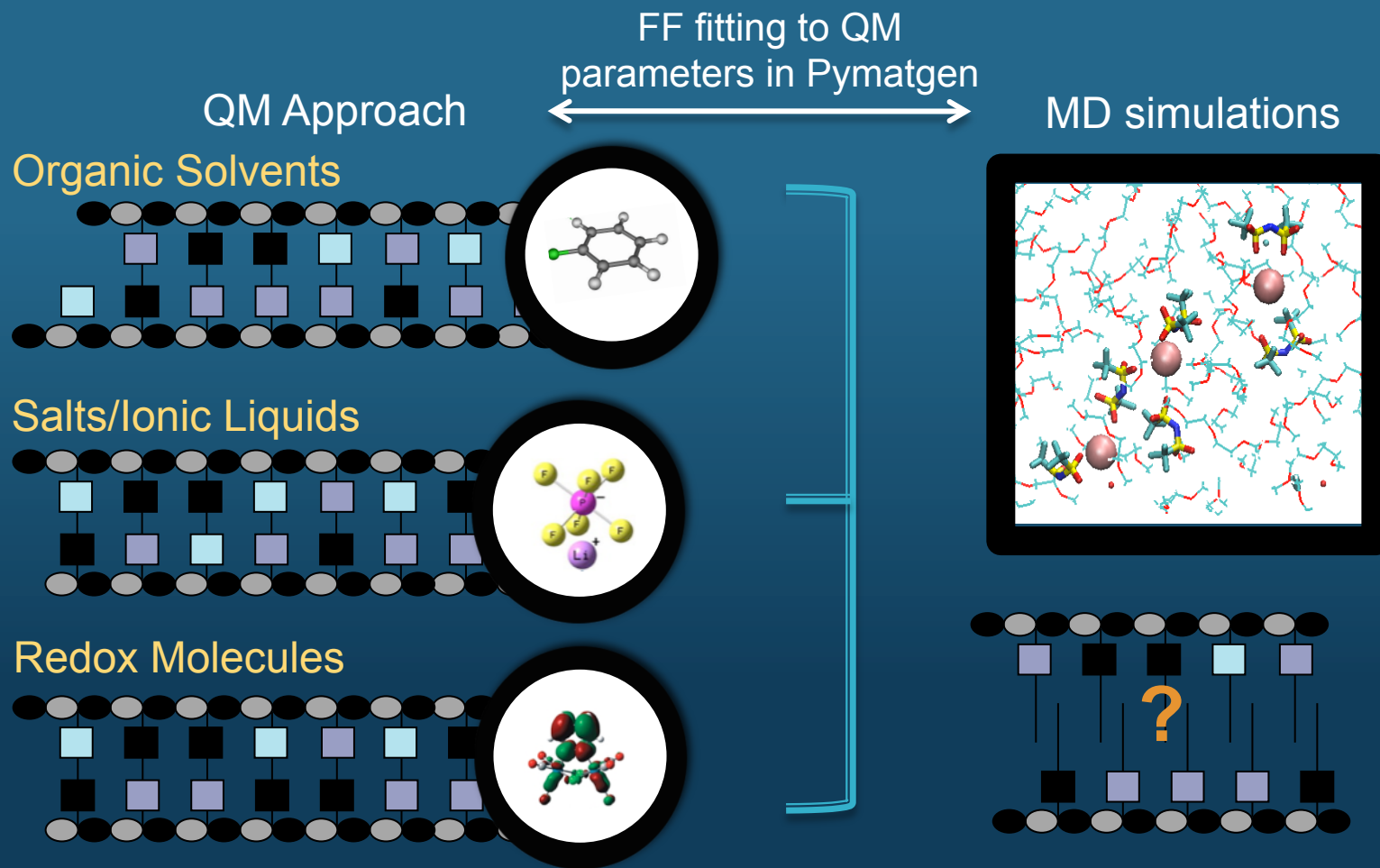
Core data



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. 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 heading "MATERIALS PROJECT" is partially visible, followed by the tagline "Accelerating materials discovery through scientific computing and innovation".

