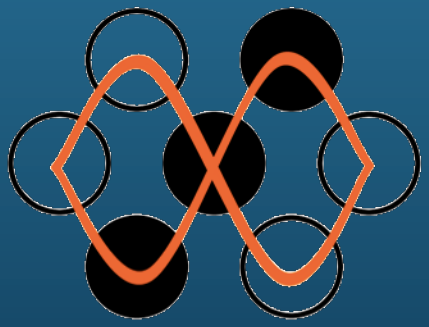
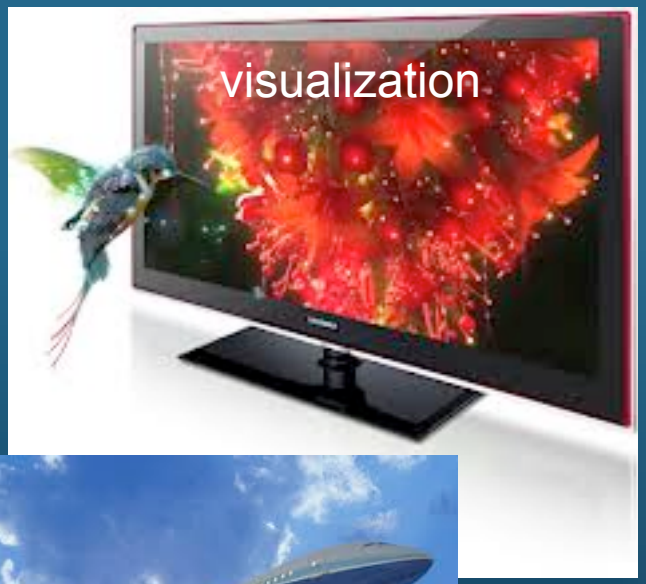
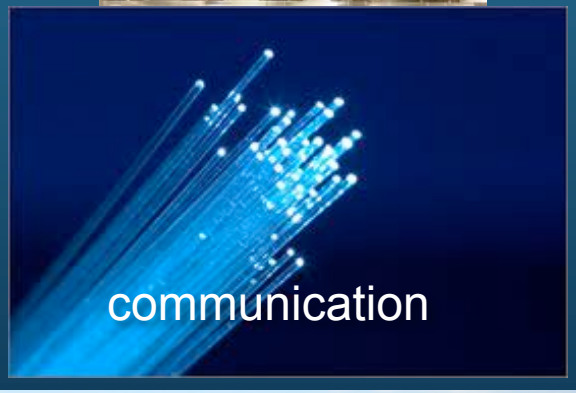


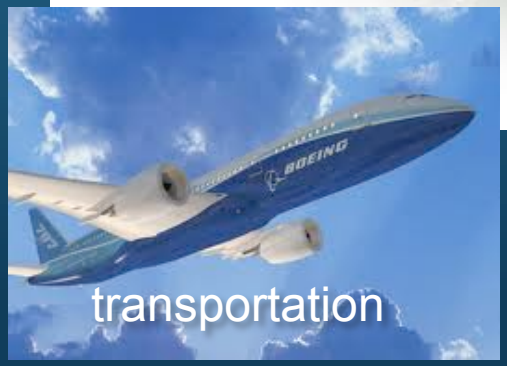
A Google for Materials?

Kristin Persson
Lawrence Berkeley National Laboratory

Engineered Materials Enable Society







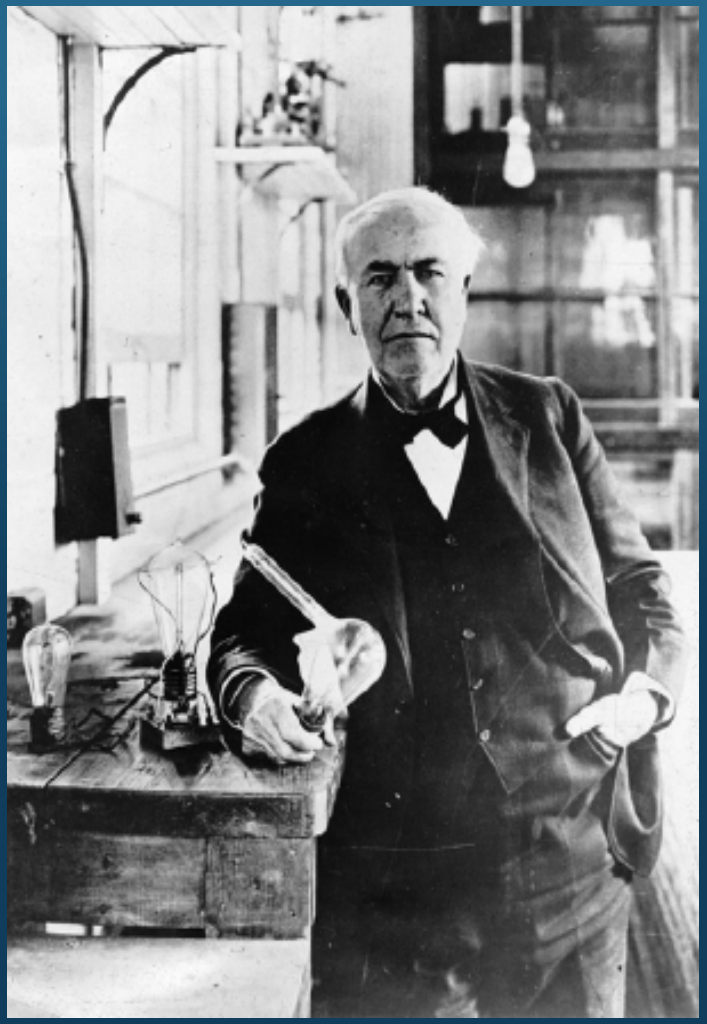
How are New Materials Invented?

"Edison Style"

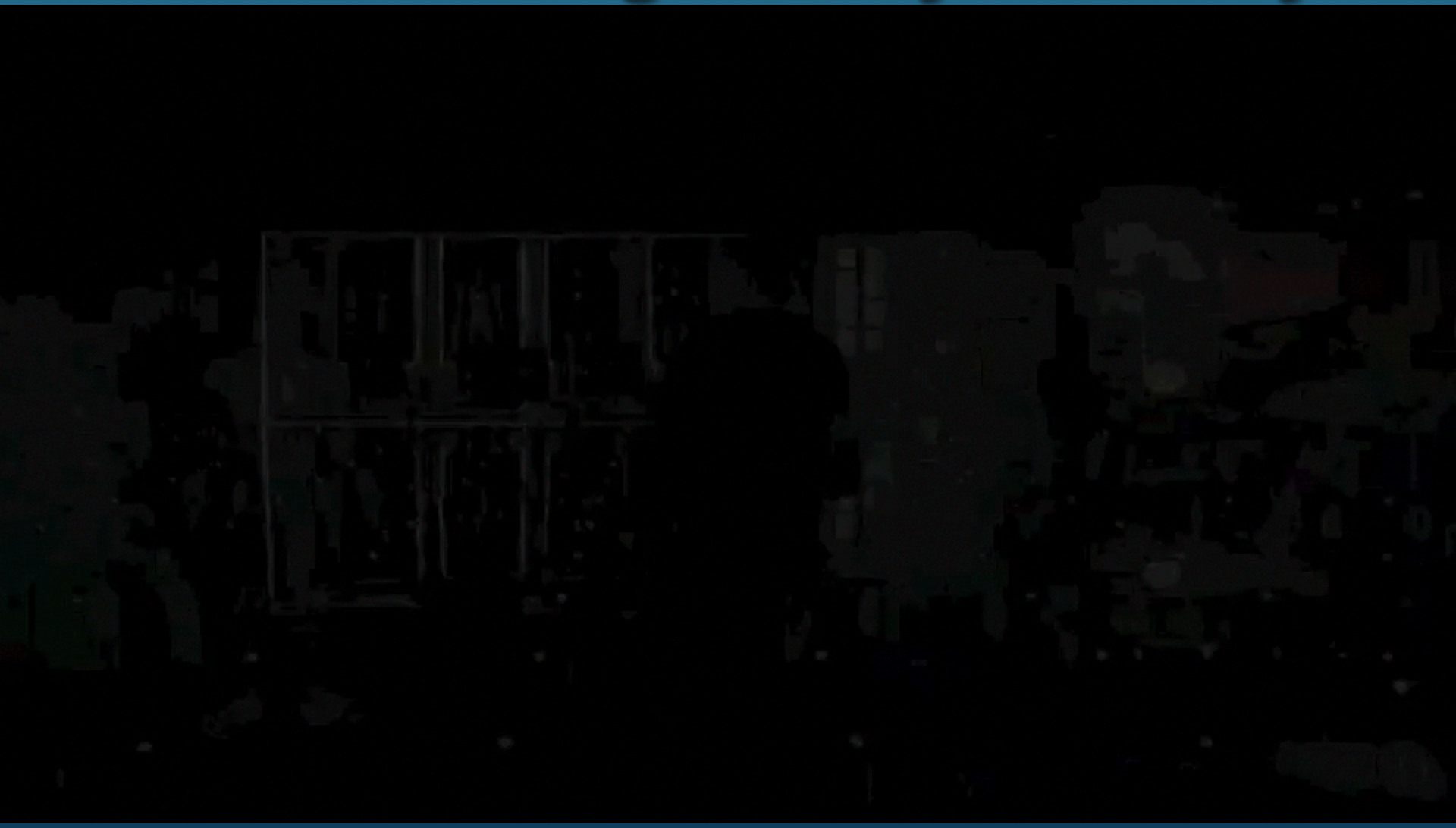
When looking for a light bulb filament, Edison tried about 3,000 materials

