The Path to Next-Generation Batteries

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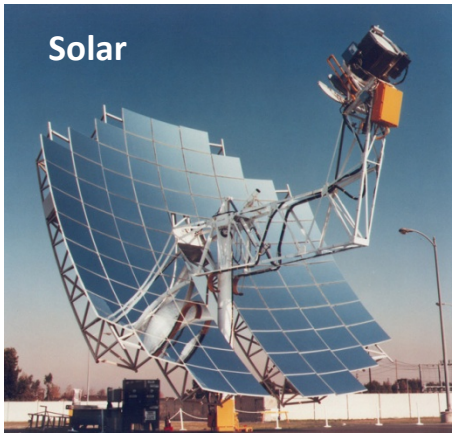
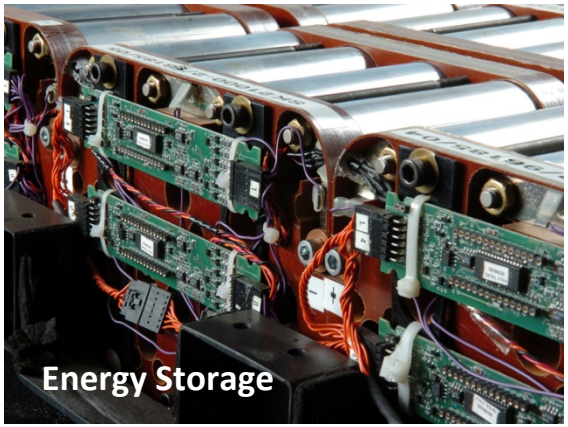
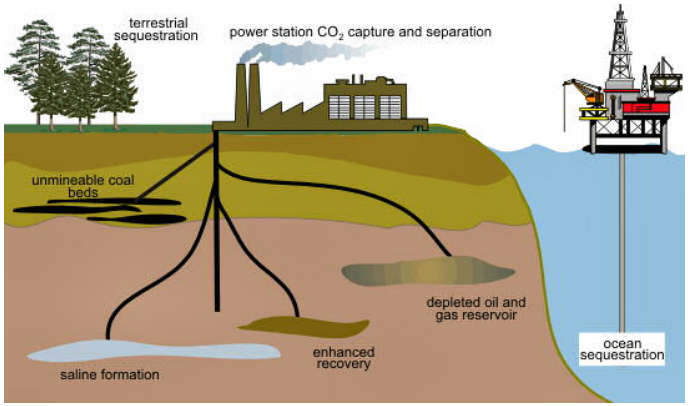
The Challenge:
How will we meet the world's future energy demands?