Below the tagline, two featured tools are shown: "Materials Explorer" for searching materials information and "Phase Diagram App" for computational phase diagrams. An inset window shows the "Explore Molecules" interface, where the formula H8C9N2 is entered. This interface includes a plot of Ionization Energy (IE) vs. Electron Affinity (EA) and a table of results.

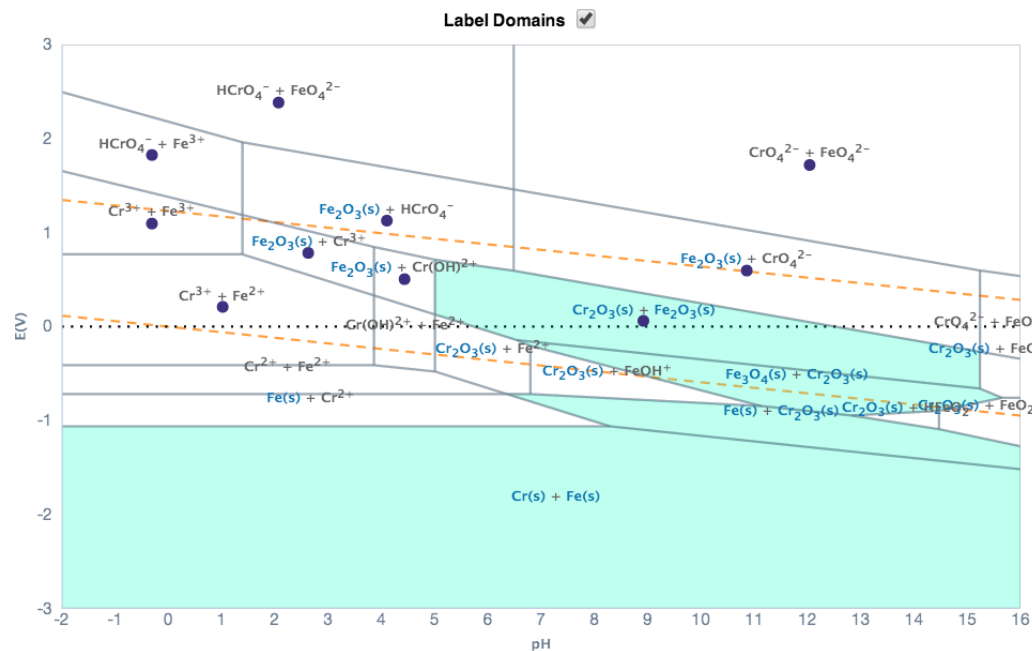
smiles	svg	EA	point group	charge	formula	IE
<chem>c1(cc2c(cc1)nccn2)C</chem>		0.409	Cs	0	H <sub>8</sub> C <sub>9</sub> N <sub>2</sub>	8.663
<chem>c1c(c2c(cc1)nccn2)C</chem>		0.451	Cs	0	H <sub>8</sub> C <sub>9</sub> N <sub>2</sub>	8.503
<chem>c1cc2c(cc1)nccn2)C</chem>		0.428	Cs	0	H <sub>8</sub> C <sub>9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

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



# > 70,000 Pourbaix Diagrams Available

[www.materialsproject.org/Pourbaix](http://www.materialsproject.org/Pourbaix)