…

And he didn't find the best one …!



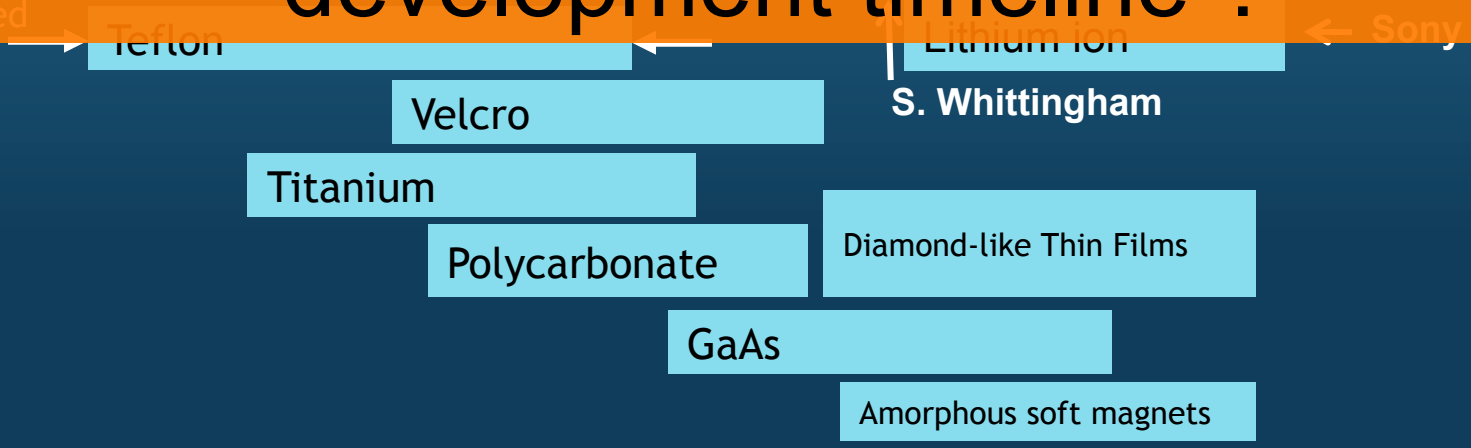
Materials Design: Hollywood Style



Reality Check

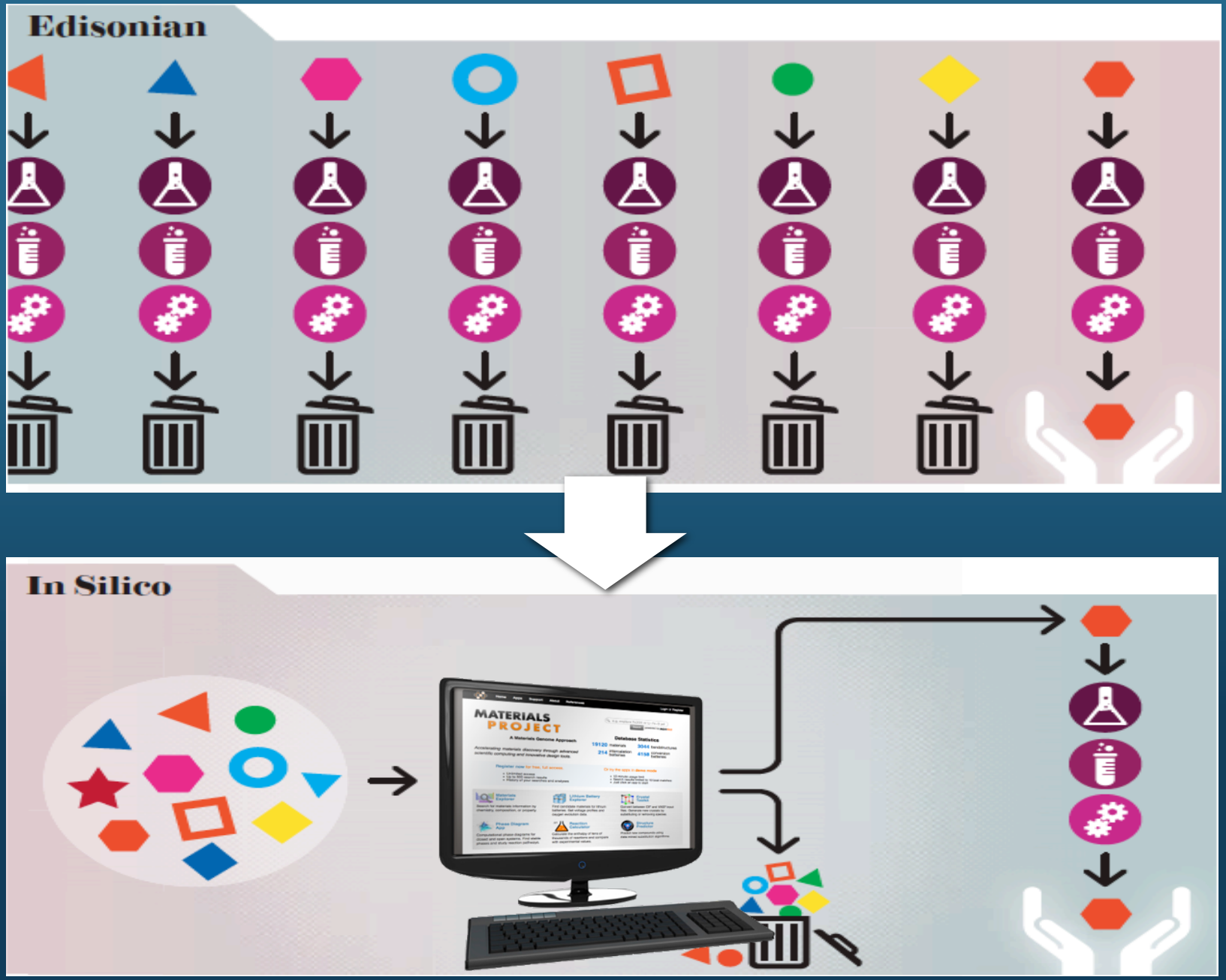
18 Years...
From new materials discovery to commercialization!

How to accelerate the innovation and development timeline ?



Materials Data from: Eagar, T.; King, M. Technology Review (00401692) **1995**, 98, 42.


