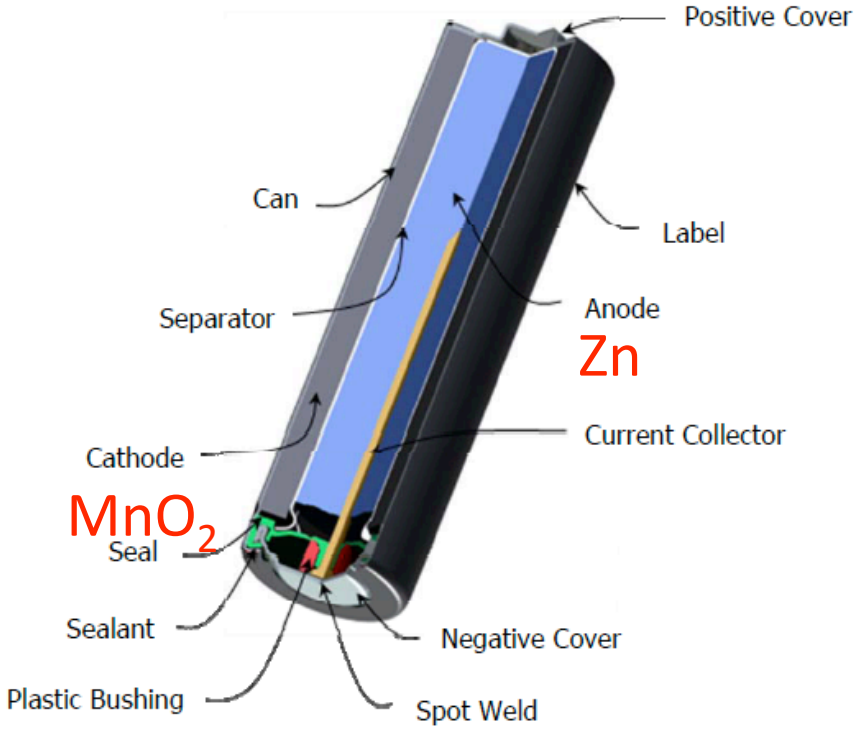
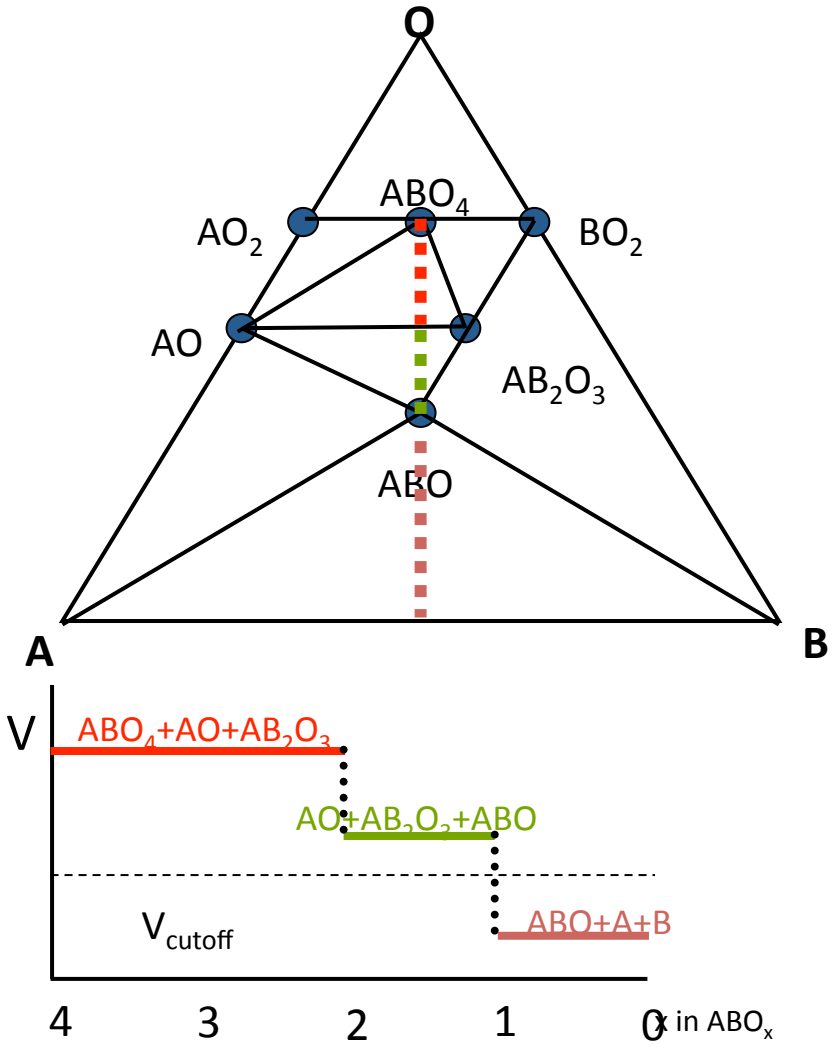
Ok – Assume we fixed the computing – Does it work?

High-throughput Materials Design: Alkaline batteries

Finding higher energy density cathode



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



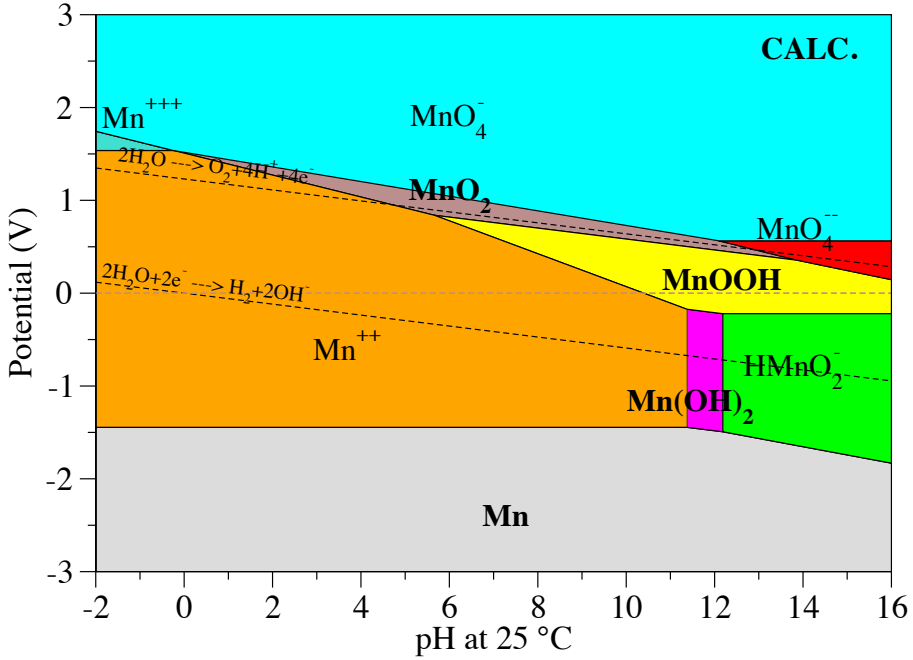
SPECS:

Higher energy density

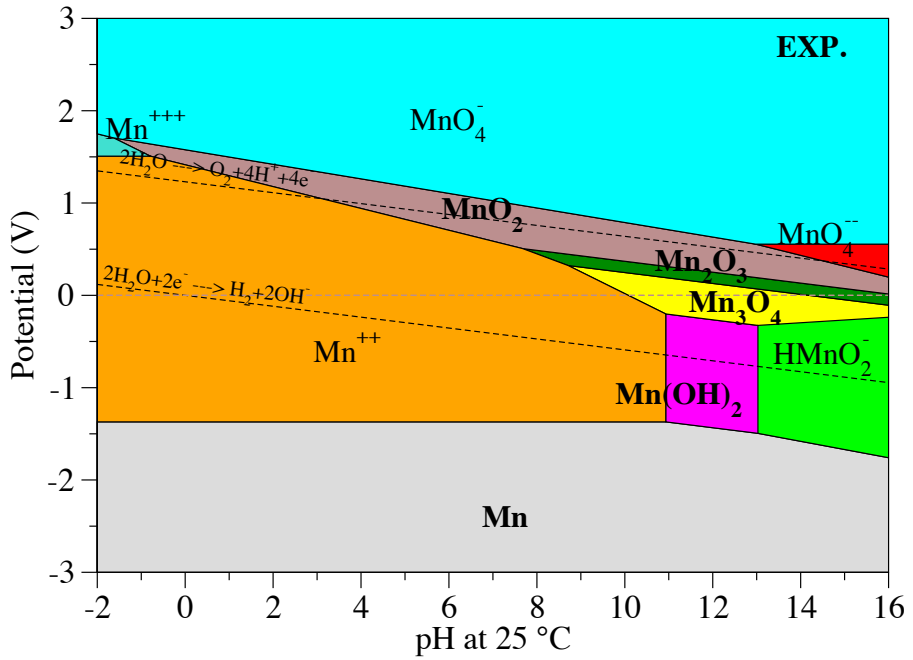
Both reactants and products stable in high molar KOH

