

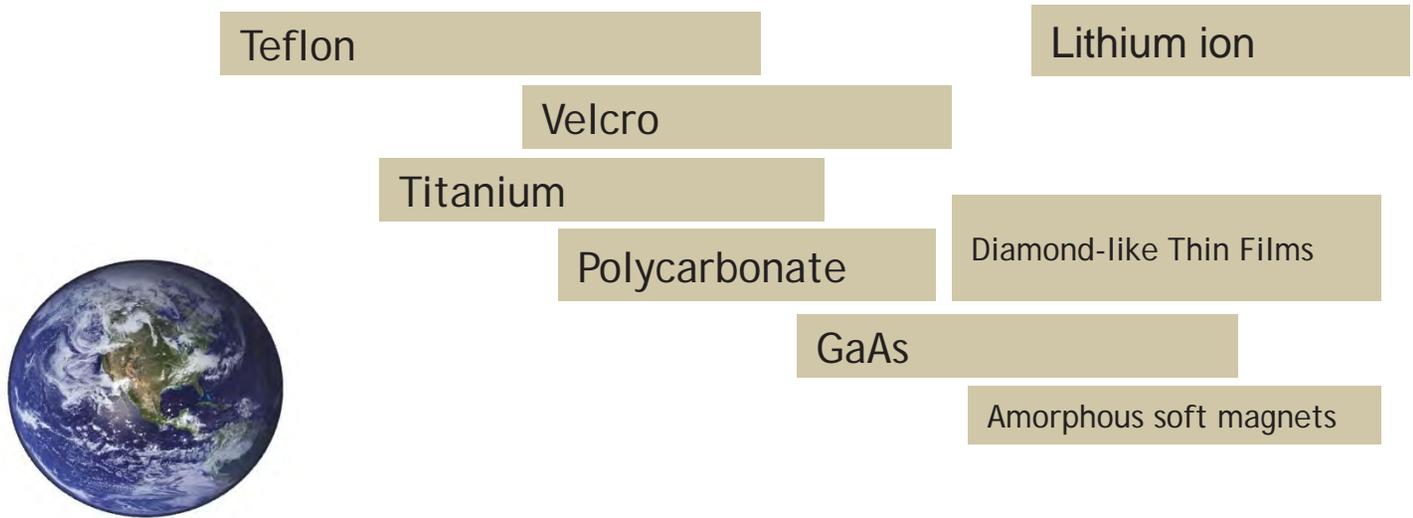
Computational Materials Design

Kristin Persson

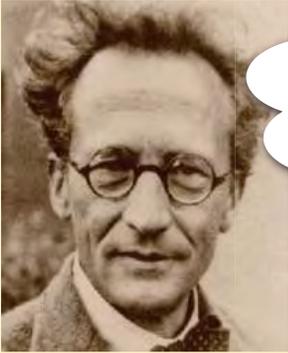
Materials Innovation Timeline



How to accelerate the innovation and development timeline ?



Theory + Computers = Predictions!

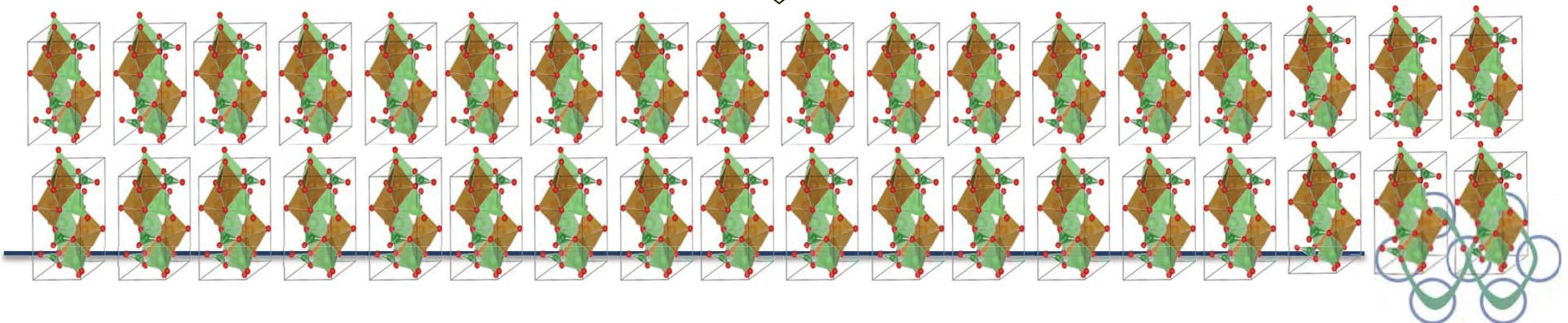
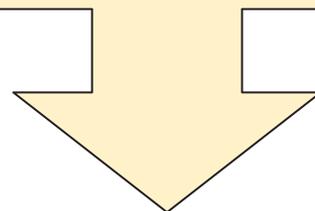


One supercomputer could crunch through ~20,000 structures in 1 day...

