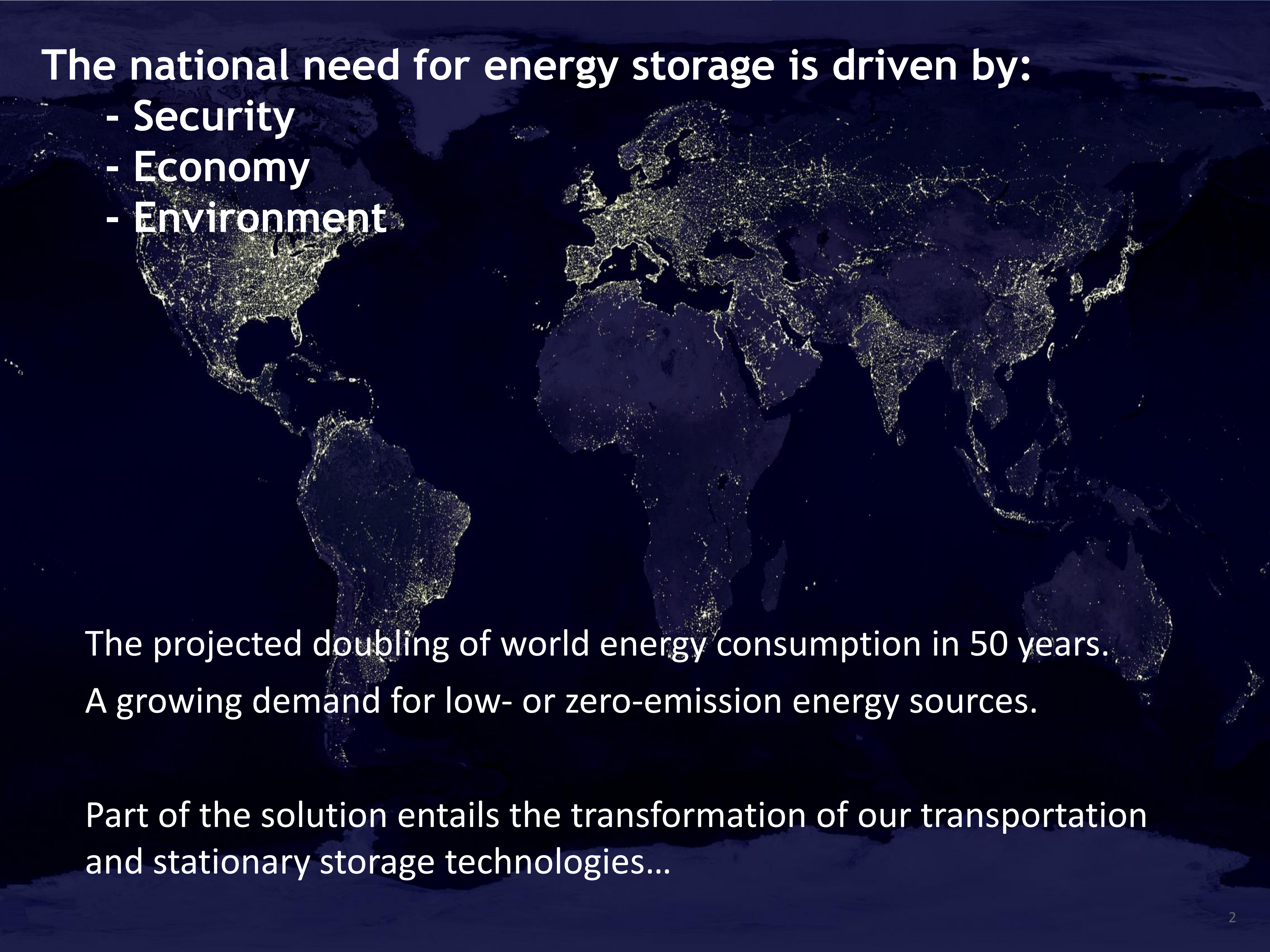
ANL Battery Program Overview

Jeff Chamberlain

July 22, 2013



The national need for energy storage is driven by:

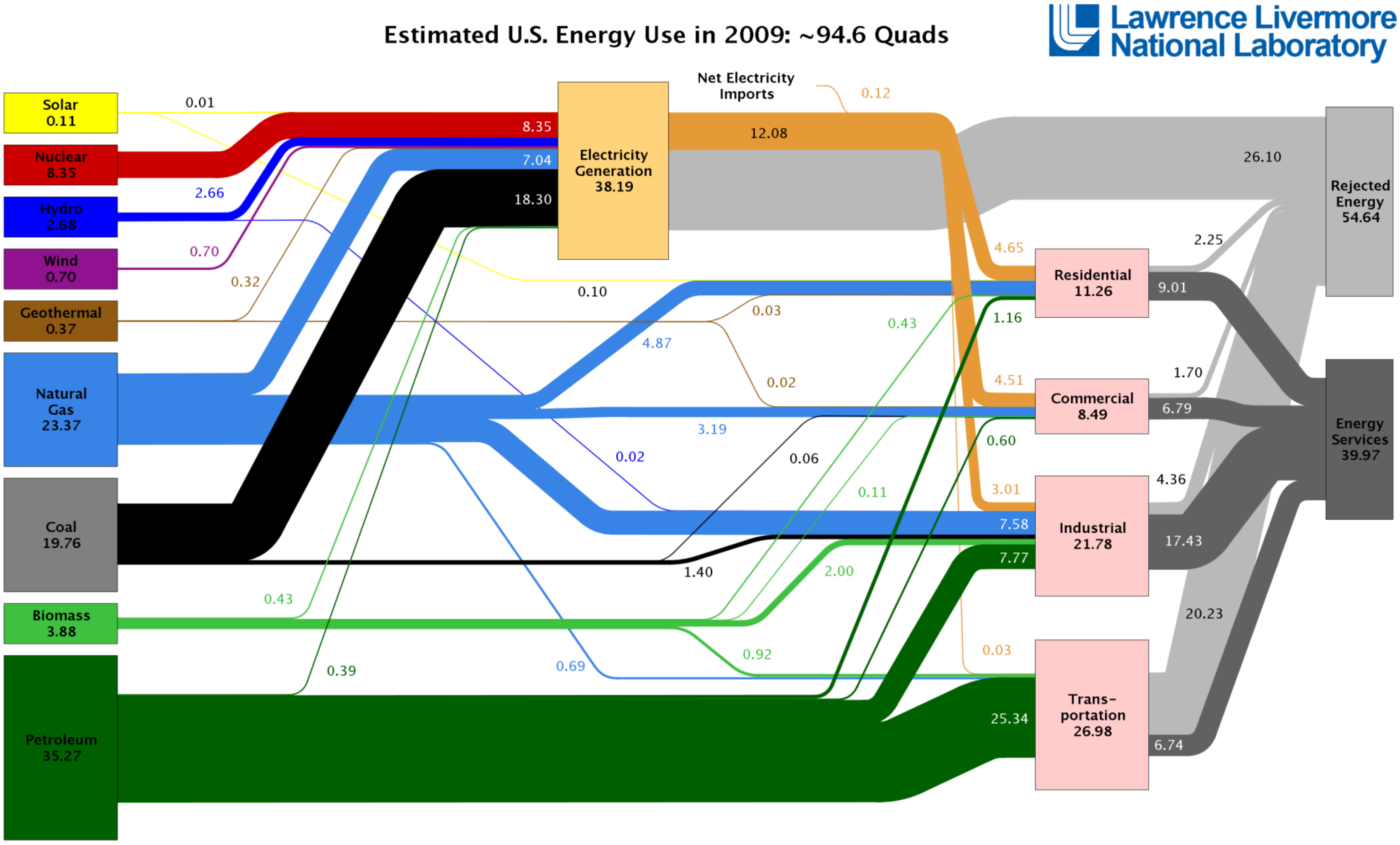
- Security
- Economy
- Environment

The projected doubling of world energy consumption in 50 years.

A growing demand for low- or zero-emission energy sources.

Part of the solution entails the transformation of our transportation and stationary storage technologies…

Energy flow chart shows relative size of primary energy resources and end uses in U.S.