Needs to model reactions at pH = 15

Our calcs



exp

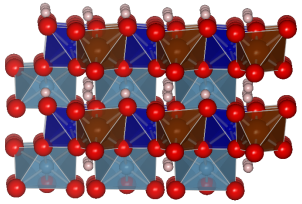


Alkaline cell reaction

$2MnO_2+H_2O+Zn \rightarrow 2MnOOH + ZnO$

M. Pourbaix, "*Atlas of Electrochemical Equilibria in Aqueous Solution*", Pergamon Press, Paris (1966).

The Screening Strategy



Database

Known compounds

30,000

permutation strategy

New compounds

~ 100,000

~ 100,000 - 200'000

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

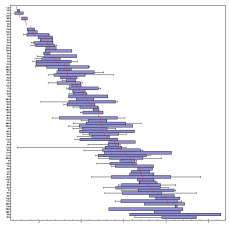
Initial screening (phenomenological)

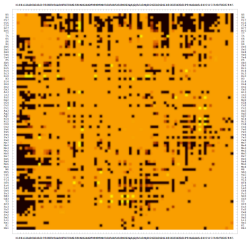
≈ 10,000 - 20'000

Computational Screening

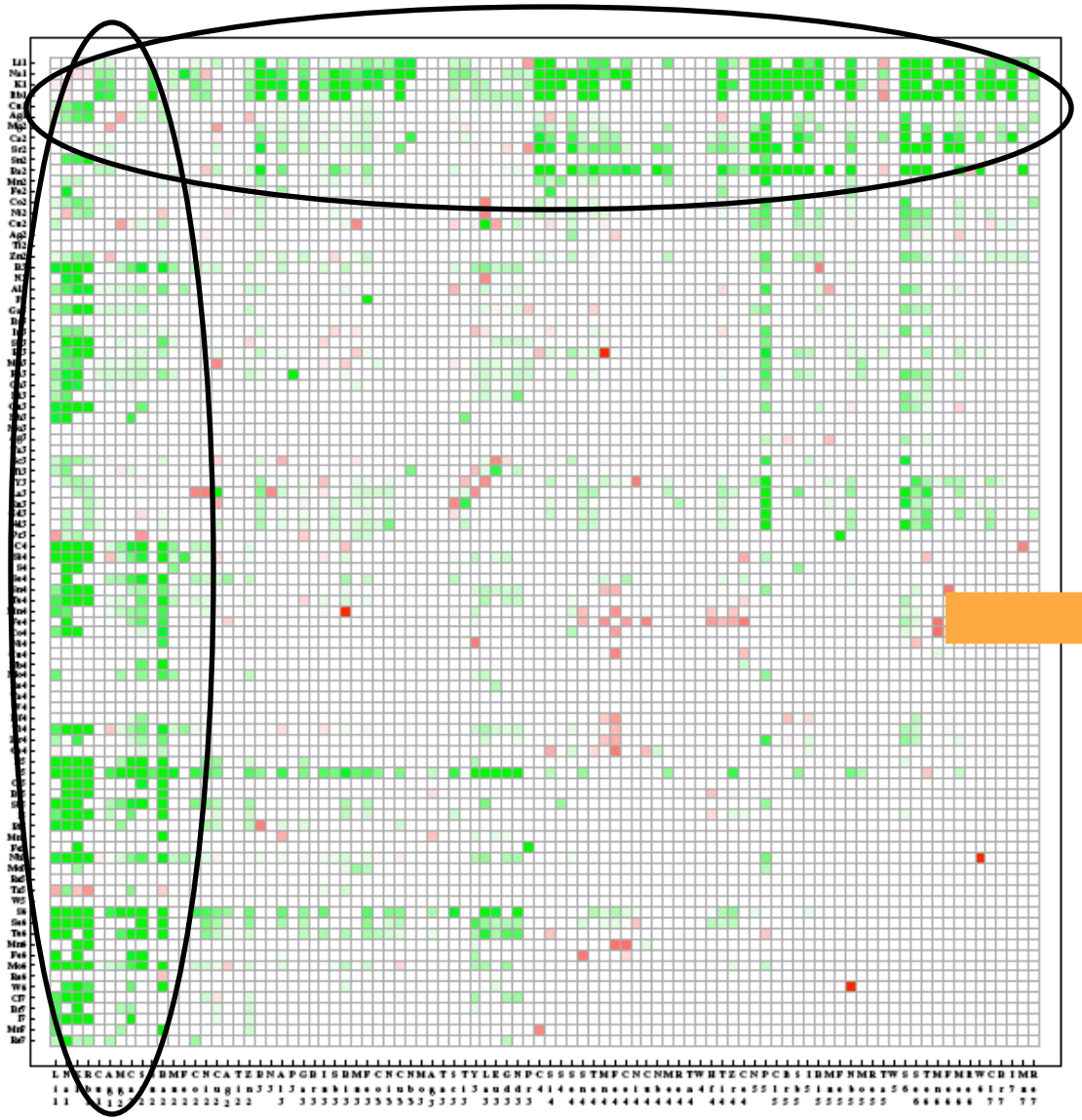
Data mining

Candidate materials





Materials Design: Solid Stability Patterns

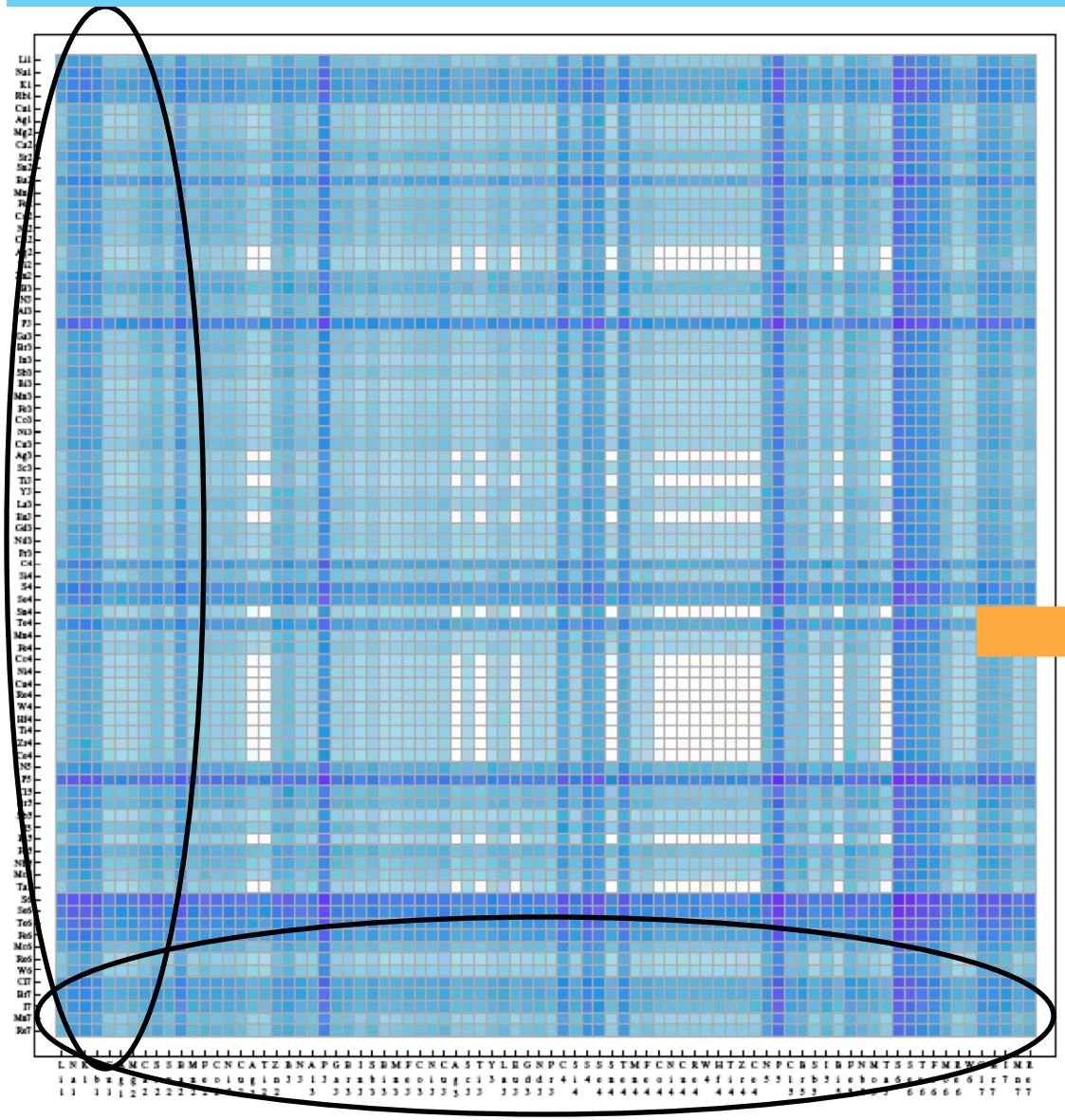


- High negative formation energy
- Negative formation energy
- Positive formation energy
- High positive formation energy

