Ab initio approaches to understanding, optimizing and discovering energy storage electrode materials

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Outline

- **How can computations help ?**
  - — What are computable properties?
  - — Application examples:
    - *Rate-limitations in graphite*
    - *Tuning particle morphology in $LiFePO_3$*
    - *Explaining the hysteresis in $LiFeF_3$ conversion reactions*
- **Discovering New Intercalation Cathodes**
  - — For Li-ion batteries
  - — Pellion Technologies: Rechargable Mg batteries
- **Towards the Materials Genome**
  - — Accelerated materials discovery for energy storage applications

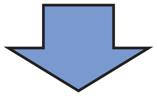
Electrode Materials from First Principles

The equations describing the basic physical interactions of matter are known

$$H\Psi = E\Psi$$

$$P_i = \frac{\exp(-\beta E_i)}{Z}$$

Quantum mechanics + statistical mechanics

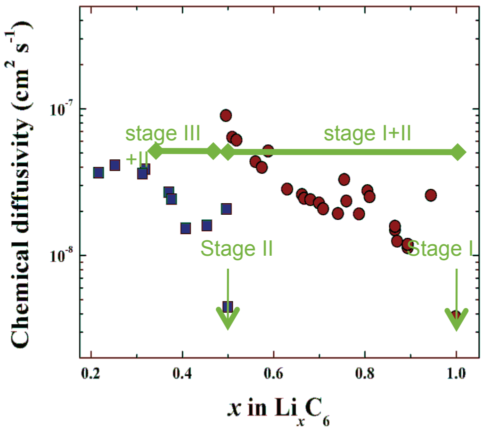


We can predict materials properties from assuming/ knowing where the atoms are….

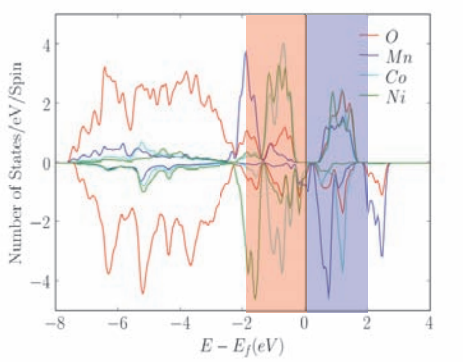
Examples: Computable Material's Properties

Ionic diffusion

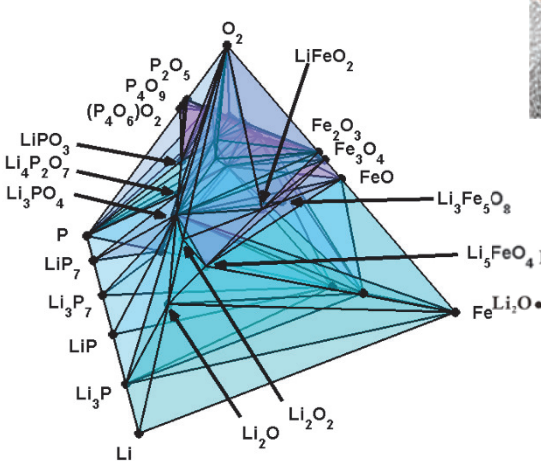
Exp: D_{Li} = ~10^{-6} $cm^2\ s^{-1}$



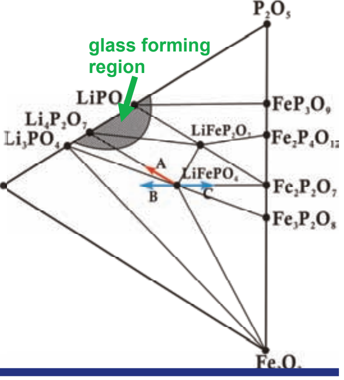
Electronic State



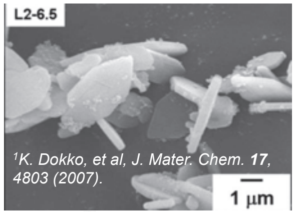
Phase diagrams



Kayyar, Qian & Luo, Appl. Phys. Lett. 95: 221905 (2009)

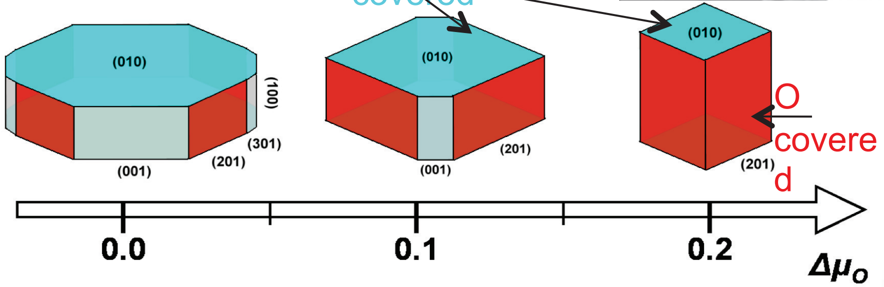


Particle morphology

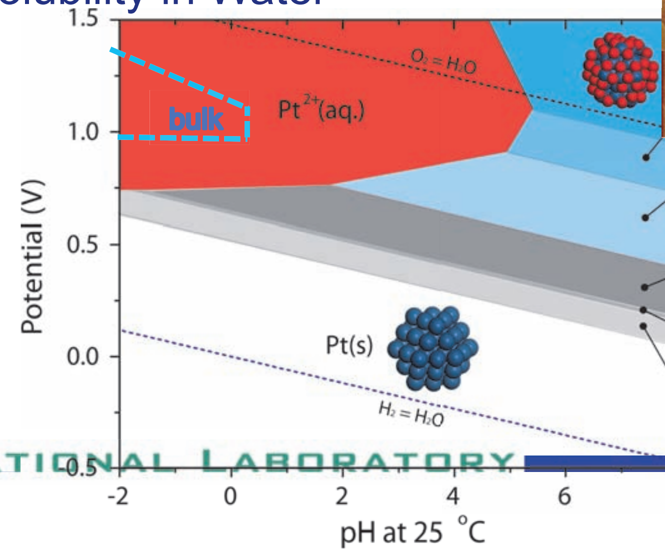


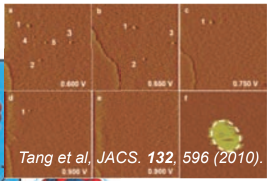
[1]K. Dokko, et al, *J. Mater. Chem.* **17**, 4803 (2007).

H_2O covered



Solubility in Water





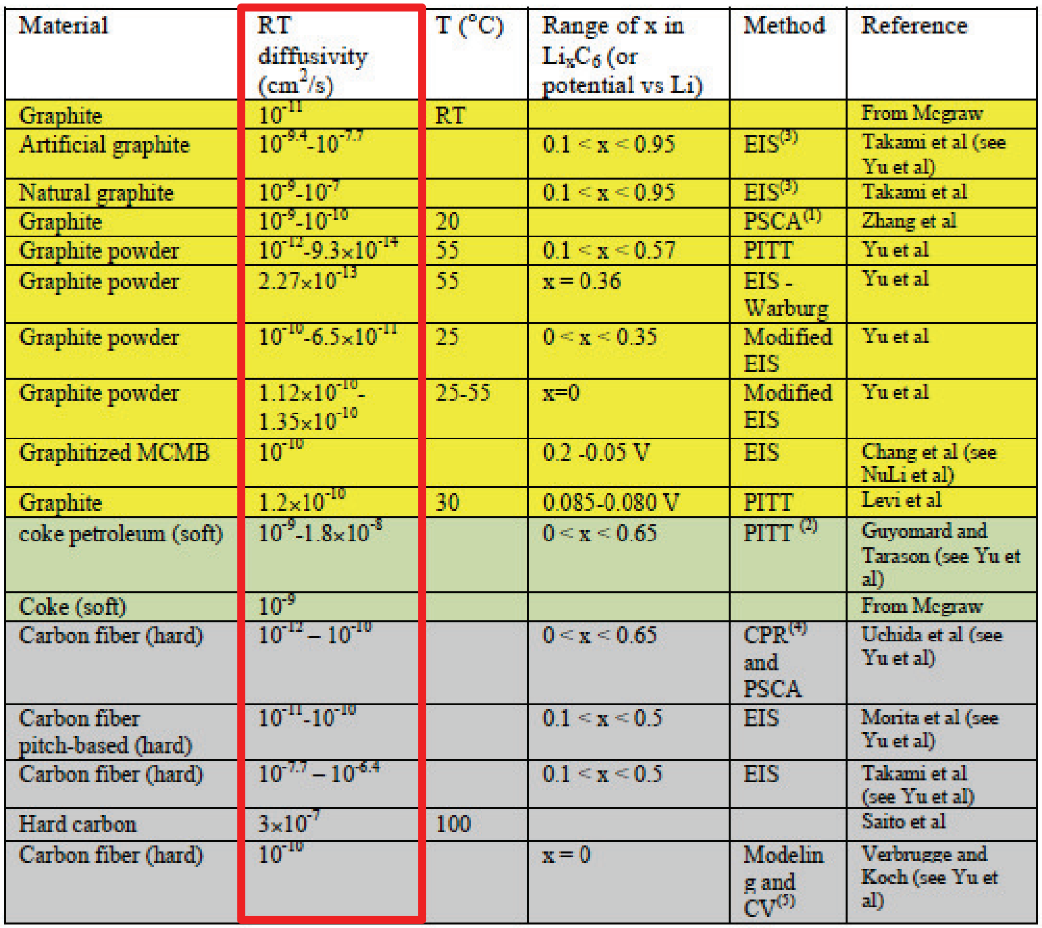
Tang et al. *JACS*. **132**, 596 (2010).

Rate limitations in graphite

Exp facts of Li-graphite

- At low temperature rate capability of carbon anode deteriorates rapidly

- Li diffusion measurements in graphite span $10^{-7} – 10^{-12}$ cm^2/s



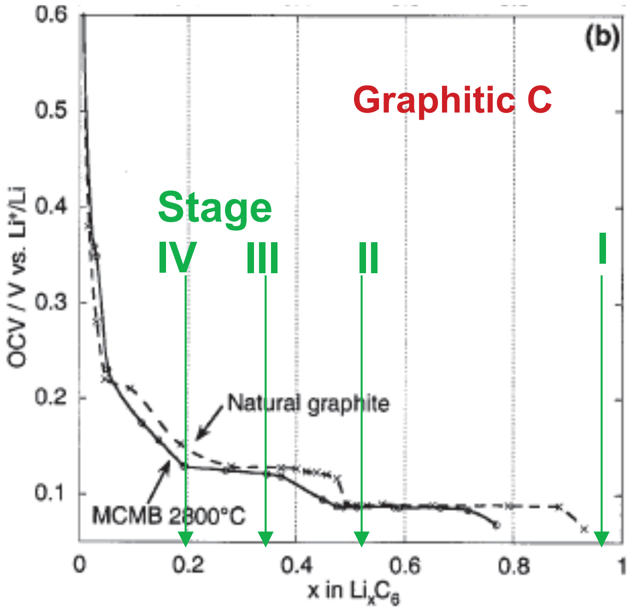
Material	RT diffusivity (cm^2/s)	T (°C)	Range of x in Li_xC_6 (or potential vs Li)	Method	Reference
Graphite	10^{-11}	RT			From Mcgraw
Artificial graphite	$10^{-9.4}$-$10^{-7.7}$		$0.1 < x < 0.95$	EIS$^{(3)}$	Takami et al (see Yu et al)
Natural graphite	10^{-9}-10^{-7}		$0.1 < x < 0.95$	EIS$^{(3)}$	Takami et al
Graphite	10^{-9}-10^{-10}	20		PSCA$^{(1)}$	Zhang et al
Graphite powder	10^{-12}-9.3×10^{-14}	55	$0.1 < x < 0.57$	PITT	Yu et al
Graphite powder	2.27×10^{-13}	55	$x = 0.36$	EIS - Warburg	Yu et al
Graphite powder	10^{-10}-6.5×10^{-11}	25	$0 < x < 0.35$	Modified EIS	Yu et al
Graphite powder	1.12×10^{-10}-1.35×10^{-10}	25-55	$x=0$	Modified EIS	Yu et al
Graphitized MCMB	10^{-10}		0.2 -0.05 V	EIS	Chang et al (see NuLi et al)
Graphite	1.2×10^{-10}	30	0.085-0.080 V	PITT	Levi et al
coke petroleum (soft)	10^{-9}-1.8×10^{-8}		$0 < x < 0.65$	PITT $^{(2)}$	Guyomard and Tarason (see Yu et al)
Coke (soft)	10^{-9}				From Mcgraw
Carbon fiber (hard)	$10^{-12} – 10^{-10}$		$0 < x < 0.65$	CPR$^{(4)}$ and PSCA	Uchida et al (see Yu et al)
Carbon fiber pitch-based (hard)	10^{-11}-10^{-10}		$0.1 < x < 0.5$	EIS	Morita et al (see Yu et al)
Carbon fiber (hard)	$10^{-7.7} – 10^{-6.4}$		$0.1 < x < 0.5$	EIS	Takami et al (see Yu et al)
Hard carbon	3×10^{-7}	100			Saito et al
Carbon fiber (hard)	10^{-10}		$x = 0$	Modeling and CV$^{(5)}$	Verbrugge and Koch (see Yu et al)

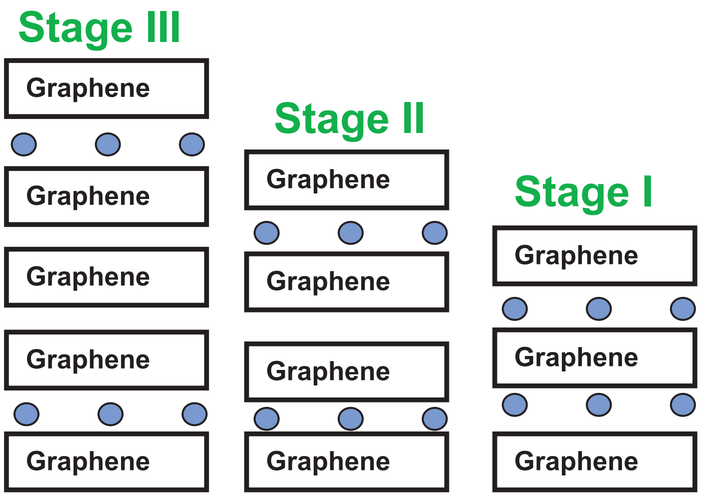
Can we find out what the Li mobility in graphite really is using first principles ?