Sustainable Energy Requires Major Innovations in Science and Technology



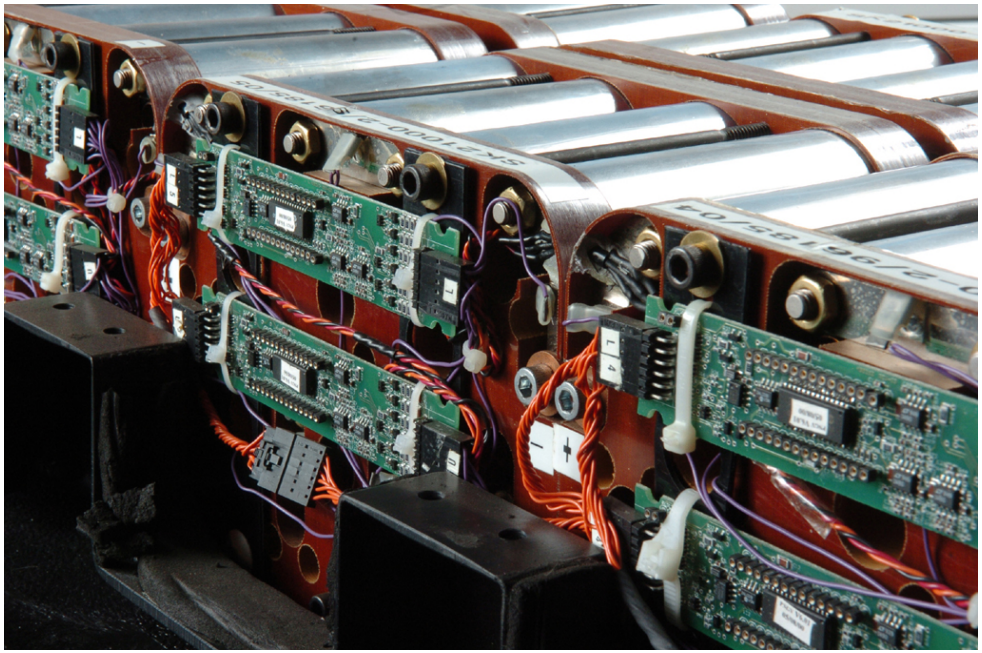


Carbon Sequestration

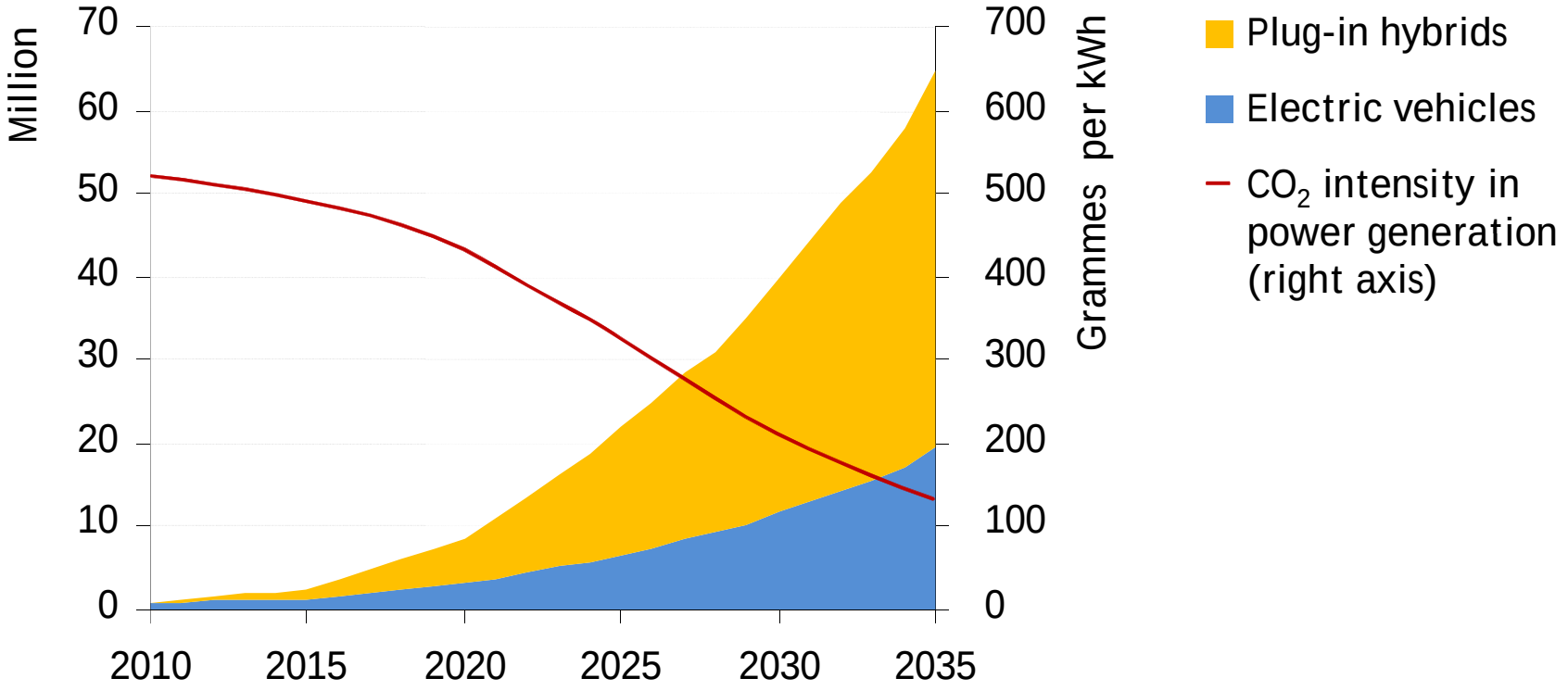


Transforming 21st Century Transportation

- Fully electrified United States transport system (cars & light trucks) will:
  - Cut US oil consumption by 1/3 (7.2 million barrels oil/day)
  - 25% well-to-wheels reduction in carbon footprint
- Need 5-10x improvement in battery energy density



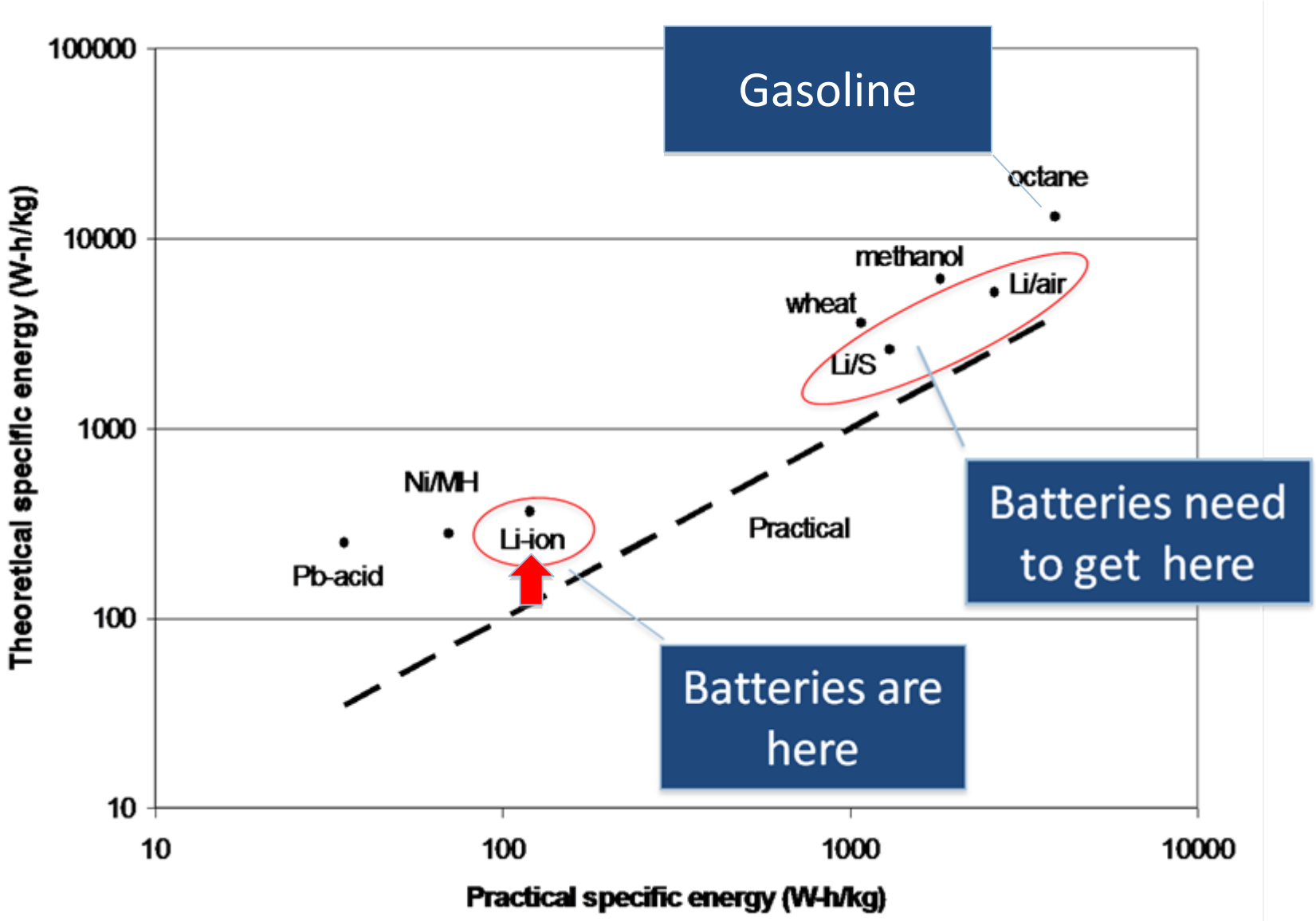
Transforming 21st Century Transportation (cont.)