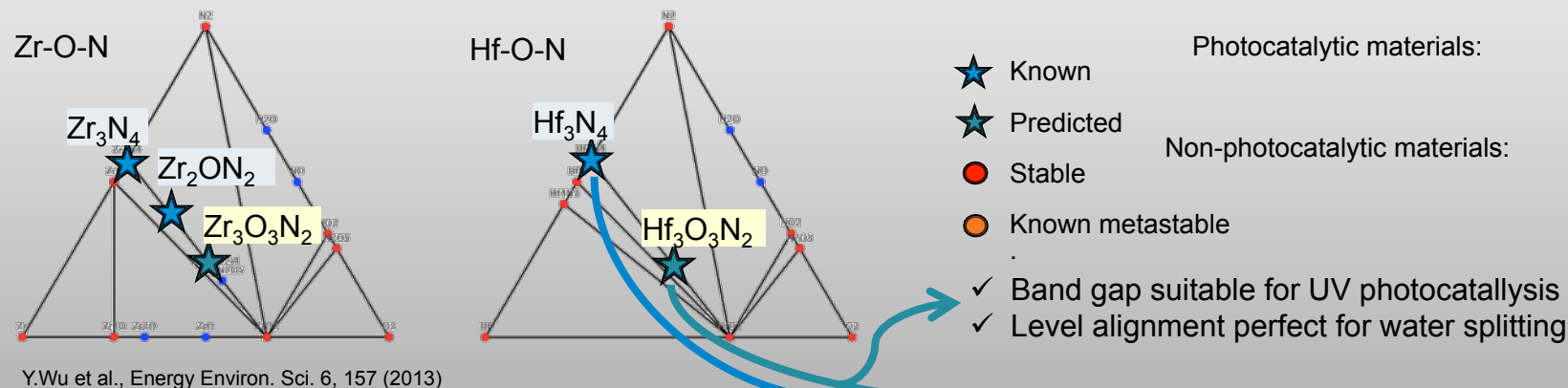


## Pourbaix Diagrams on the Materials Project

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

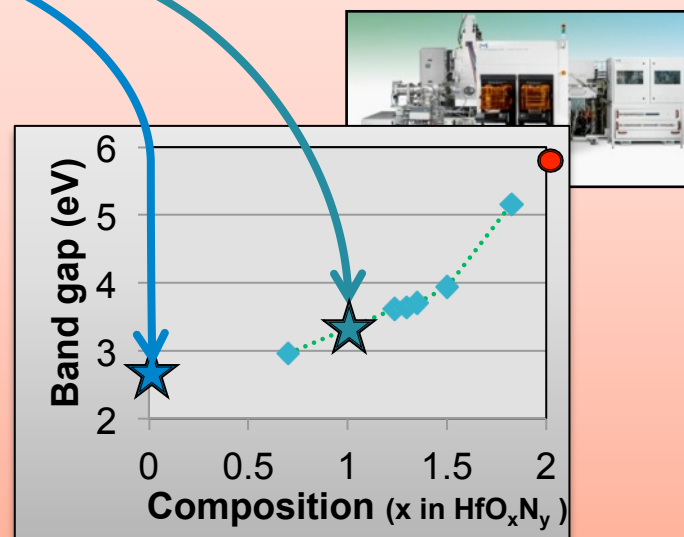
# Intermolecular : New Materials for Photocatalysis

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

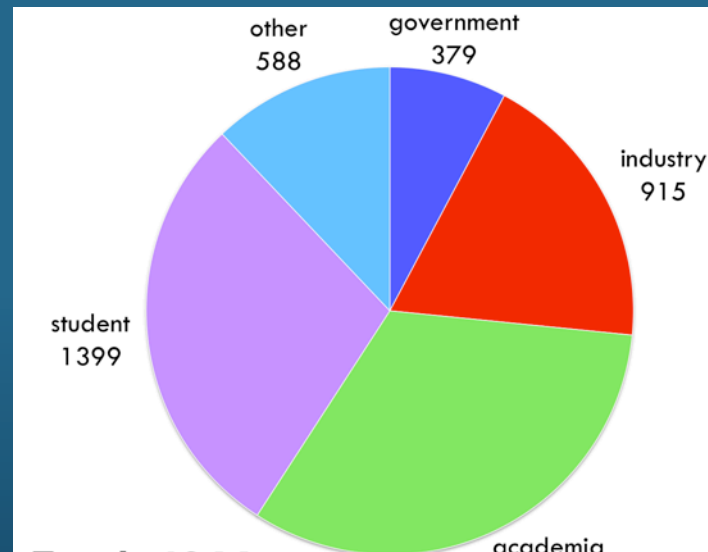
- ❑ **Grants:** 2012 DOE Center, JCESR, U Madison NSF Center, JCAP

- ❑ **Users:** > 5600 and counting...