Exp facts of Li-graphite

Graphite intercalates in stages

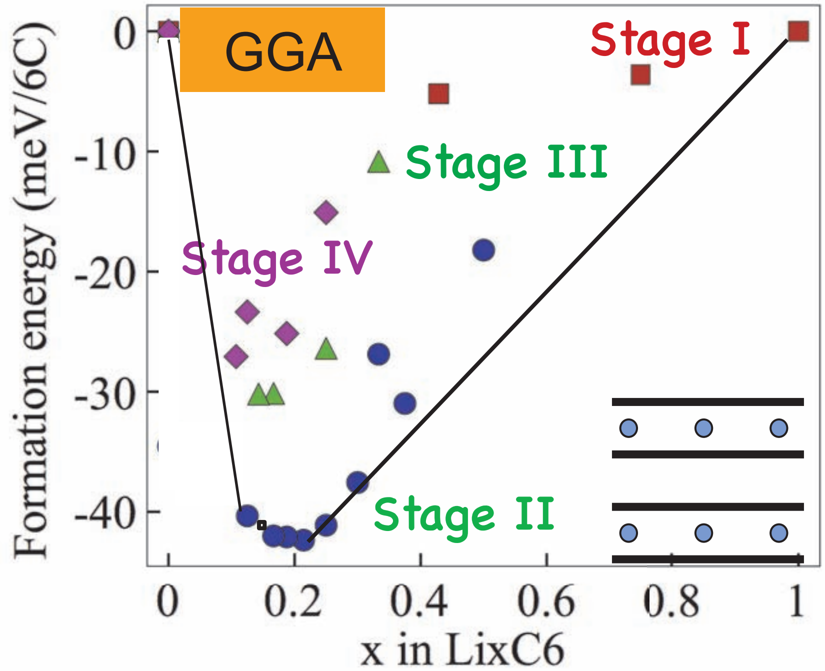
Reynier, et. al. JES 151, A422, 2004

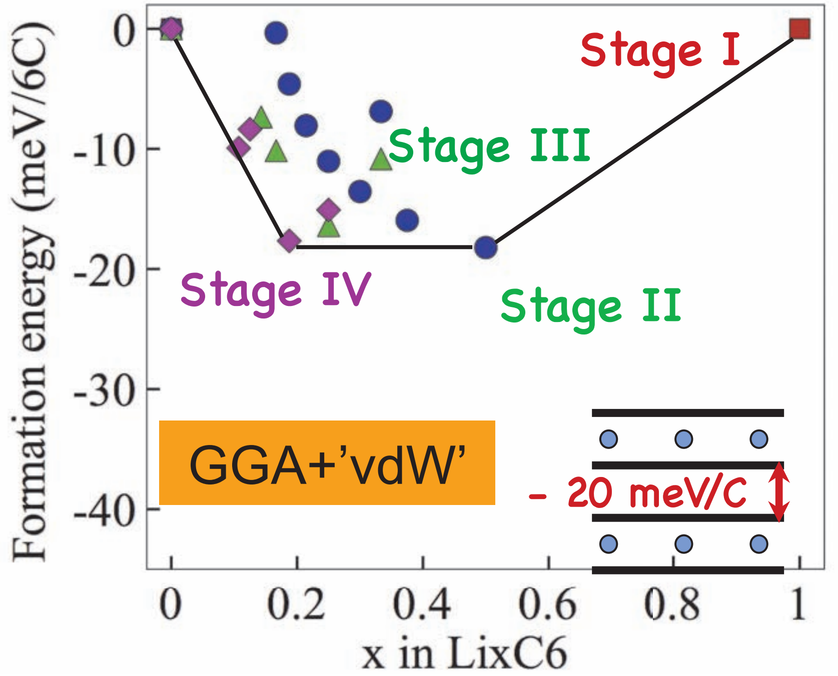




All possible Li-graphite decorations

Compound formation energies ⇨ voltage = - dE/dx

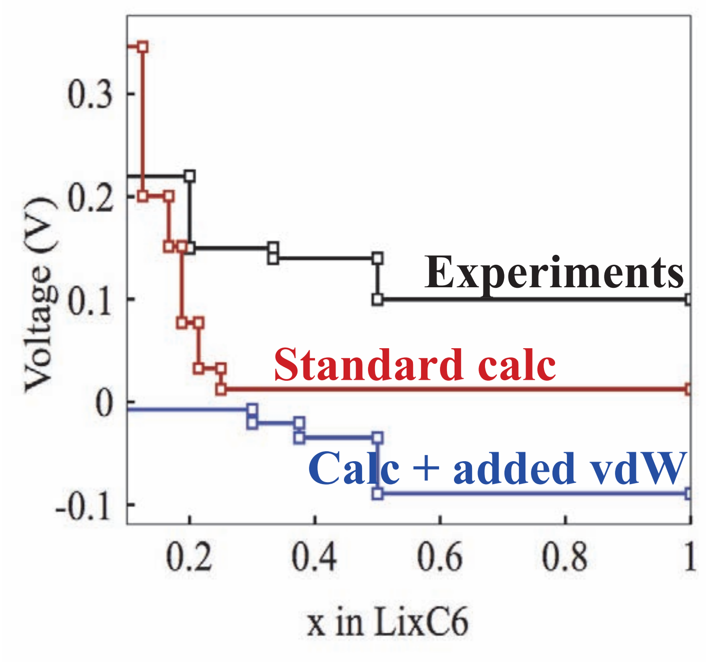




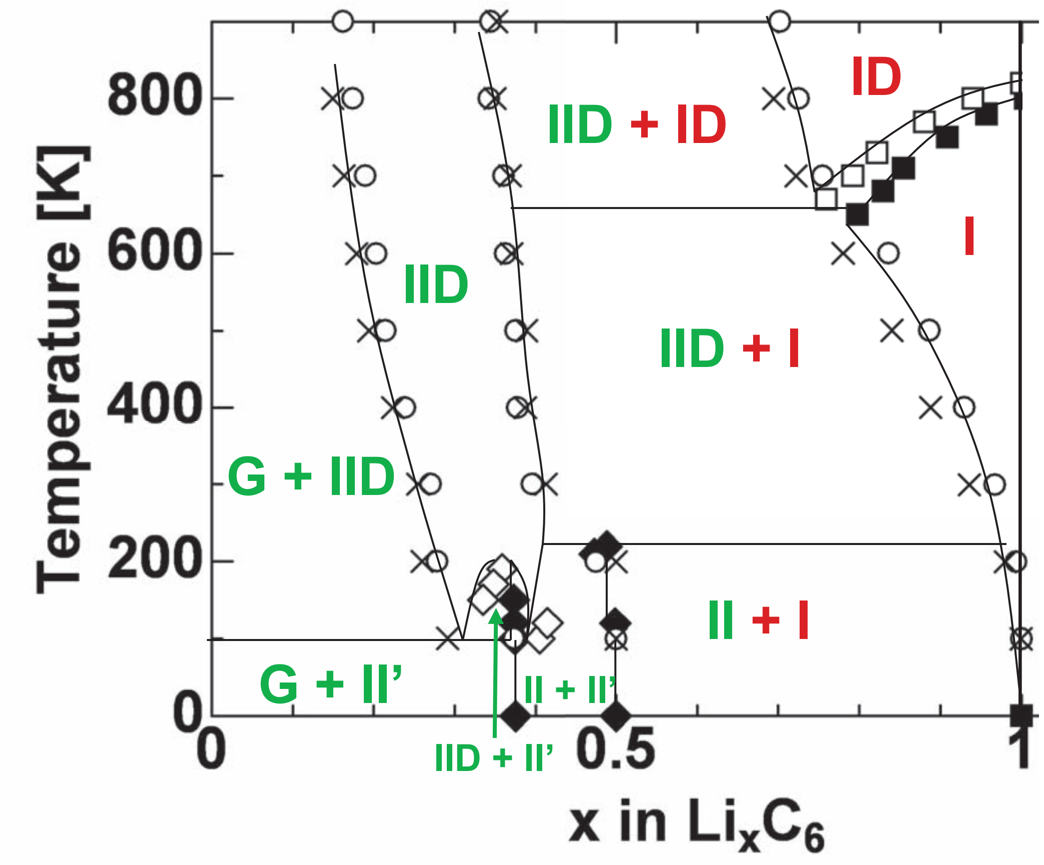
Correct staging is obtained by adding vdW to empty layers

The right Li-C interactions

Correct **form** of voltage curve

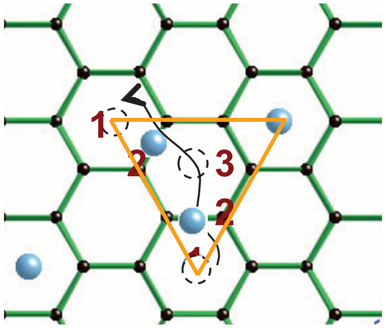


Correct stage I and stage II **order-disorder** temperatures



Predicting how fast Li moves in graphite

Li hop (from above)



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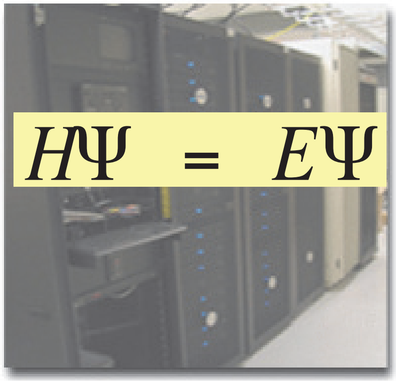
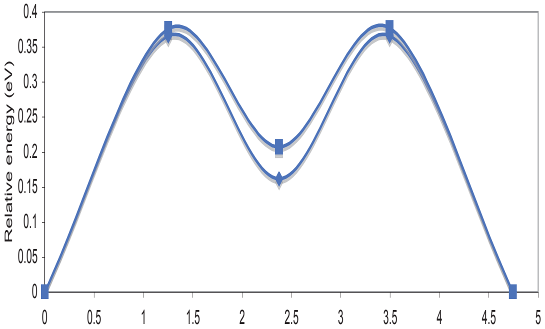


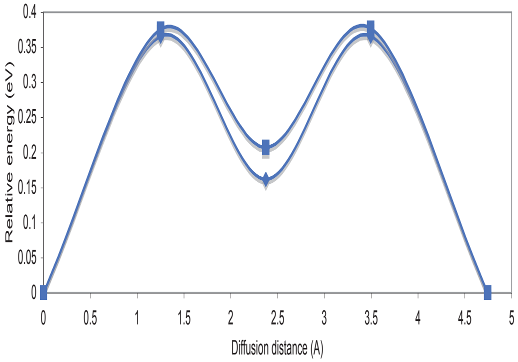
$$H\Psi = E\Psi$$

Li hop activation barriers



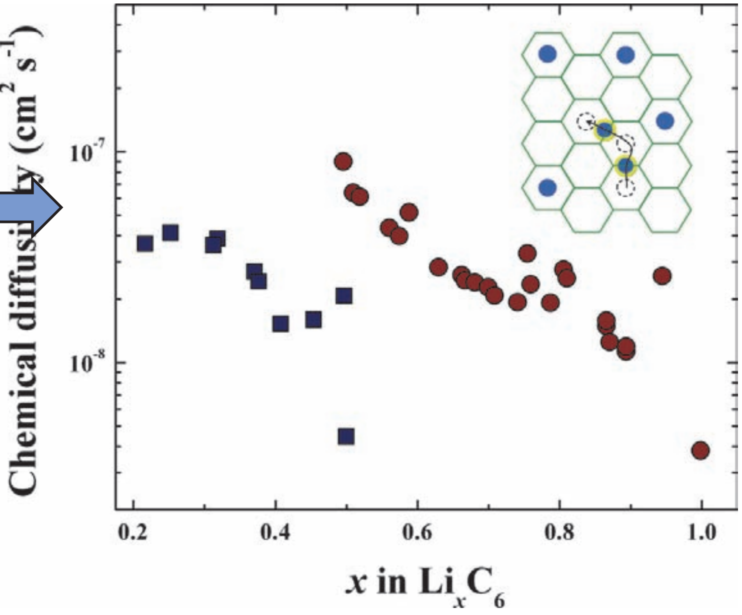
Li diffusivity in graphite

Li hop activation barriers



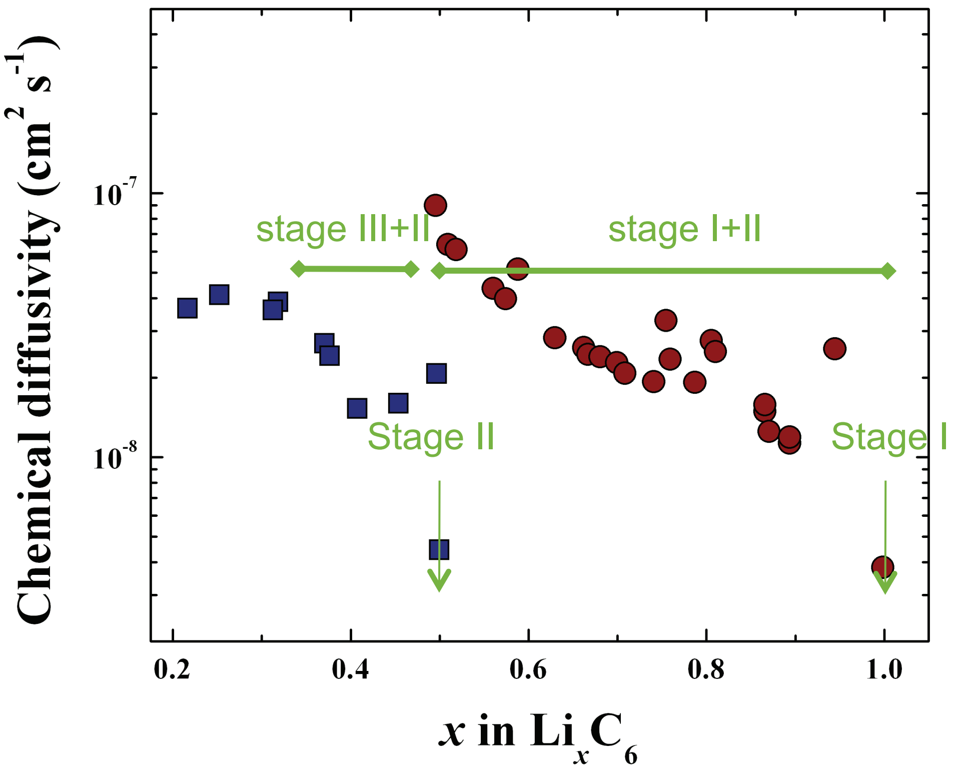
+

$$P_i = \frac{\exp(-\beta E_i)}{Z}$$

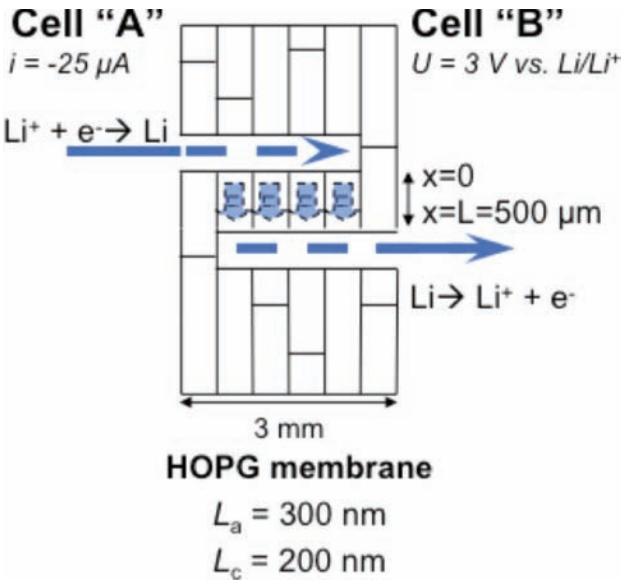


Surprising Results

Calc



Exp



$D = 4.4 \times 10^{-6} \pm 0.1 \times 10^{-6}$ cm^2 s^{-1}

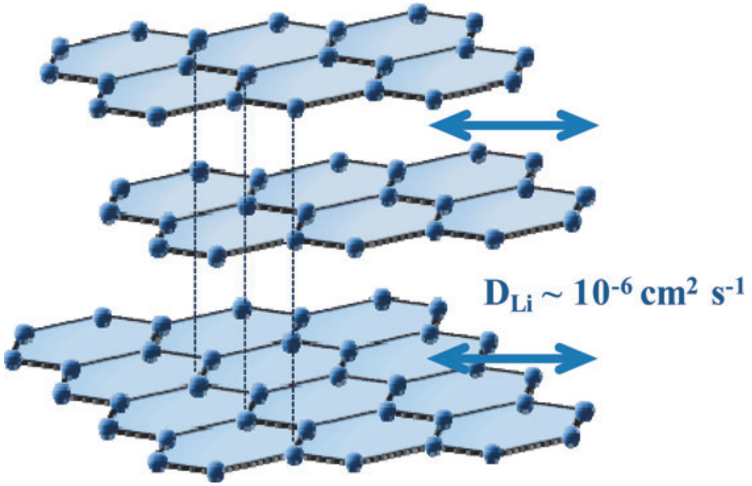
[1] K. Persson, V. A. Sethuraman, L. J. Hardwick, Y. Hinuma, Y. S. Meng, A. van der Ven, V. Srinivasan, R. Kostecki and G. Ceder, J Phys Chem Lett 1176–1180, 2010.

K. Persson, Y. Hinuma, Y. S. Meng, A. Van der Ven, and G. Ceder, *Thermodynamic and Kinetic Properties of the Li – Graphite System from First-Principles Calculations*, Physical Review B 82, 125416, 2010.

Carbon can be super fast!

Computations predicted in-plane Li diffusivity of ~10^{-7} cm^2/s

Charge/discharge 45 nm graphite particle in **0.2 ms**!



Same month experiments published ~1000C rate in single carbon particle

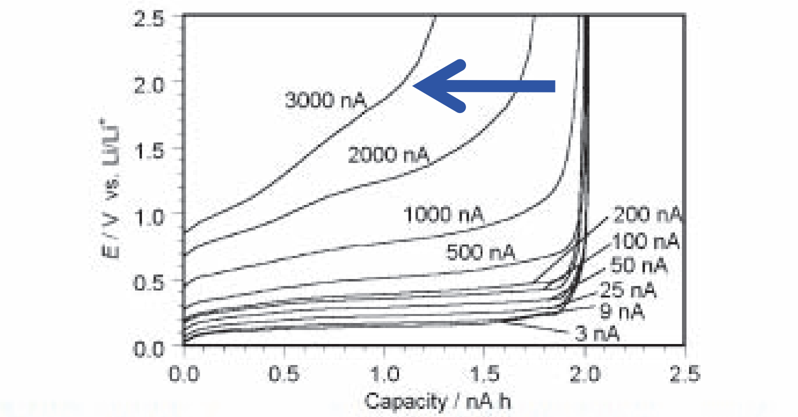


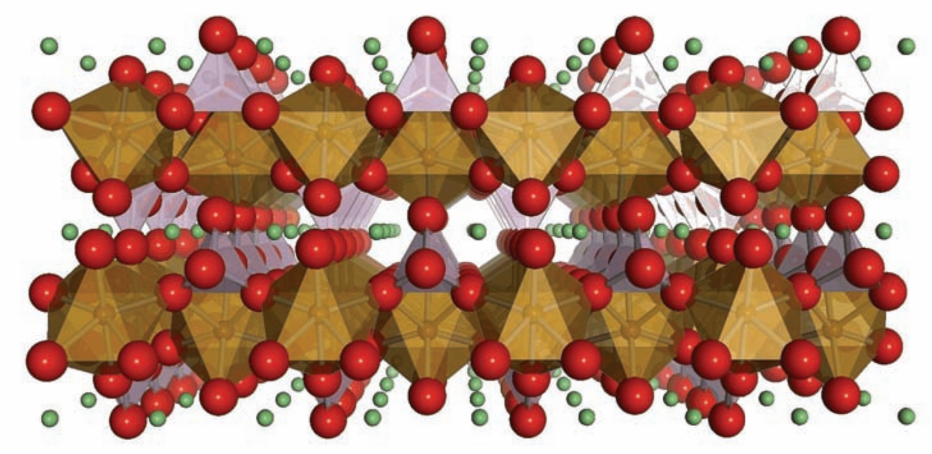
Figure 3. Discharge curves of a single MCMB particle (diameter: 18 μm) measured at various currents. Prior to each discharge, the MCMB particle was fully lithiated by charging at a low current of 3 nA.

Dokko et al, J Phys Chem C, 114, 18, 2010

These studies show that 'normal' ***low rate*** *behavior of carbon anodes is* ***not due to graphite***
We may be able to engineer the electrodes to be better!

Tuning the particle morphology of $LiFePO_4$

Motivation: morphology optimization of $LiFePO_4$



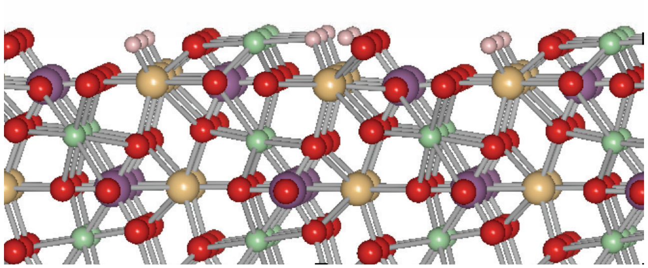
- $LiFePO_4$ performance very dependent on particle size and shape
- Morphology dependent on facet growth-rate, strain, temperature etc[1]
- Maximize *ac* facet for optimized Li intercalation into particle

Can we understand particle morphology development through first-principles calculations and tune it by changing water conditions?

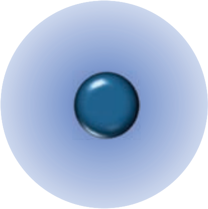
[1] Chen, Song and Richardson, ESSL 9, A295 (2006).

How do we compute particle shape?

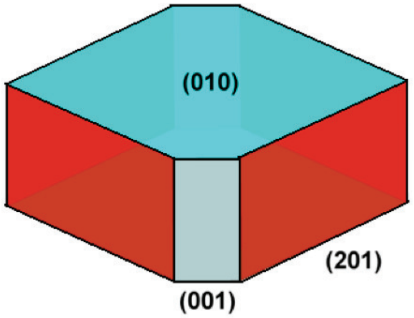
How can we study electrode material surfaces and relevant processes with ab initio modeling?