International Energy Agency projects plug-in hybrids and electric vehicles reach 39% of new sales by 2035

International Energy Agency: World Energy Outlook 2010

Major Gaps Remain in Energy Storage Technology



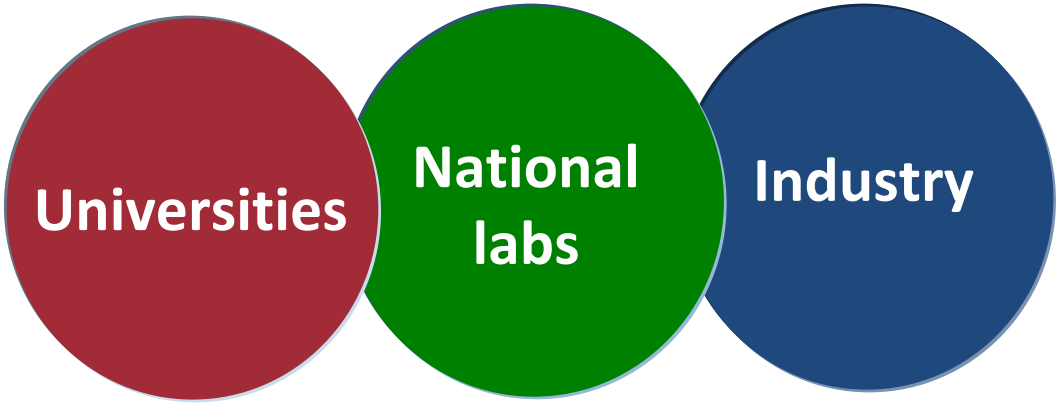
A Vision for Excellence in Energy Storage Research

Discovery Research → Use Inspired Research → Applied R&D → Technology Demo → Technology Deployment

Basic Science
Understand and control materials through rational design, identify and exploit new electrochemical phenomena

Technology Development
Develop materials that approach theoretical maximum energy density, power density, safety, throughput efficiency, and life

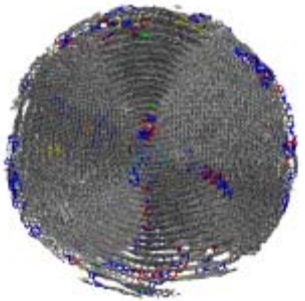
Engineering
Develop low-cost materials and thin film manufacturing processes and novel control systems; integrate technologies for adoption into electric transportation and grid applications



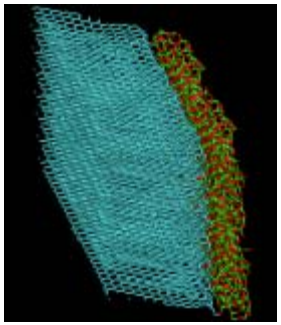
… requires strong partnerships among national laboratories, academia, and industry across the innovation pipeline

Science Challenges for Electrical Energy Storage

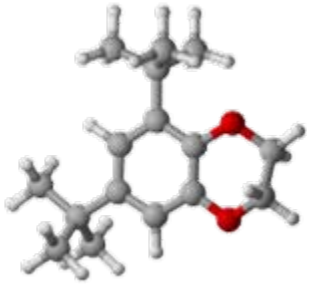
- Materials that maximize energy storage capacities as well as promote charge transport
- Electrocatalytic materials to control electron transfer, bond breaking, and bond formation
- Understand and control electrochemical phenomena in solids and interfaces
- Control of ion and electron transport in extremely heterogeneous media
- Electrolytes that maximize charge transport kinetics with excellent redox and thermal stability
- Control of complex reactions and intercalation products to enable safe energy release