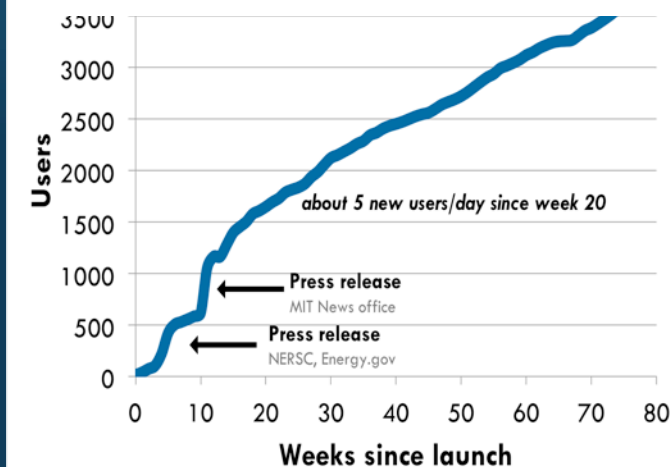
- ❑ **Course-ware :** UC San Diego, UC Davis, UC Irvine, U Michigan, John-Hopkins, Cornell, ...

- ❑ **Partner institutions:** UC Berkeley, UC San Diego, MIT, Duke, U Wisconsin, U Kentucky, U Louvain Belgium, Cambridge UK, Caltech, ...

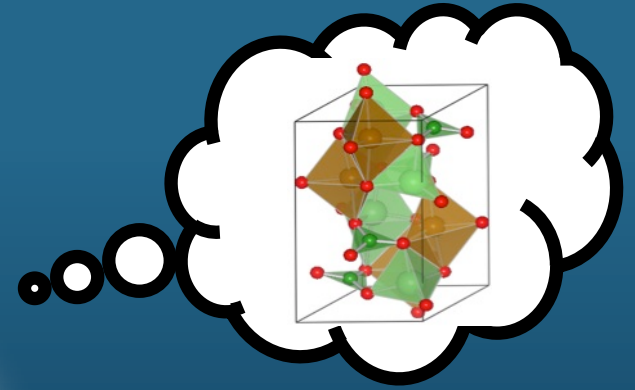
- ❑ **Companies:** Toyota, Sony, Bosch, 3M, Honda, Samsung, LG Chem, Dow Chemicals, GE Global Research, Intermolecular, Applied Materials, Energizer, Advanced Materials, General Motors, Corning, DuPont, Nippon Steel, L'Oreal USA, Caterpillar, HP, Unilever, Lockheed Martin, Texas Instruments, Ford, Bose, Sigma-Aldrich, Siemens, Raytheon, Umicore, Seagate, ...



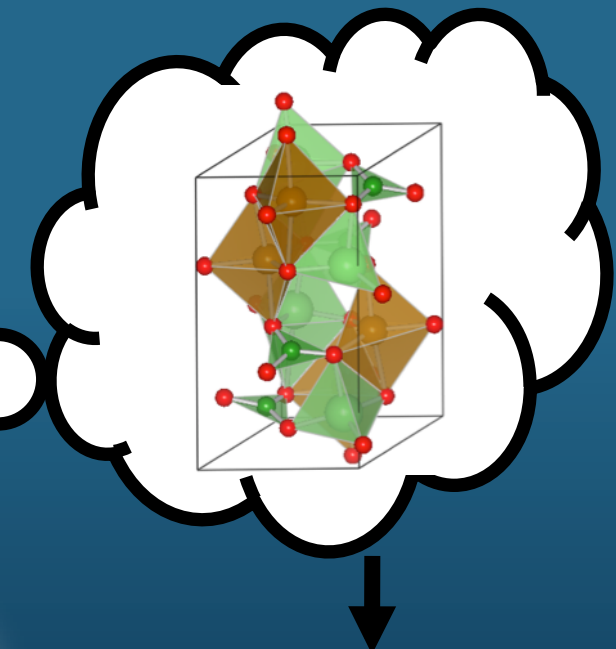
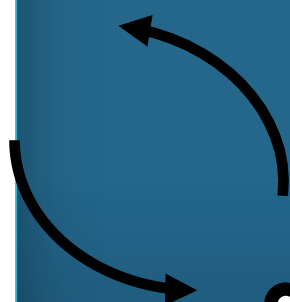
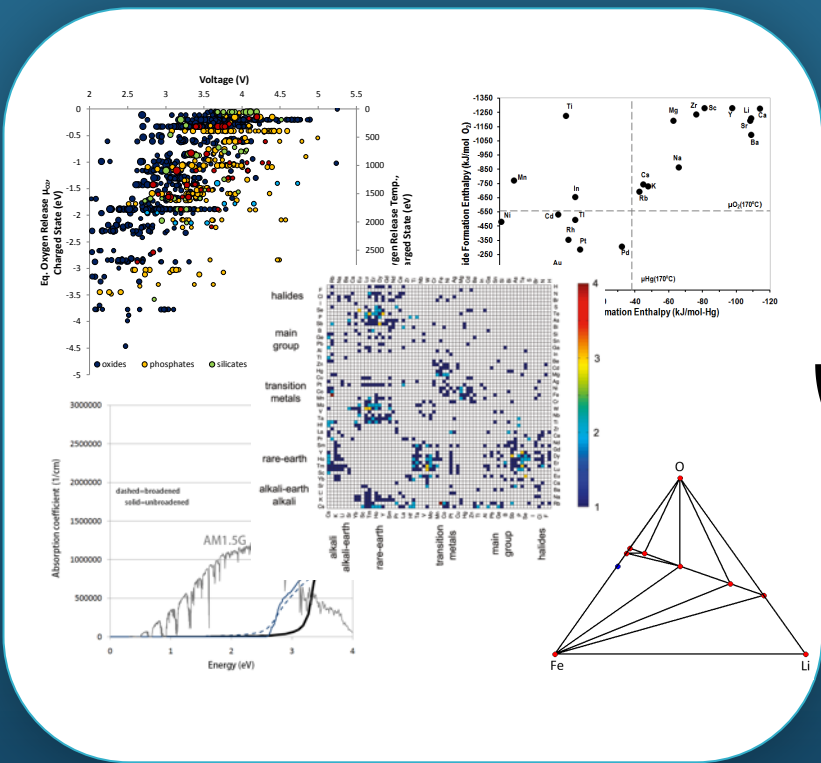
**As of today: 5622 users**