Which cation stabilizes another cation

Design stable solids

Materials Design: KOH Instability



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

Which cations dissolve

Design stable solids at high pH

Candidate Compounds and Design Rules

> 130,000 compounds considered
- 30,000 known from ICSD
- > 100,000 new generated

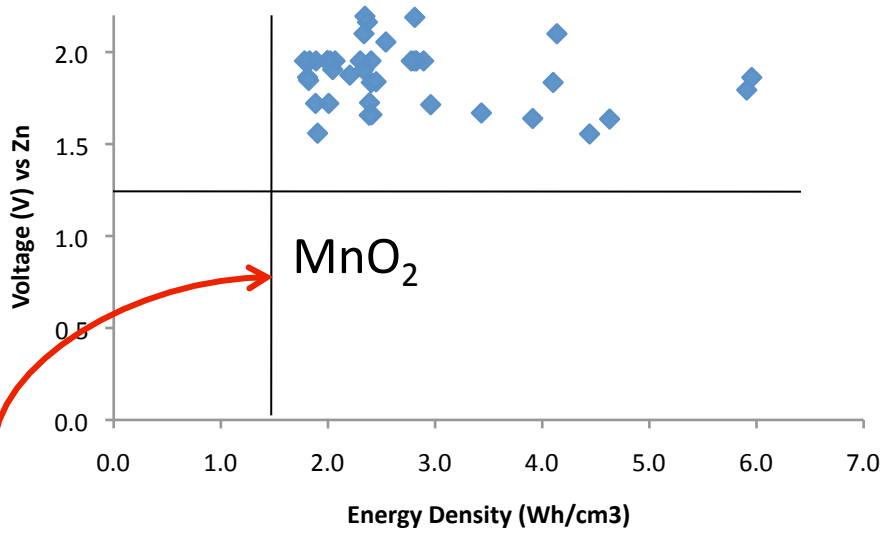
Tier 1

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

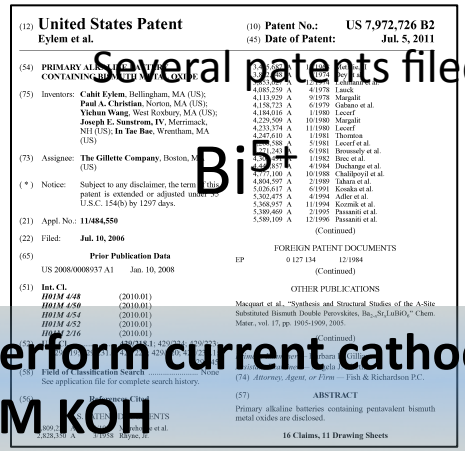
Tier 2

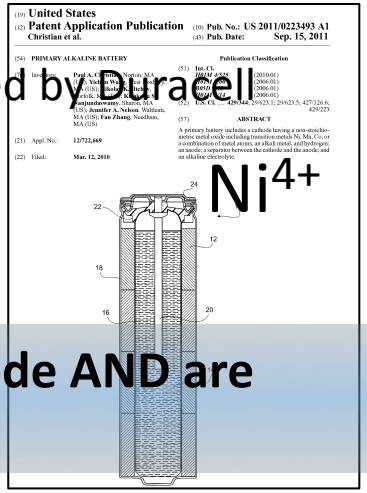
≈ 200 compounds
- ✓ Reactant stable in air
- ✓ Reactant stable in 9N KOH
- ✓ Product stable in 9N KOH

Predicted alkaline cathode material performance



Several patents filed by Duracell





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

But what about Bismuth availability?

✓Not too expensive (~$20-30/kg)
✓Low global production (by-product of lead refinement)
✓NO domestic production…

World Mine Production and Reserves:

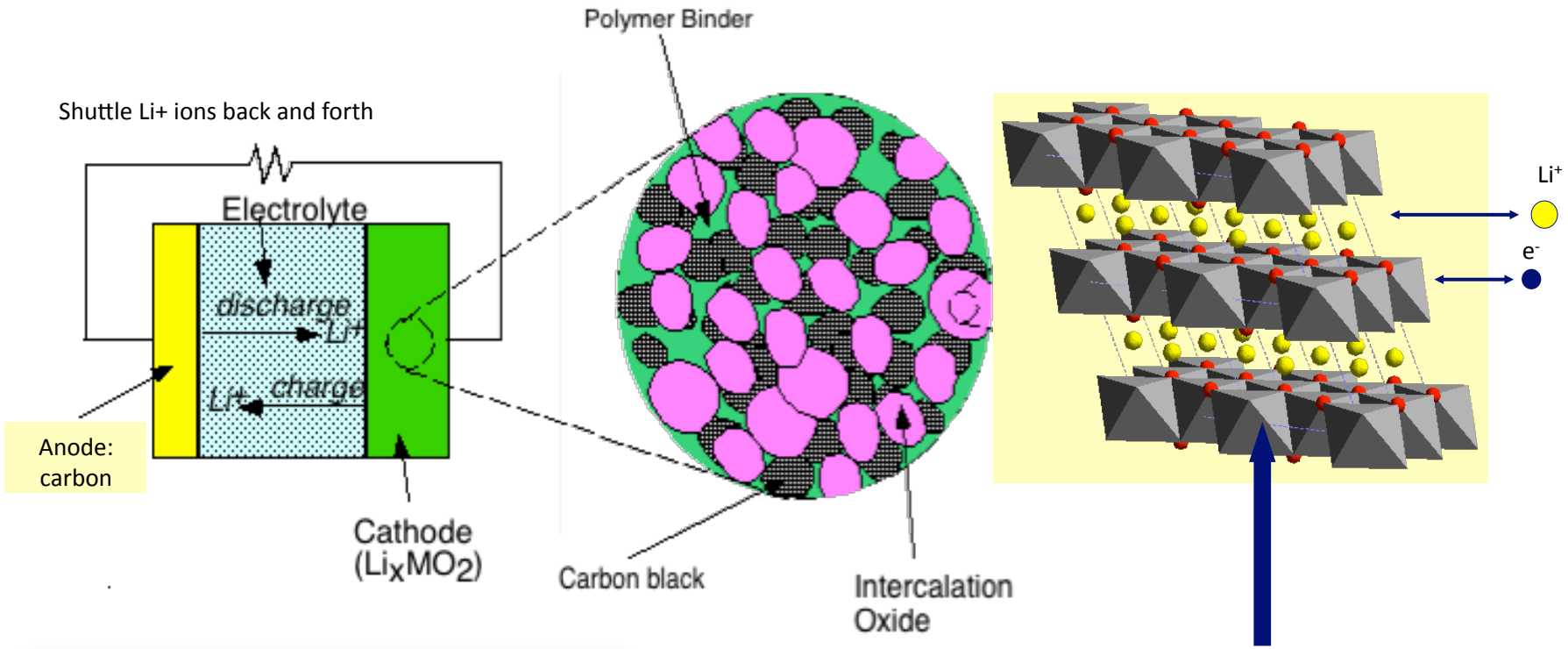
	Mine production		Reserves[2]
	2010	2011[e]	
United States	—	—	—
Bolivia	90	100	10,000
Canada	90	100	5,000
China	6,500	6,000	240,000
Kazakhstan	150	—	NA
Mexico	850	1,000	10,000
Peru	1,100	1,100	11,000
Other countries	120	200	39,000
World total (rounded)	8,900	8,500	320,000

Project focused on high energy novel materials, which was successful – however, driving force not enough to develop – just patents …

Company Strategy

High-throughput Materials Design: Li-ion batteries

In Silico Materials Design: Li ion batteries



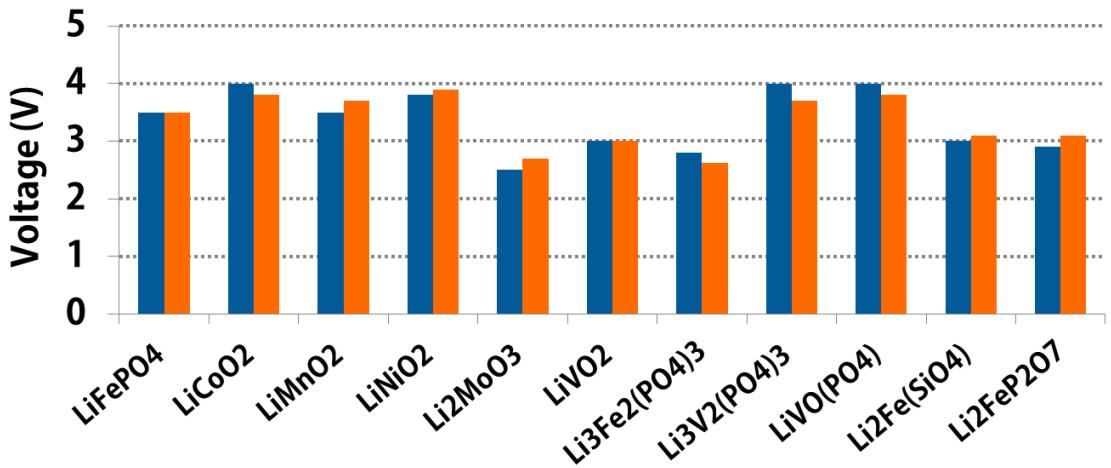
Li-ion is a family of chemistries, differentiated by cathode