New materials for Li ion storage

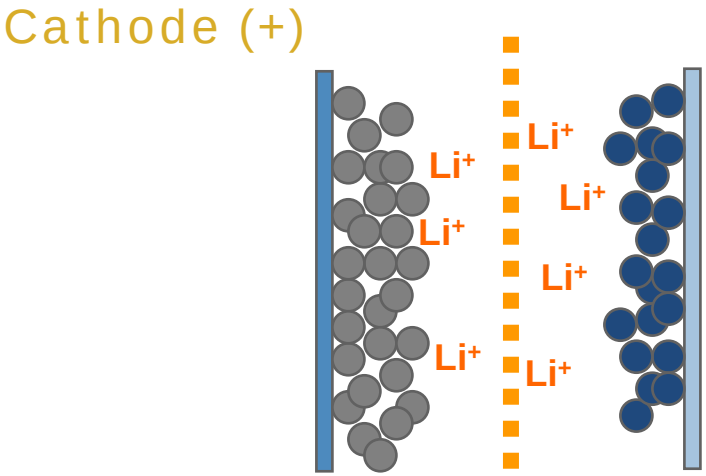


Protective films for anodes and cathodes



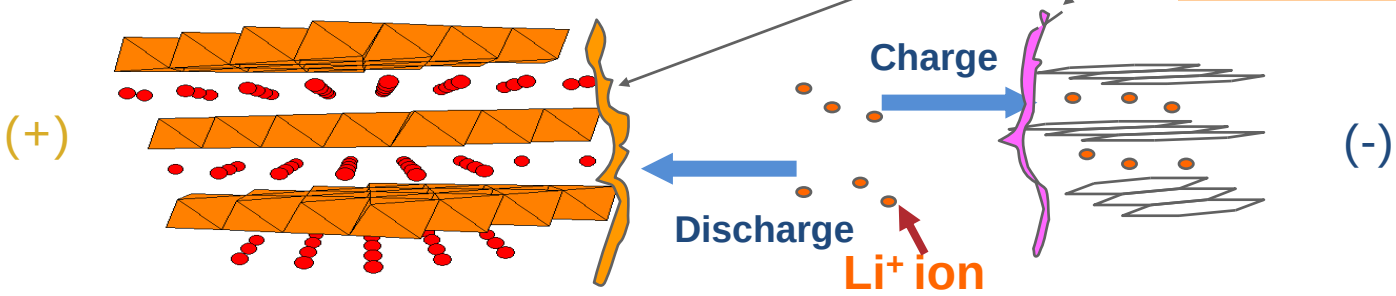
Shuttles for overcharge protection

How Lithium-ion Battery Works



Cell performance impacted by structured electrode materials and effective solid electrolyte interface (SEI)

Solid Electrolyte Interface protect electrode from reacting with electrolyte



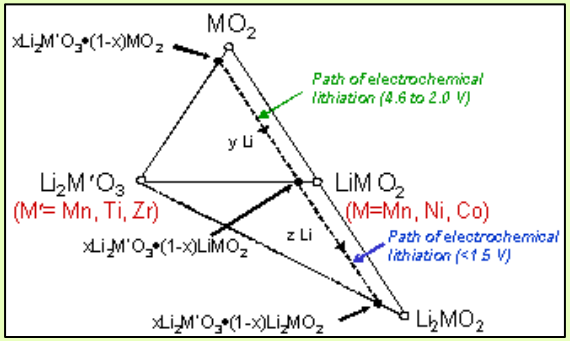
Positive Electrode: Layered oxides
Such as $LiCoO_2$, $LiNiO_2$

$$LiNi_{1-x}Co_xO_2 <-> yLi^+ + Li_{1-y}Ni_{1-x}Co_xO_2$$

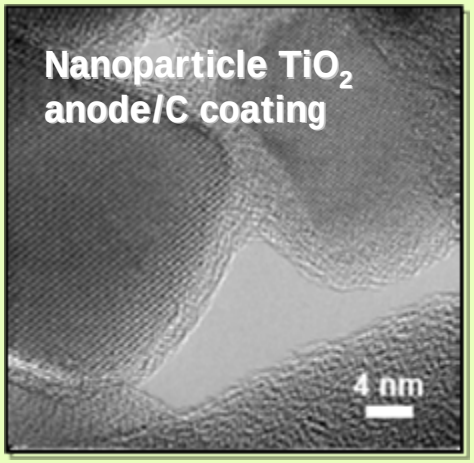
Negative Electrode: Carbon

$$6C + Li <---> C_6Li$$

From Fundamental Research to Cars on the Road

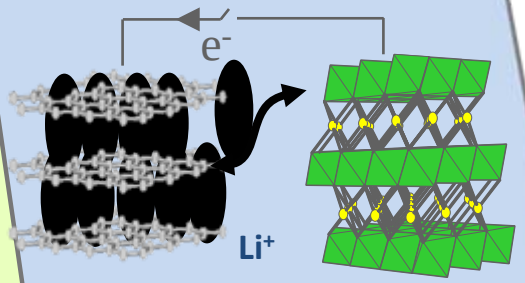


Discovery of new materials for stable, high-capacity cathodes

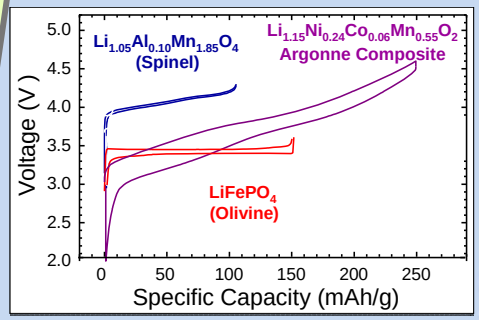


Tailoring electrode-electrolyte interface using nanotechnology

Li_xC_6 (Anode) $xLi_2MnO_3•(1-x)LiMO_2$ (Cathode)



Creating high-energy Li-ion cells with double cathode capacity, enhanced stability

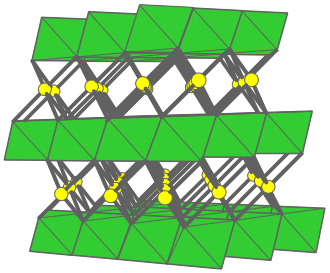


GM VOLT

Licenses to materials and cell manufacturers and automobile companies

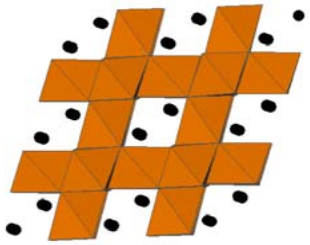
Scientists Develop Fundamental Knowledge of the Material Properties