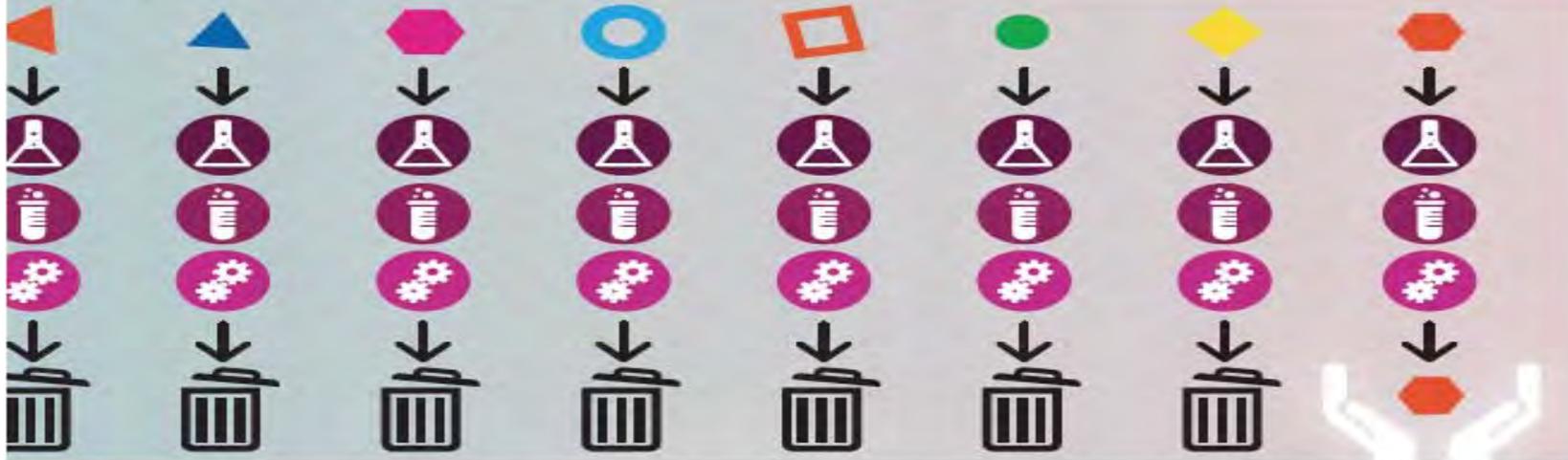
+



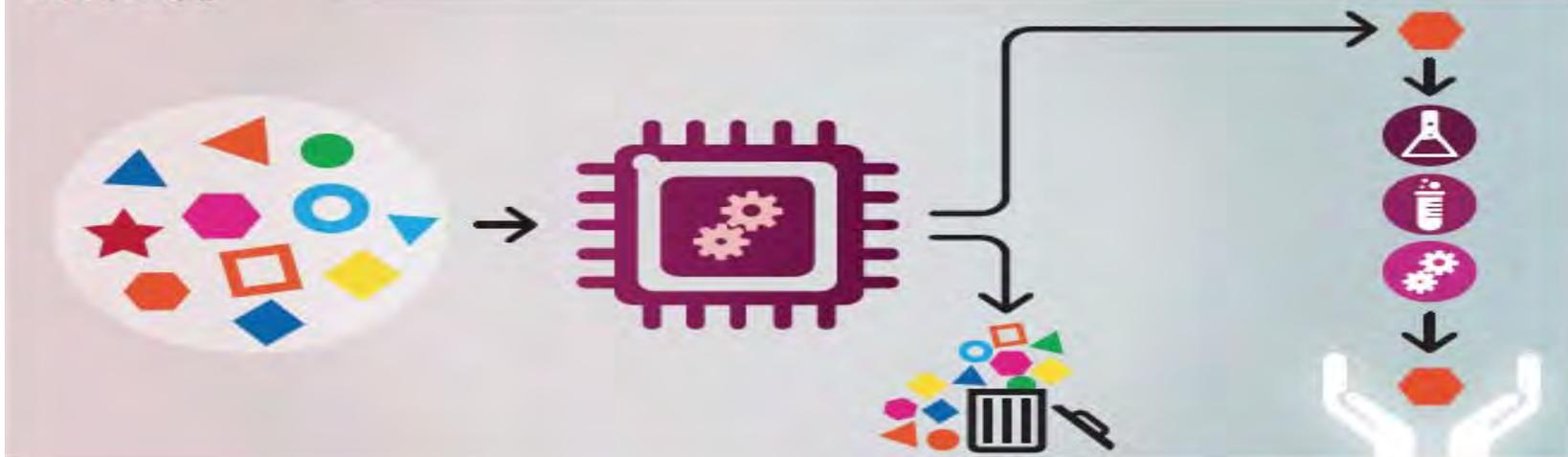
$$i\hbar \frac{d\Psi(\{r_i\};t)}{dt} = \hat{H} \Psi(\{r_i\};t)$$



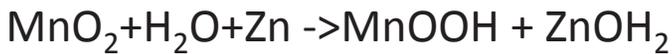
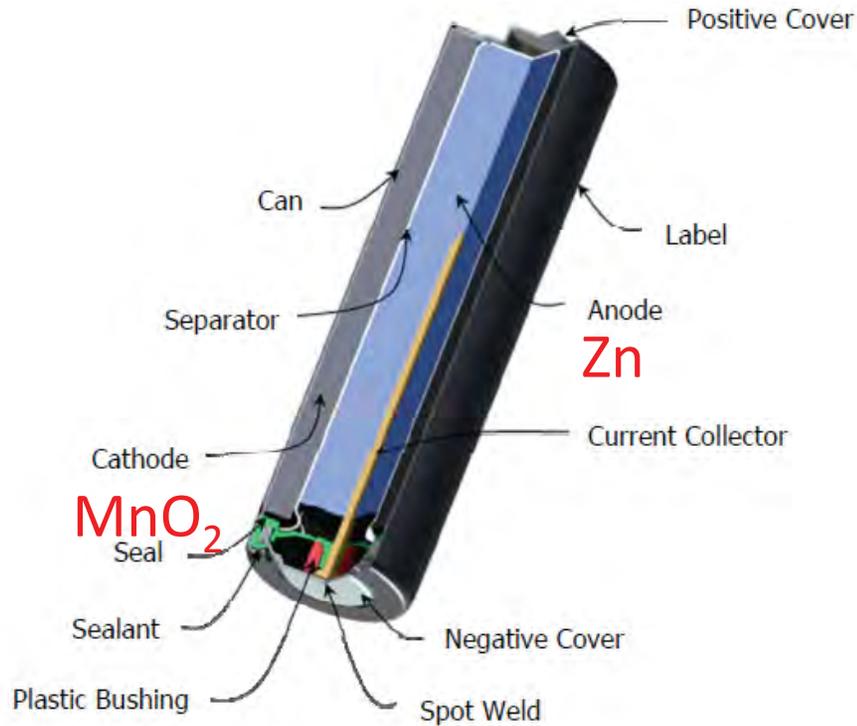
Edisonian



In Silico



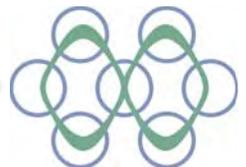
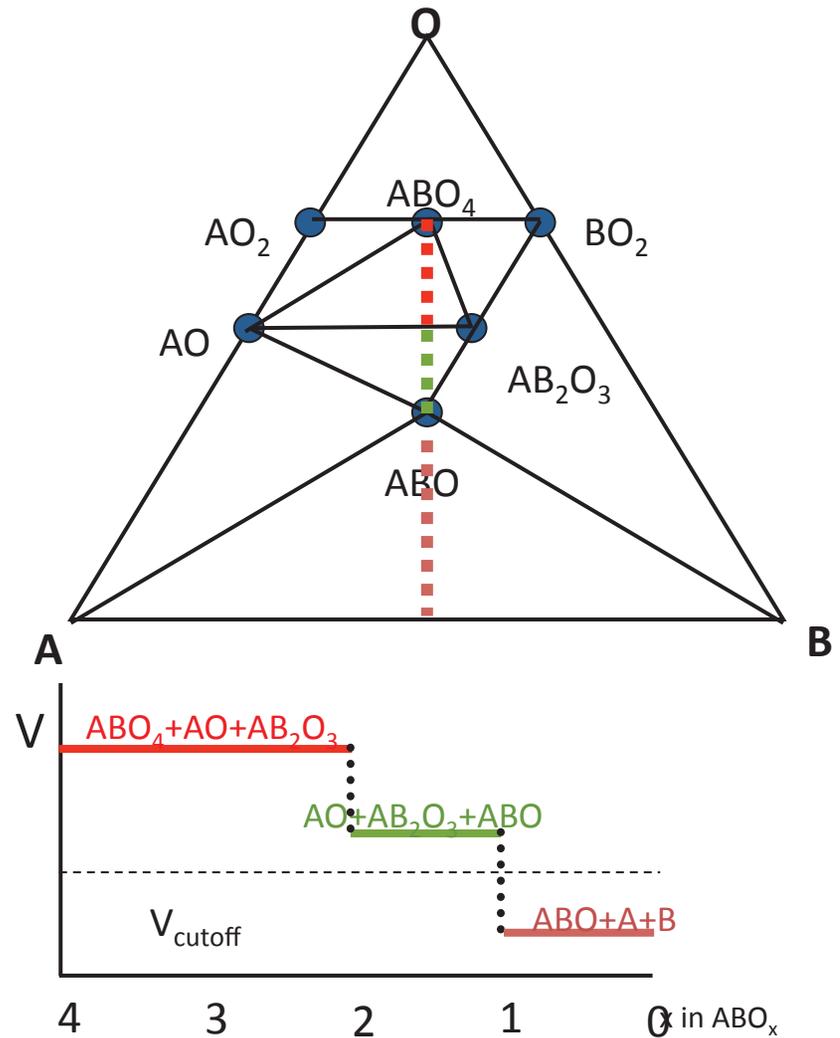
Finding higher energy density cathode