Thought provoking Hopper could crunch through ~20k structures in 1 day…
$H\psi = E\psi$


Edisonian
In Silico
MATERIALS
PROJECT

Novel Materials for Alkaline batteries

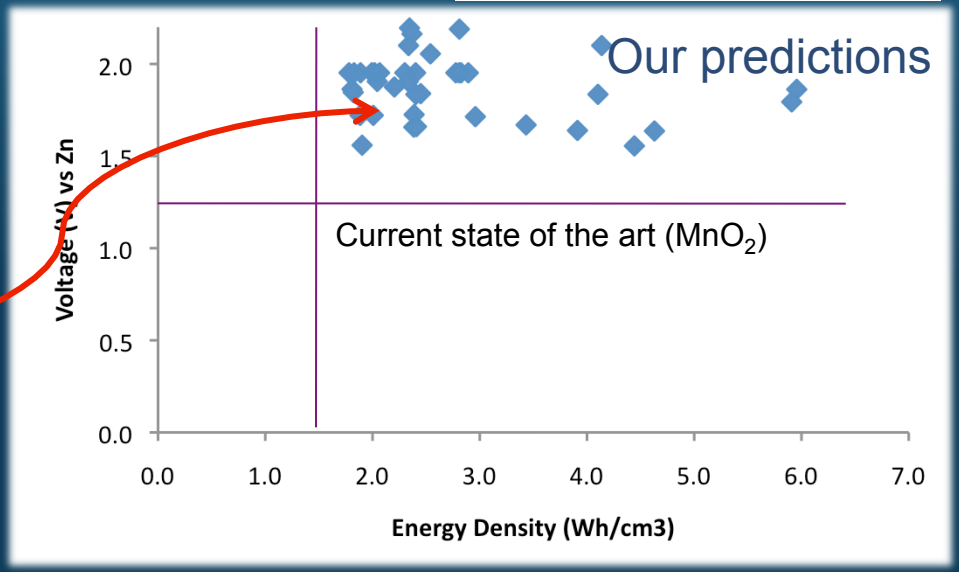
> 130,000 compounds screened

Screening I

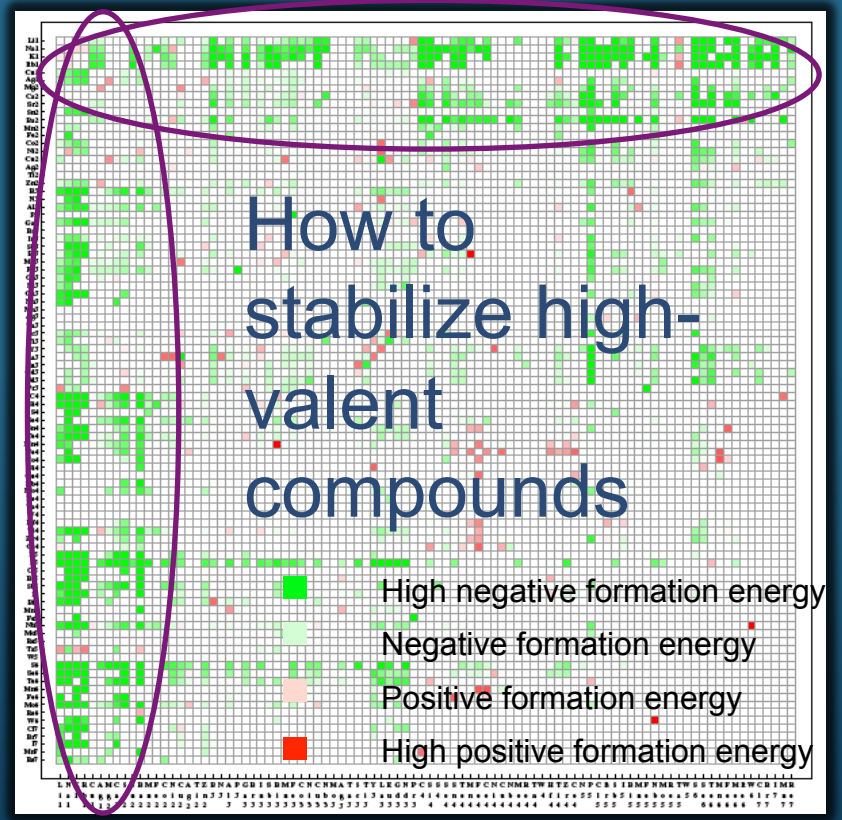
> 1500 compounds
- ✓ Capacity > 1 Ah/cc
- ✓ 1.1 V < Ave voltage < 2.2 V
- ✓ Energy density > 1.7Wh/cc

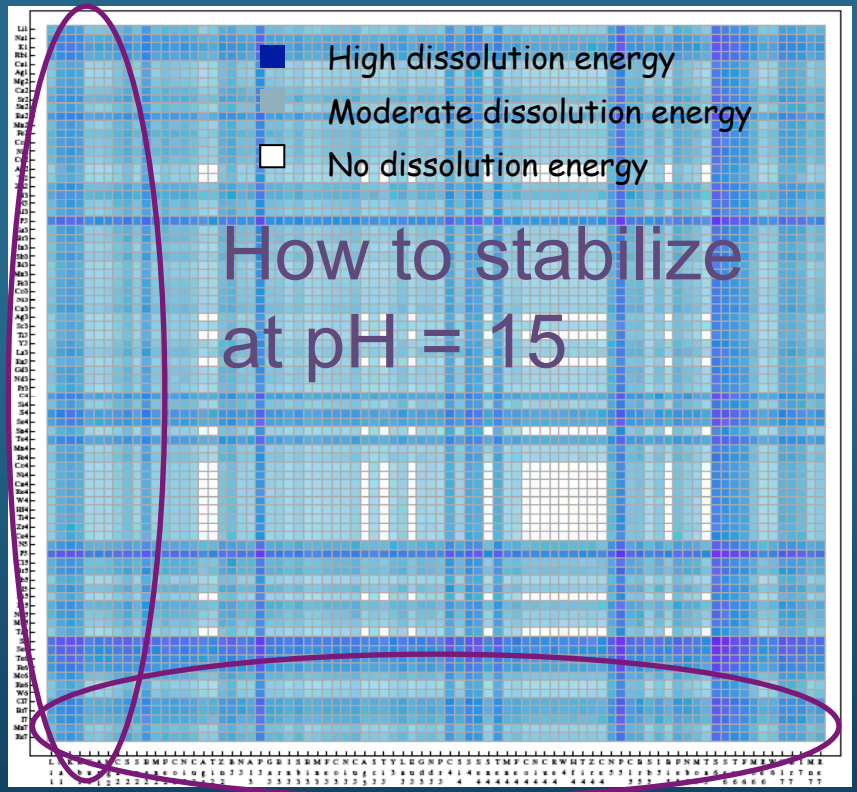
Screening II

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

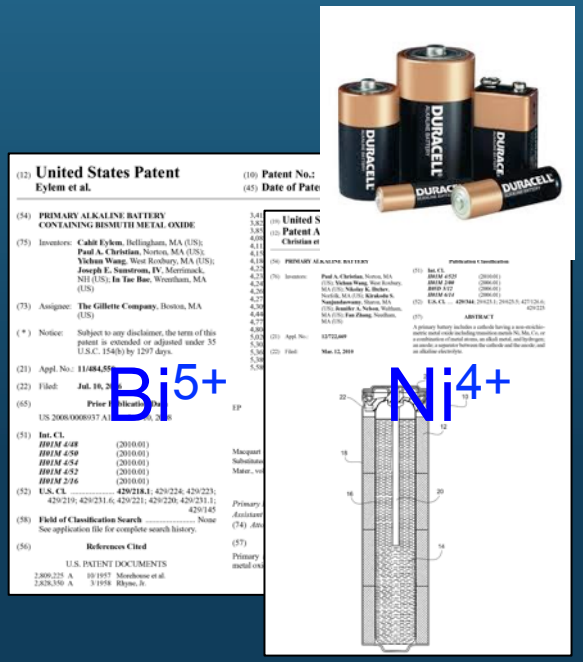




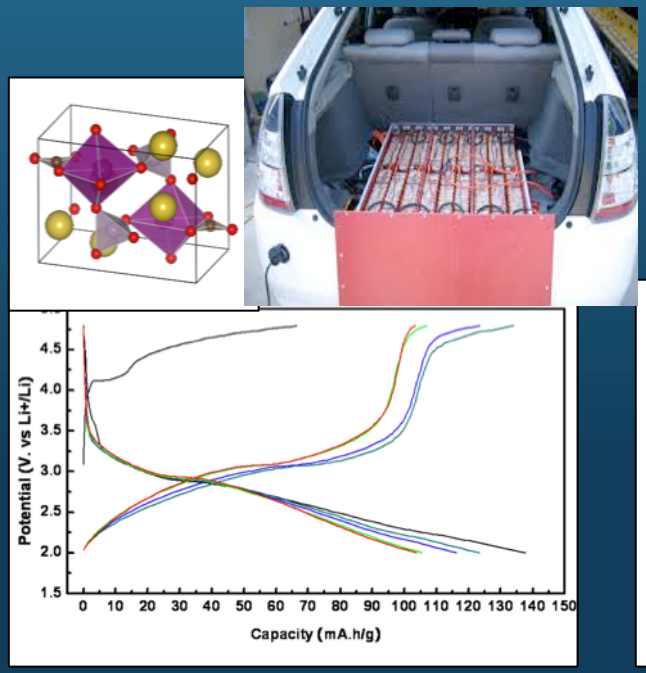
Design rules: how to stabilize high energy compounds, which corrosion-resistant elements to add…