Stable surfaces w absorbent species



Dissolution



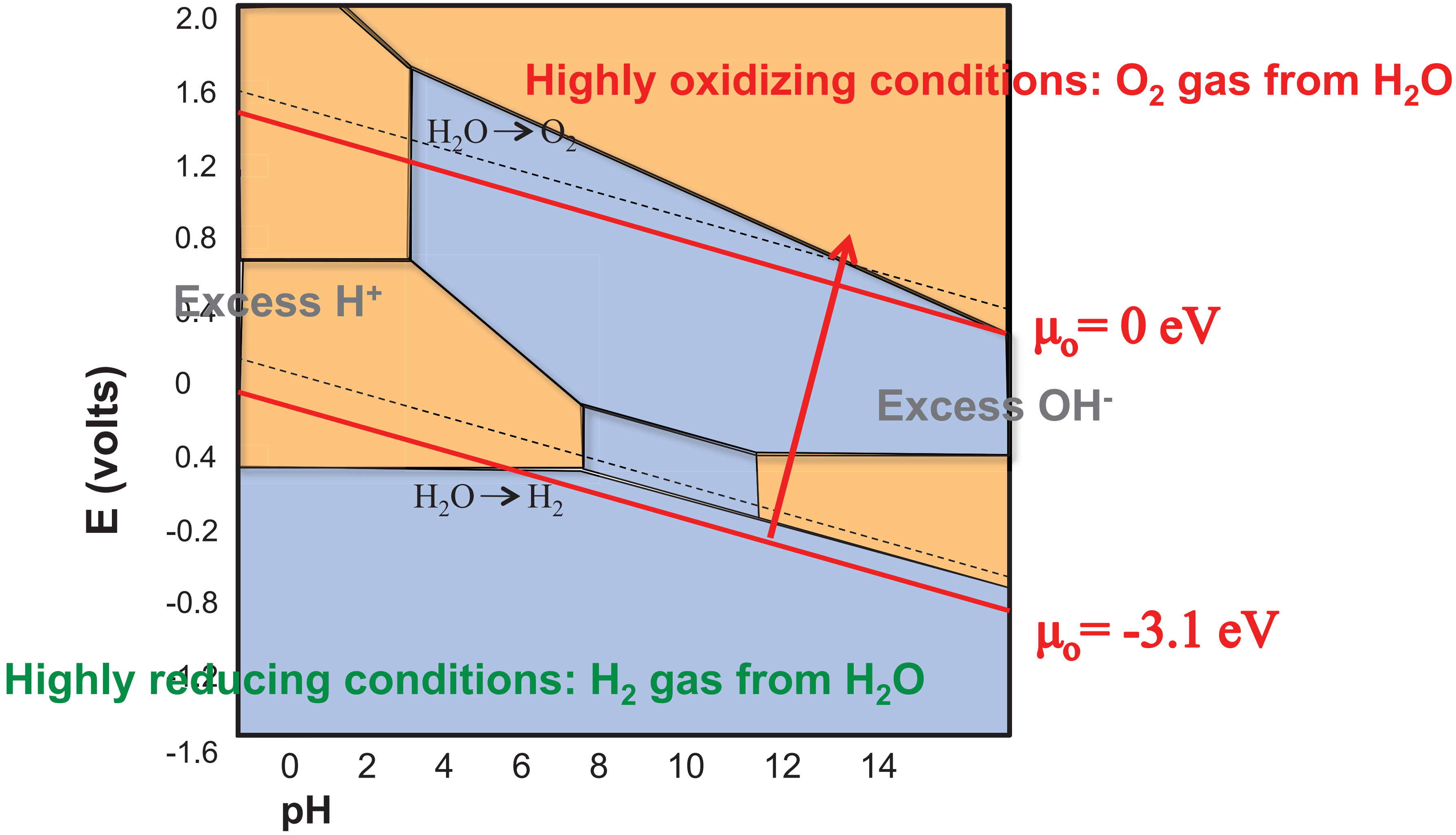
Particle morphology

Ability to predict

- **Preferred absorbed species** on different surface facets
- **Stable surface facets** in equilibrium with different aqueous environments including dissolution
- **Particle morphology** as function of aqueous environment

Water map: Pourbaix diagram

We consider all reactions to be in equilibrium with water



Highly oxidizing conditions: O_2 gas from H_2O

$\mu_o = 0$ eV

$\mu_o = -3.1$ eV

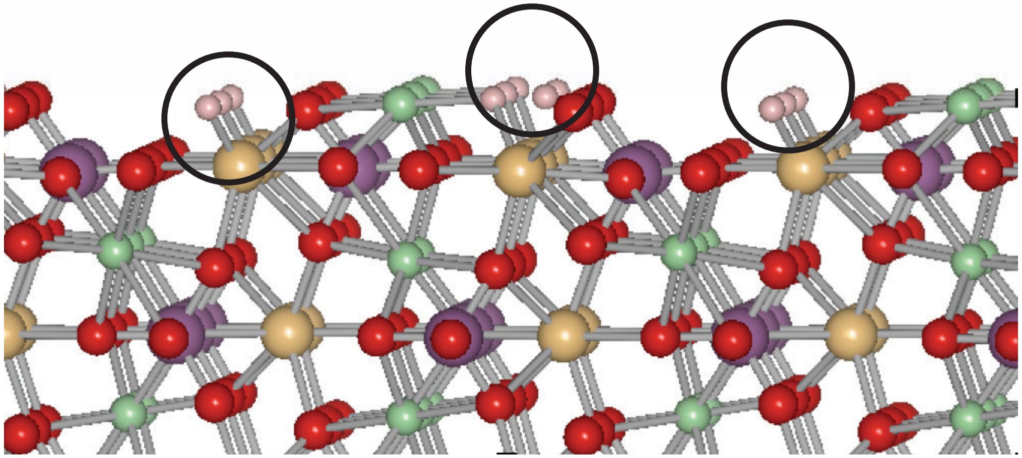
Highly reducing conditions: H_2 gas from H_2O

Surfaces + Absorbants

Stable surface facets are calculated

Surface energies with H, O, OH and H_2O termination for all relevant crystal facets

H_2O / O^{2-} / H^+ / OH^- ?

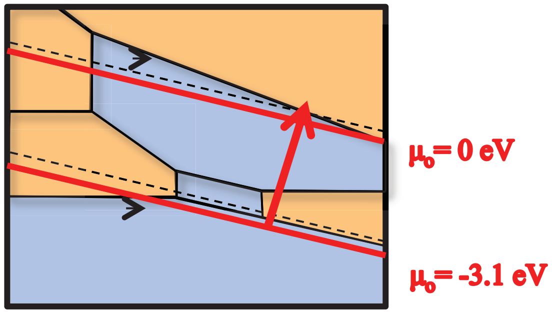


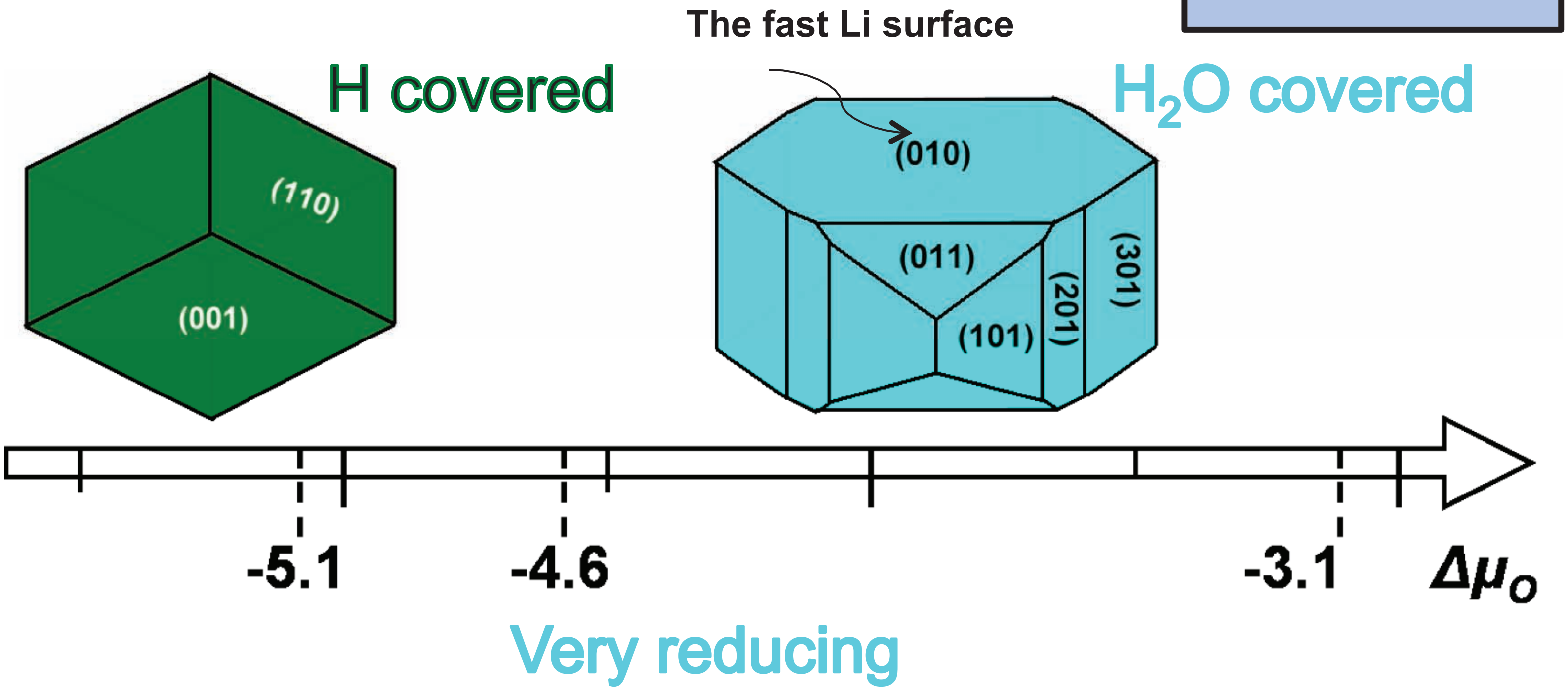
H on under-coordinated Li and O

Reducing conditions

Equilibrium particle shapes can be predicted as function of solution pH, oxygen chemical potential and Li$^+$ concentration

For each oxygen chemical potential, the Wulff shape is constructed, given the ***thermodynamically*** stable surface absorbents.



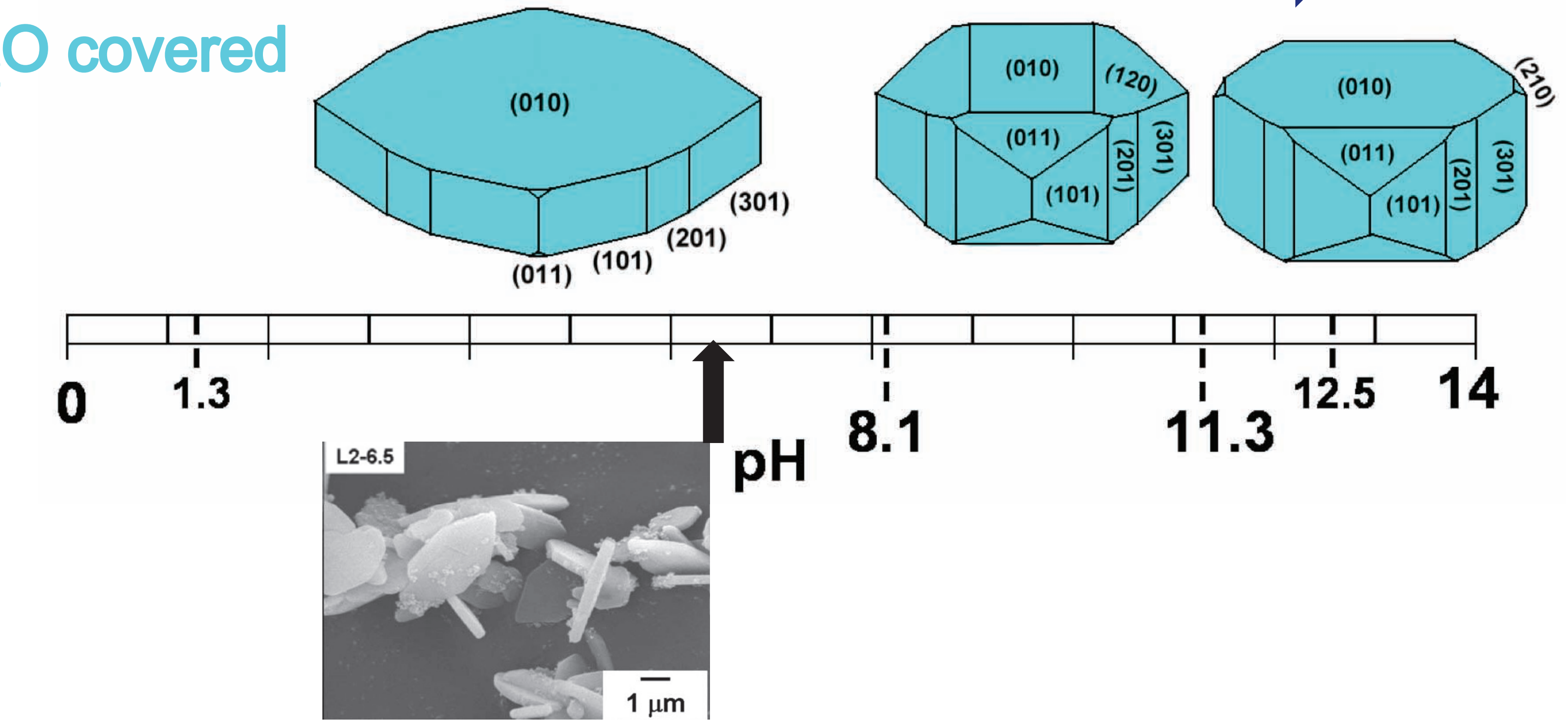


‘Normal’ Water Conditions

For $0 < \mu_O < -3.1$ shape change is due to Li ions dissolving from the surfaces which affects the surface energies and therefore the shape. Supported by exp[1]

Li dissolution drives shape change

H_2O covered



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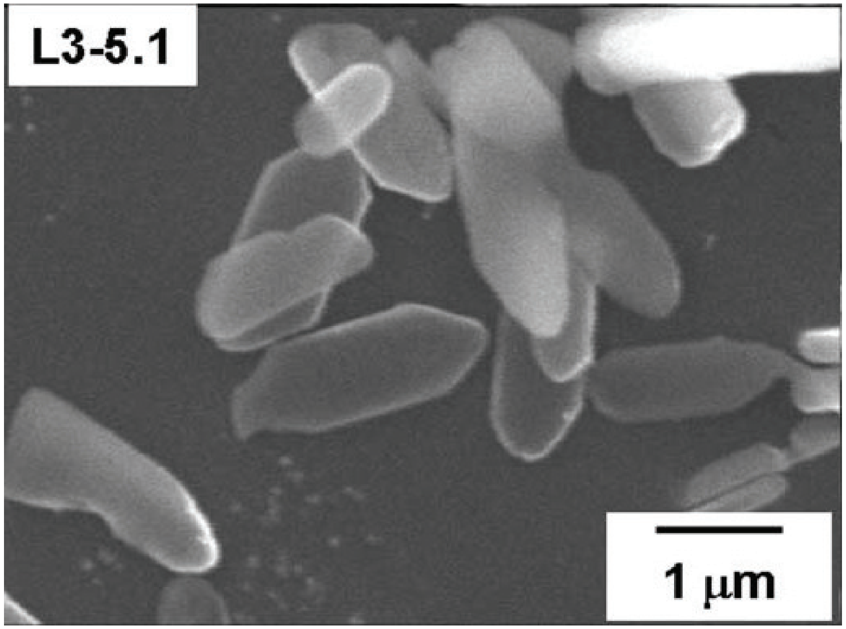
[1] K. Dokko, S. Koizumi, H. Nakano, and K. Kanamura, J. Mater. Chem. **17**, 4803 (2007).

Compare to Exp

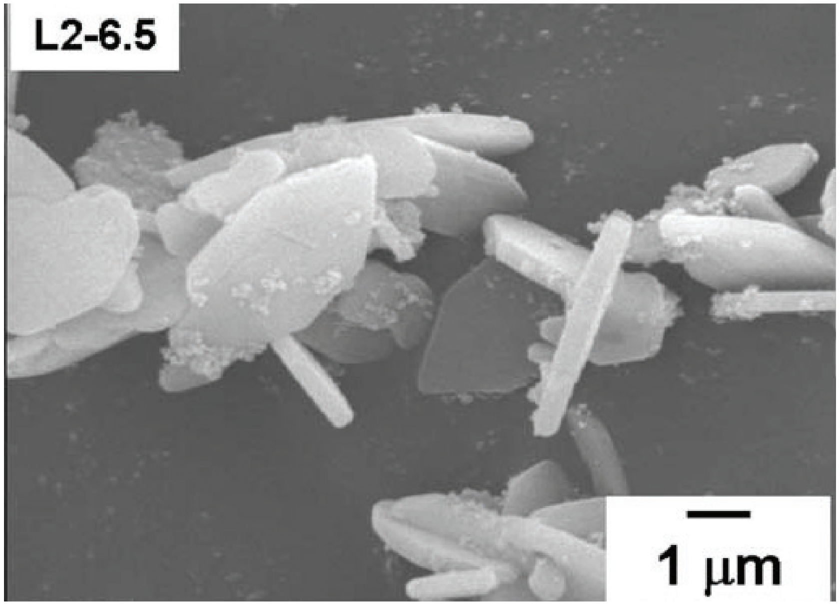
Increasing the **Li concentration** enables the same shape particle be synthesized **at lower pH**

pH = 5.1



[Li$^+$] = 3 M

pH = 6.5

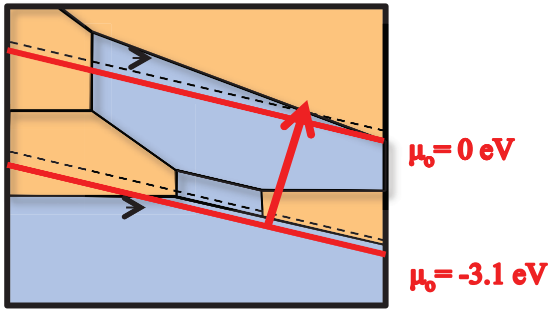


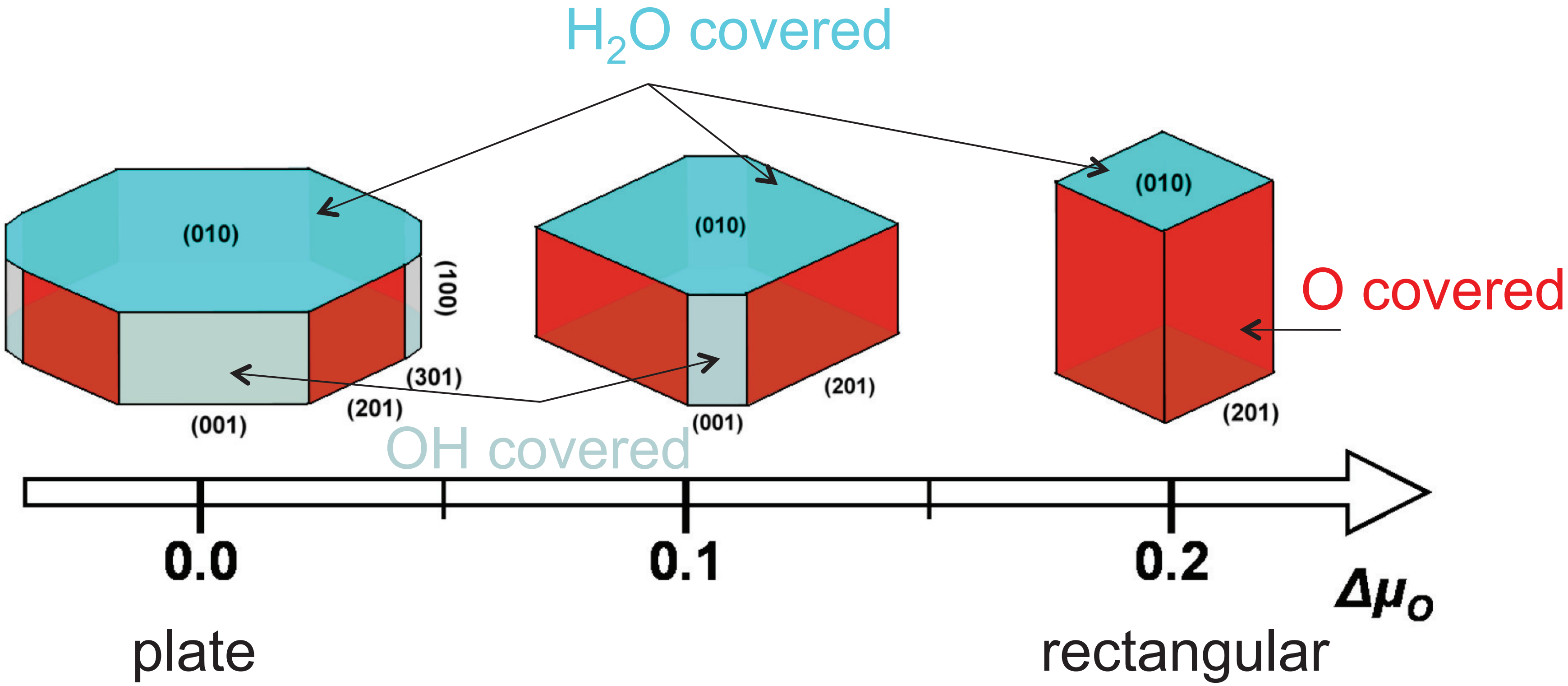
[Li$^+$] = 2 M

[1] K. Dokko, S. Koizumi, H. Nakano, and K. Kanamura, J. Mater. Chem. **17**, 4803 (2007).