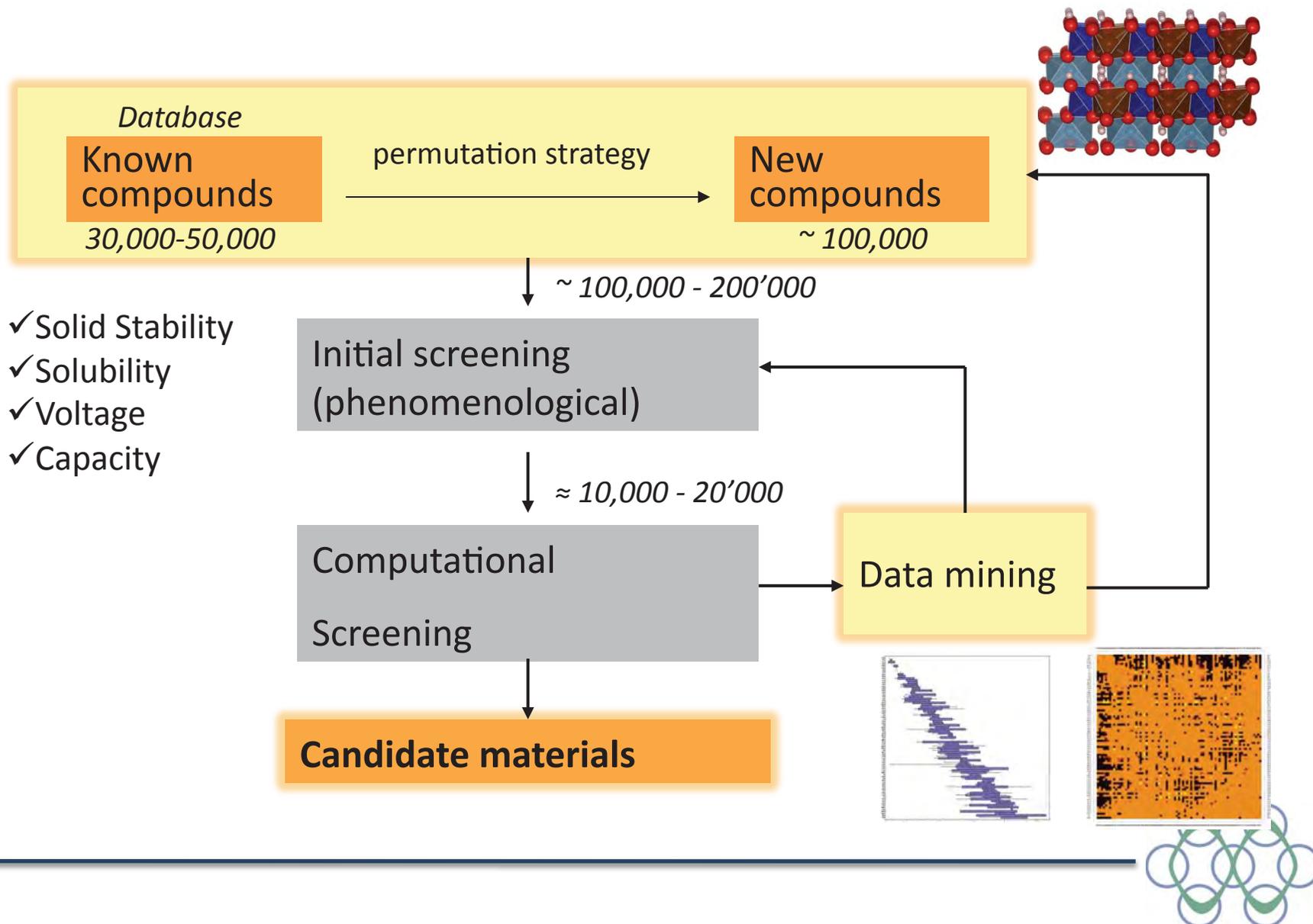
SPECS:

Higher energy density

Both reactants and products stable in high molar KOH



The Screening Strategy



Novel Materials for Alkaline batteries

> 130,000 compounds considered

- 30,000 known from ICSD
- > 100,000 new generated



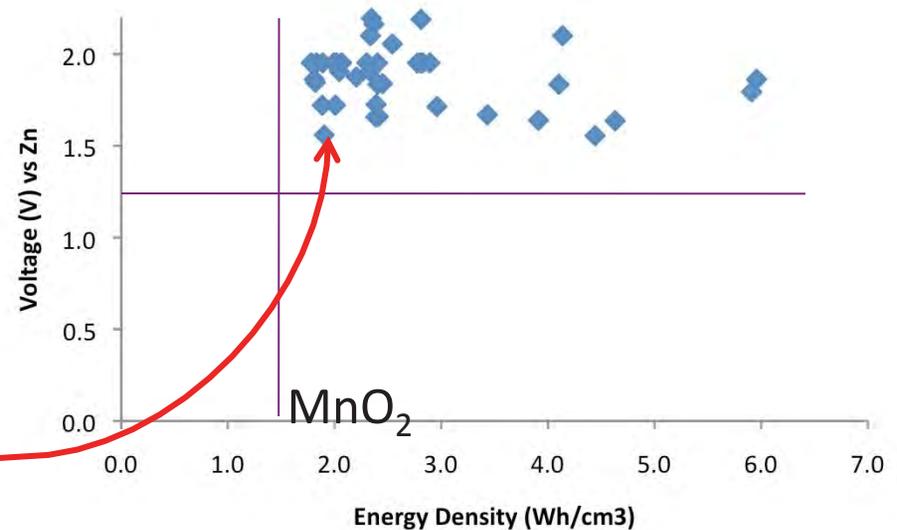
> 1500 compounds

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



≈ 200 compounds

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



(53) United States Patent	(56) Patent No.:	US 7,972,726 B2
Eylem et al.	(45) Date of Patent:	Jul. 5, 2011
(54) PRIMARY ALKALINE BATTERY CONTAINING BISMUTH METAL OXIDE	2,415,607 A	12/1908 Marlin, II
(75) Inventors: Cahn Eylem, Billingham, MA (US); Paul A. Christian, Norwin, MA (US); Yikim Wang, West Roxbury, MA (US); Joseph E. Swanson, IV, Merrimack, NH (US); In Tae Bae, Wrentham, MA (US)	2,415,610 A	7/27/14 Day et al.
(73) Assignor: The Gillette Company, Boston, MA (US)	4,005,226 A	12/17/74 Johnson et al.
(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted pursuant to 35 U.S.C. 154(b) by 1297 days.	4,113,297 A	8/19/78 Margalit
(21) Appl. No.:	4,174,725 A	6/19/79 Galbraith et al.
(22) Filed:	4,184,019 A	2/10/80 Leland
(23) Prior Publication Data	4,229,509 A	10/1980 Margalit
(24) Foreign Patent Documents	4,273,293 A	11/1980 Leland
(25) Int. Cl.	4,247,610 A	1/1981 Thomson
(26) Int. Cl.	4,009,505 A	2/1982 Leland et al.
(27) Int. Cl.	4,079,247 A	1/1982 Day et al.
(28) Int. Cl.	4,194,207 A	4/1984 Decharge et al.
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(30) Int. Cl.	4,273,293 A	11/1980 Leland
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United States Patent Application Publication

(11) Patent No.: US 2012/022493 A1

(12) Pub. Date: Sep. 15, 2011

(13) PRIMARY ALKALINE BATTERY

(14) Inventors: Paul A. Christian, Norwin, MA (US); Yikim Wang, West Roxbury, MA (US); Joseph E. Swanson, IV, Merrimack, NH (US); In Tae Bae, Wrentham, MA (US); Fan Zhang, Norwalk, CT (US)

(15) Int. Cl. (2010.01): H01M 4/08

(16) Int. Cl. (2010.01): H01M 4/50

(17) Int. Cl. (2010.01): H01M 4/52

(18) Int. Cl. (2010.01): H01M 2/16

(19) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(20) Field of Classification Search: None

(21) Notice: See application file for complete search history.

(22) References Cited

(23) U.S. PATENT DOCUMENTS

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(24) FOREIGN PATENT DOCUMENTS

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(25) OTHER PUBLICATIONS

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(26) ABSTRACT

Primary alkaline batteries containing pentavalent bismuth metal oxides are disclosed.

16 Claims, 11 Drawing Sheets

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(36) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(37) Field of Classification Search: None

(38) Notice: See application file for complete search history.

(39) References Cited

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(52) Int. Cl. (2010.01): H01M 2/16

(53) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(54) Field of Classification Search: None

(55) Notice: See application file for complete search history.

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(68) Int. Cl. (2010.01): H01M 4/52

(69) Int. Cl. (2010.01): H01M 2/16

(70) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(71) Field of Classification Search: None

(72) Notice: See application file for complete search history.

(73) References Cited

(74) U.S. PATENT DOCUMENTS

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(85) Int. Cl. (2010.01): H01M 4/52

(86) Int. Cl. (2010.01): H01M 2/16

(87) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(88) Field of Classification Search: None

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(90) References Cited

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(92) FOREIGN PATENT DOCUMENTS

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(94) ABSTRACT

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(104) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

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(118) Int. Cl. (2010.01): H01M 4/50

(119) Int. Cl. (2010.01): H01M 4/52

(120) Int. Cl. (2010.01): H01M 2/16

(121) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(122) Field of Classification Search: None

(123) Notice: See application file for complete search history.

(124) References Cited

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(126) FOREIGN PATENT DOCUMENTS

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(136) Int. Cl. (2010.01): H01M 4/52

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(151) Int. Cl. (2010.01): H01M 4/08

(152) Int. Cl. (2010.01): H01M 4/50

(153) Int. Cl. (2010.01): H01M 4/52

(154) Int. Cl. (2010.01): H01M 2/16

(155) U.S. Cl. (2010.01): 429/218.4; 429/224; 429/225; 429/219; 429/231.6; 429/231.7; 429/231.8; 429/245

(156) Field of Classification Search: None

(157) Notice: See application file for complete search history.

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(174) Notice: See application file for complete search history.

(175) References Cited

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Primary alkaline batteries containing pentavalent bismuth metal oxides are disclosed.

16 Claims, 11 Drawing Sheets

(180) Patent Application Publication

(181) Pub. No.: US 2012/022493 A1

(182) Pub. Date: Sep. 15, 2011

(183) PRIMARY ALKALINE BATTERY

(184) Inventors:

ICSD

Other experimental databases

User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)



Analysis

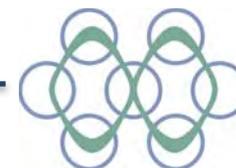
Web apps

Materials API

Workflow Manager

Post-processing and error-checking

Supercomputing Resources



ICSD

Other experimental databases

User submissions

Input processing & transformations

pymatgen

- Robust materials analysis



Custodian

- Self-healing error recovery



Fireworks

- Smart workflow management



StructureNotationalLanguage (SNL)