Proof of concept – it's just the beginning…

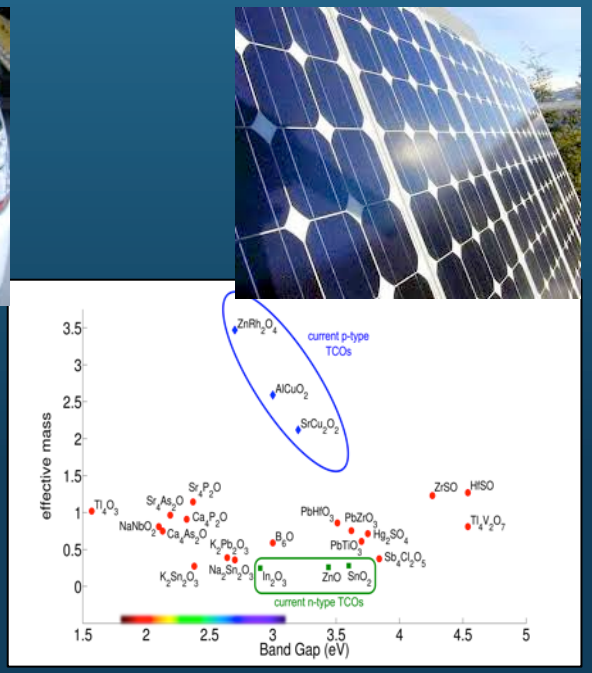
Completely new materials predicted and synthesized based on computational predictions



2005:
Novel stable alkaline batteries



2011:
Novel class of Li ion electrodes



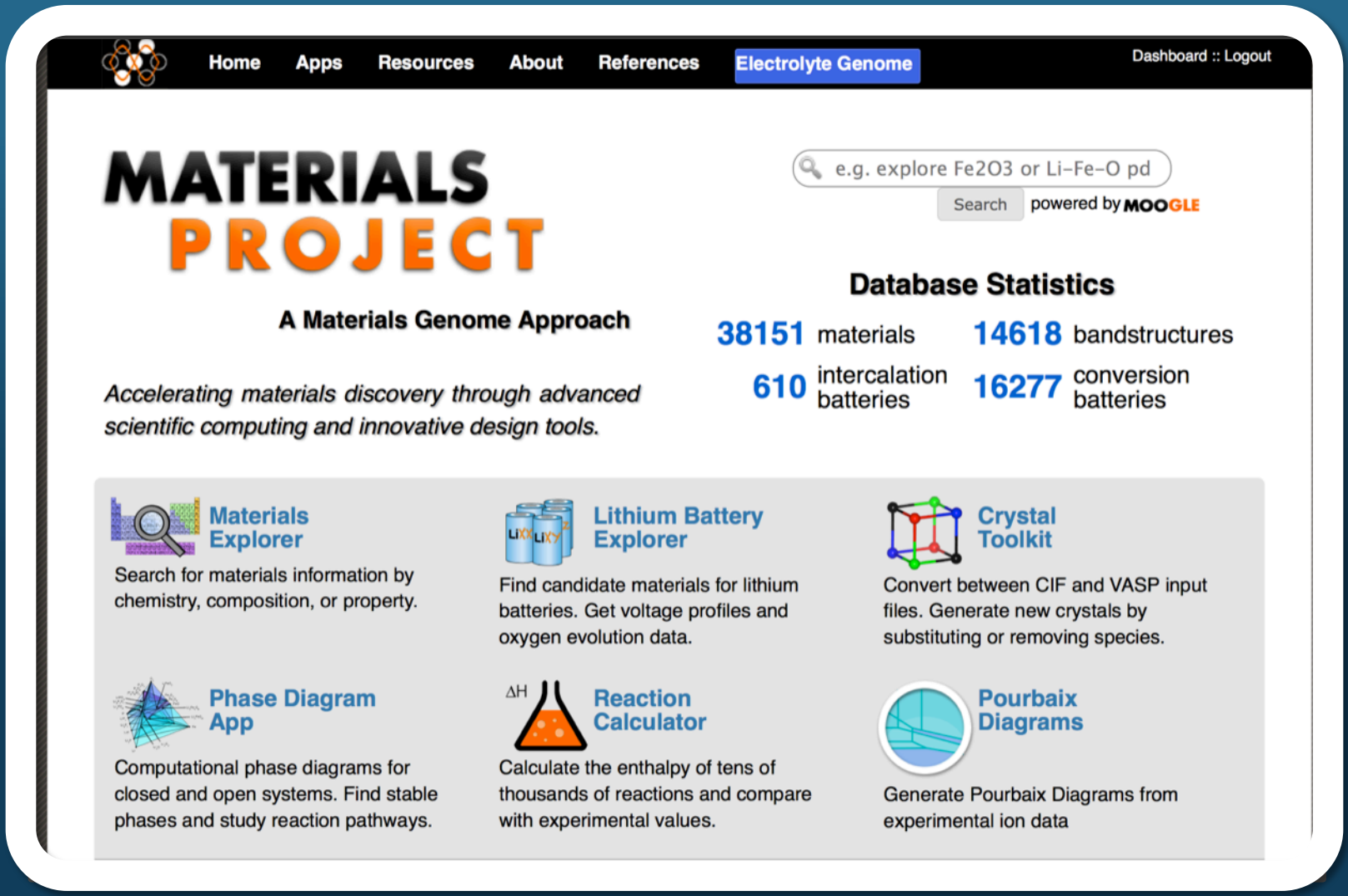
2013:
Improved transparent conductors

Materials Design in the Information Age

Materials Design in the Information Age

Today's Status:

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

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First-Of-Its-Kind Search Engine Will Speed Materials Research

November 3, 2011 - 1:05pm

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.

"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."

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 **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 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