Cathode needs to host and exchange large amounts of Li^+ and electrons at high rate and remain stable

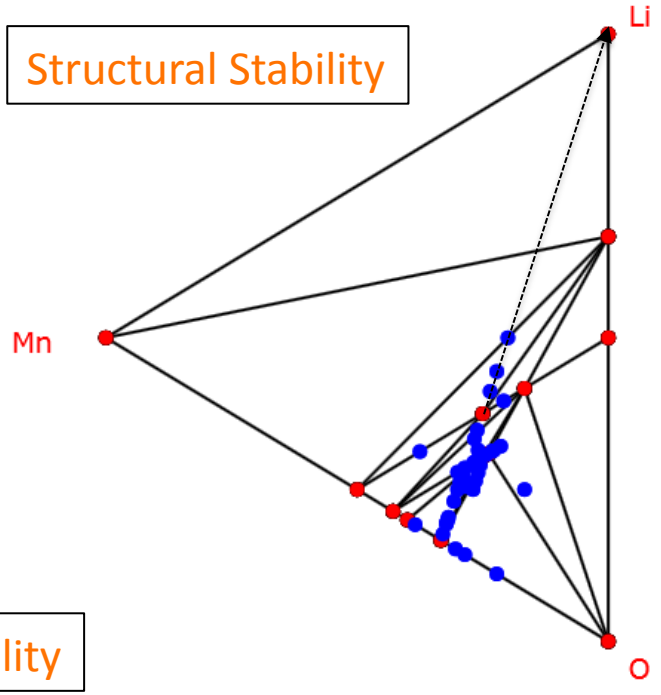
Need: good capacity, voltage, rate, stability, safety, cost, ….