Analysis

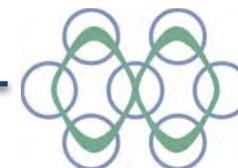
Web apps

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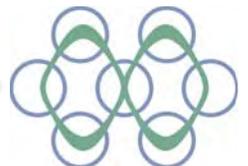
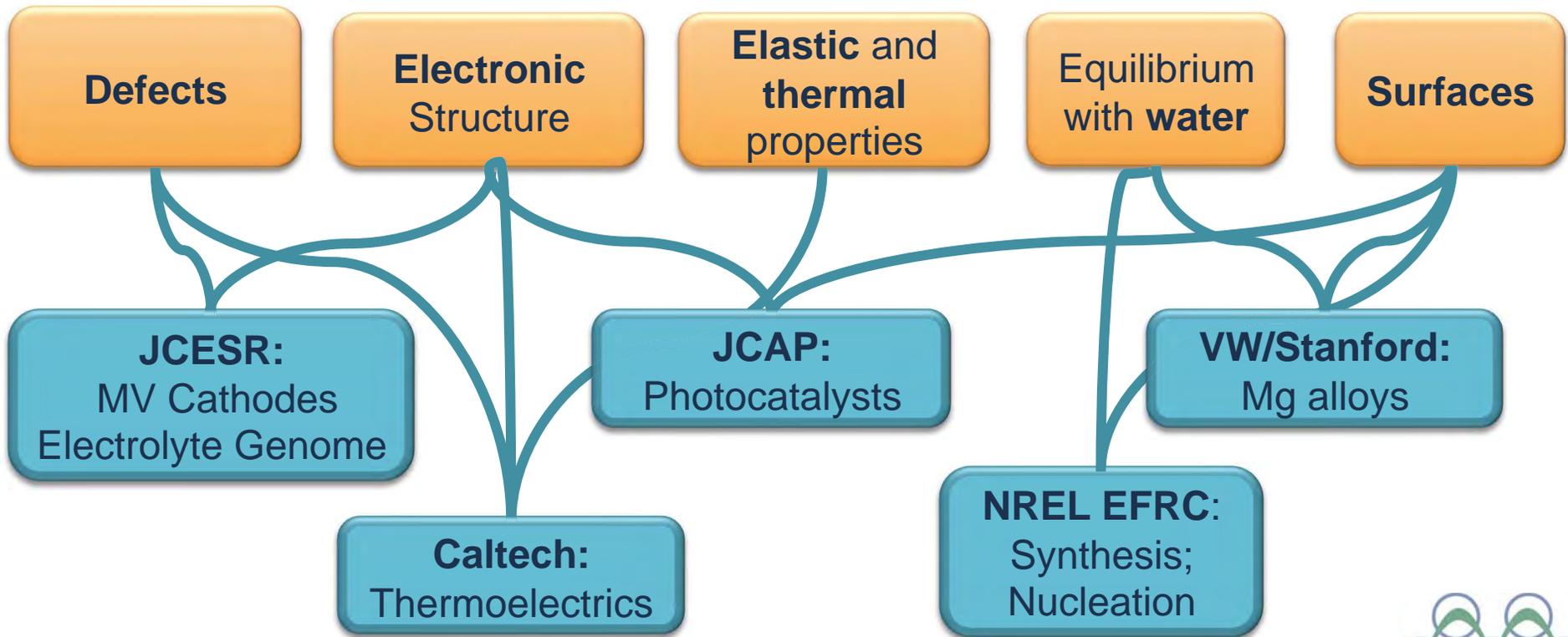


Leveraging the MP Infrastructure

pymatgen

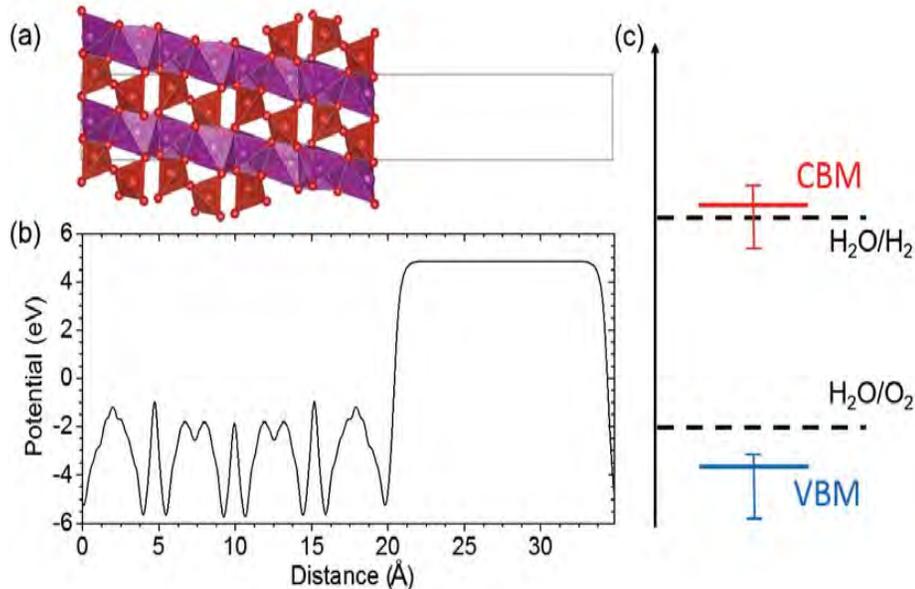
Fireworks

Custodian

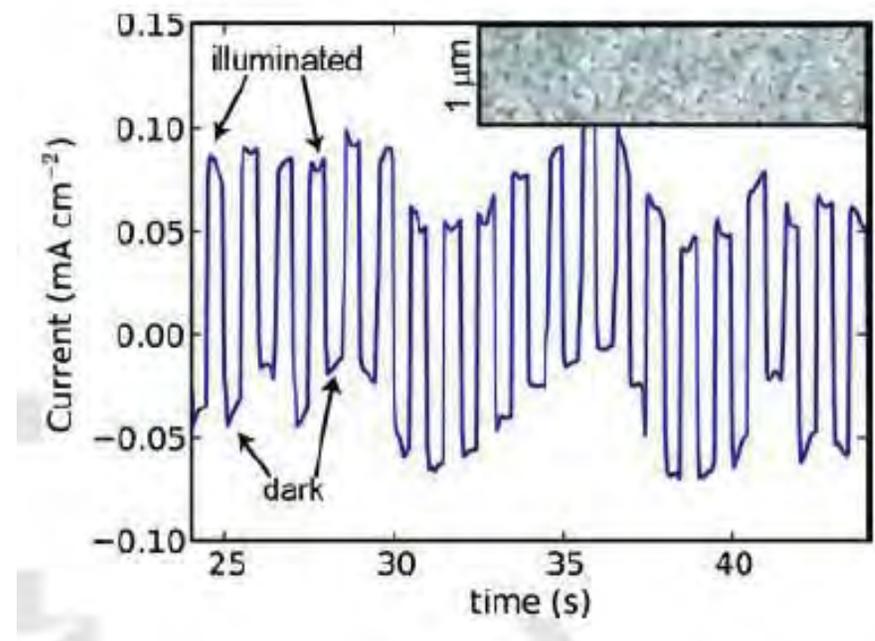


Novel corrosion-resistant oxide lightabsorber found: $\beta\text{-Mn}_2\text{V}_2\text{O}_7$

Collaboration with JCAP; material synthesis and testing by John Gregoire



Predicted near optimal band edge energies for hydrogen evolution reaction and oxygen evolution reaction; band gap of 1.8 eV.



385-nm illumination in 0.1 M NaOH (aq) with 50 \AA 10^{-3} M $[\text{Fe}(\text{CN})_6]^{3-/4-}$ redox couple.

Evidence of excellent photoabsorbing capability and corrosion resistance

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.