Ordered Rocksalt
Layered
$LiMO_2$
(**M=Co, Ni, Mn**)



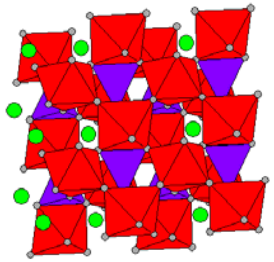
- **Capacity limited to ~ 0.5 Li per M atom (i.e., ~140 mAh/g)**
- **Co^{4+} and Ni^{4+} unstable/highly oxidizing**
- **Structure destabilized at low Li content**
- **Layered $LiMnO_2$ transforms to spinel**

Spinel
LiM_2O_4
(**M=Mn**)



- **Capacity limited to <0.5 Li/Mn at 4 V**
- **Robust M_2O_4 spinel framework; 3-D channels**
- **High rate capability**
- **Jahn-Teller (Mn^{3+}) distortion at 3 V**
- **Solubility problems at high potentials**

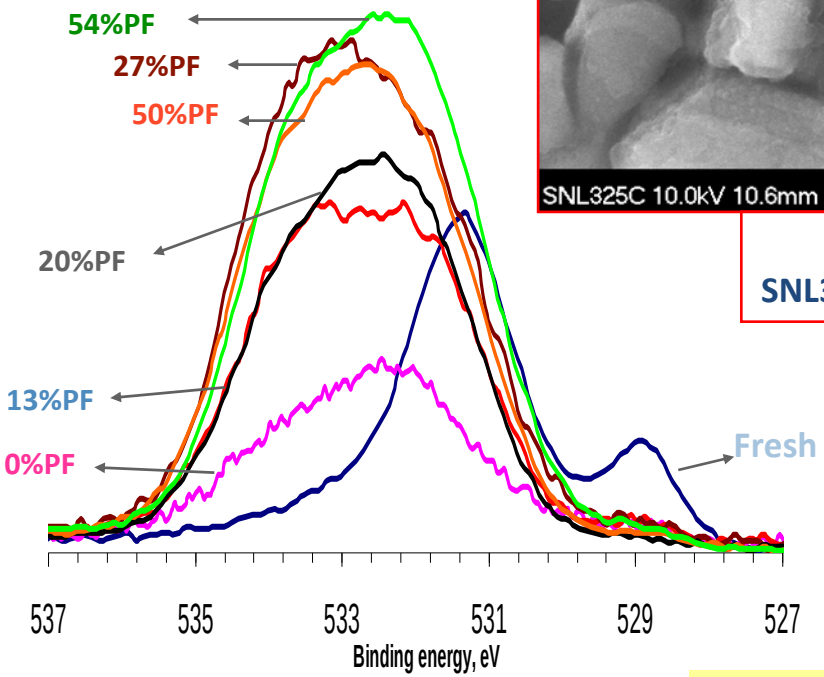
Olivine
$LiMPO_4$
(**M=Fe, Mn**)

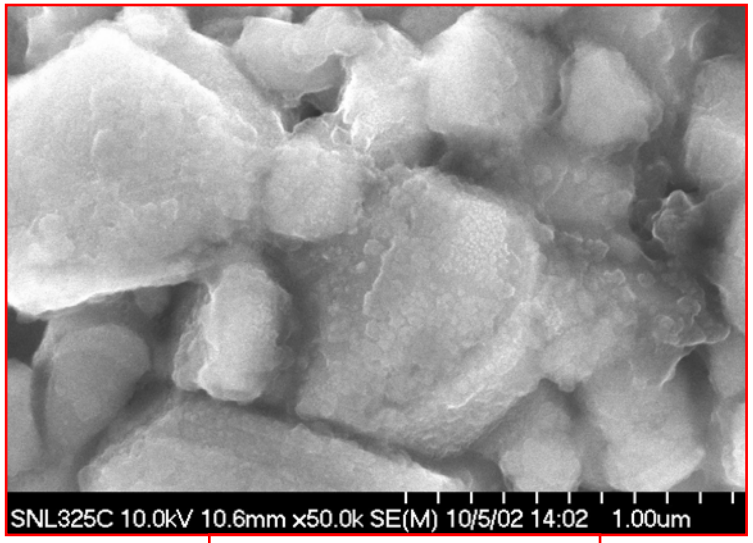


- **Capacity limited to 1 Li/Fe; P inactive**
- **Excellent structural and thermal stability**
- **1-D channels**
- **Poor electronic and Li-ion conductivity**
- **Poor packing density**

Fundamental Knowledge Combined with Analysis of the Challenges (e.g. Cathode Surface Film Changes over Time)

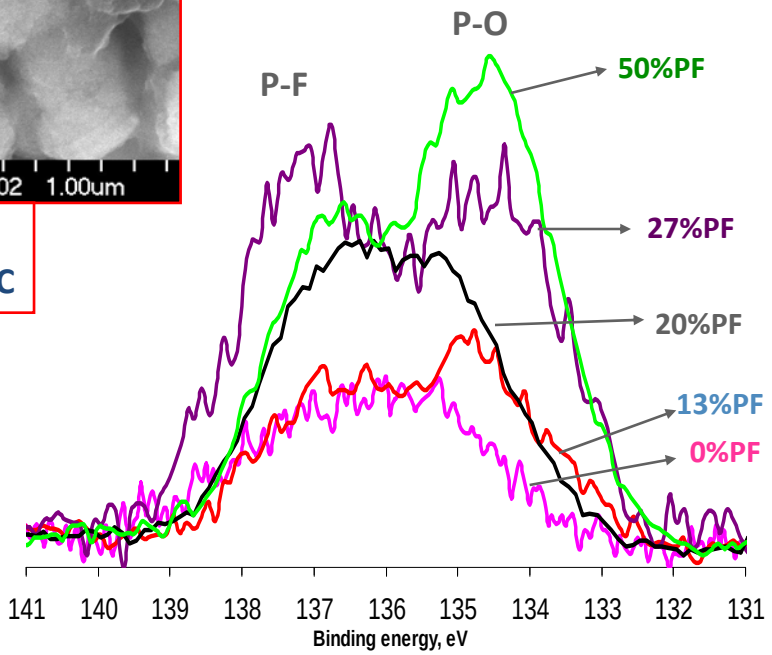
O1s XPS spectra show ROR/ROLi peak growth on aging