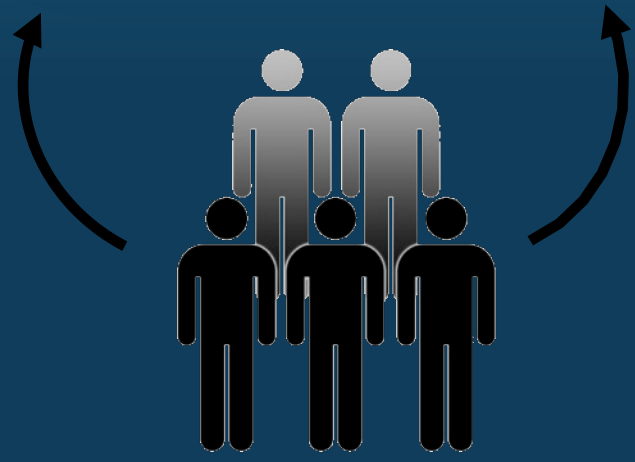
From single entities...







... towards a materials genome



“Con  
fi

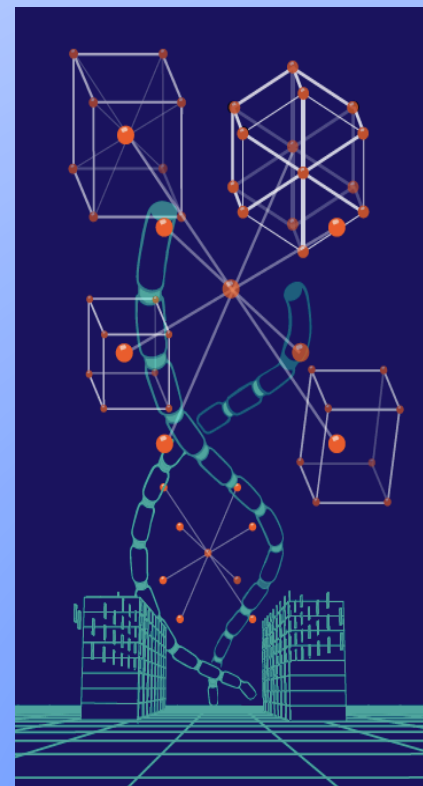
# Thank you for your attention!

## Thanks to sponsors:



## 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