Home

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

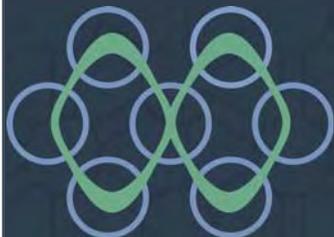
November 3, 2011 - 1:05pm

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,



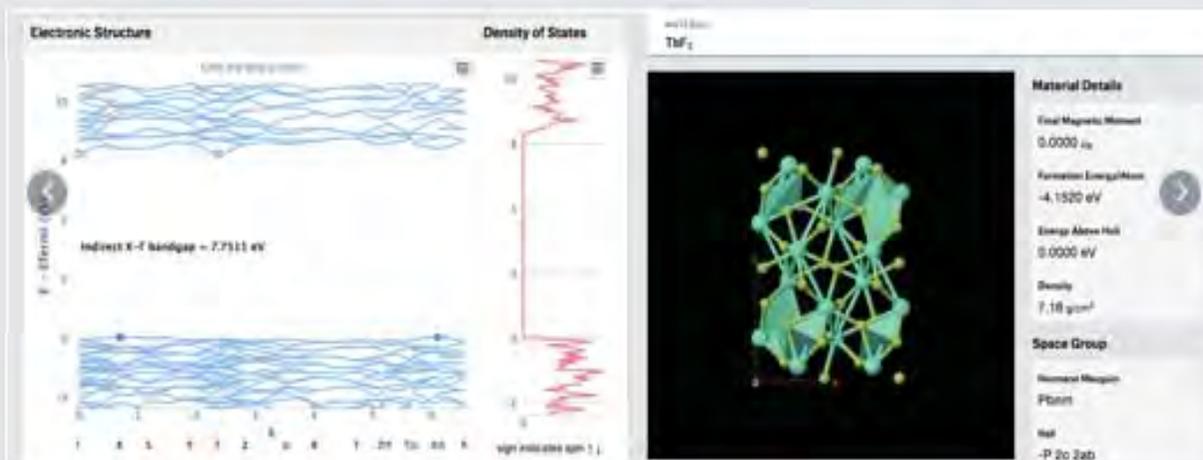


The Materials Project

Harnessing the power of supercomputing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Learn more](#)

[Sign In or Register](#) to start using



EXPLORE MATERIALS

Search for materials information by chemistry, composition, or property

EXPLORE BATTERIES

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

VISUALIZE STABILITY

Generate phase and pourbaix diagrams to find stable phases and study reaction pathways.

INVENT STRUCTURES

Design new compounds with our structure editor and substitution algorithms

CALCULATE

Calculate the enthalpy of 10,000+ reactions and compare with experimental values

+40,000

+28,000

+2,000

+18,000

Database Statistics

58097

COMPOUNDS

28340

BANDSTRUCTURES

2185

LI INTERCALATION ELECTRODES

18226

LI CONVERSION ELECTRODES

MP Apps

Electronic structure

Structure

Phase diagrams

Li-ion properties

Aqueous stability

Design Center

Porous Nanomaterials

...

The screenshot displays the Materials Project (MP) web interface. At the top, there is a search bar with the text "Search for materials information by chemistry, composition, or property". Below the search bar, the "Explore Materials" section shows a search for "Fe Li S". The periodic table is visible, with elements Fe, Li, and S highlighted. Below the periodic table, there are buttons for "Nelements" and "Elements". The search results are displayed in a table with columns: Materials Id, Formula, Spacegroup, Formation Energy (eV), E Above Hull (eV), Band Gap (eV), Nsites, Density (gm/cc), and Volume. The table shows 10 entries, with the first entry being mp-756173 with formula Li_5FeS_4 and spacegroup Pmmn. To the right of the table, there is a sidebar with various filters and controls, including "Band Gap (eV)", "Energy Above Hull", "Formation Energy", "# unit cell sites", "Density", "Volume", "Crystal Systems", "Spacegroup Number", "Spacegroup Symbol", and "Has bandstructure".

Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	Nsites	Density (gm/cc)	Volume
mp-756173	Li_5FeS_4	Pmmn	-1.069	0.062	0.014	20	1.99	365.138
mp-776781	Li_5FeS_4	Pbca	-1.067	0.064	0.022	80	1.991	1459.637
mp-753585	$\text{Li}_{14}\text{Fe}_2\text{S}_9$	$\bar{P}3$	-1.136	0.071	0	25	1.944	424.896
mp-754210	Li_8FeS_4	$P4_2/nmc$	-1.099	0.09	0.022	22	2.023	370.556
mp-776797	Li_5FeS_4	Pbca	-1.033	0.098	0.022	80	2.076	1400.237
mp-768400	Li_8FeS_6	$P6_3cm$	-1.07	0.103	0.021	30	1.866	540.747
mp-756094	LiFeS_2	$\bar{P}3m1$	-0.704	0.116	0	4	3.652	57.712
mp-756489	Li_8FeS_4	$P6_3mc$	-1.072	0.117	0	22	2.106	356.072
mp-756187	Li_2FeS_2	$P4_2/mcm$	-0.886	0.124	0.263	10	2.346	189.512
mp-768214	Li_3FeS_3	$P2_1/c$	-0.917	0.126	0.008	28	2.422	474.135





Battery Explorer

EXPLORE MATERIALS: Search for materials information by chemistry, Cell composition, or property

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

VISUALIZE STABILITY: Generate phase and Pourbaix diagrams to find stable phases and study reaction pathways.

INVENT STRUCTURES: Design new compounds with our structure editor and substitution algorithms.

CALCULATE: Calculate the enthalpy of 10,000+ reactions and compare with experimental values.

Database Statistics

54808 8748 25541 2091 16128

COMPOUNDS POURBAIX DIAGRAMS BANDSTRUCTURES LI INTERCALATION ELECTRODES LI CONVERSION ELECTRODES



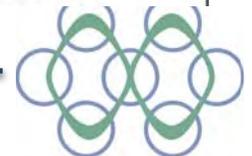
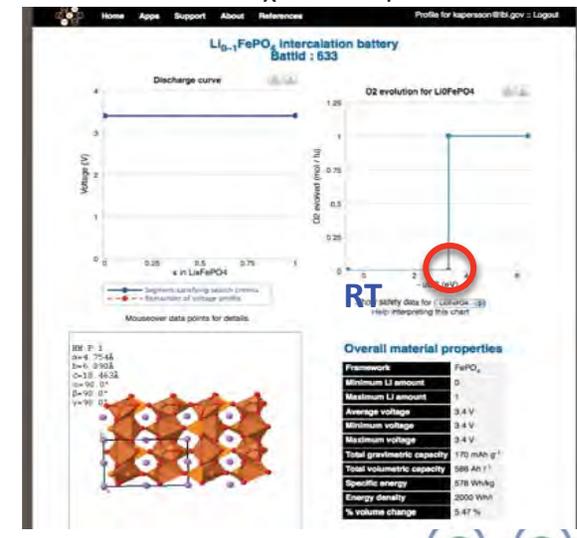
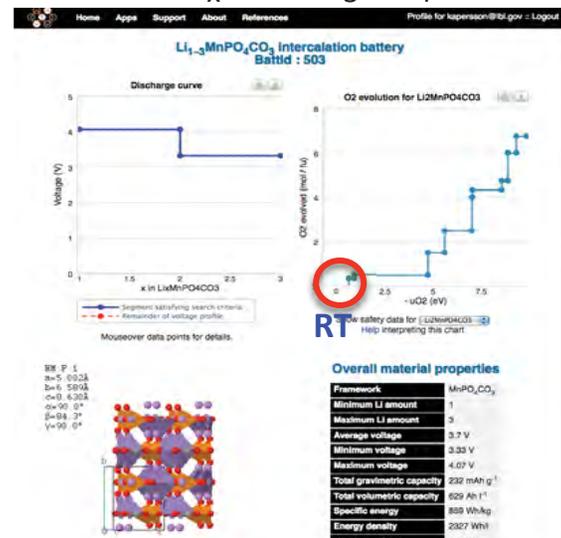
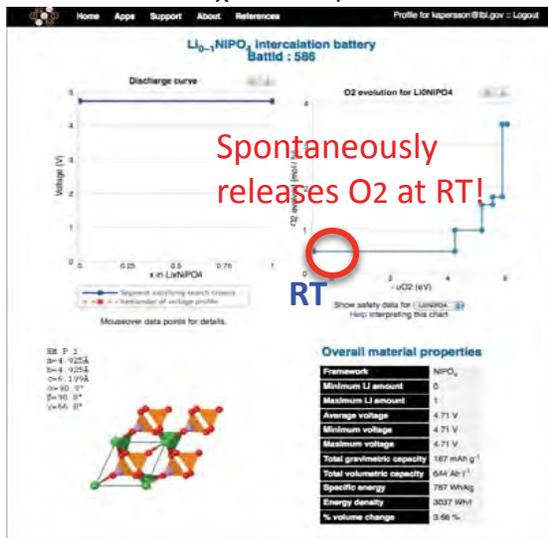
Explore Batteries