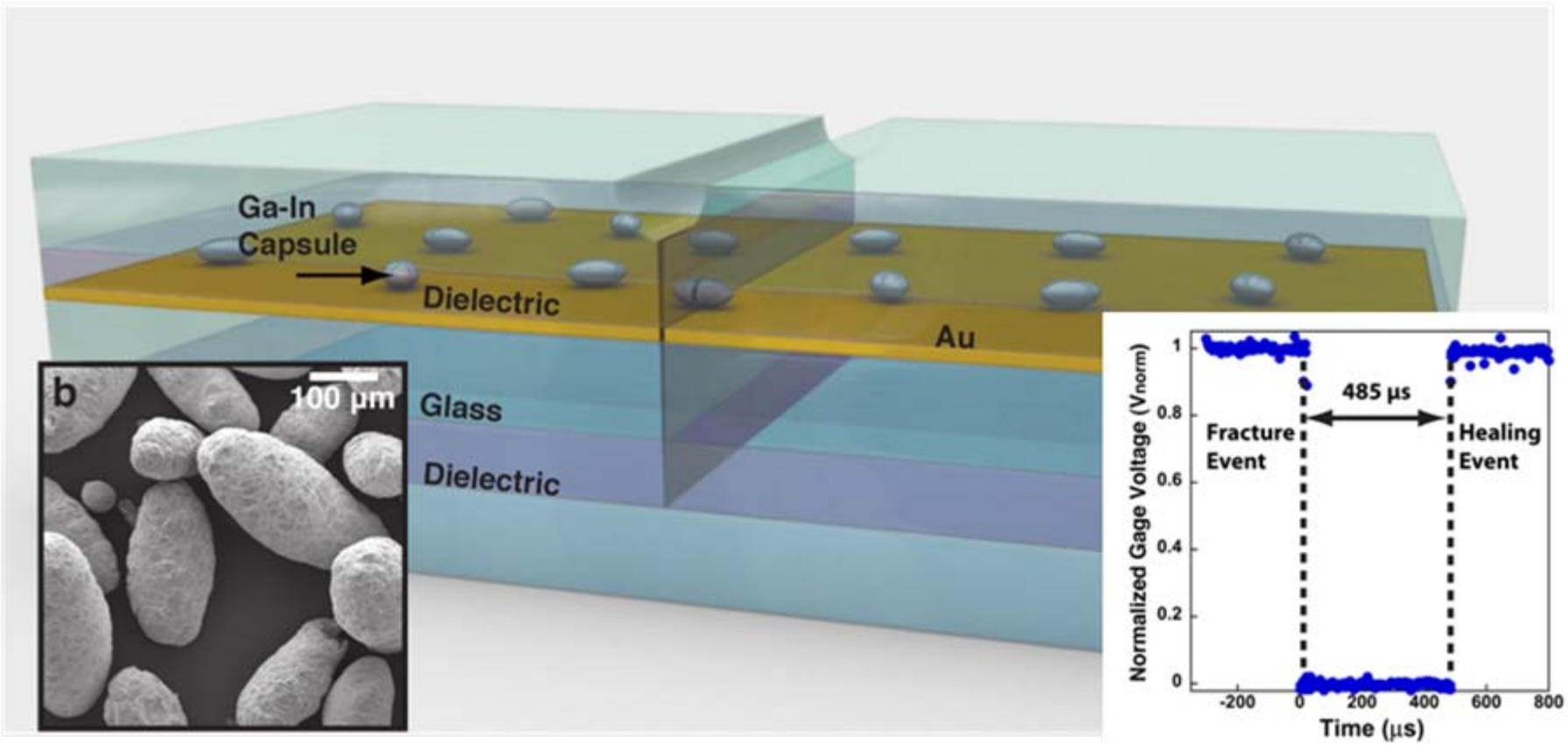
SEM image
SNL325, 45°C, 80%SOC

P2p XPS spectra show P-O bond changes on aging



XPS analysis area: 1 sq. mm.

New Interfaces could Make Li-ion Batteries Self-healing, Safer



Center for Electrical Energy Storage, J. Moore, N. Sottos, S. White (UIUC), K. Amine (ANL)