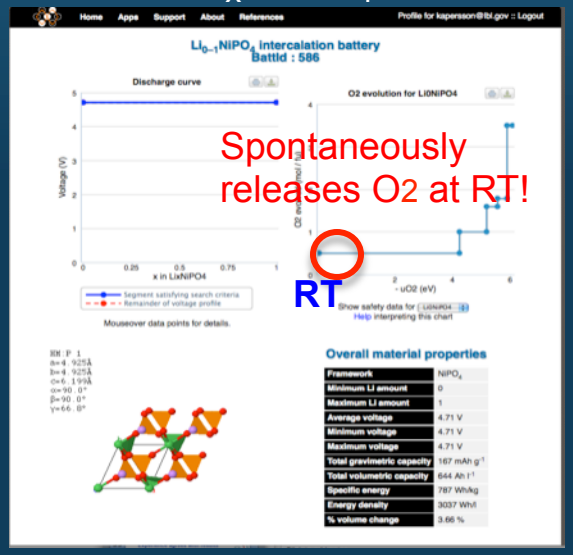
safer

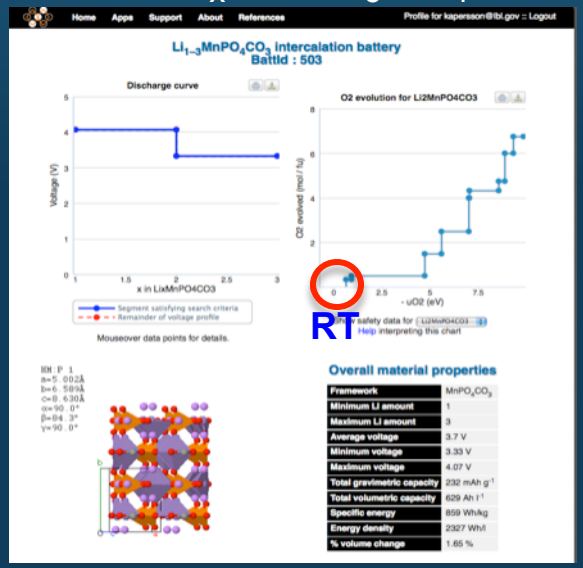
safer

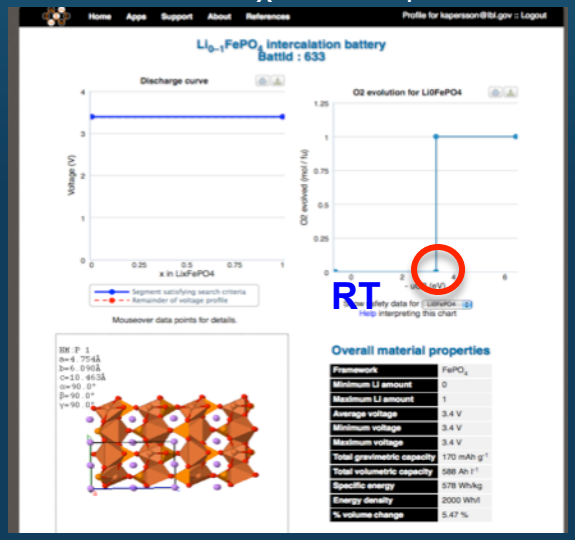
Li_xNiPO_4

$Li_xMnCO_3PO_4$

Li_xFePO_4







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

ICSD Other experimental databases User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)

pymatgen

- Robust materials analysis

Custodian

- Self-healing error recovery

Fireworks

- Smart workflow management

Analysis

Web apps

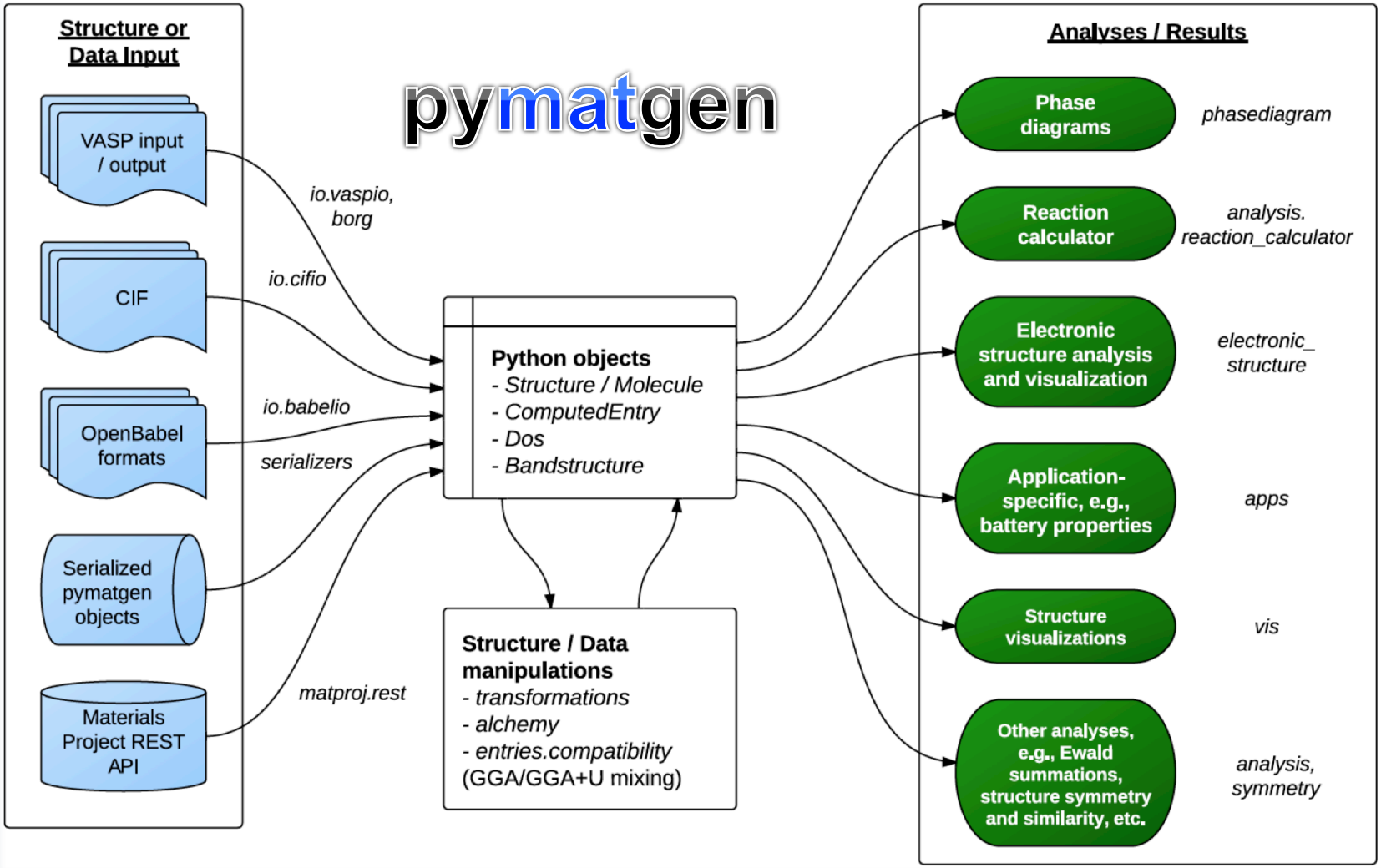
Materials API

Workflow Manager

Post-processing and error-checking

Supercomputing Resources

Open Source Codes

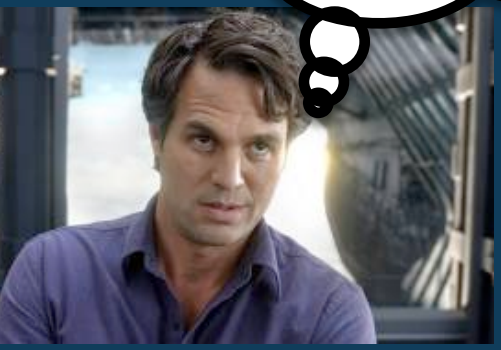


Building robust software that lasts… :

All pymatgen classes and methods come with unit tests

All code have proper documentation

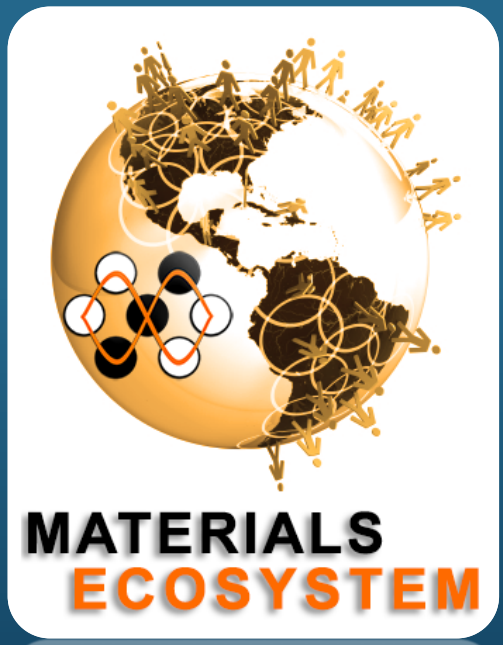
Does anyone remember how to run ‘GoBabyMonte.c’ ???



Nah – Bob left in 2004….