LiFePO₄

Reduced Cell Formula	Spacegroup	Average Voltage	Capacity Grav	Capacity Vol	Specific E Wh/kg	E Density Wh/l	Stability Charge	Stability Discharge
Al _{0.33} - _{0.33} FeO ₄	Fd3m	2.98	308	1272	887	2657	0.18	0
Zn ₀ - _{0.33} FeO ₄	Fd3m	2.94	222	1140	565	2846	0.21	0
Ca ₀ - _{0.33} FeO ₄	Pnmb	4.29	248	1152	1065	4838	0.29	0
Mg ₀ - _{0.33} FeO ₄	Fd3m	3.8	268	1135	1019	4314	0.21	0
Li _{0.5} - _{0.5} FeO ₄	C2	4.02	87	382	349	1575	0.17	0
Li _{0.5} - _{0.5} FeO ₄	C2	4.11	208	810	848	3331	0.12	0
Li _{0.5} - _{0.5} FeO ₄	I4/mmd	3.93	263	1192	1112	4092	0.14	0
Li _{0.75} - _{0.75} FeO ₄	Pcab	3.77	217	835	818	3084	0.12	0

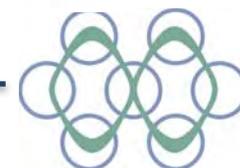
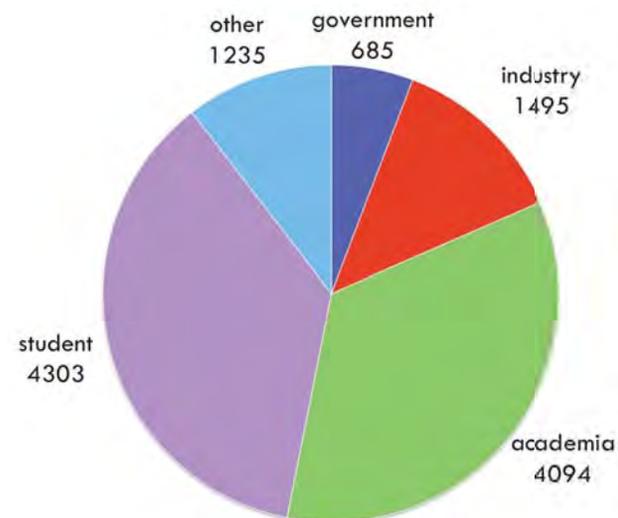
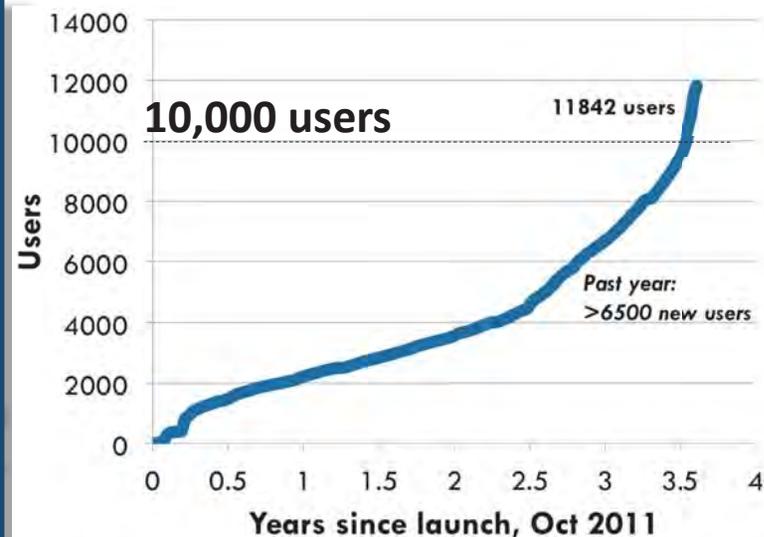
safer