Argonne NATIONAL LABORATORY

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

NORTHWESTERN
UNIVERSITY

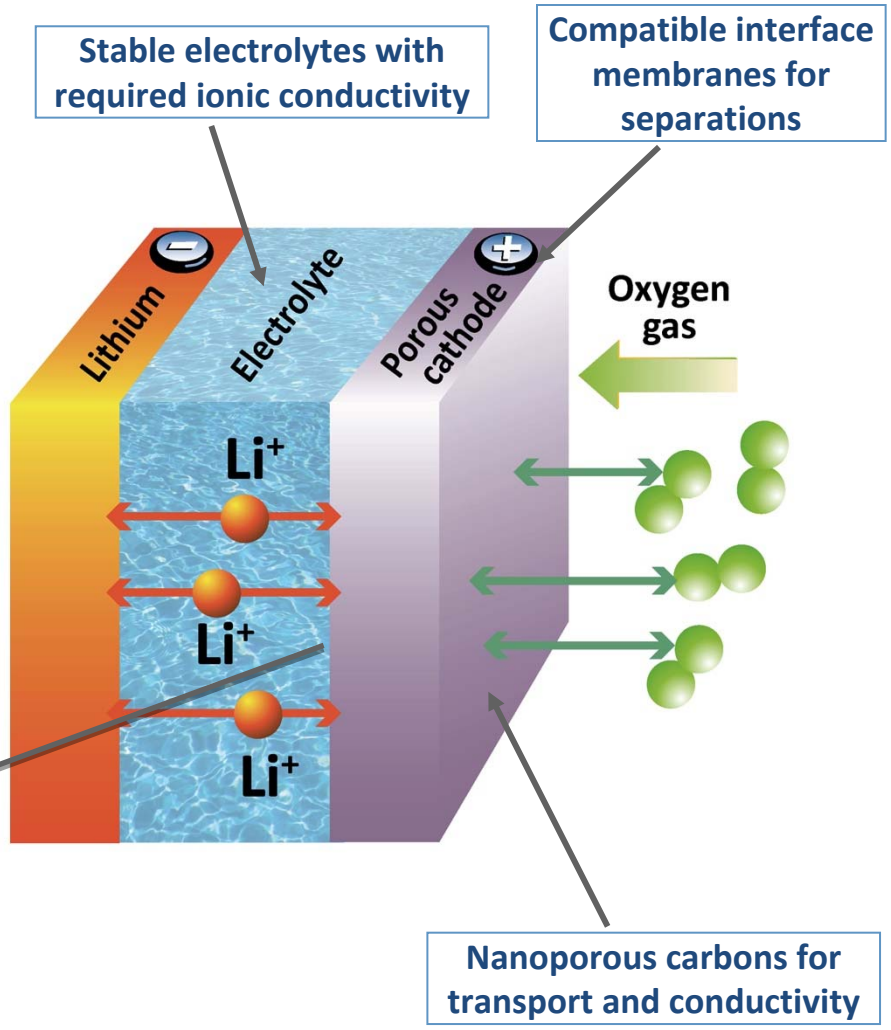
The Future Beyond Lithium-ion: Lithium-air

Theoretical 10x increase in energy density

- **Specific energy: 11,000 Wh/kg**

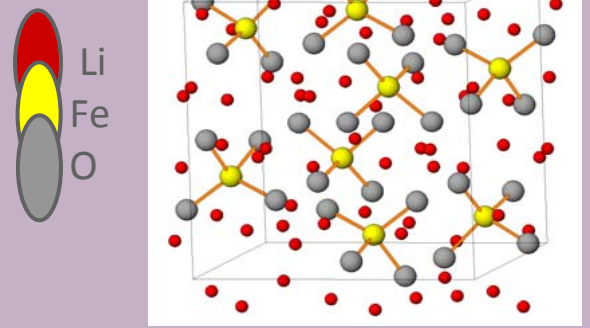
  (Gasoline: 13,000Wh/kg)

- **500-mile electric vehicles**
- **Fundamental science challenges in new cathode materials, catalysts**



New catalyst for cathode

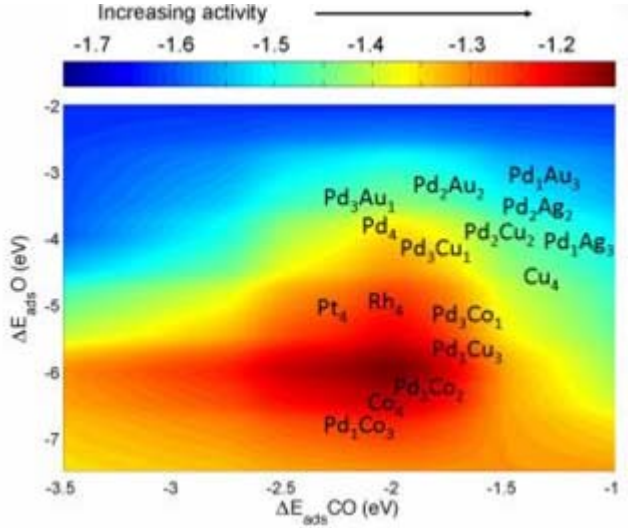
Li_5FeO_4 (Pbca)



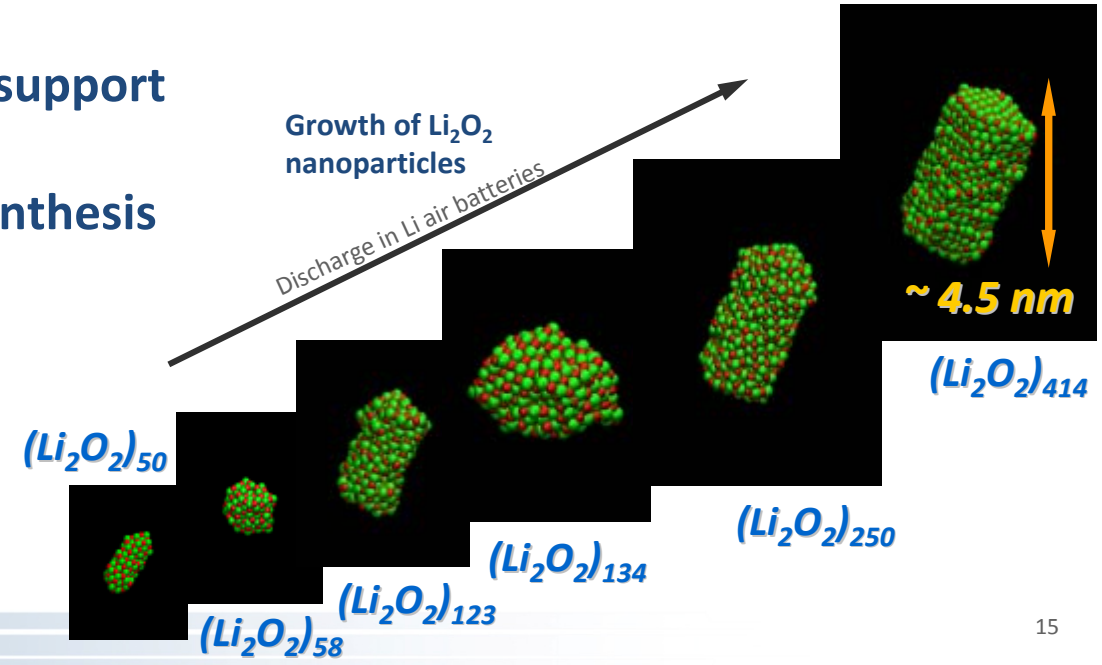
Johnson, Amine et al., Argonne National Laboratory