Most are Computable

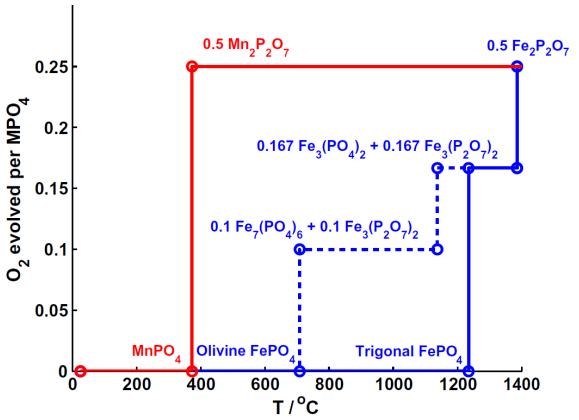
Voltage



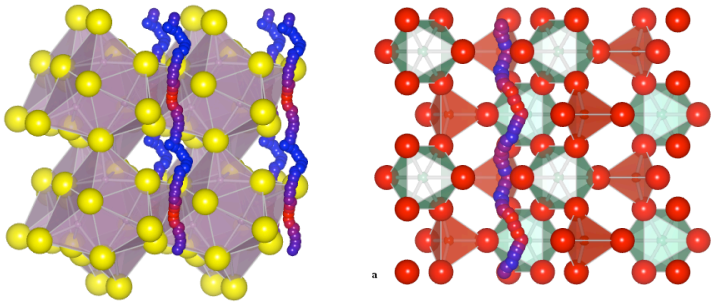
Structural Stability



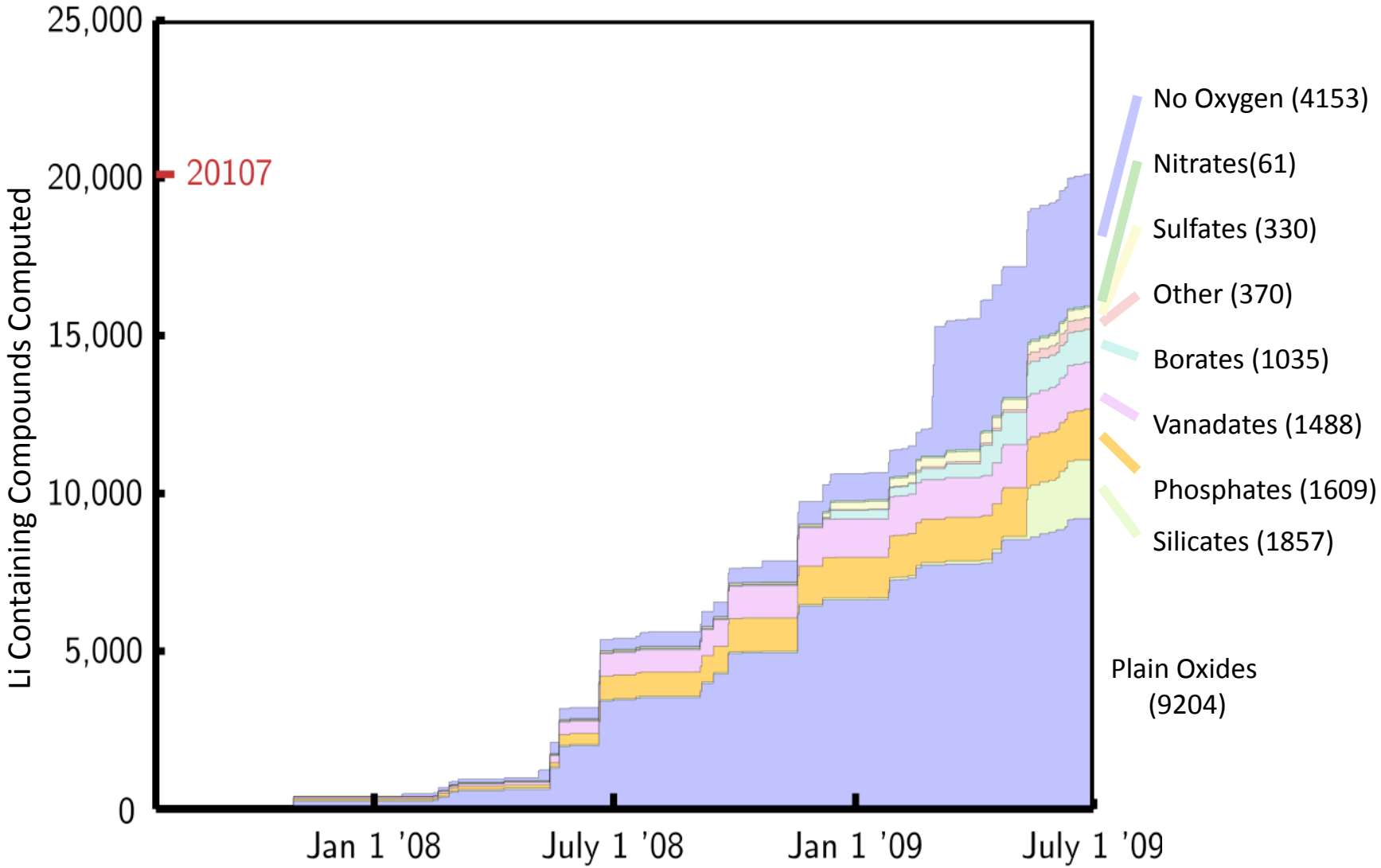
O2 release: safety



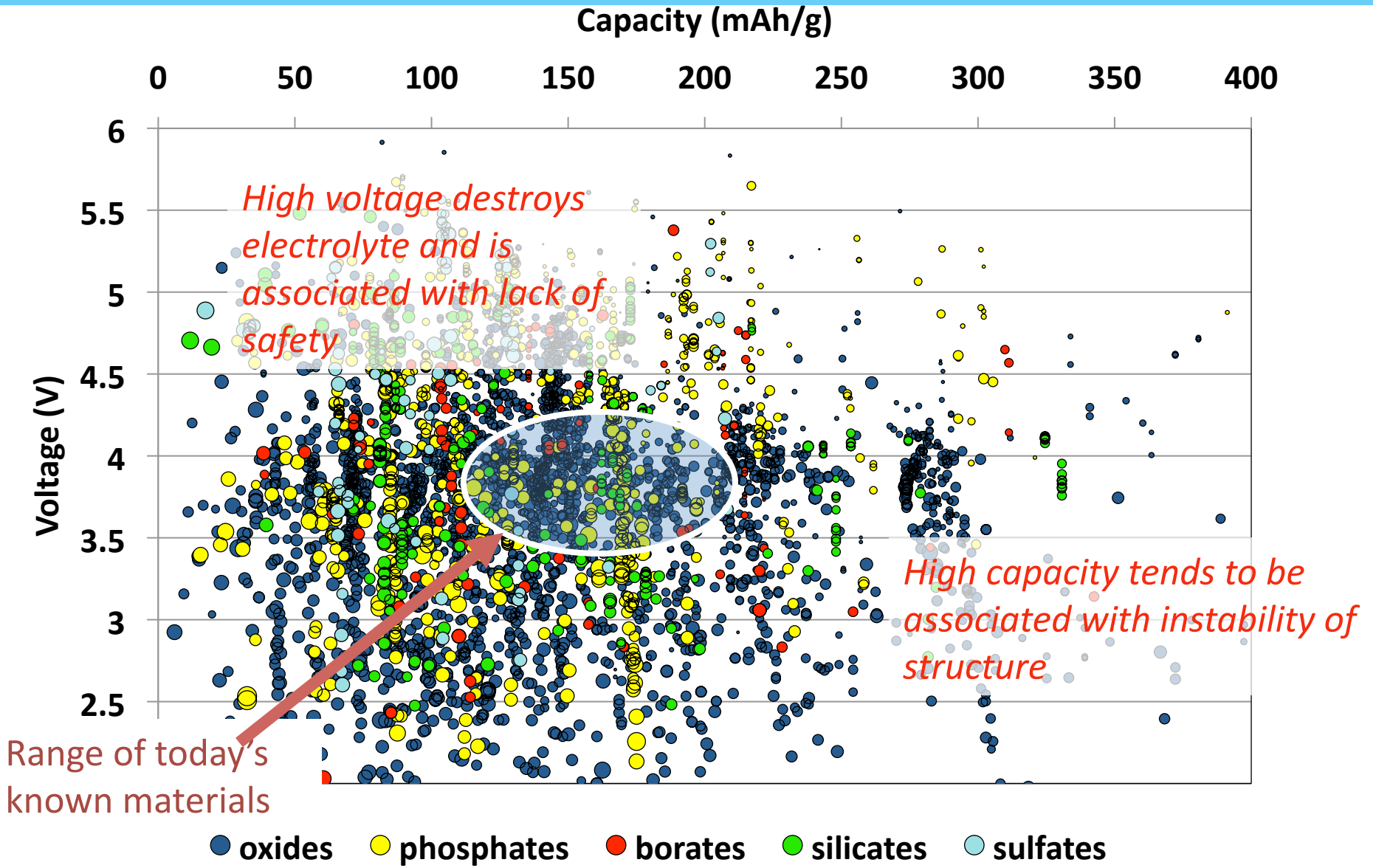
Li mobility



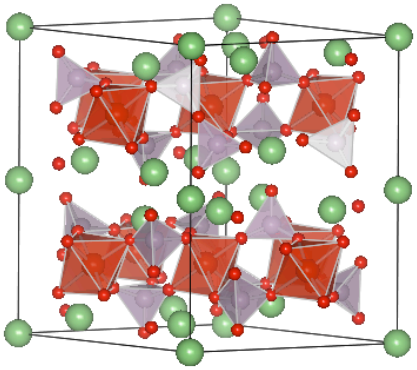
About 25,000 battery compounds investigated so far



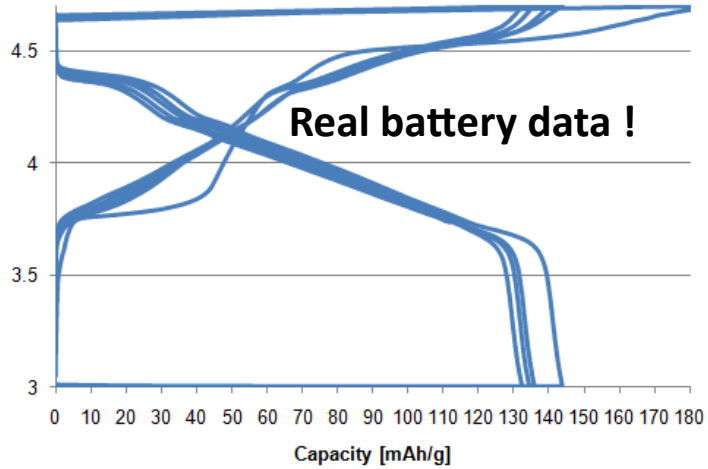
Target Design Spaces



New Li-ion Cathode Materials Discovered

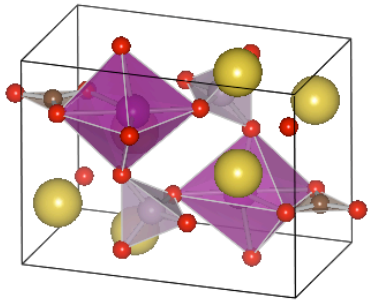


New phosphate discovered @MIT through computations



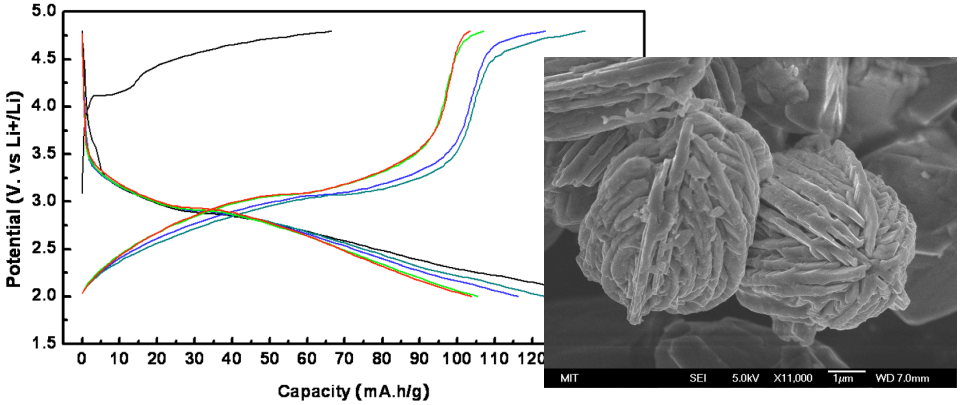
Courtesy of Ceder at al, MIT

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



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

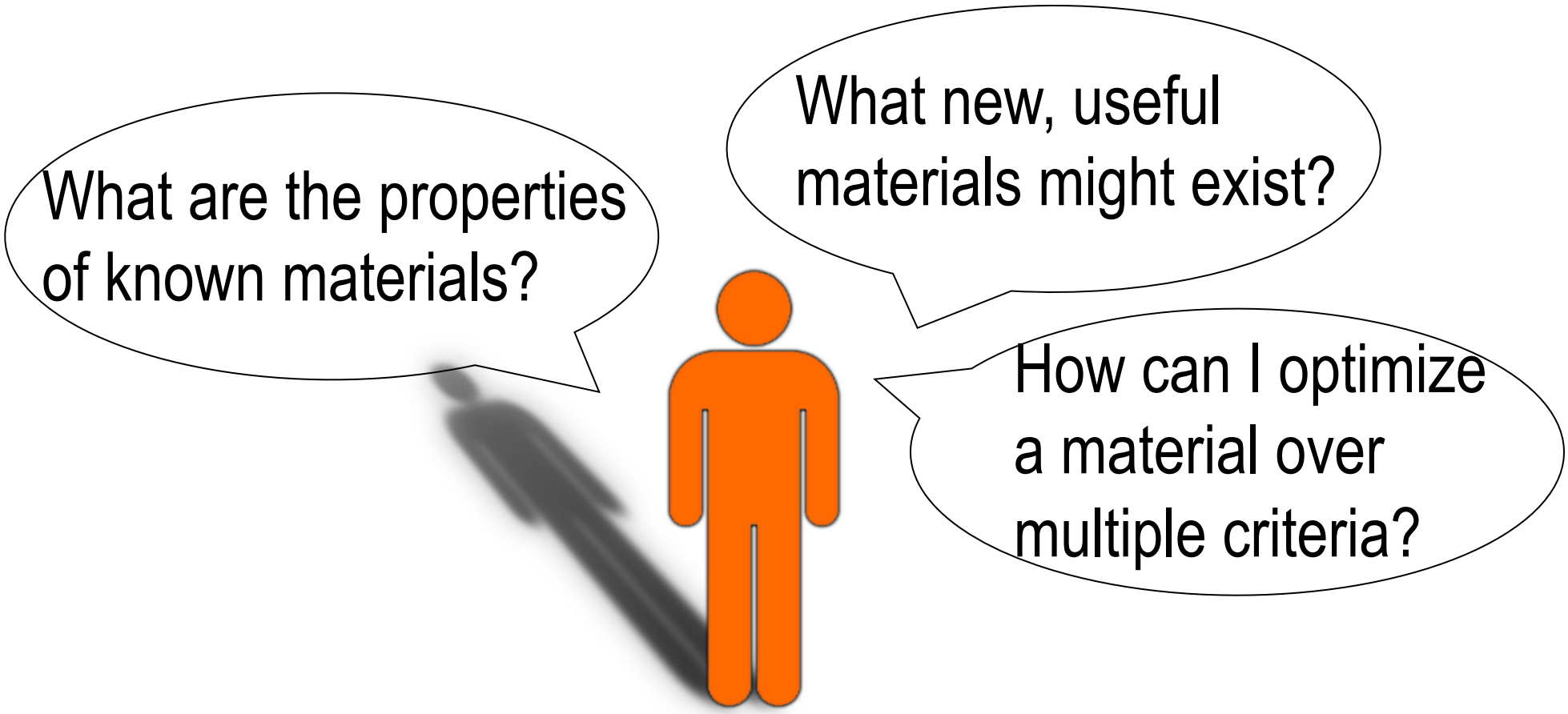
"Sidorenkites": $Li_3M(CO_3)(PO_4)$ (M = Fe, Mn, Ni, Co)