Oxidizing conditions drive pillar-shape

For $0 < \mu_O < 0.2$ eV different absorbing species affect the shape





Explaining the hysteresis in conversion reactions

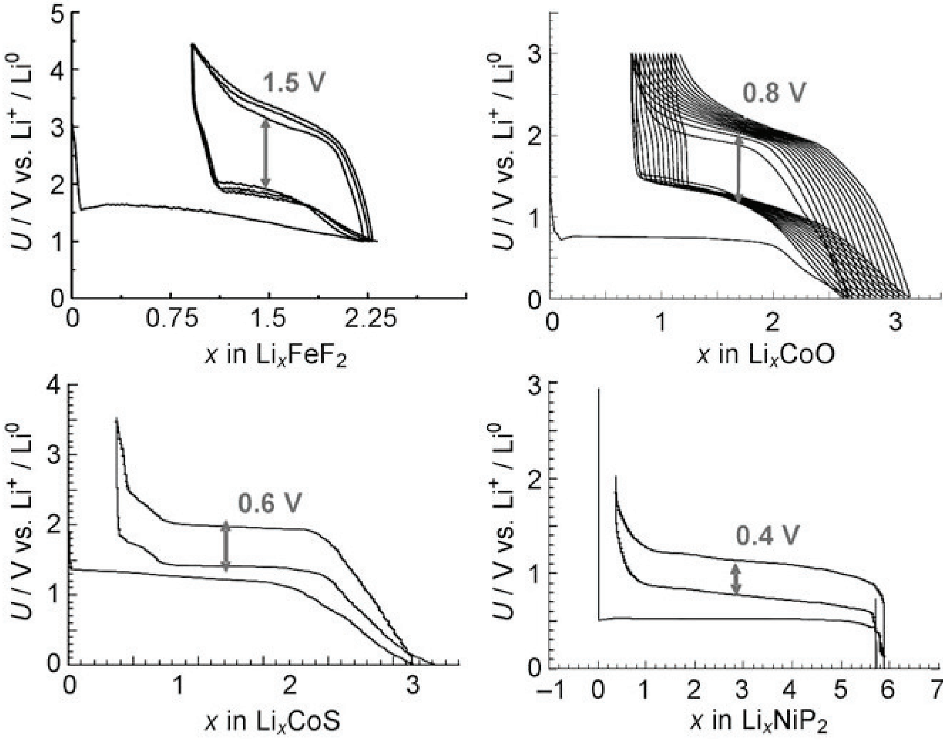
Hysteresis in conversion reactions

Conversion reactions: e.g. $TM\text{-}O_x + 2xLi \rightarrow TM_{(nano)} + xLi_2O$

All conversion reactions show hysteresis; from 0.3 V (hydrides) to 1.5 V (fluorides):

fluorides

oxides



sulphides

phosphides

From Bruce P. et al, AngChem 2006

Possible explanations

To design conversion materials without hysteresis, we need to understand the cause:

~~Electronic conductivity?~~

Poor ionic mobility?
~~Li transport?~~
cation/anion transport?

Bond breaking?

Nucleation/growth?

Hysteresis shows Arrhenius-type limiting kinetics, not ohmic[1]

Good electronic conductivity in Fe_3O_4 still produces hysteresis [1]

High power conversion reactions has been seen[1] but hysteresis remains

Hysteresis scales with ionicity – larger for fluorides than oxides and phosphides[2]

Stable cycling has been obtained despite hysteresis. If the same bonds reform the path to do so has to be different…

Relaxation to constant potential takes VERY long time, up to months

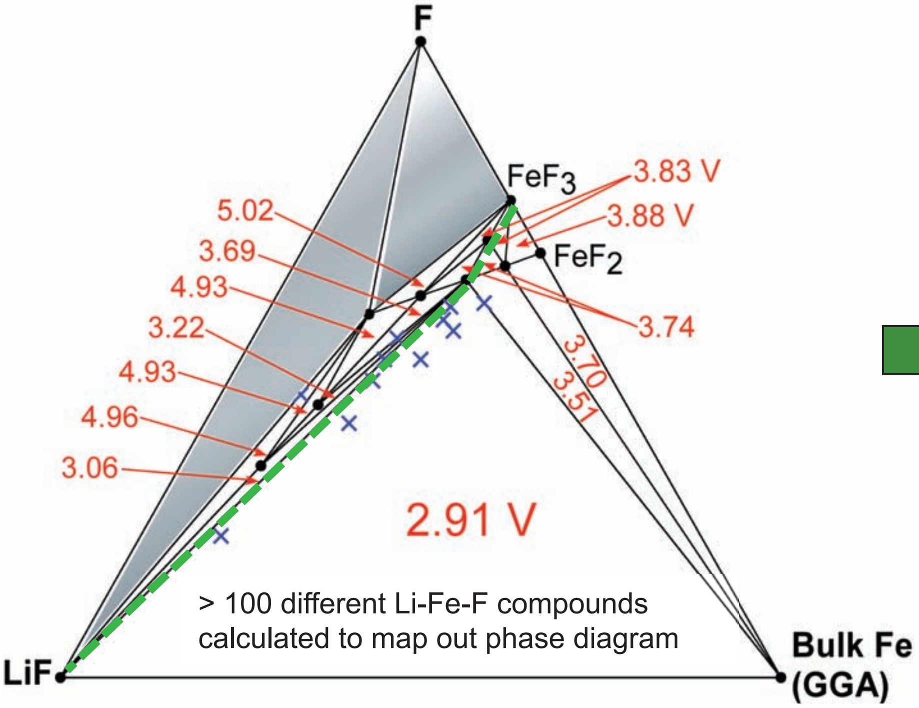
processes are non-equilibrium!

[1] Taberna et al, Nat Mat 2008
[2] Bruce AngChem 2006

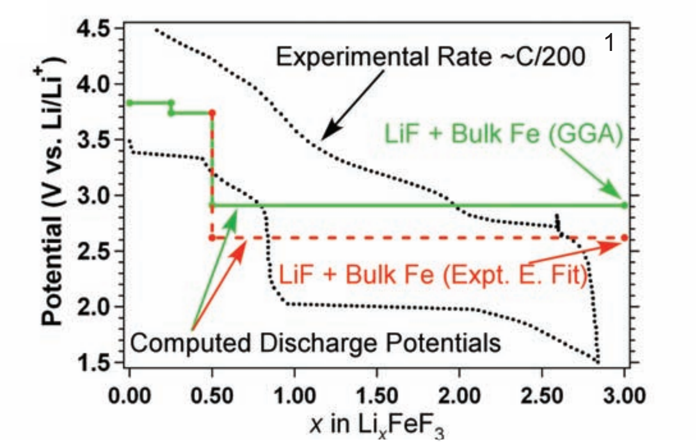
Li-Fe-F Phase Diagram

Different transport properties of the involved chemical species induces different reaction path on conversion and re-conversion ?

If thermodynamic equilibrium ⟶ voltage profile same during charge and discharge



> 100 different Li-Fe-F compounds calculated to map out phase diagram



[1] Courtesy of Badway, F.; Cosandey, F.; Pereira, N.; Amatucci, G. G. *J. Electrochem. Soc.* **2003**, *150*, A1318, A1209.

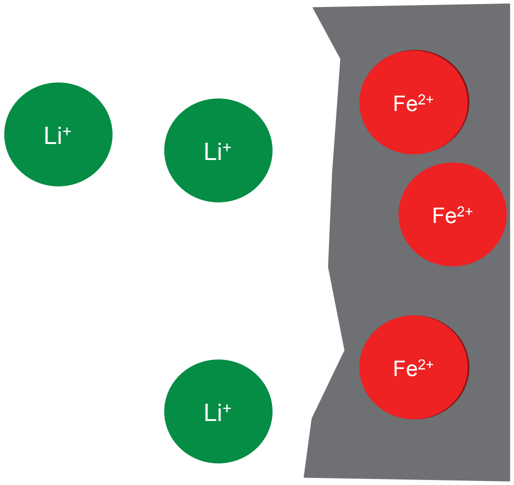
Published in R. E. Doe, K. A. Persson, Y. S. Meng, G. Ceder, Chemistry of Materials, 20, 5274, 2008.

Kinetics during Reduction of FeF3

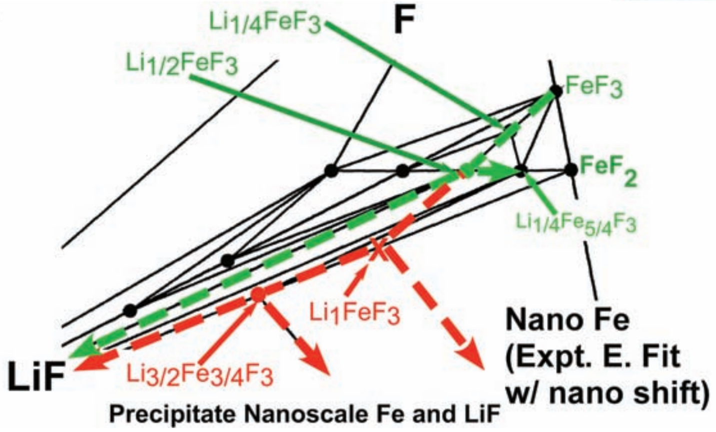
Consider diffusion during conversion

If Fe diffuses much slower than Li^+, then maximum reduction in Li_xFeF_3 will occur rather than Fe precipitation.

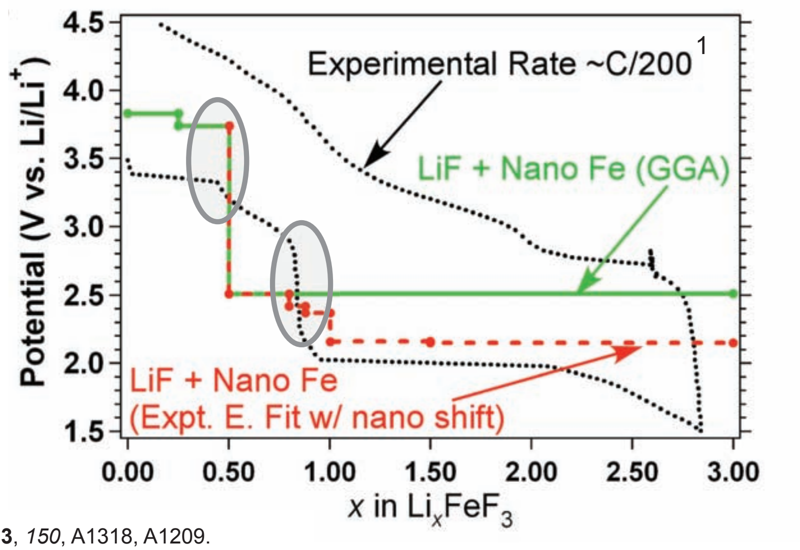
‘Kinetic’ Reduction Path



Assuming Fe limited diffusion favors complete reduction to Fe^{2+}



Phase diagram path yields voltage profile



Kinetically favored path (in red), as well as thermodynamically, assuming precipitation to nano Fe

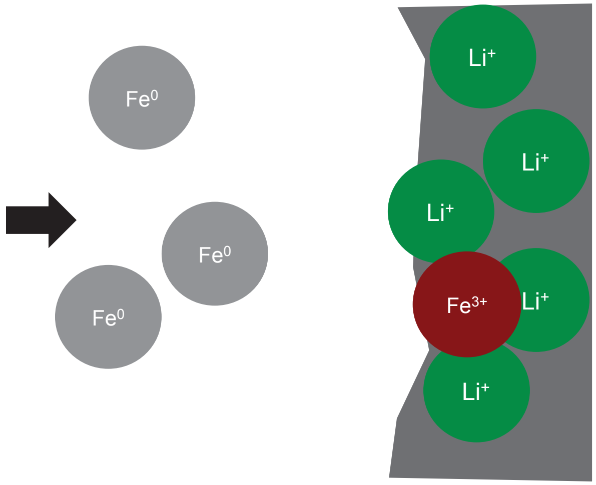
[1] Courtesy of Badway, F.; Cosandey, F.; Pereira, N.; Amatucci, G. G. *J. Electrochem. Soc.* **2003**, *150*, A1318, A1209.

Kinetics during Oxidization

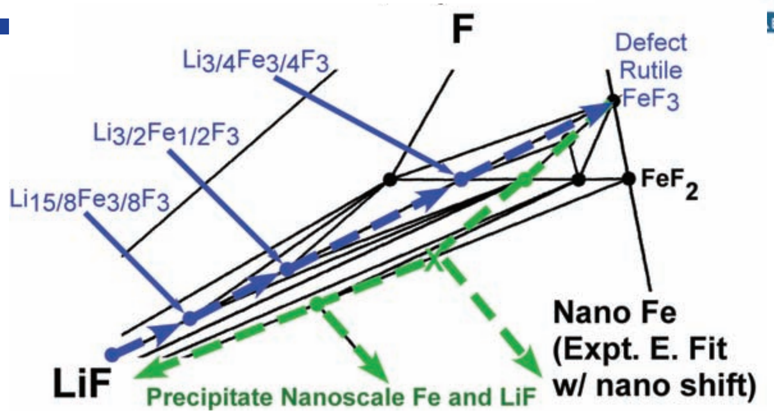
Consider diffusion during **re**-conversion

Fe migrates slowly into LiF and Li^+ moves quickly out, so maximum oxidation in Li_xFeF_3 will occur.

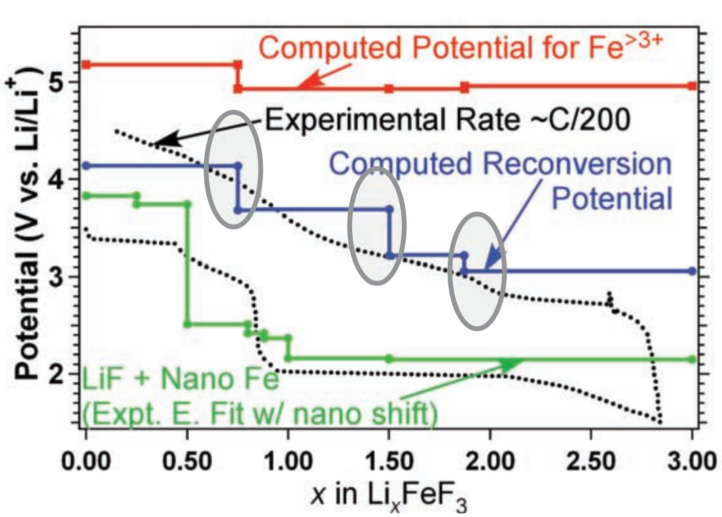
‘Kinetic’ Oxidation Path



Assuming Fe limited diffusion favors complete oxidation to Fe^{3+}



Phase diagram path yields voltage profile

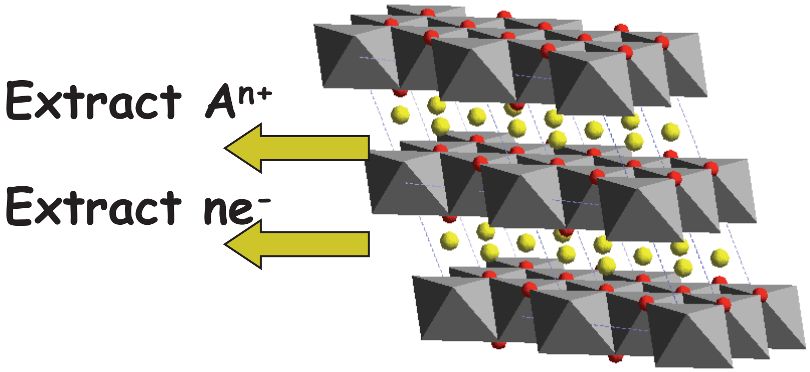


Kinetically favored path (in blue) agrees reasonably well with experiments[1]

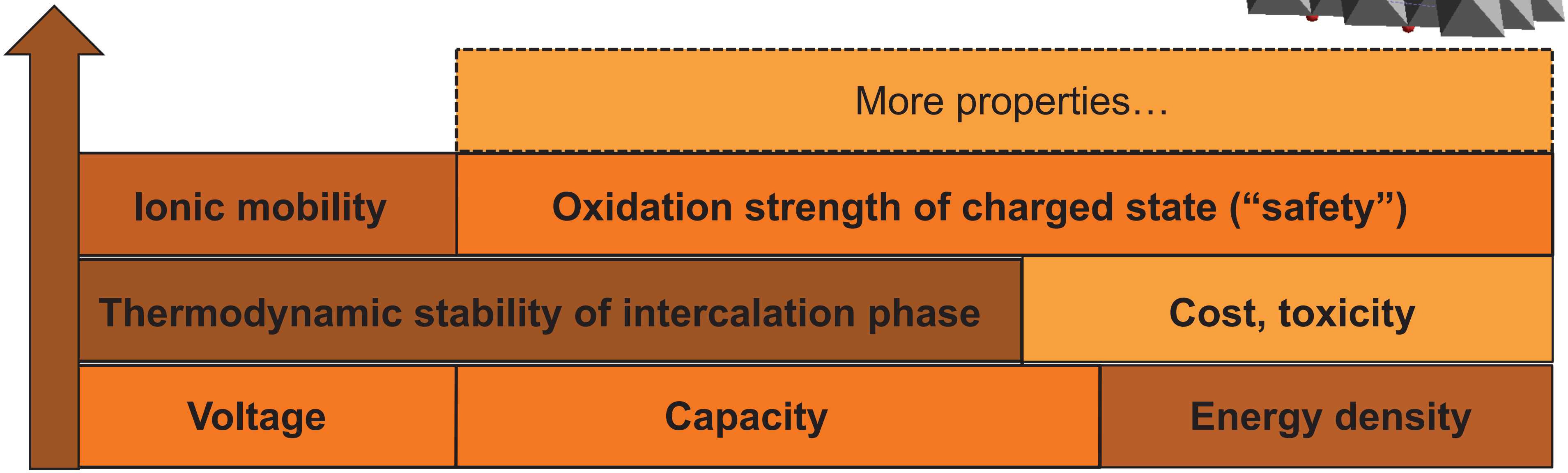
[1] Courtesy of Badway, F.; Cosandey, F.; Pereira, N.; Amatucci, G. G. *J. Electrochem. Soc.* **2003**, *150*, A1318, A1209.