World Wide Usage

MATERIALS PROJECT



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

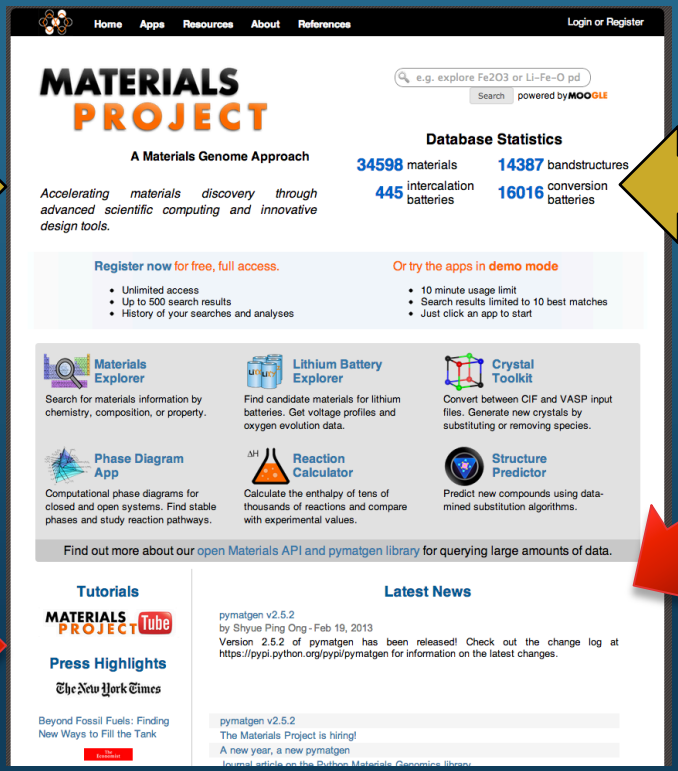
Improved accessibility of data

More developers of analyses and apps

Increased data value

Separate databases

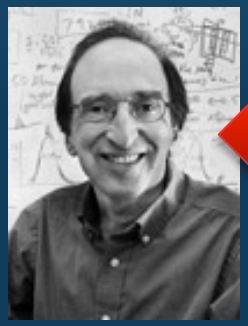
User not in group, sees only core data



Core data

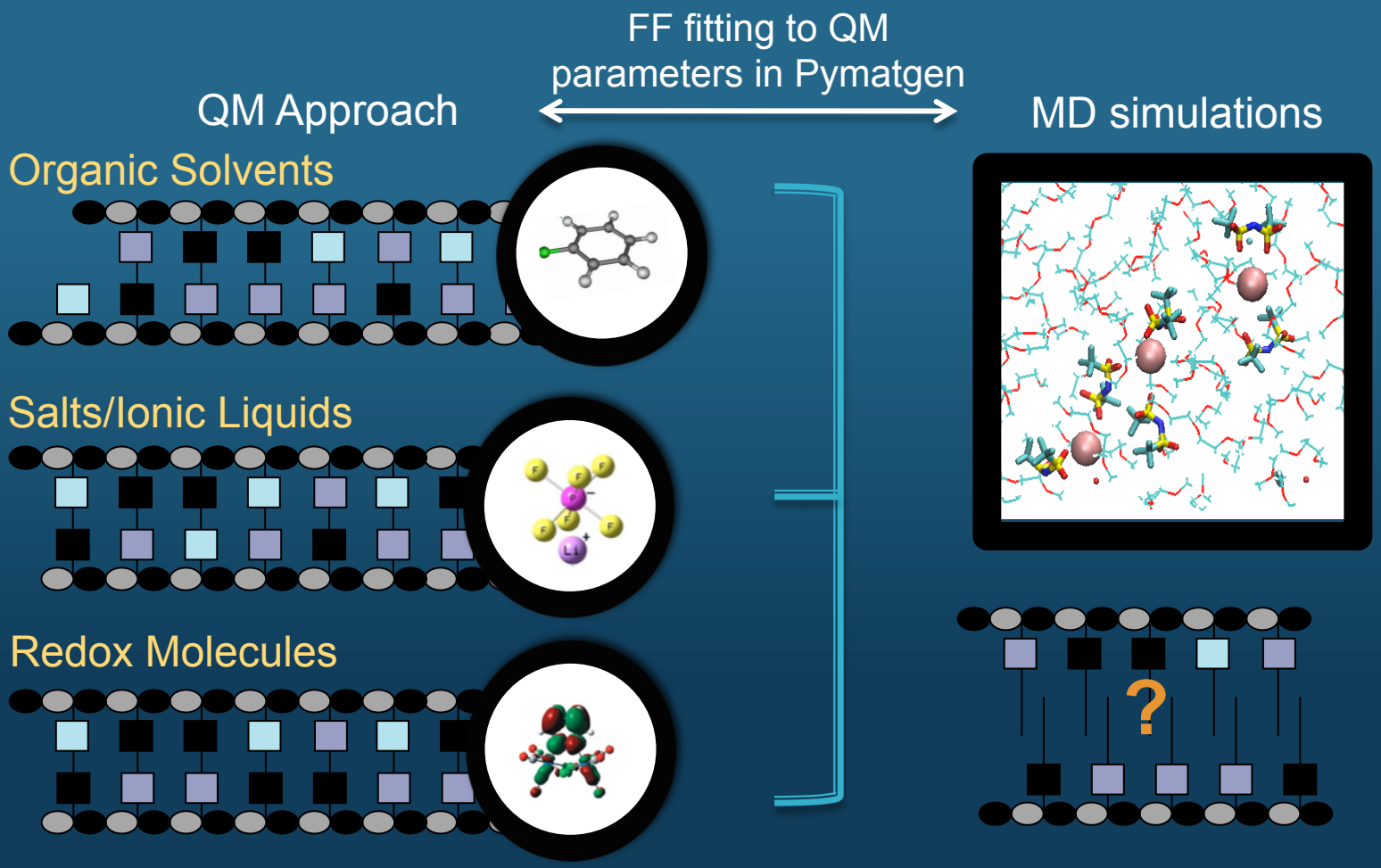
Unified View

Sandbox can be shared by a group of users



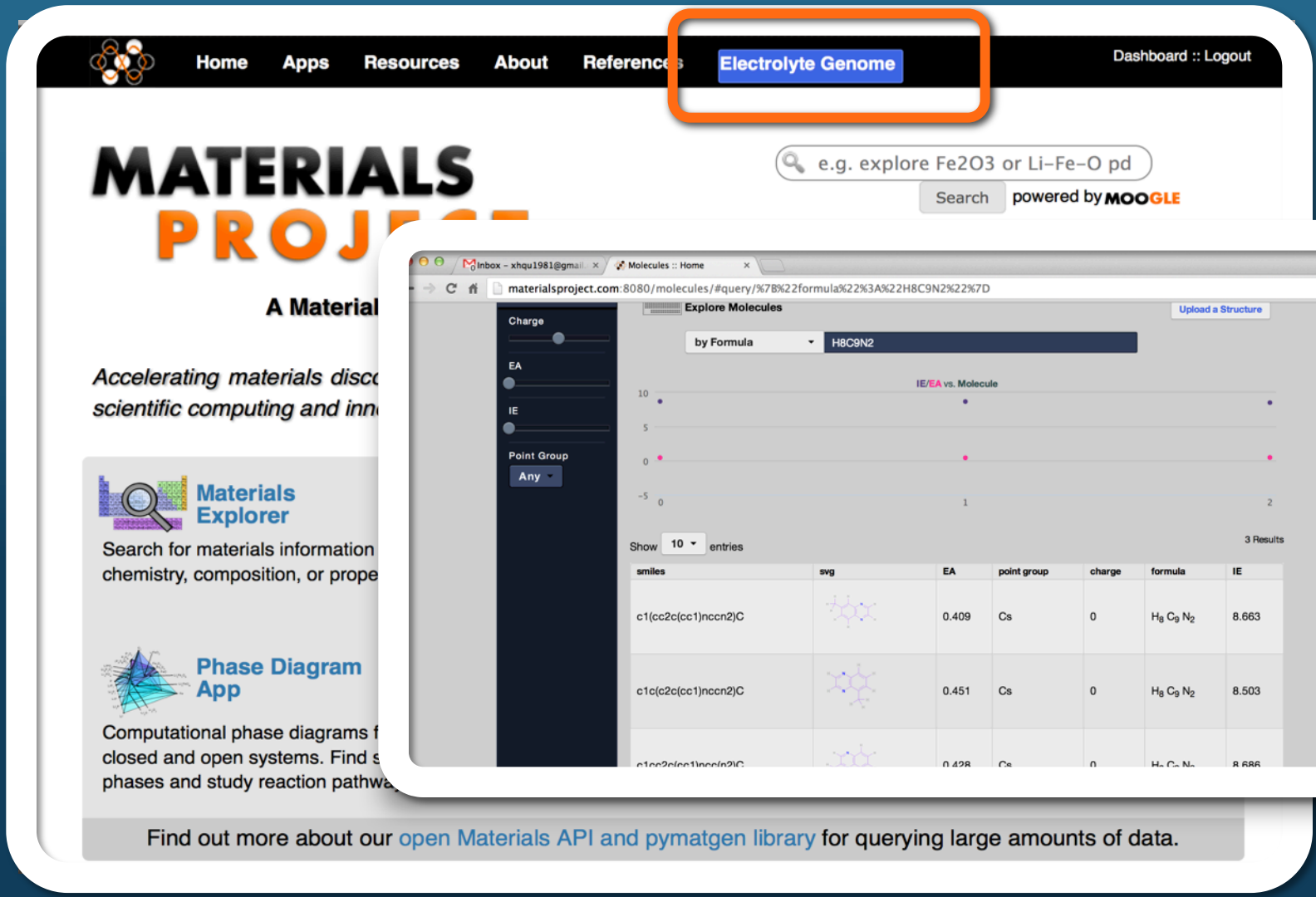
User in group, sees a unified view of <u>both</u> sandbox and core data