Courtesy of Ceder at al, MIT

The Materials Project:
A Growing Public Resource

Bringing information to YOU



Often, 'experience' of individuals is the only guide

The MATERIALS PROJECT

a materials genome approach

Formerly the "Materials Genome Project"

A public Project to compute "all" properties of all inorganic materials

carboncycle2.0

BERKELEY LAB

www.materialsproject.org

The MATERIALS PROJECT

Goals

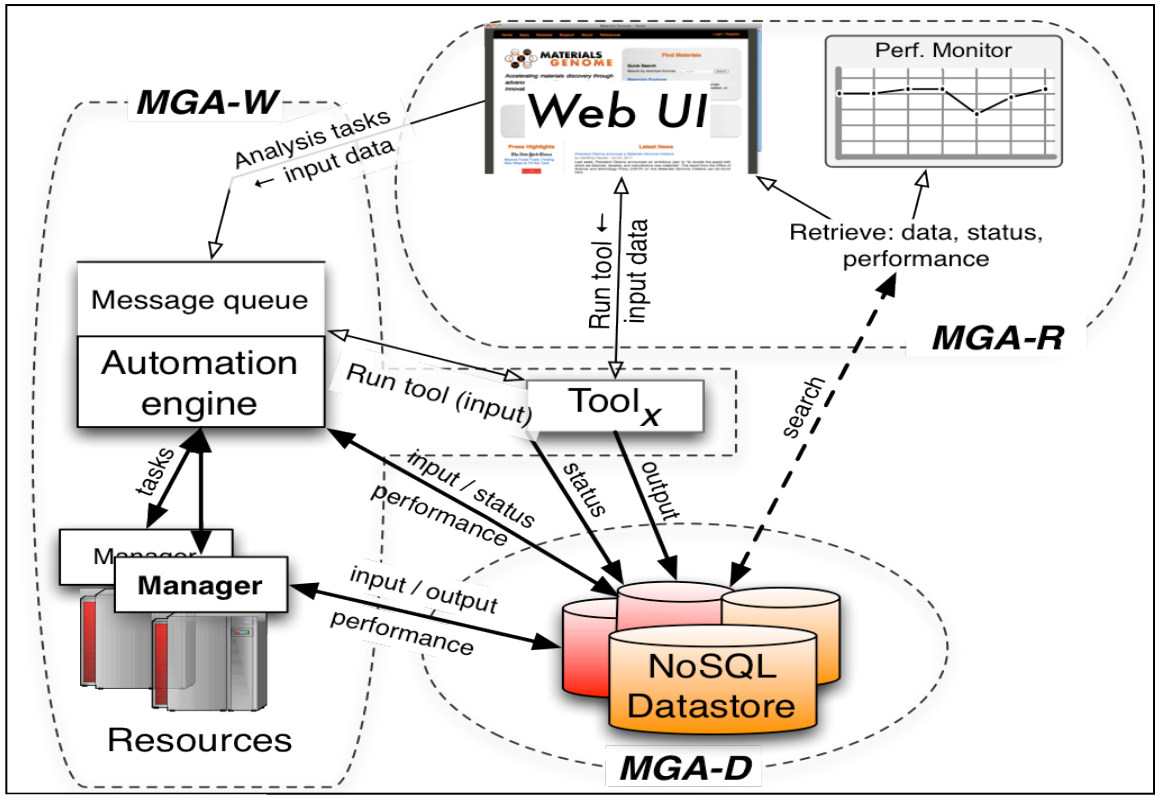
- Fill in ‘missing’ property data on all known compounds
- Assist researchers in predicting new materials
- Provide interactive analysis tools and codes
- Enable rapid screening and data mining

MATERIALS GENOME

The MATERIALS PROJECT

Large machinery under the hood to manage:

- ✓Input data
- ✓Runs
- ✓Output
- ✓Analyses
- ✓Web interface



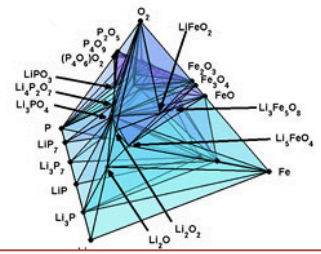
LBNL NERSC
Kathy Yelick
David Skinner
Shreyas Cholia
Daniel Gunter
Annette Greiner

MIT
Gerbrand Ceder
Shyue Ping Ong
Geoffroy Hautier

LBNL CRD
David Bailey
Anubhav Jain

LBNL EETD
Kristin Persson
Michael Kocher

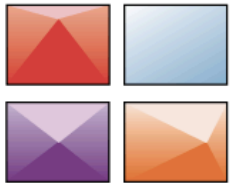
- Over 20,000 compounds and growing daily
- Multiple tools based on computed data



PhaseDiagramApp

The Phase Diagram App uses density functional theory calculations from our database to generate **0K compositional and grand potential phase diagrams** of 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 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!

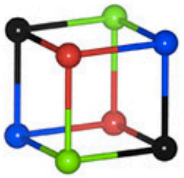
MaterialsExplorer

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".



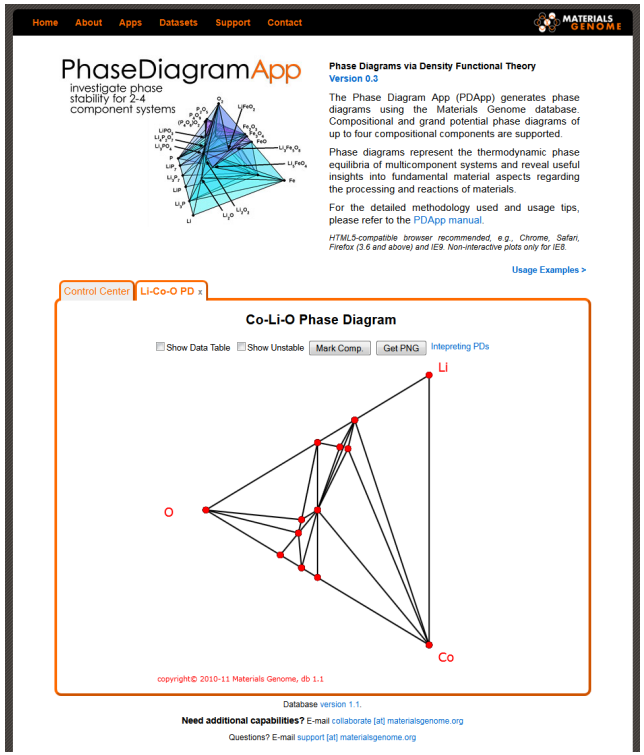
CrystalToolkit

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.

www.materialsproject.org

The MATERIALS PROJECT

Data

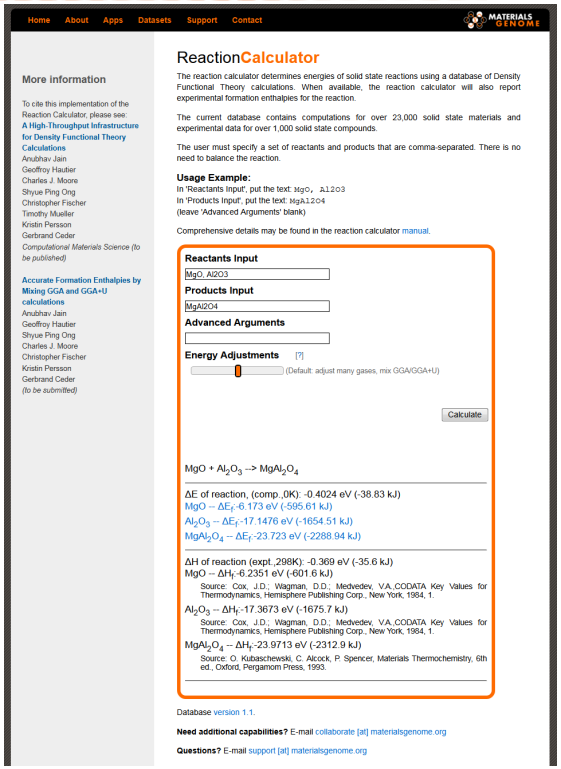


Phase diagrams

with available data:

28,300

SYSTEMS



Reaction energies

already available online:

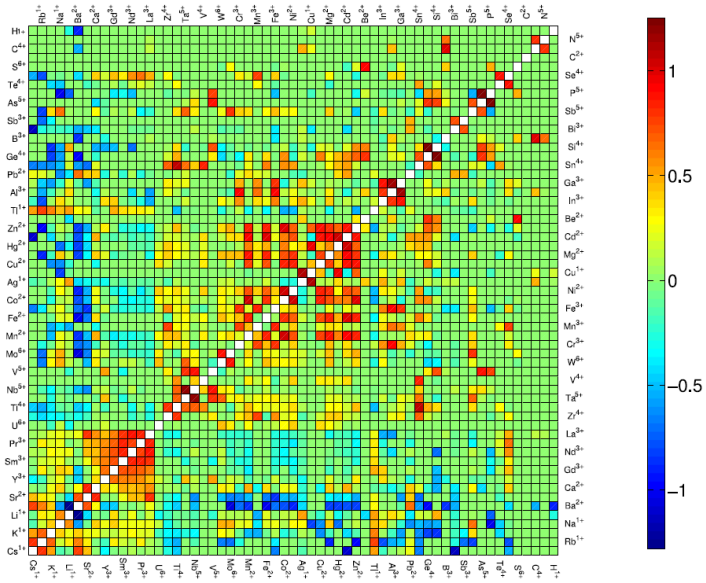
>35,000

REACTIONS

The MATERIALS PROJECT

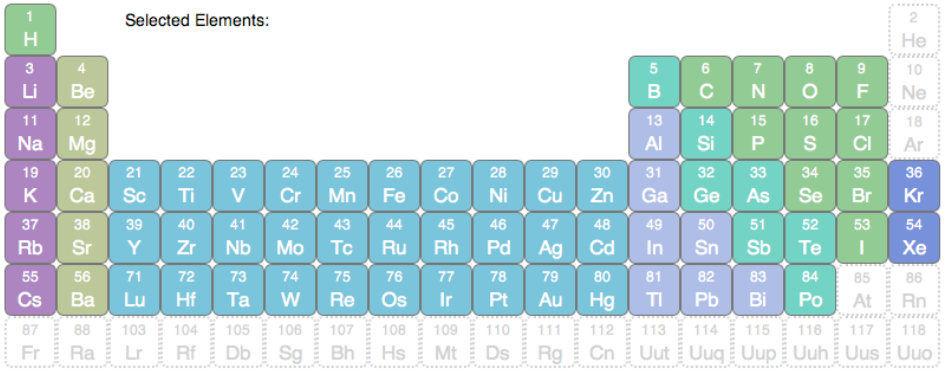
Structure Predictor

Predict new compounds using data-mined substitution algorithms.



Hautier, Fischer, Erlacher, Jain, Ceder
Inorganic Chemistry (2010)

Step 1: Select elements



MATERIALS PROJECT | Home | Apps | Support | About | References | kapersson@lbl.gov | Logout

StructurePredictor Result 255

Selected species	Nb:[5] O:[-2] Ti:[4]
Threshold	-4
Created at	Oct. 18, 2011, 8:48 a.m.
Completed at	Oct. 18, 2011, 4:05 p.m.
Computational time	10275 sec
Number of crystals	23

Candidate Structures

Show 50 entries Search:

Ranking	ID	Score	Chemical Formula	Number of Sites	CIF
1	189	-3.8932	$Ti_2Nb_2O_9$	26	Crystal Structure (CIF) [Download Link]
2	190	-3.8932	$Ti_2Nb_2O_9$	52	Crystal Structure (CIF) [Download Link]
3	173	-3.8022	$Ti_4Nb_{18}O_{53}$	150	Crystal Structure (CIF) [Download Link]
4	183	-3.8022	$TiNb_2O_7$	20	Crystal Structure (CIF) [Download Link]
5	184	-3.7108	$TiNb_2O_7$	60	Crystal Structure (CIF) [Download Link]
6	175	-3.6103	$Ti_4Nb_2O_{13}$	19	Crystal Structure (CIF) [Download Link]
7	188	-3.5608	$Ti_2Nb_2O_9$	52	Crystal Structure (CIF) [Download Link]
8	172	-3.5032	$Ti_2Nb_{10}O_{29}$	41	Crystal Structure (CIF) [Download Link]
9	177	-3.4582	$Ti_4Nb_2O_{13}$	38	Crystal Structure (CIF) [Download Link]
10	186	-3.3965	$TiNb_2O_7$	20	Crystal Structure (CIF) [Download Link]
11	192	-3.3965	$TiNb_4O_{12}$	17	Crystal Structure (CIF) [Download Link]
12	182	-3.3950	$TiNb_2O_7$	1080	Crystal Structure (CIF) [Download Link]
13	187	-3.3950	$TiNb_2O_7$	40	Crystal Structure (CIF) [Download Link]
14	181	-3.3448	$TiNb_2O_7$	1080	Crystal Structure (CIF) [Download Link]
15	194	-3.3448	$Ti_6Nb_4O_{20}$	116	Crystal Structure (CIF) [Download Link]
16	191	-3.3046	$TiNb_4O_{12}$	68	Crystal Structure (CIF) [Download Link]
17	174	-3.1551	$Ti_3Nb_2O_{11}$	32	Crystal Structure (CIF) [Download Link]
18	176	-3.1551	$Ti_4Nb_2O_{13}$	76	Crystal Structure (CIF) [Download Link]
19	179	-3.0800	$TiNb_2O_7$	20	Crystal Structure (CIF) [Download Link]

The MATERIALS PROJECT

Safety

?

LithiumBatteryExplorer

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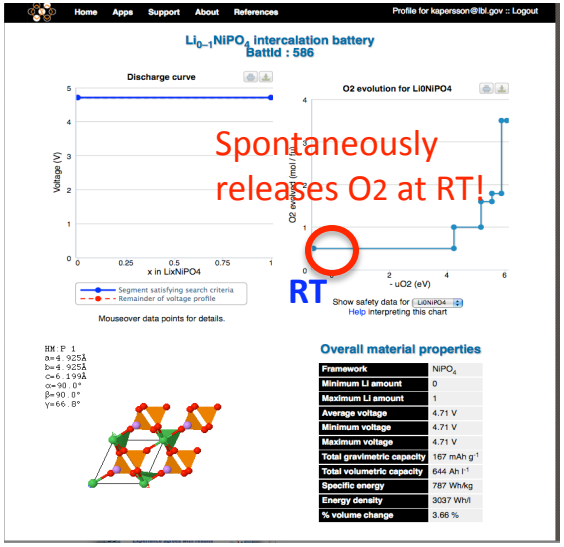
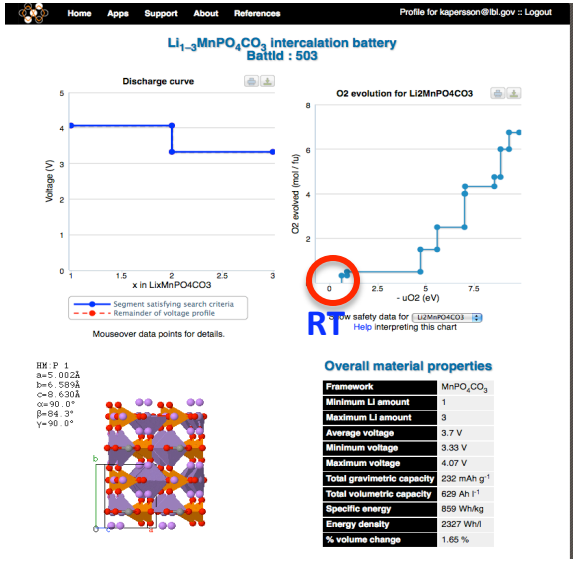
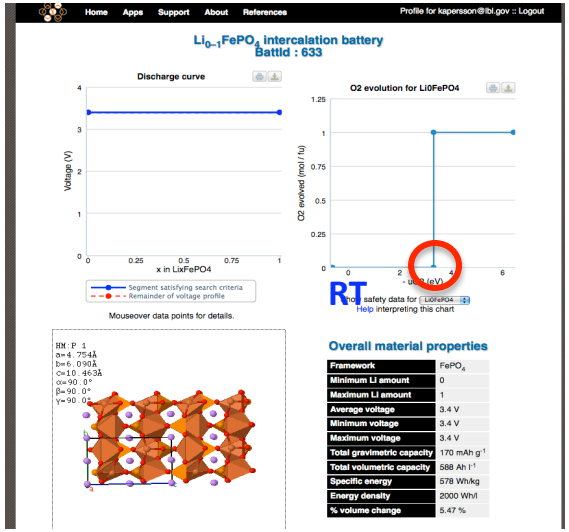
Oxygen release correlates with oxygen chemical potential of cathode