Discovering New Intercalation Cathodes

Computable Screening Criteria



Adding another property increases computation screening power



More properties…

Ionic mobility

Oxidation strength of charged state (“safety”)

Thermodynamic stability of intercalation phase

Cost, toxicity

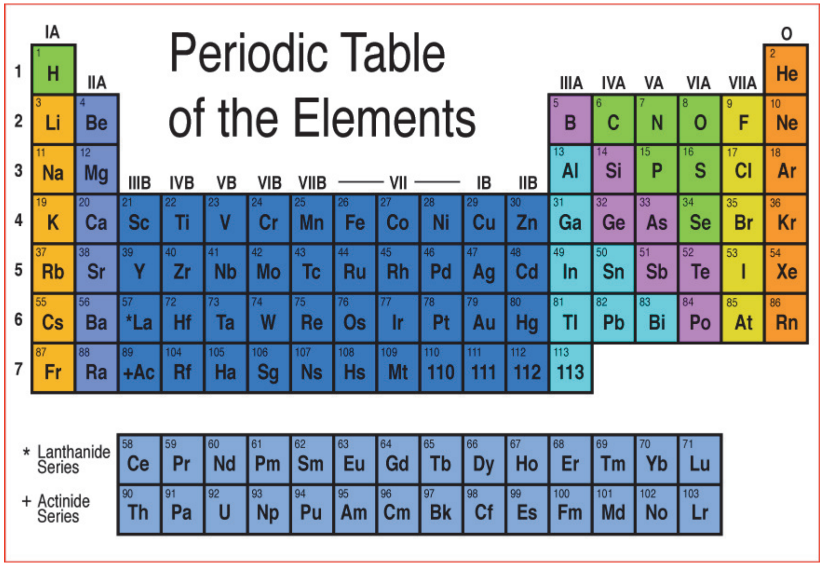
Voltage

Capacity

Energy density

If we can compute one material…can we do all?

Can we compute all computable properties for all materials ?



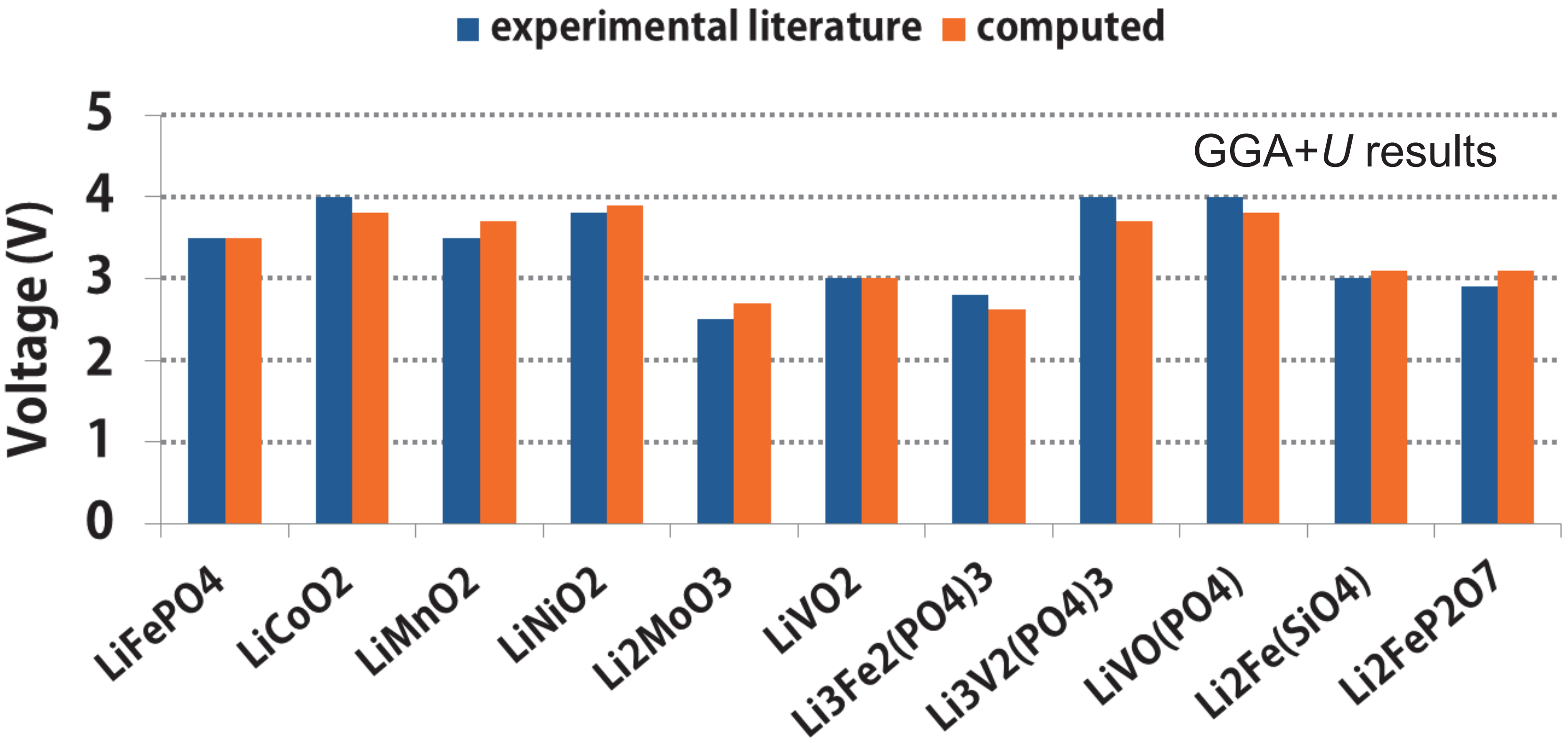
Periodic Table of the Elements

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	O
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 *La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 +Ac	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110 110	111 111	112 112	113 113					

* Lanthanide Series	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
+ Actinide Series	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

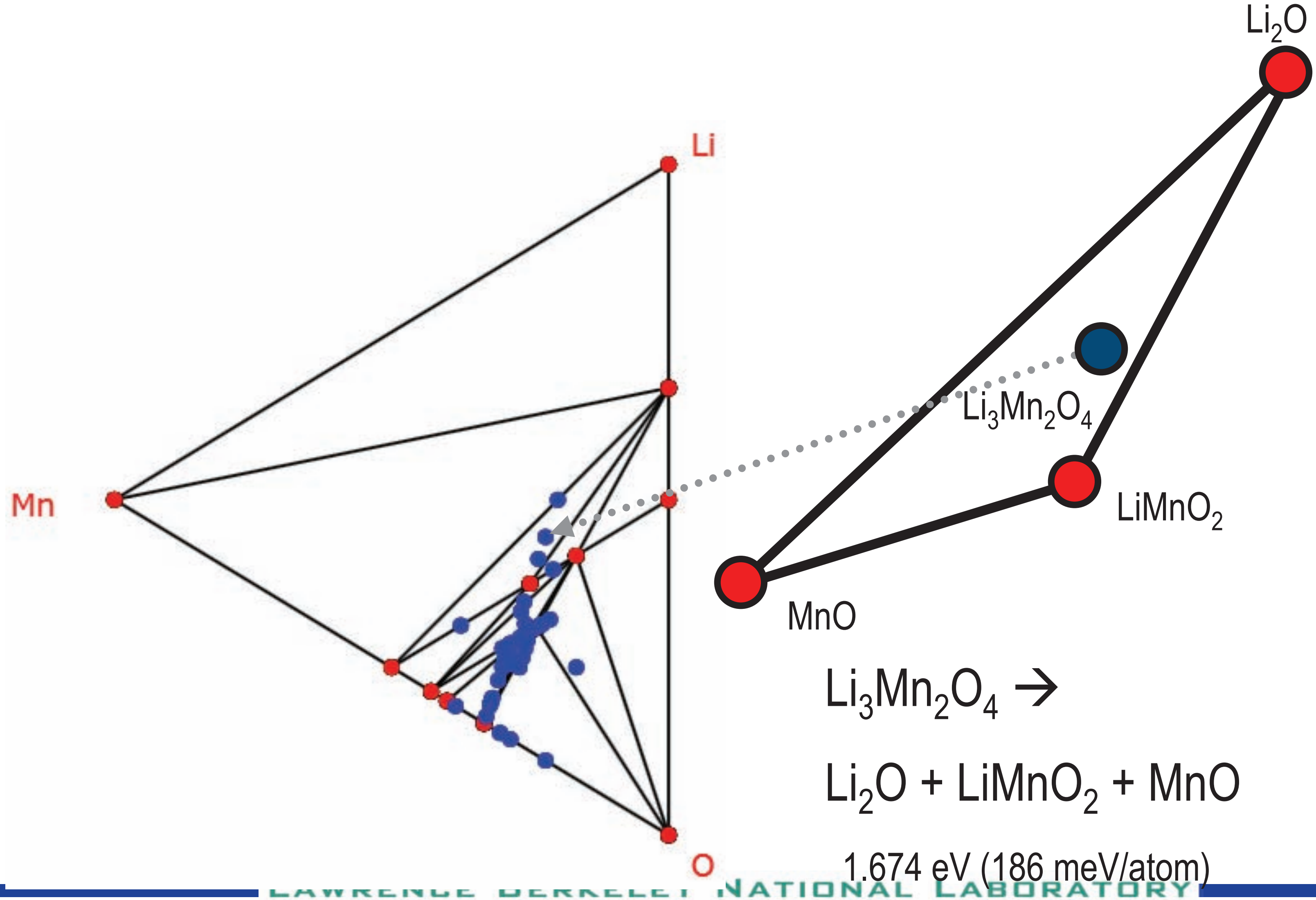
Yes, computing can be scaled!

DFT+U predicts voltage to about 0.1-0.2V



+U is fit to binaries - method is predictive outside its fitted compound

Structural stability – will we able to synthesize our prediction?



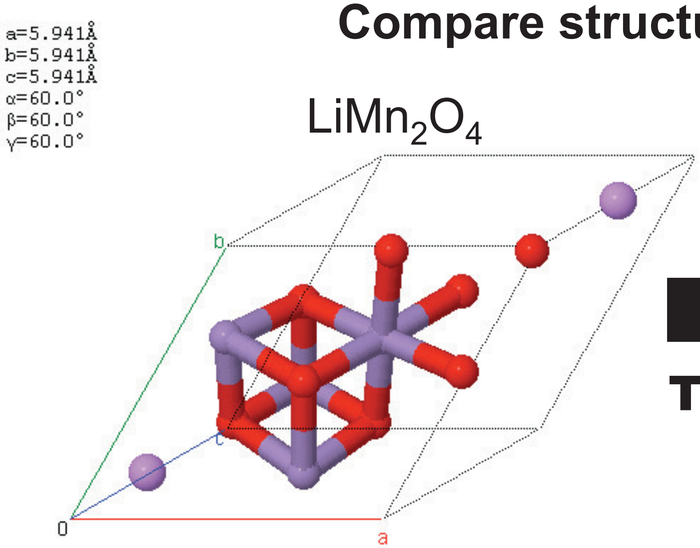
$Li_3Mn_2O_4$ →

Li_2O + $LiMnO_2$ + MnO

1.674 eV (186 meV/atom)

Structural stability –
is the reaction topotactic?

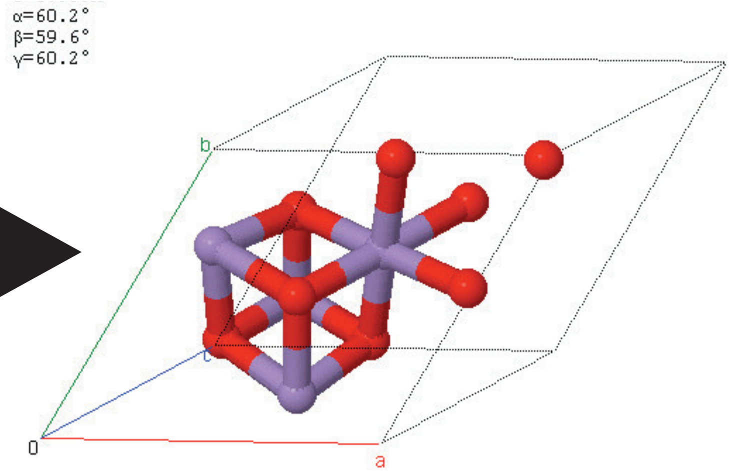
Compare structures removing the mobile ion