A ‘Genomic’ Approach to Electrolytes



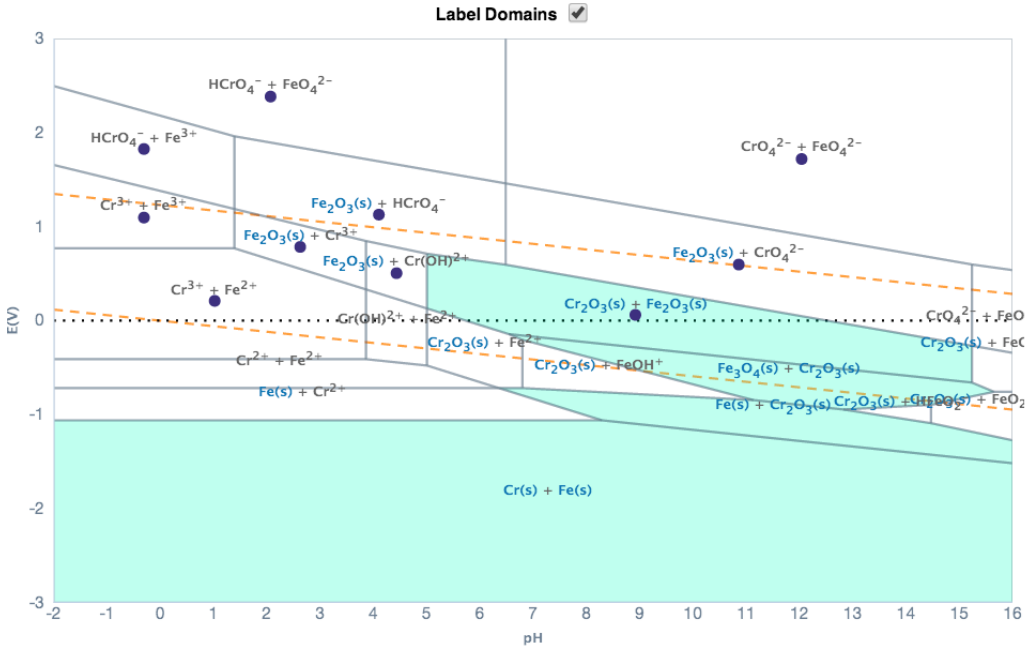
Substitution, mutation and selection to arrive at optimal electrolytes and redox molecules

JCESR Sandbox: The Electrolyte Genome



> 70,000 Pourbaix Diagrams Available

www,materialsproject.org/Pourbaix

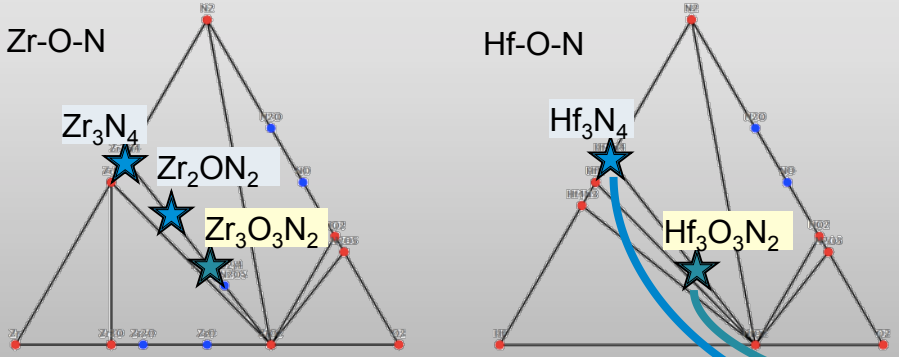


Pourbaix Diagrams on the Materials Project

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



Y.Wu et al., Energy Environ. Sci. 6, 157 (2013)

Photocatalytic materials:

- Known
- Predicted

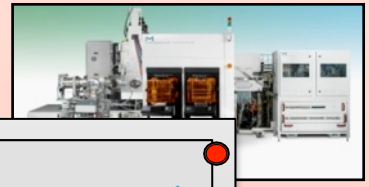
Non-photocatalytic materials:

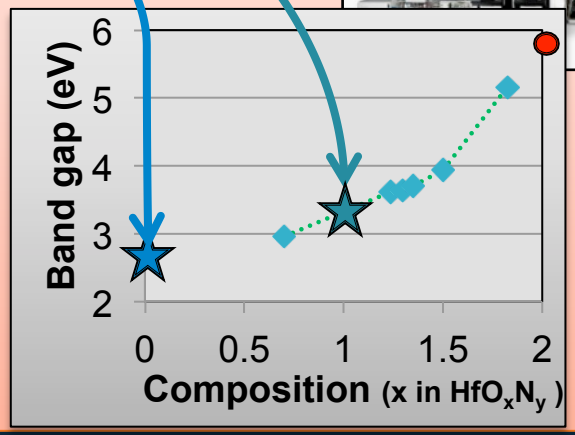
- Stable
- Known metastable

- ✓ Band gap suitable for UV photocatallysis
- ✓ Level alignment perfect for water splitting

Materials developed by Intermolecular show properties matching these predictions

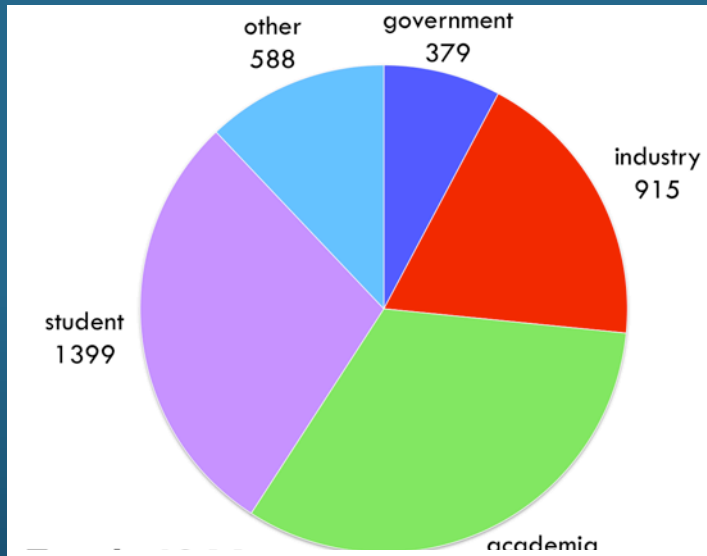
- ✓ Focus on materials with multiple applications
- ✓ Synthesis methods developed
- ✓ Range of O:N compositions scanned
- ✓ Optical characterization data match the predicted band gap
- ✓ Future workflow could focus on optimizing the water splitting capabilities