Li_xNiPO_4 → safer → $Li_xMnCO_3PO_4$ → safer → Li_xFePO_4



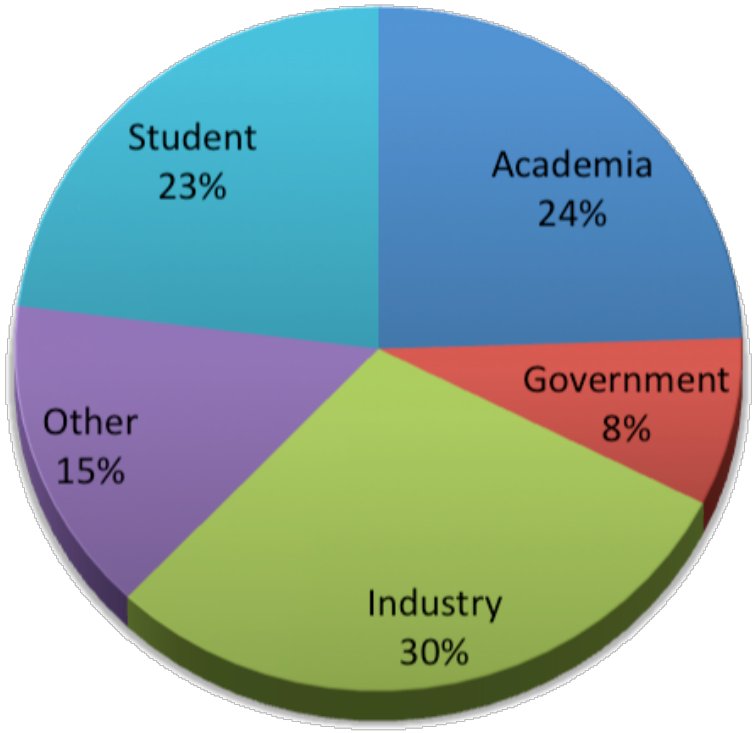




The MATERIALS PROJECT

Usage

Launched Oct 11 2011



- ❑ >2,000 registered users
- ❑ > 6000 phase diagrams generated
- ❑ > 7000 structure predictions executed

Lawrence Berkeley National Laboratory
Kristin Persson
David Bailey
Michael Kocher
Anubhav Jain
Daniel Gunter

Massachusetts Institute of Technology
Gerbrand Ceder
Shyue Ping Ong
Evgueni Chtykov

National Energy Research Scientific Computing Center
David Skinner
Shreyas Cholia
Annette Greiner

UCL Université Catholique de Louvain, Belgium
Geoffroy Hautier

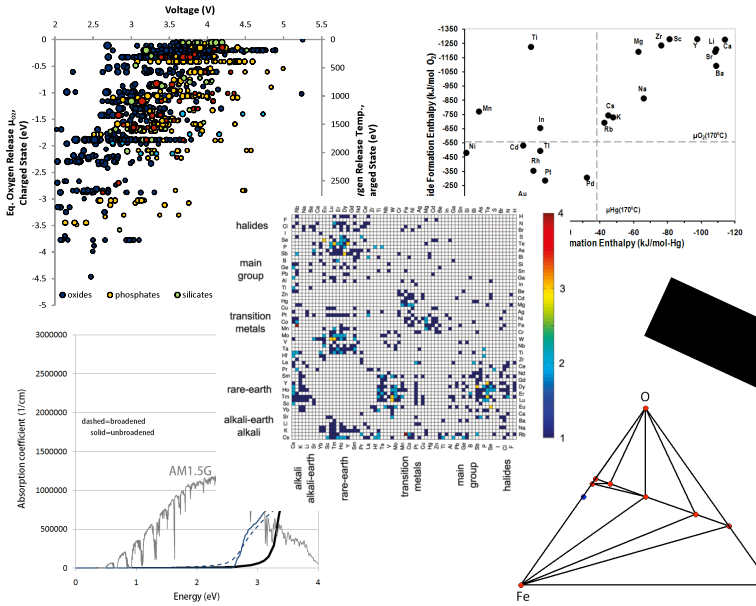
University of Kentucky
Alan Dozier
Matthew J. Beck

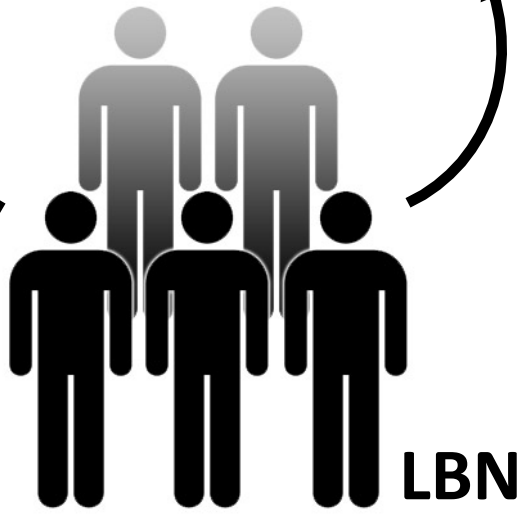
University of California, Berkeley
Mark Asta

NUS National University of Singapore
Stefan Adams

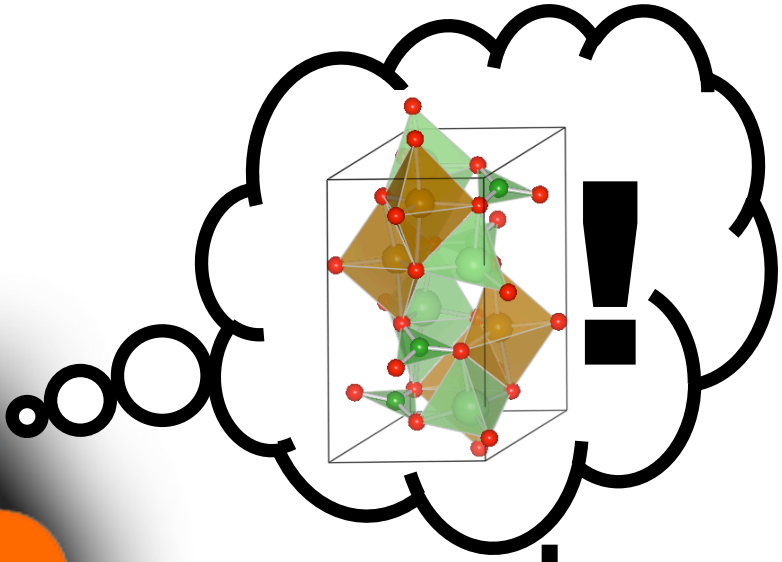
www.materialsproject.org

The Materials Genome Revolution





LBNL/MIT + partners

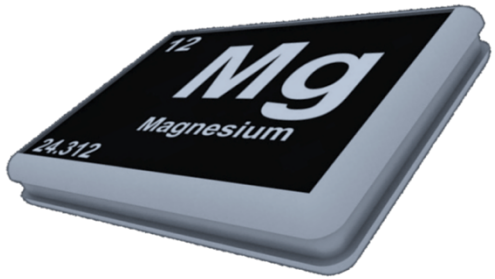


“bringing science solutions to the world”

The MATERIALS PROJECT

Current and Planned Application areas

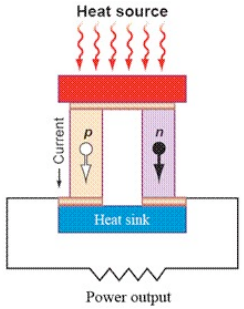
- Alkaline battery cathodes
- Li-ion battery electrodes
- Na-ion battery electrodes
- Electrolytes
- Rechargeable Mg-ion batteries



- Solid State Ion conductors

- Hg capture from gas streams

- Corrosion/Stability in Water
- Photocatalysts
- Thermoelectrics



- Surface energies and nanoparticles

Applications are often created in collaboration with companies

The Google of Materials Properties is arriving

- Materials are the cornerstone of many applications
- Materials properties can be predicted by computations: **ab initio + other methods**.
- We will reach the point where properties of all materials are computed: **A Materials Genome**

www.materialsproject.org

The MATERIALS PROJECT

Recognition

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 End