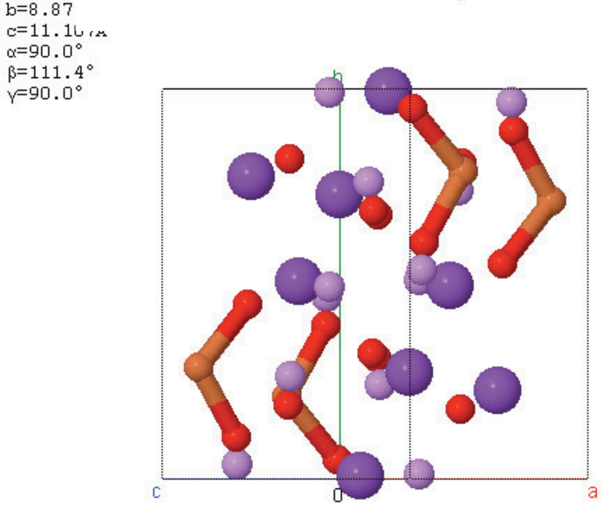


$LiMn_2O_4$

remove Li

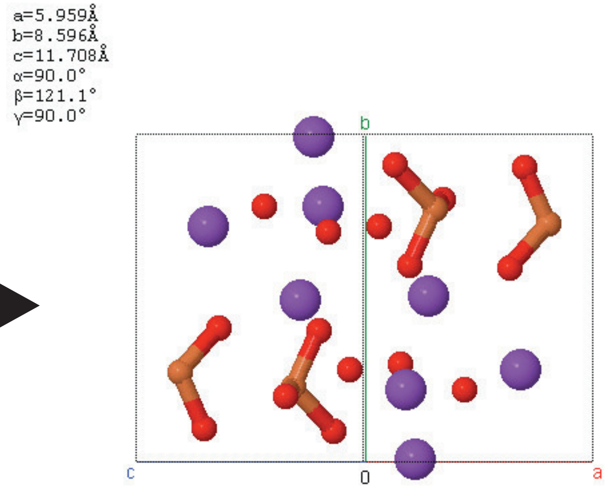
TOPOTACTIC





remove Li

NON - TOPOTACTIC

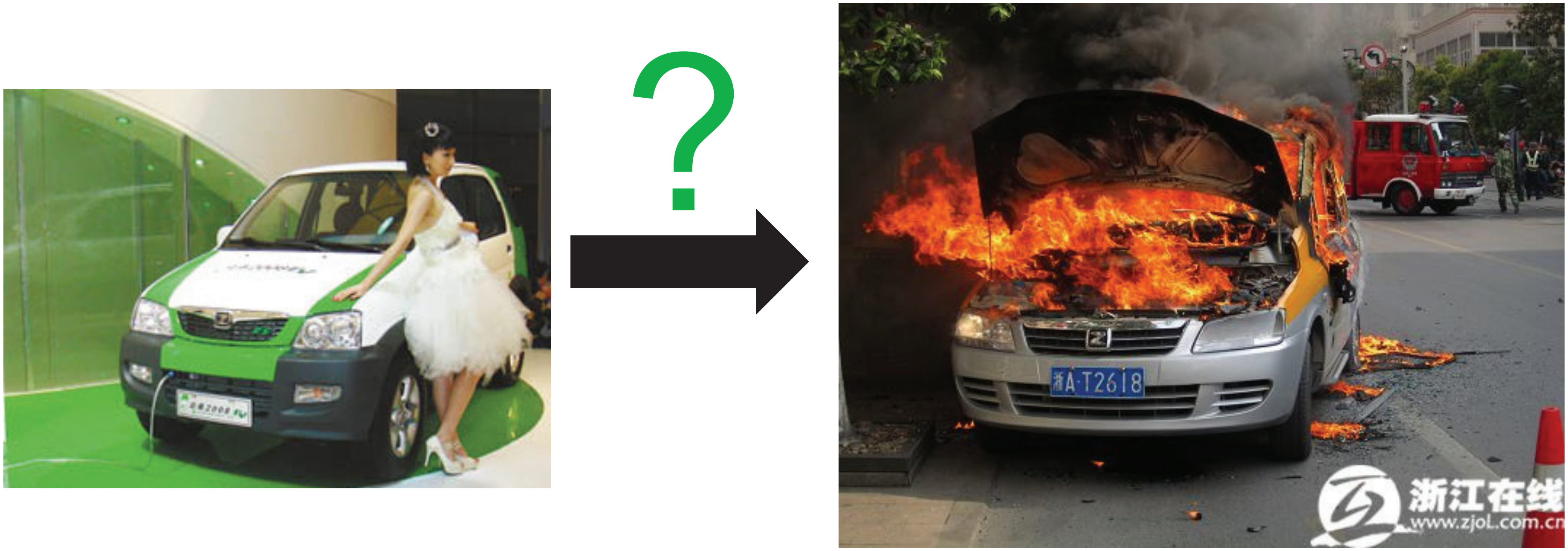


$Li_3K_2FeO_4$

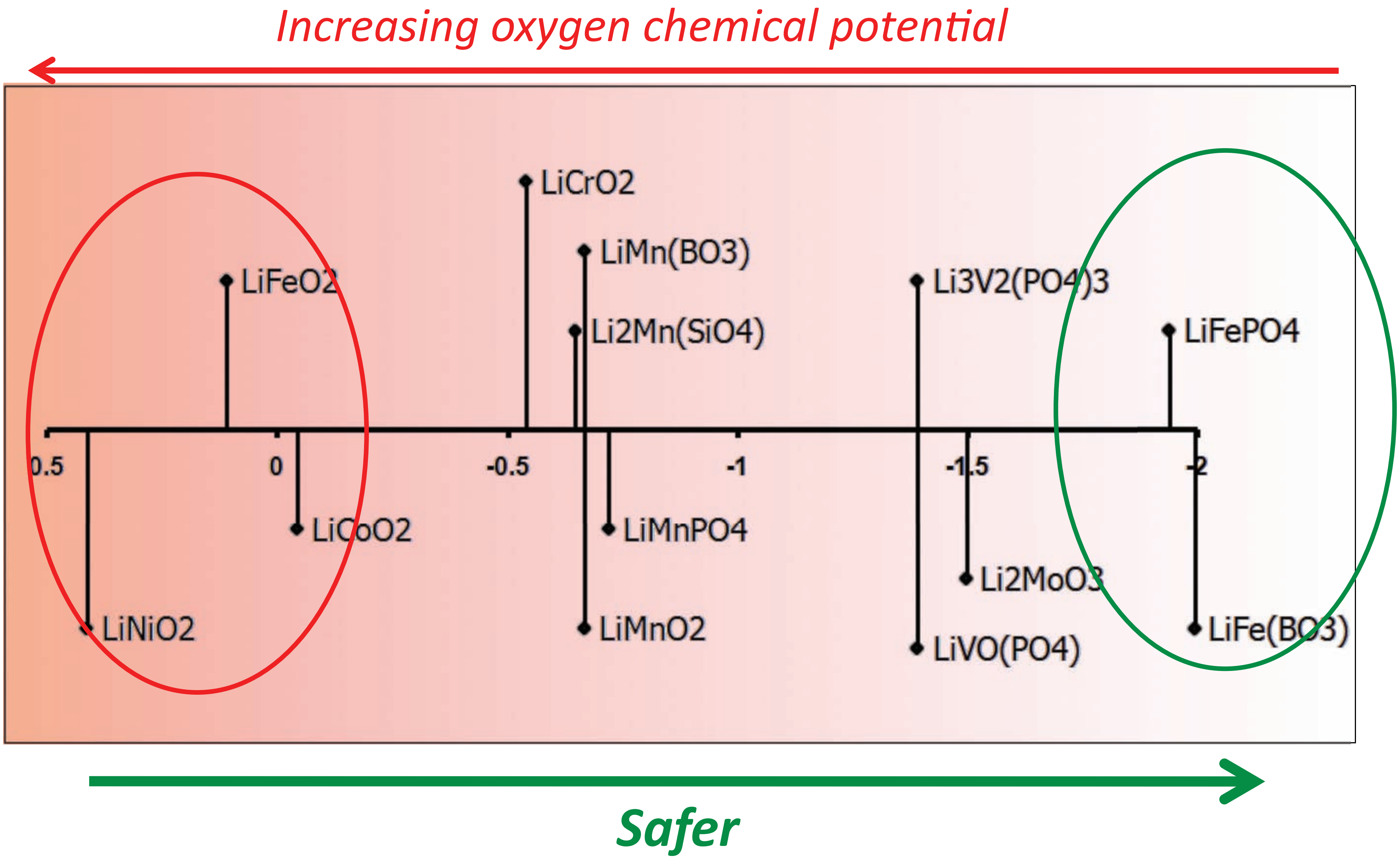
Cathode safety

How to compute safety?

- **Oxygen release correlates with oxygen chemical potential of cathode**

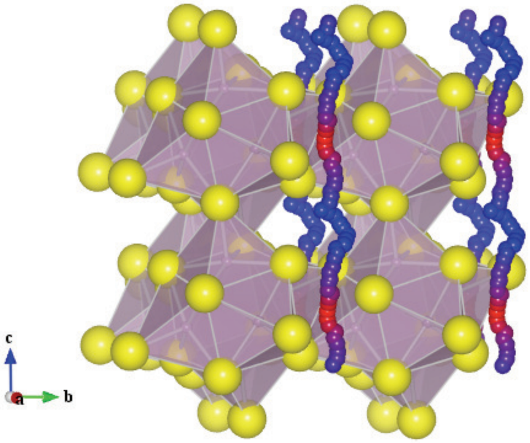


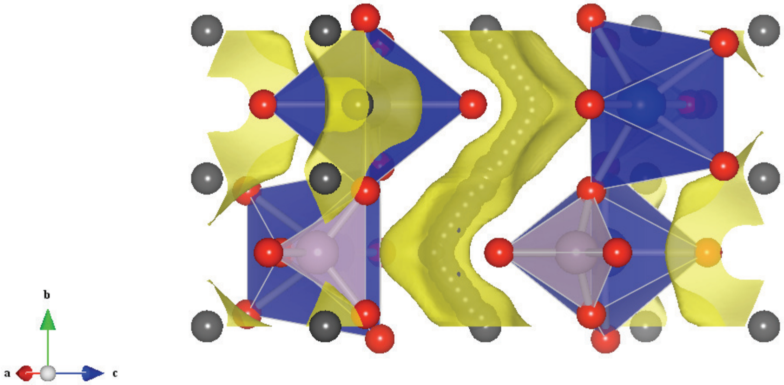
Experience agrees with results

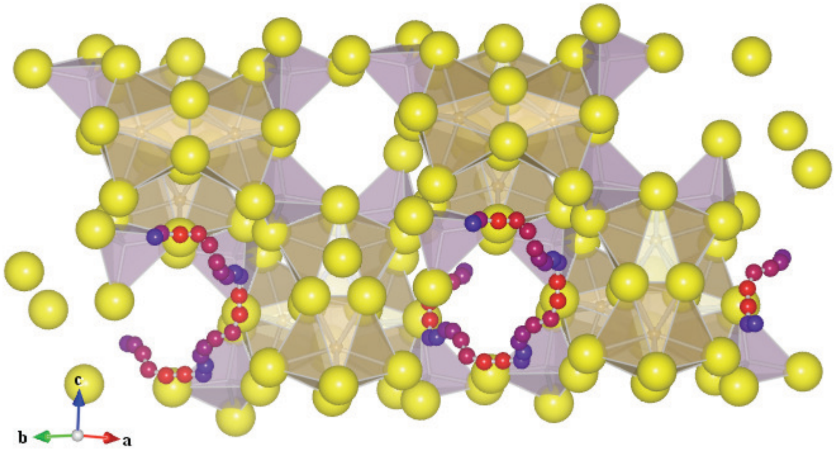


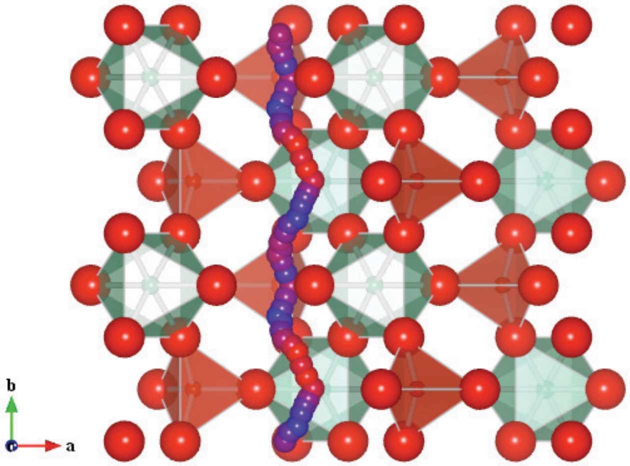
Ionic mobility

Developed ability to automatically find diffusion paths for Li/Mg/… in structures.



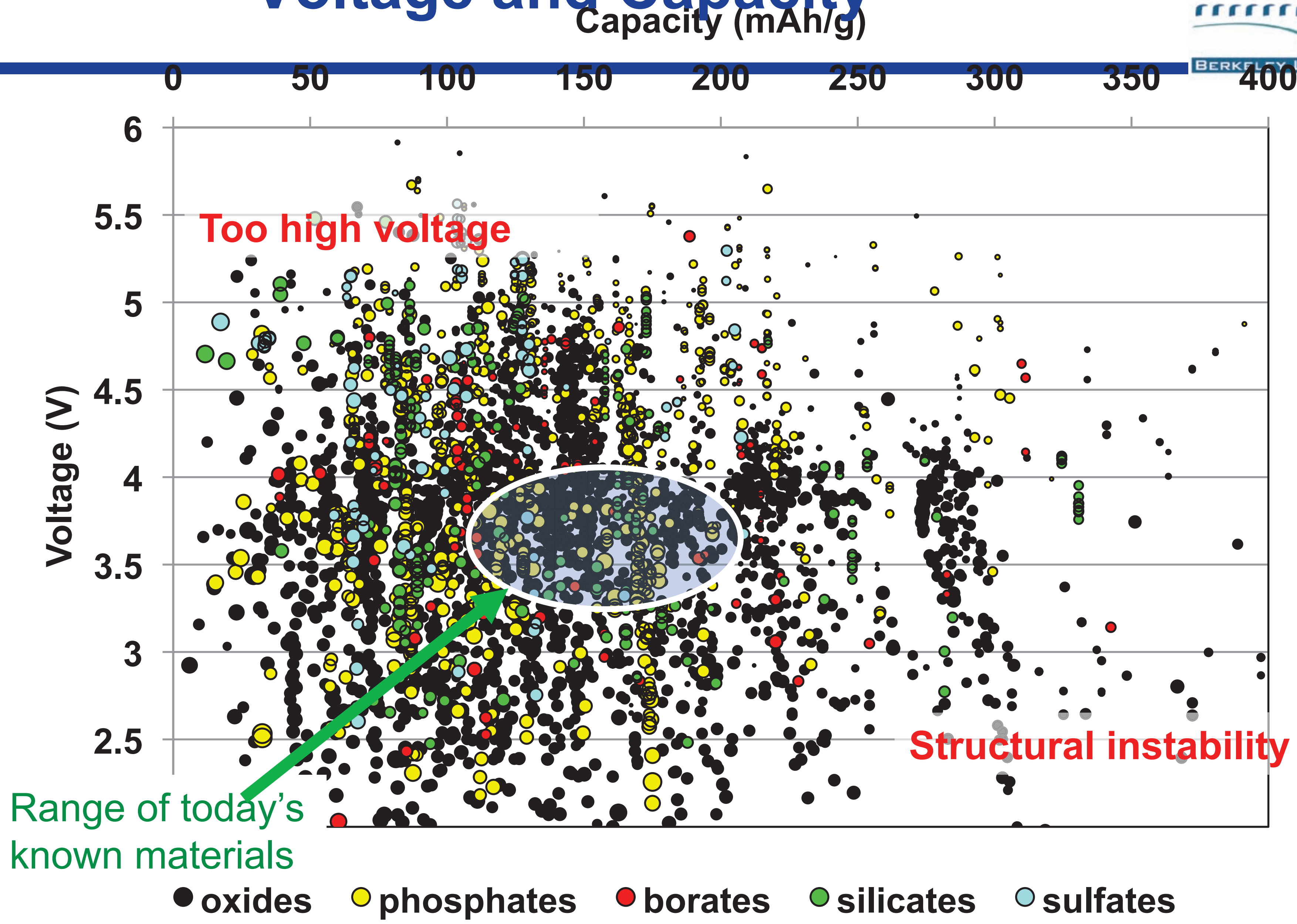




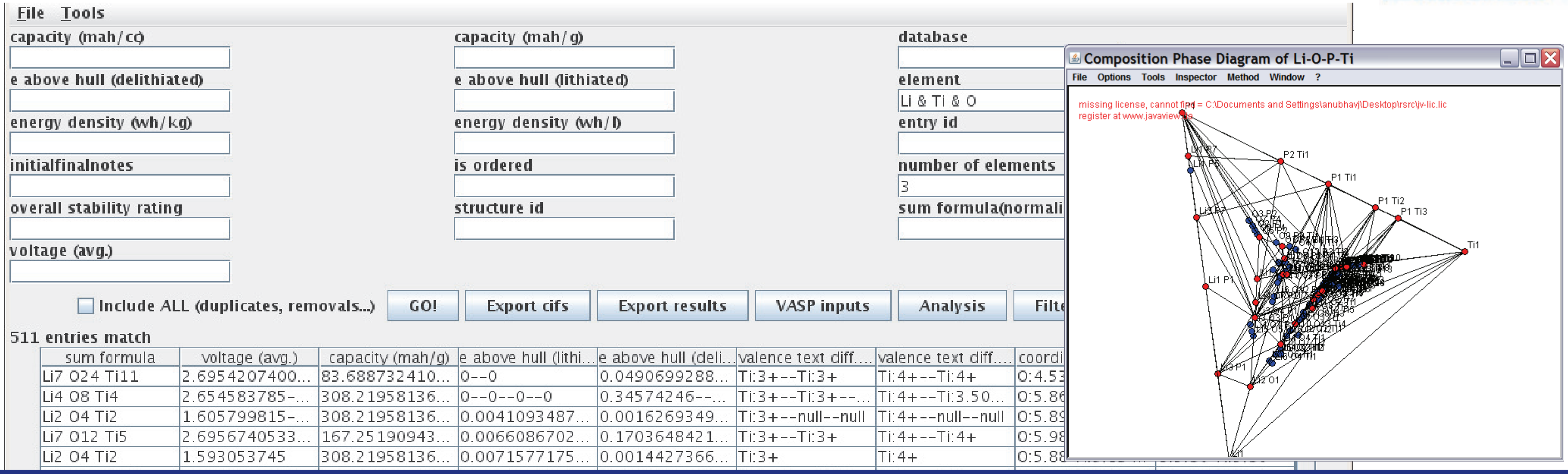


Evaluated thousands of known structures...

Voltage and Capacity



Organized in Materials Properties Database…



capacity (mah/cc):

e above hull (delithiated):

energy density (wh/kg):

initialfinalnotes:

overall stability rating:

voltage (avg.):

capacity (mah/g):

e above hull (lithiated):

energy density (wh/l):

is ordered:

structure id:

database:

element: Li & Ti & O

entry id:

number of elements: 3

sum formula(normali

☐ Include ALL (duplicates, removals...)

511 entries match

sum formula	voltage (avg.)	capacity (mah/g)	e above hull (lithi...	e above hull (deli...	valence text diff....	valence text diff....	coordi
Li7 O24 Ti11	2.6954207400...	83.688732410...	0--0	0.0490699288...	Ti:3+--Ti:3+	Ti:4+--Ti:4+	O:4.53
Li4 O8 Ti4	2.654583785-...	308.21958136...	0--0--0--0	0.34574246--...	Ti:3+--Ti:3+--...	Ti:4+--Ti:3.50...	O:5.86
Li2 O4 Ti2	1.605799815-...	308.21958136...	0.0041093487...	0.0016269349...	Ti:3+--null--null	Ti:4+--null--null	O:5.89
Li7 O12 Ti5	2.6956740533...	167.25190943...	0.0066086702...	0.1703648421...	Ti:3+--Ti:3+	Ti:4+--Ti:4+	O:5.98
Li2 O4 Ti2	1.593053745	308.21958136...	0.0071577175...	0.0014427366...	Ti:3+	Ti:4+	O:5.88

Composition Phase Diagram of Li-O-P-Ti

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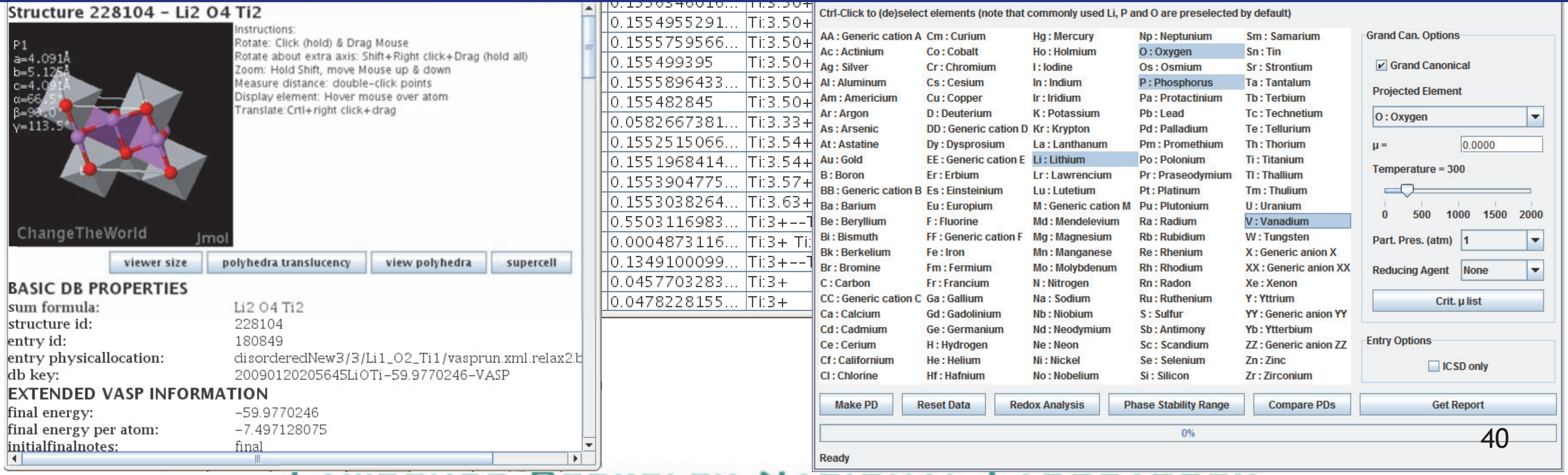
register at www.javaview.de

Collaboration with MIT: Made possible by Gillette (P&G), Bosch and Umicore and BATT


Structure 228104 - Li2 O4 Ti2

Instructions:
Rotate: Click (hold) & Drag Mouse
Rotate about extra axis: Shift+Right click+Drag (hold all)
Zoom: Hold Shift, move Mouse up & down
Measure distance: double-click points
Display element: Hover mouse over atom
Translate: Crtl+right click+drag

BASIC DB PROPERTIES

sum formula: Li2 O4 Ti2
structure id: 228104
entry id: 180849
entry physicallocation: disorderedNew3/3/Li1_O2_Ti1/vasprun.xml.relax2.b
db key: 20090120205645LiOTi-59.9770246-VASP

EXTENDED VASP INFORMATION

final energy: -59.9770246
final energy per atom: -7.497128075
initialfinalnotes: final