Computational Chemistry and Materials Science: Designing What You Make

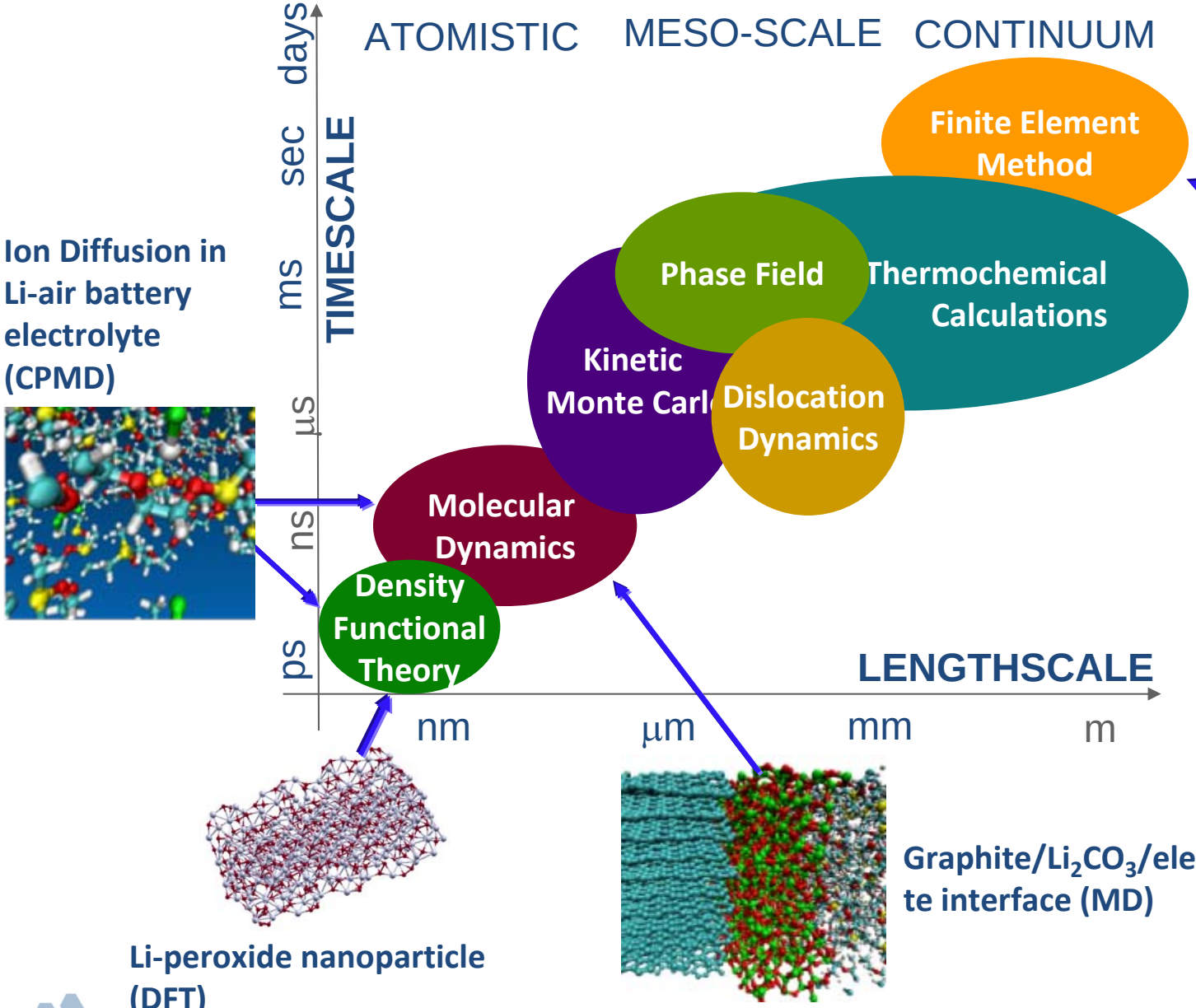
- New and improved *ab initio* methods
- Simpler models with same/better accuracy as *ab initio*
- Effective means of multiscale computation
- Software engineering and code support
- Computation to aid materials synthesis
- Path to exascale computation



Volcano plots for screening of catalysts for Li-air batteries



Multi-scale Theory and Computation – "Battery Computer Simulator"



Summary

- Must create an innovation ecosystem made up of national laboratories, universities, and industry (in a public-private partnership) to transform energy storage and enable transportation electrification and integration of renewables on the grid

- Must address basic science challenges to achieve the necessary technology breakthroughs

- Must use multi-scale theory and computation to create new materials and chemistries, address the basic science challenges, and drive innovation


Discussion