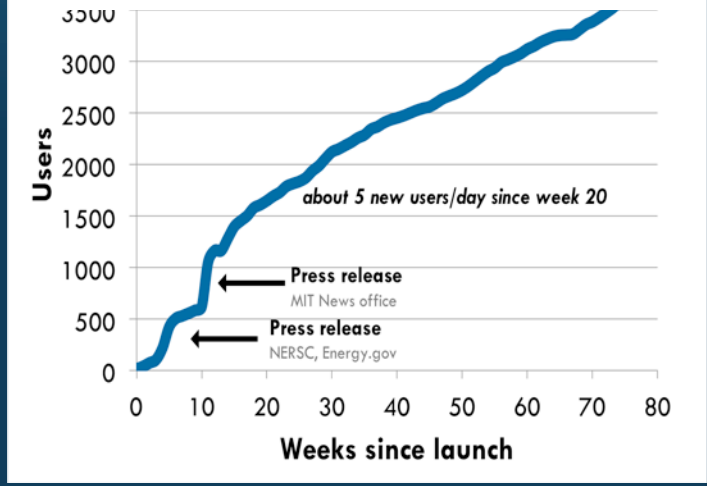


A Rapidly Growing Resource

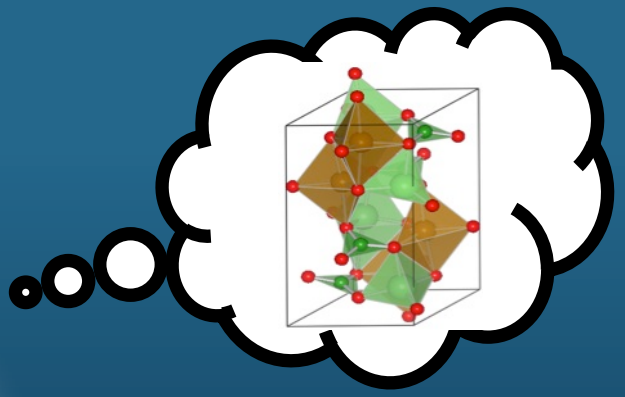
- Launched online Oct 2011
- Grants: 2012 DOE Center, JCESR, U Madison NSF Center, JCAP
- Users: > 5600 and counting…
- Course-ware : UC San Diego, UC Davis, UC Irvine, U Michigan, John-Hopkins, Cornell, …
- **Partner institutions:** UC Berkeley, UC San Diego, MIT, Duke, U Wisconsin, U Kentucky, U Louvain 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, …

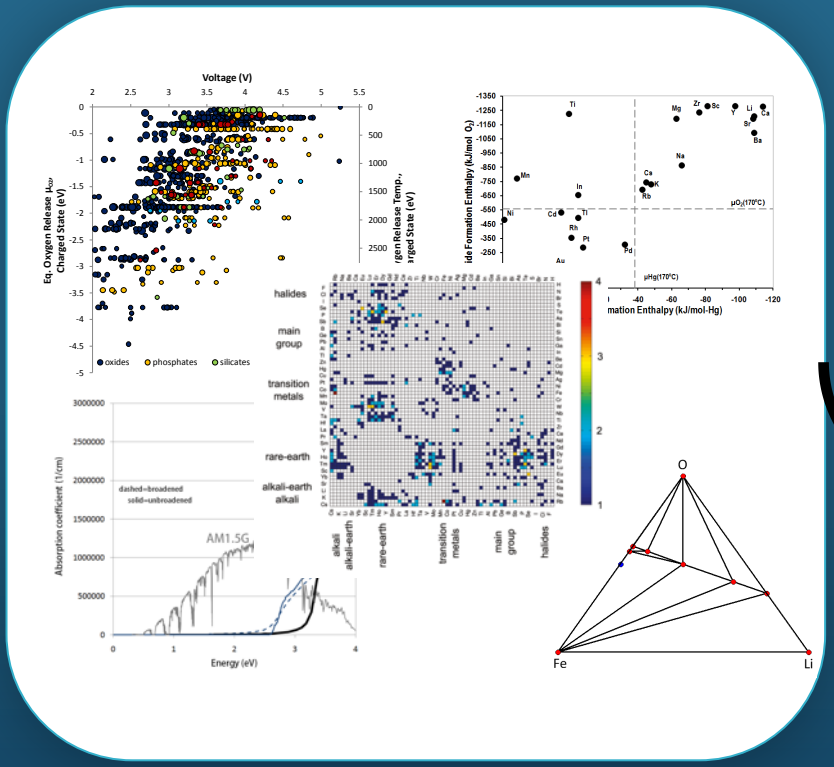


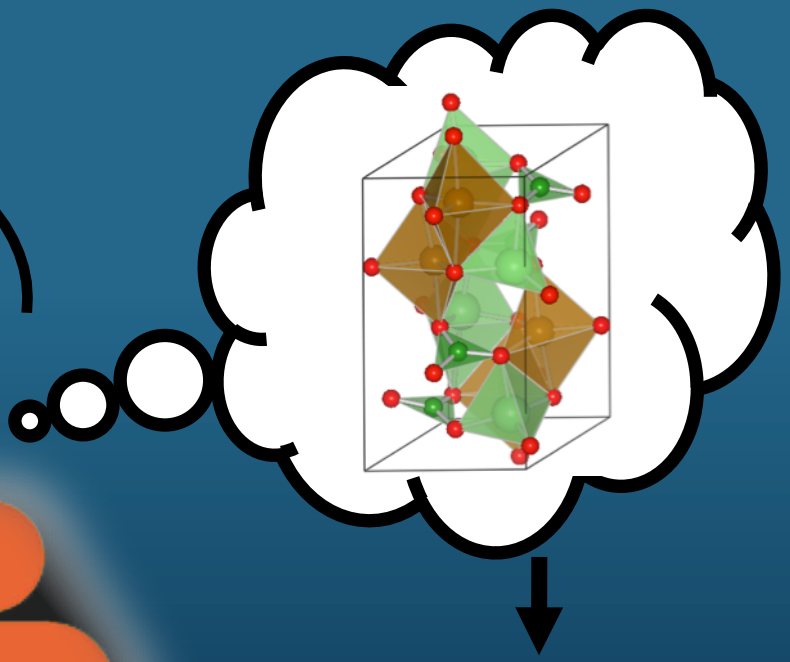
As of today: 5622 users

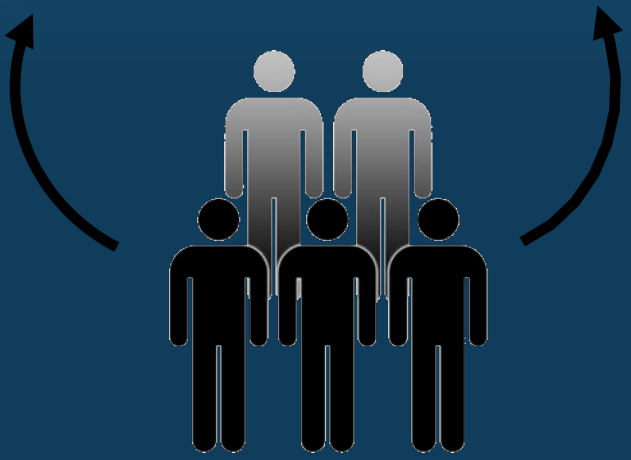


From single entities…









… towards a materials genome

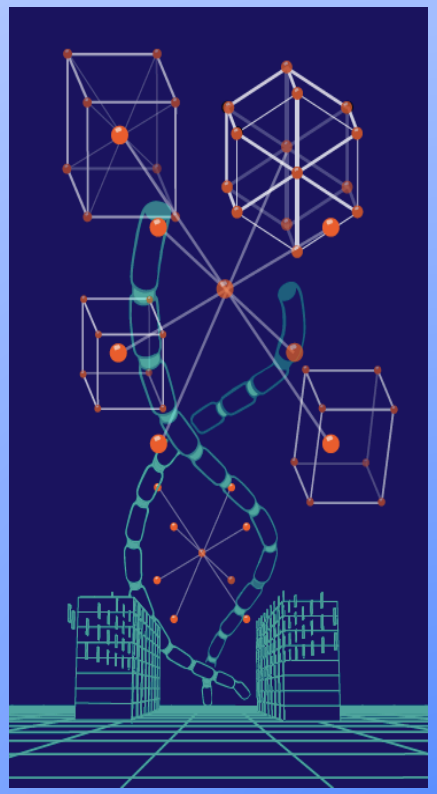
Thank you for your attention!

Thanks to sponsors:

U.S. DEPARTMENT OF ENERGY

NERSC

NSF



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

"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