0.1554955291...	Ti:3.50+
0.1555759566...	Ti:3.50+
0.155499395	Ti:3.50+
0.1555896433...	Ti:3.50+
0.155482845	Ti:3.50+
0.0582667381...	Ti:3.33+
0.1552515066...	Ti:3.54+
0.1551968414...	Ti:3.54+
0.1553904775...	Ti:3.57+
0.1553038264...	Ti:3.63+
0.5503116983...	Ti:3+--T
0.0004873116...	Ti:3+ Ti:
0.1349100099...	Ti:3+--T
0.0457703283...	Ti:3+
0.0478228155...	Ti:3+

Ctrl-Click to (de)select elements (note that commonly used Li, P and O are preselected by default)

AA : Generic cation A
Ac : Actinium
Ag : Silver
Al : Aluminum
Am : Americium
Ar : Argon
As : Arsenic
At : Astatine
Au : Gold
B : Boron
BB : Generic cation B
Ba : Barium
Be : Beryllium
Bi : Bismuth
Bk : Berkelium
Br : Bromine
C : Carbon
CC : Generic cation C
Ca : Calcium
Cd : Cadmium
Ce : Cerium
Cf : Californium
Cl : Chlorine
Cm : Curium
Co : Cobalt
Cr : Chromium
Cs : Cesium
Cu : Copper
D : Deuterium
DD : Generic cation D
Dy : Dysprosium
EE : Generic cation E
Er : Erbium
Es : Einsteinium
Eu : Europium
F : Fluorine
FF : Generic cation F
Fe : Iron
Fm : Fermium
Fr : Francium
Ga : Gallium
Gd : Gadolinium
Ge : Germanium
H : Hydrogen
He : Helium
Hf : Hafnium
Hg : Mercury
Ho : Holmium
I : Iodine
In : Indium
Ir : Iridium
K : Potassium
Kr : Krypton
La : Lanthanum
Li : Lithium
Lr : Lawrencium
Lu : Lutetium
M : Generic cation M
Md : Mendelevium
Mg : Magnesium
Mn : Manganese
Mo : Molybdenum
N : Nitrogen
Na : Sodium
Nb : Niobium
Nd : Neodymium
Ne : Neon
Ni : Nickel
No : Nobelium
Np : Neptunium
O : Oxygen
Os : Osmium
P : Phosphorus
Pa : Protactinium
Pb : Lead
Pd : Palladium
Pm : Promethium
Po : Polonium
Pr : Praseodymium
Pt : Platinum
Pu : Plutonium
Ra : Radium
Rb : Rubidium
Re : Rhenium
Rh : Rhodium
Rn : Radon
Ru : Ruthenium
S : Sulfur
Sb : Antimony
Sc : Scandium
Se : Selenium
Si : Silicon
Sm : Samarium
Sn : Tin
Sr : Strontium
Ta : Tantalum
Tb : Terbium
Tc : Technetium
Te : Tellurium
Th : Thorium
Ti : Titanium
Tl : Thallium
Tm : Thulium
U : Uranium
V : Vanadium
W : Tungsten
X : Generic anion X
XX : Generic anion XX
Xe : Xenon
Y : Yttrium
YY : Generic anion YY
Yb : Ytterbium
ZZ : Generic anion ZZ
Zn : Zinc
Zr : Zirconium

Grand Can. Options

☑ Grand Canonical

Projected Element: O : Oxygen

μ = 0.0000

Temperature = 300

Part. Pres. (atm): 1

Reducing Agent: None

Entry Options

☐ ICSD only

Ready

Three cathode materials discovered using high-throughput DFT

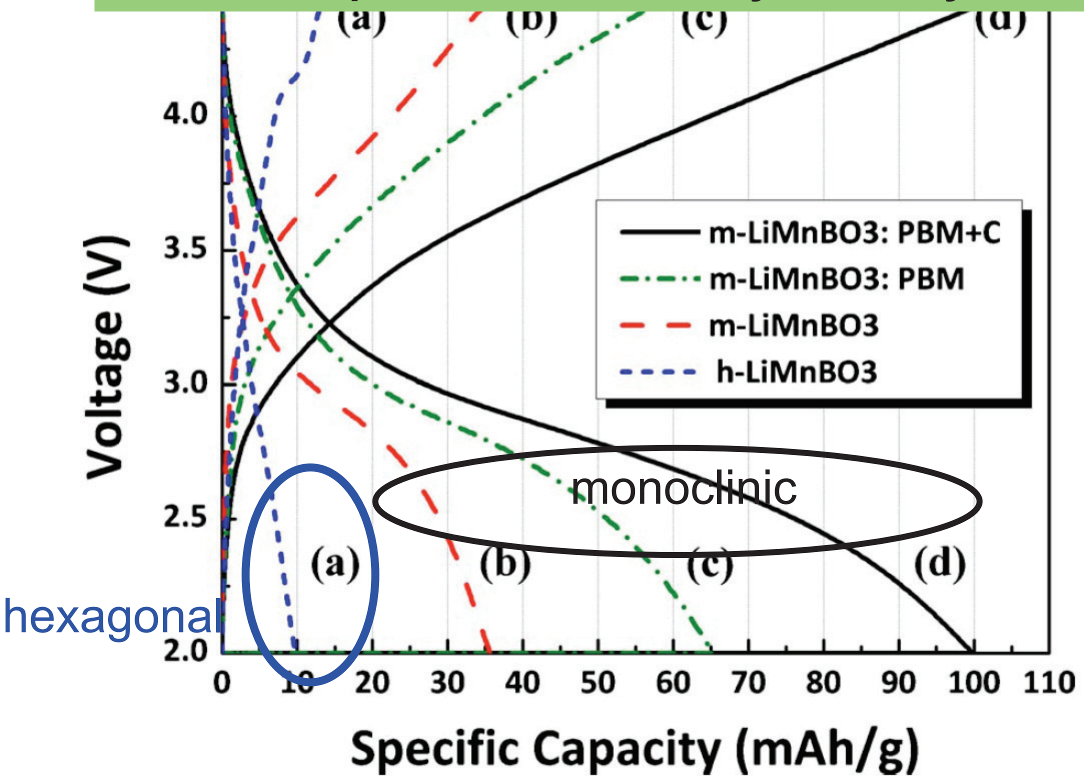
Chemistry	Novelty	Energy density vs. $LiFePO_4$	% of theoretical capacity achieved in the lab to date
$LiMnBO_3$	Compound known (new electrochem.)	50% greater	~45%
$Li_3M(PO_4)(CO_3)$ M=Fe, Mn, ...	New	40% greater	~45%
$Li_9V_3(P_2O_7)_3(PO_4)_2$	New	20% greater	~65%

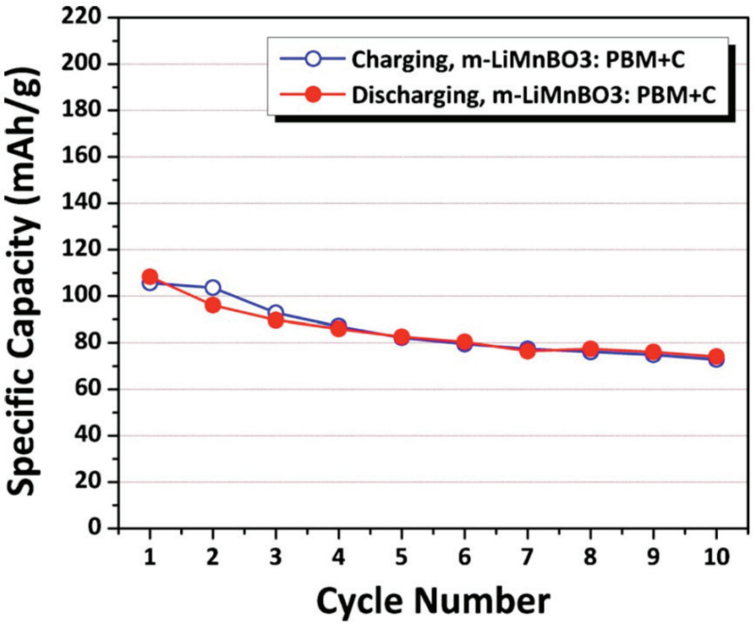
All three systems synthesized in Ceder group at MIT during the last 18 months

Alternate crystal structure of $LiMnBO_3$ exhibits good performance

Chemistry	Novelty	Energy density vs. $LiFePO_4$	% of theoretical capacity achieved in the lab to date
$LiMnBO_3$	Compound known (new electrochem.)	50% greater	~45%

Monoclinic phase less thermodynamically unstable and lower Li activation barriers

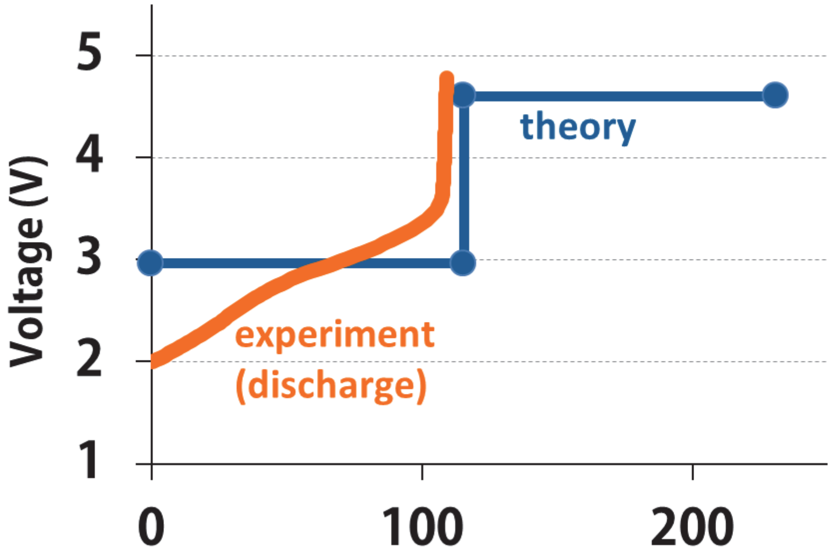


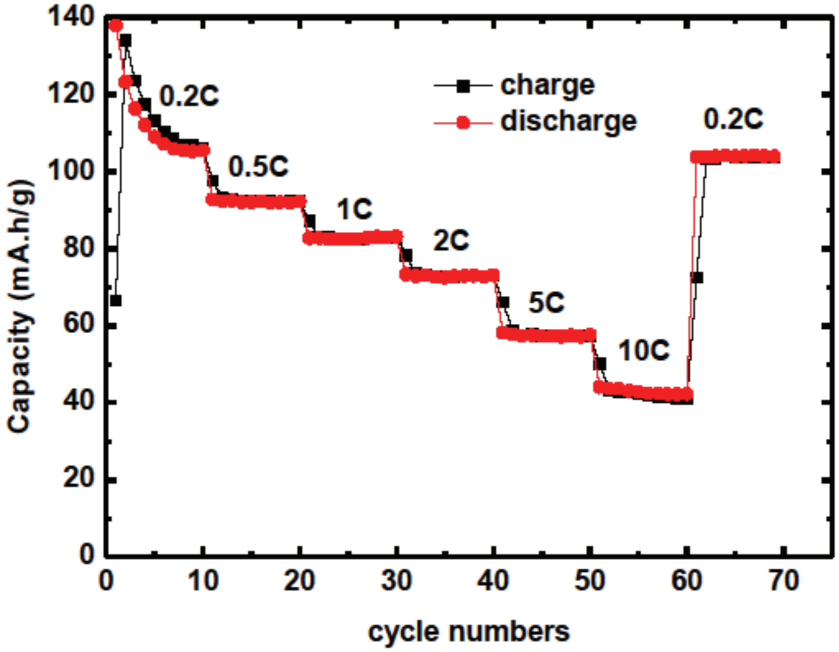


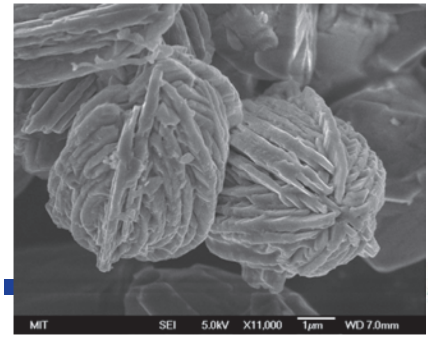
Courtesy of Kim, Moore, Kang, Hautier, Jain, Ceder
J. Electrochem. Soc. (2011)

Previously unknown lithium metal carbonophosphates as cathodes

Chemistry	Novelty	Energy density vs. $LiFePO_4$	% of theoretical capacity achieved in the lab to date
$Li_3M(PO_4)(CO_3)$ M=Fe, Mn, …	New	40% greater	~45%



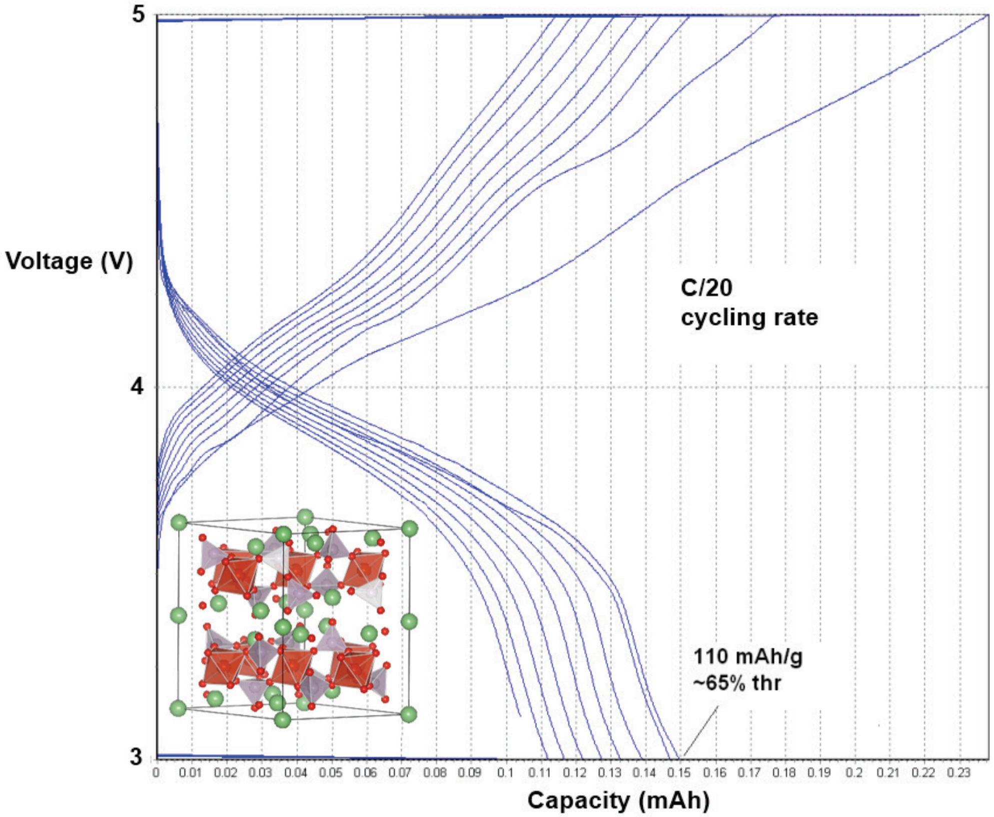




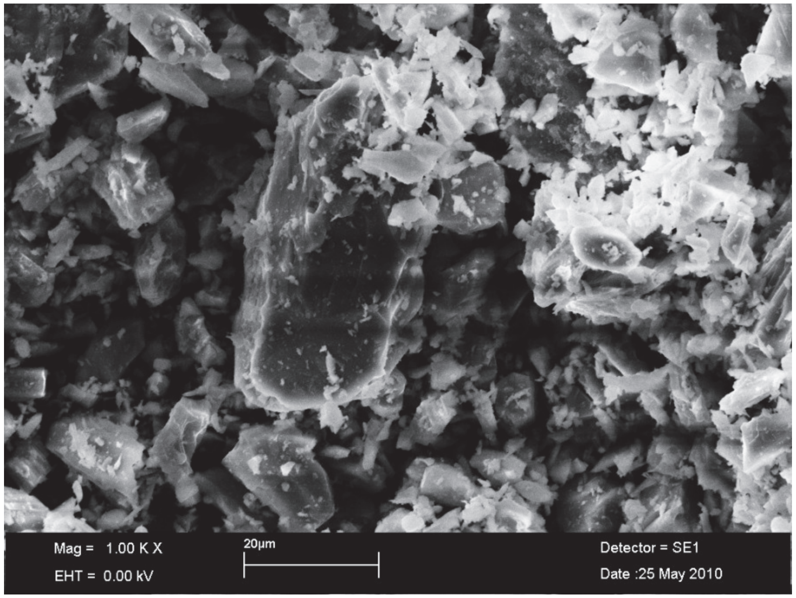
Courtesy of Chen*, Hautier*, Jain, Moore, Kang, Doe, Wu, Zhu, Ceder manuscript in submission

New polyanion material exhibits good electrochemical performance

Chemistry	Novelty	Energy density vs. $LiFePO_4$	% of theoretical capacity achieved in the lab to date
$Li_9V_3(P_2O_7)_3(PO_4)_2$	New	20% greater	~65%



Courtesy of Jain, Ceder (in submission)



large (~20 micron) particle size needs to be reduced

Pellion Technologies:
Rechargeable Mg intercalation batteries

Why Mg ?

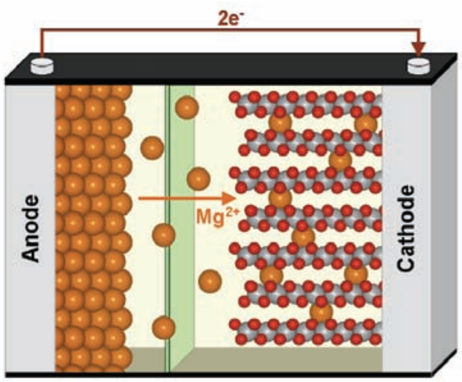
☐ **CAPACITY**: Mg is divalent (Mg^{2+}) thereby displace double the charge per ion compared to Li^{+}. **3x in volumetric energy**, **2x** in gravimetric

☐ **ANODE**: Mg metal can be used as anode (2300 mAh/g)

☐ **ELECTROLYTES** have been developed for stable Mg deposition (**Aurbach : > 2000 cycles**)

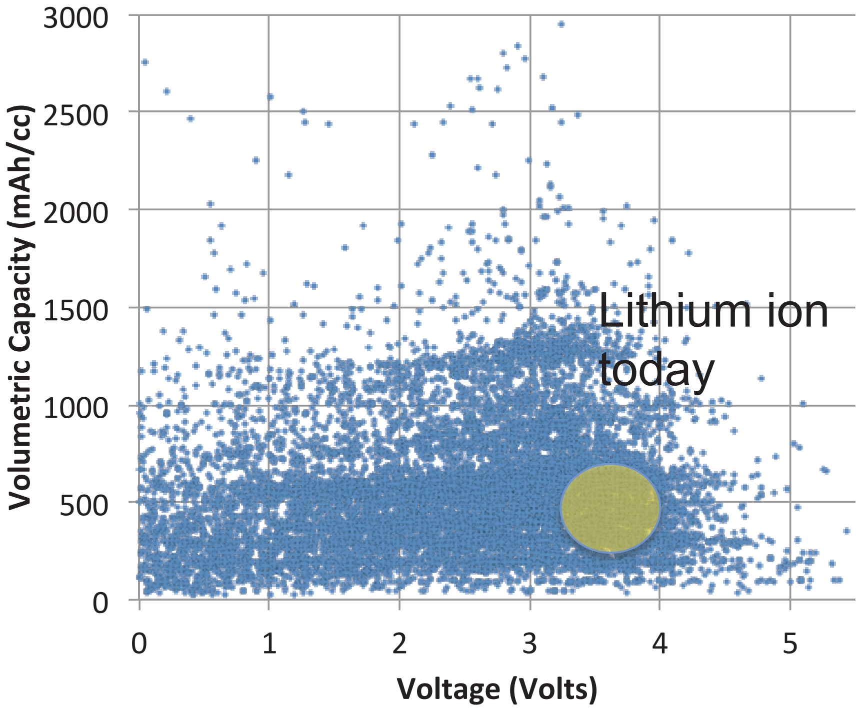
☐ **COST**: Mg is much less expensive than Li

☐ **RESOURCE SUPPLY**: Mg is 8th most abundant element in Earth's crust. Has variety of sources.