safer

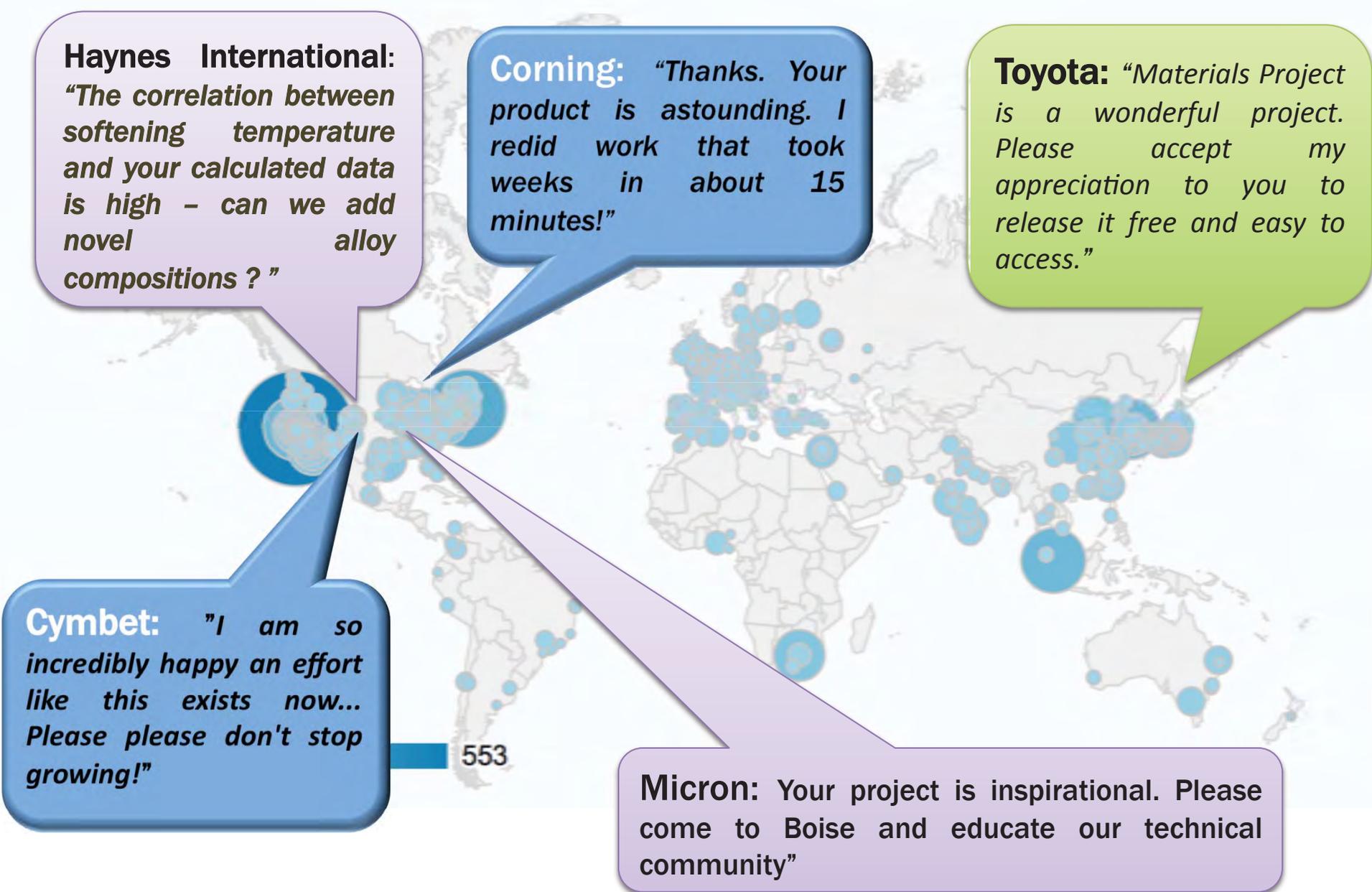


The Materials Project Impact

- ❑ **Launched online Oct 2011**
- ❑ **Users:** ~12,000 registered
- ❑ 8 million records downloaded through API
- ❑ **Active Partnerships:** JCAP, JCESR, NREL-EFRC, Minnesota MGI Center on Porous Materials; U Leuven, U Wisconsin-Madison (MaterialsHub), EPFL, ...
- ❑ **Course-ware :** UC San Diego, UC Davis, UC Irvine, U Michigan, Johns-Hopkins, Cornell, MIT, UC Santa Barbara...
- ❑ **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, ...



World-Wide Resource

A world map with several blue circles of varying sizes indicating global locations. Five callout boxes are connected to specific locations on the map by lines. The callouts contain testimonials and questions from various international organizations.

Haynes International:
"The correlation between softening temperature and your calculated data is high - can we add novel alloy compositions?"

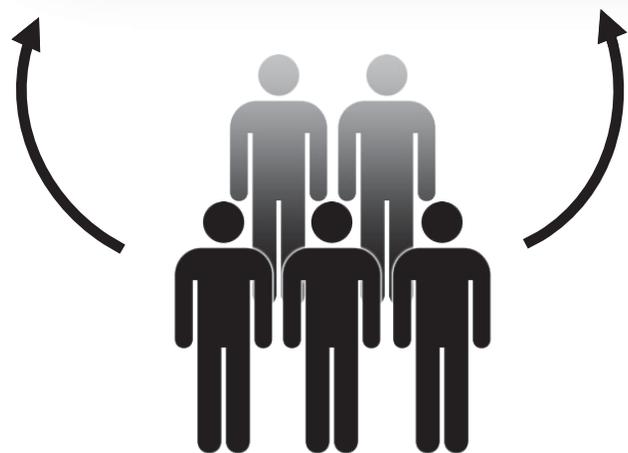
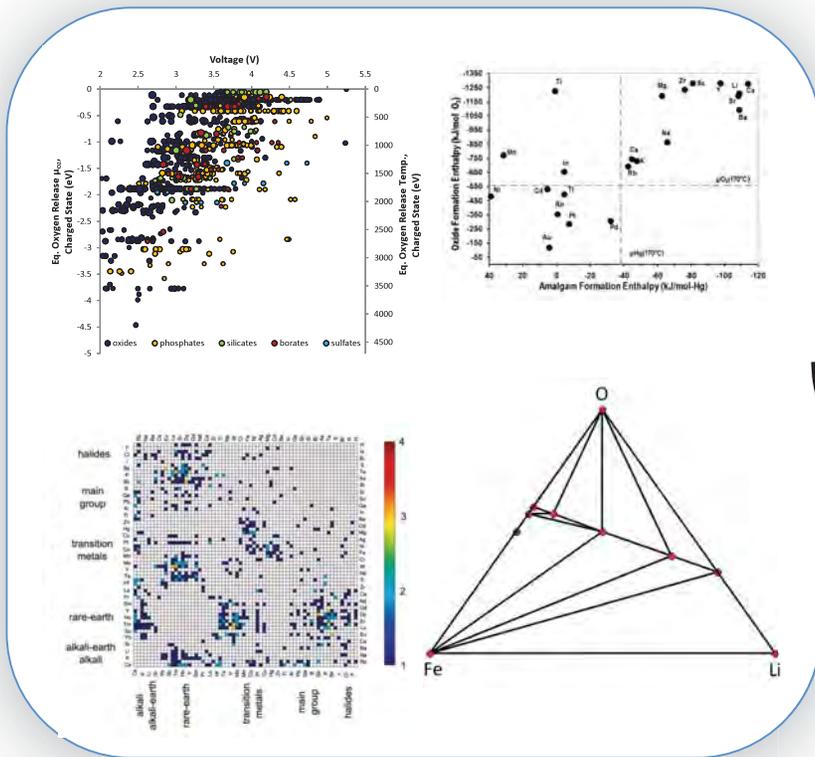
Corning: *"Thanks. Your product is astounding. I redid work that took weeks in about 15 minutes!"*

Toyota: *"Materials Project is a wonderful project. Please accept my appreciation to you to release it free and easy to access."*

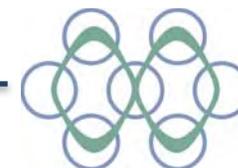
Cymbet: *"I am so incredibly happy an effort like this exists now... Please please don't stop growing!"*

553

Micron: Your project is inspirational. Please come to Boise and educate our technical community"



... towards a materials genome



Thanks to BES DOE and NERSC