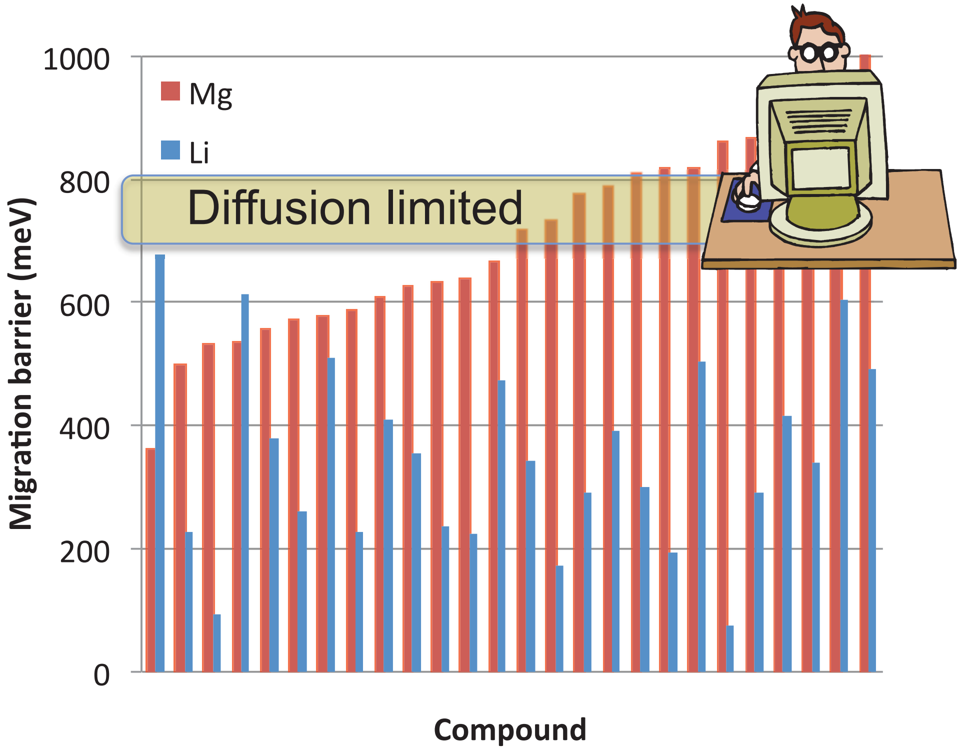


Need a high-energy cathode that works with electrolyte and anode

Mg Cathode Computational Screening

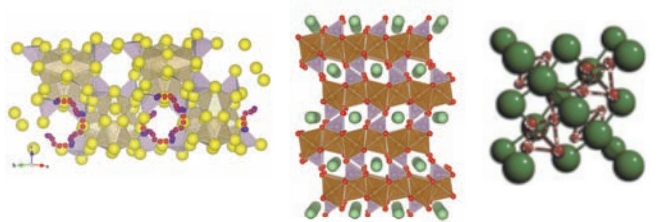


Mg Voltage and Capacity of ≈ 9,600 compounds computed

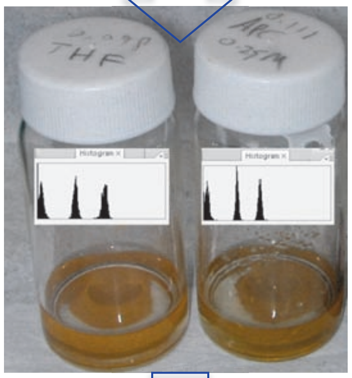


Accurate diffusion barriers demonstrate fast Mg kinetics for some materials

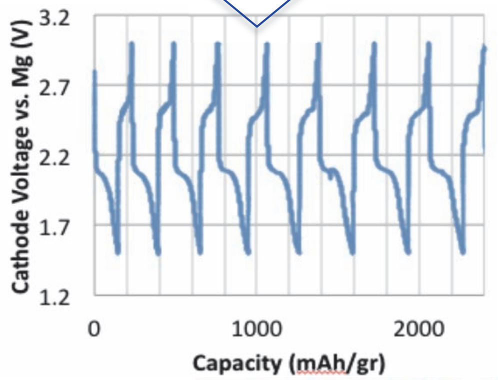
Computations – Experiments in sync



Computationally screened 9600 compounds



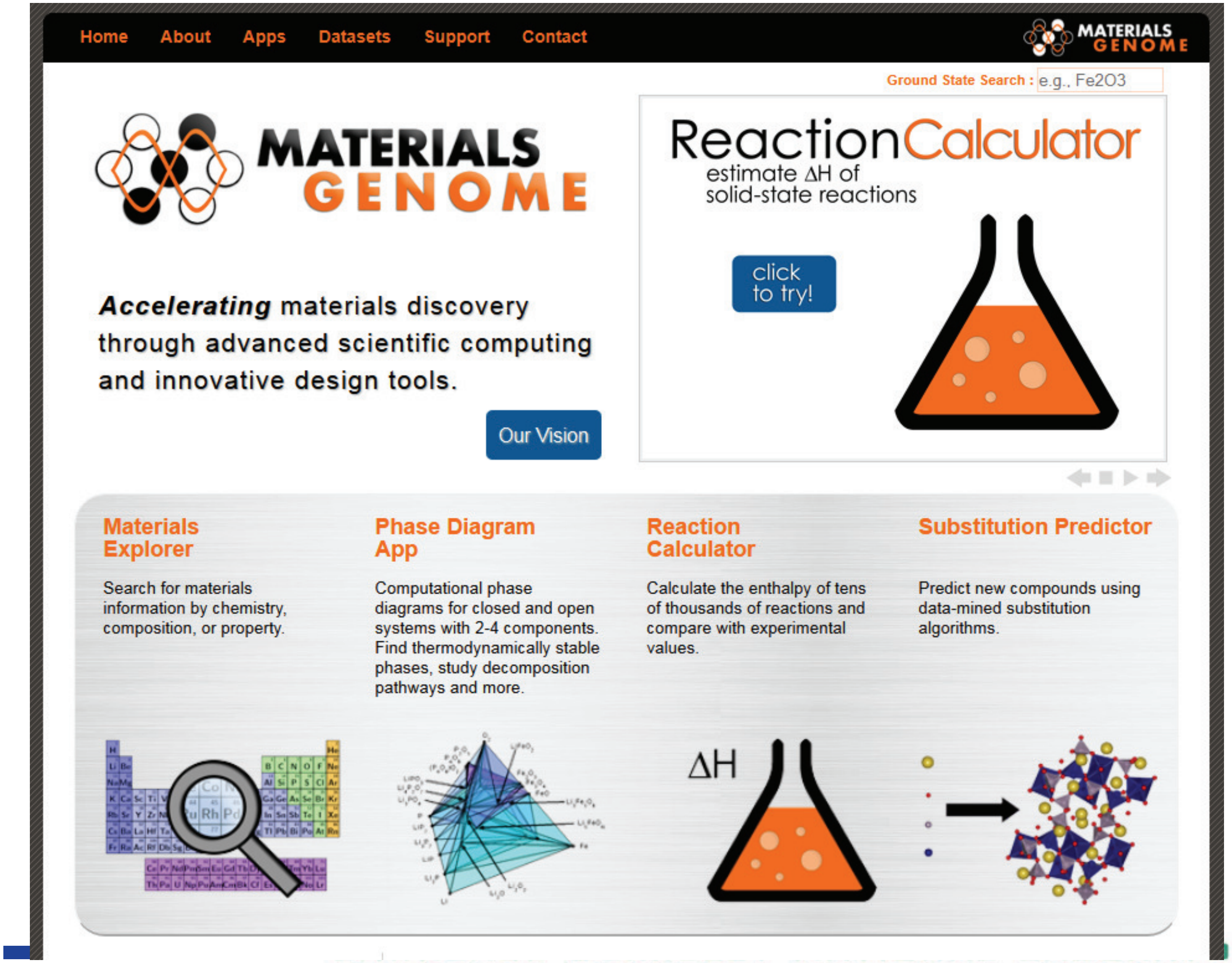
Successfully synthesized 15 different candidate cathode compounds (> 100 samples)



Cathodes currently under electrochemical testing…

Towards a Materials Genome

www.materialsgenome.org alpha version is online!



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

ReactionCalculator

estimate ΔH of solid-state reactions

Materials Explorer

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

Phase Diagram App

Computational phase diagrams for closed and open systems with 2-4 components. Find thermodynamically stable phases, study decomposition pathways and more.

Reaction Calculator

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

Substitution Predictor

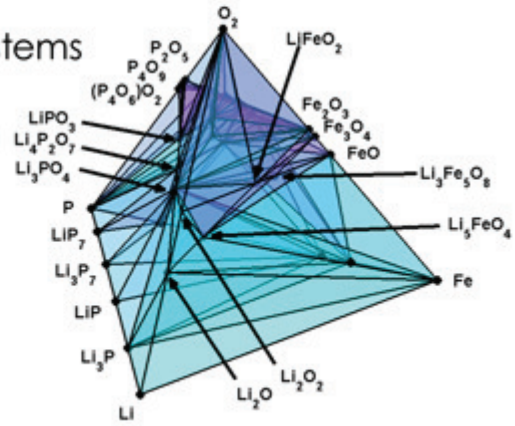
Predict new compounds using data-mined substitution algorithms.

Current Apps – More Coming

PhaseDiagramApp

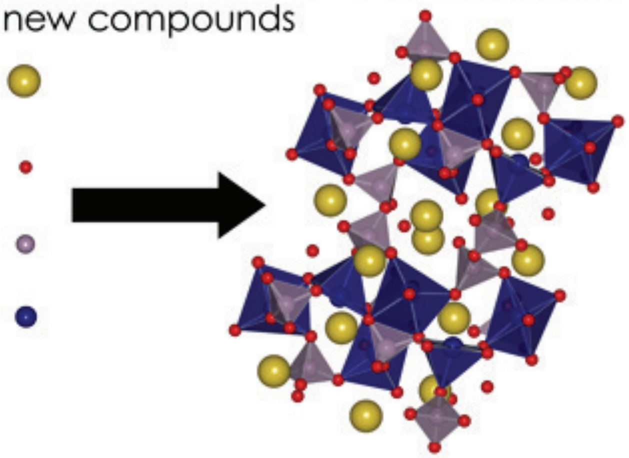
investigate phase
stability for 2-4
component systems

28,300
SYSTEMS



SubstitutionPredictor

predict new compounds



ReactionCalculator

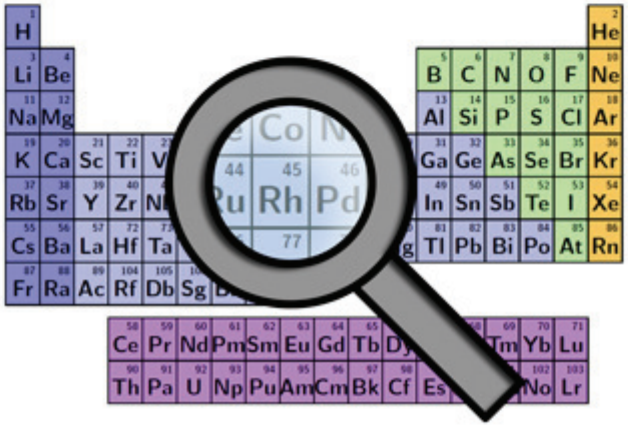
estimate ΔH of
solid-state reactions

>35,000
REACTIONS

Y NAT

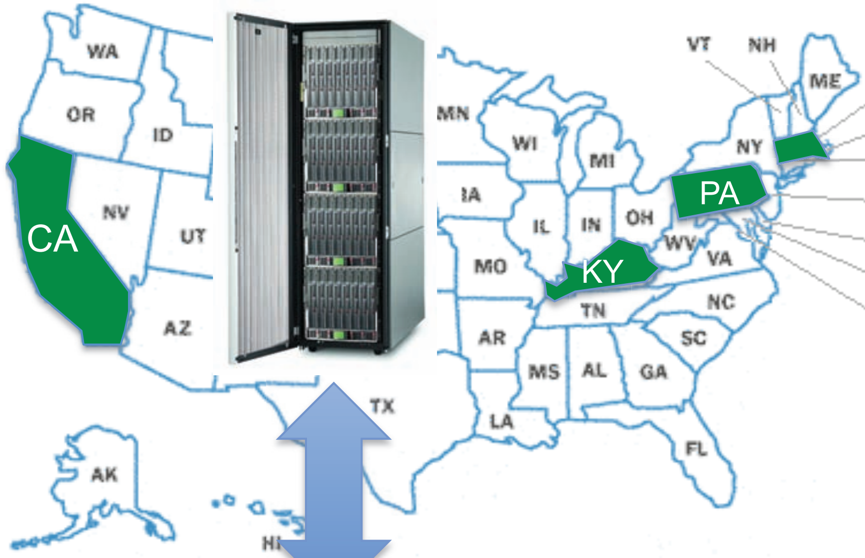
MaterialsExplorer

search the database



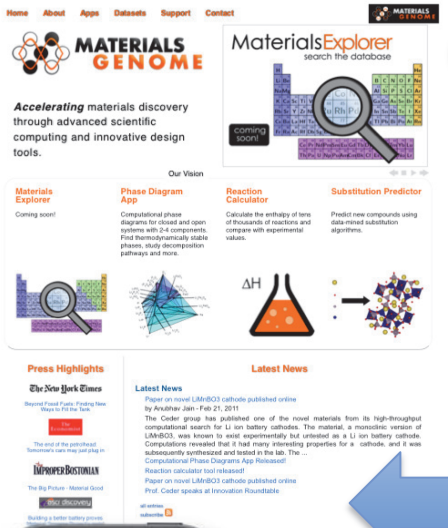
Leveraging the Information Age

Becoming the Discovery Engine of Materials Science



(DataBase)

Calculating ~400 compounds/day



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MATERIALS GENOME

MaterialsExplorer
search the database

coming soon!

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

Our Vision

Materials Explorer
Coming soon!

Phase Diagram App
Computational phase diagrams for closed and open systems with 2-4 components. Find thermodynamically stable phases, study decomposition pathways and more.

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

Substitution Predictor
Predict new compounds using data-mined substitution algorithms.

ΔH

Press Highlights

The New York Times
Beyond Fossil Fuels: Finding New Ways to Fill the Tank

The Economist
The end of the petrolhead. Tomorrow's cars may just plug in

Improper Bostonian
The Big Picture - Material Good

asci discovery
Building a better battery proves

Latest News

Latest News

Paper on novel LiMnBO3 cathode published online
by Anubhav Jain - Feb 21, 2011
The Ceder group has published one of the novel materials from its high-throughput computational search for Li ion battery cathodes. The material, a monoclinic version of LiMnBO3, was known to exist experimentally but untested as a Li ion battery cathode. Computations revealed that it had many interesting properties for a cathode, and it was subsequently synthesized and tested in the lab. The ...

Computational Phase Diagrams App Released!
Reaction calculator tool released!
Paper on novel LiMnBO3 cathode published online
Prof. Ceder speaks at Innovation Roundtable

all entries
subscribe

Which compounds have {x,y,z,…} properties

Invert the design problem

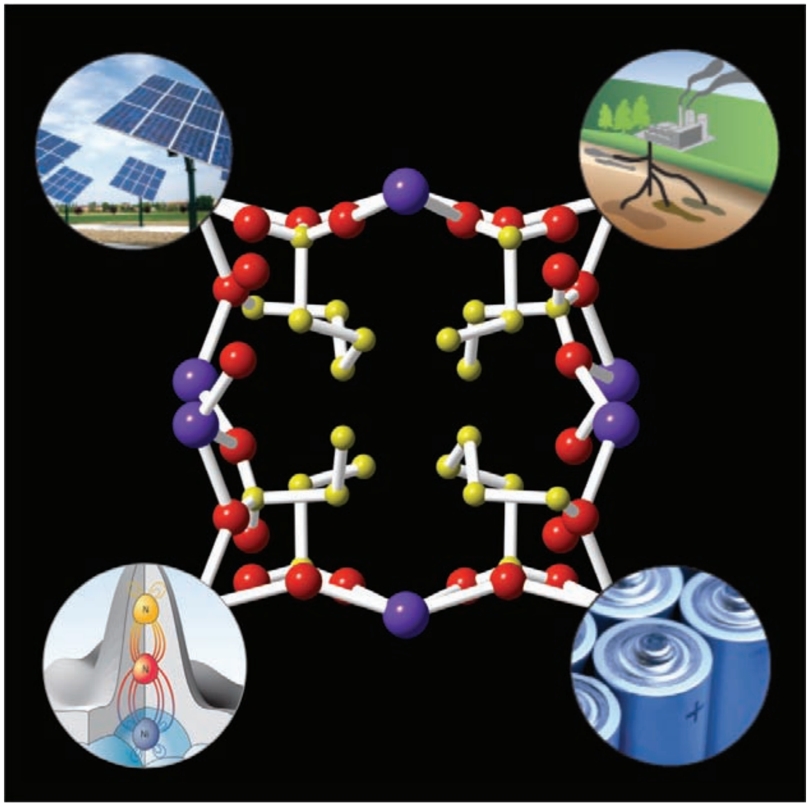
Share the information

….Towards a Materials Genome

Computing all properties of all inorganic materials

MIT
Gerbrand Ceder
Anubhav Jain
Shyue Ping Ong
Geoffroy Hautier

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



LBNL EETD
Kristin Persson
Michael Kocher

LBNL CRD
Juan Meza
David Bailey
Alex Kaiser
Maciej Haranczyk

The End