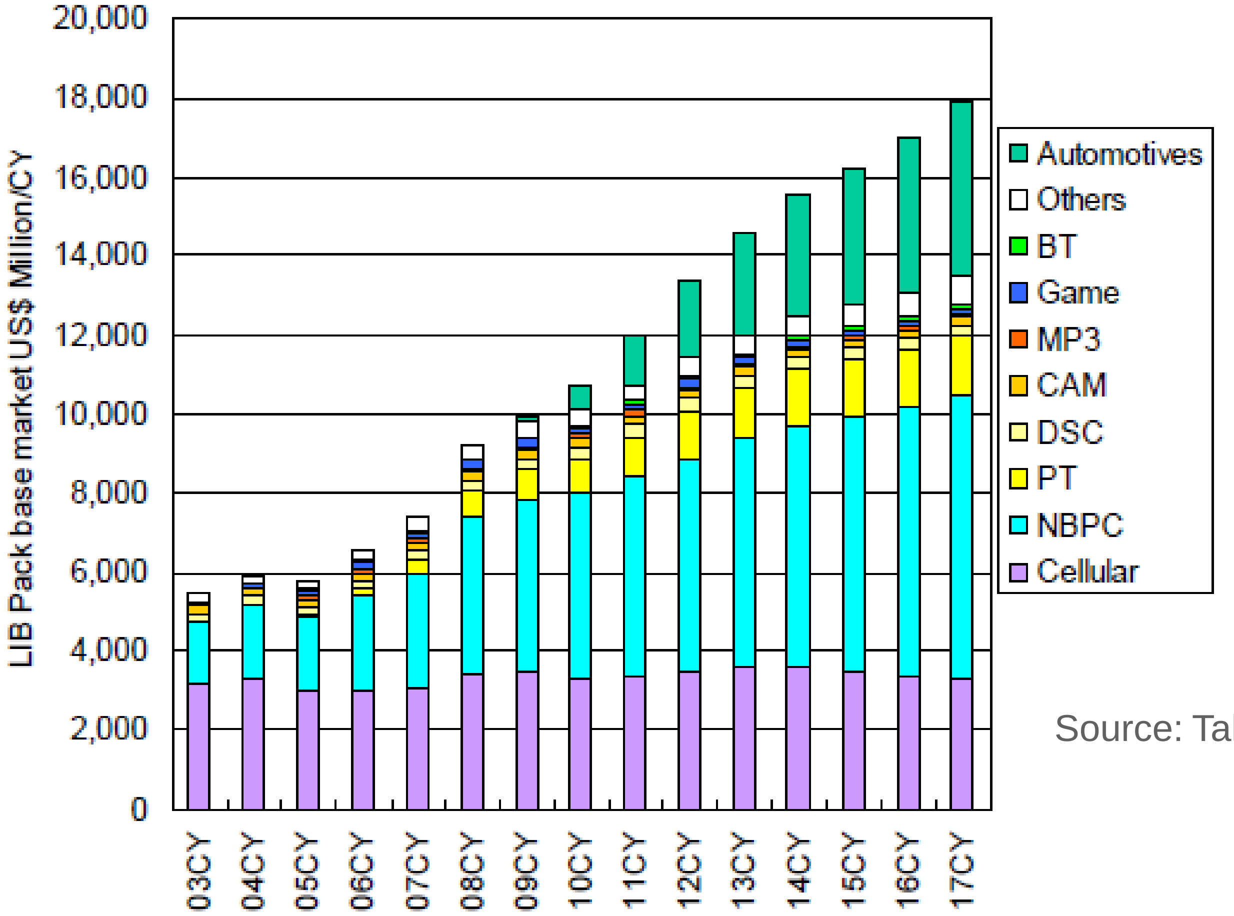


Estimated U.S. Energy Use in 2009: ~94.6 Quads

Lawrence Livermore National Laboratory

Source: LLNL 2010. Data is based on DOE/EIA-0384(2009), August 2010. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports flows for non-thermal resources (i.e., hydro, wind and solar) in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 80% for the residential, commercial and industrial sectors, and as 25% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

Economic Drivers are Enormous: transportation

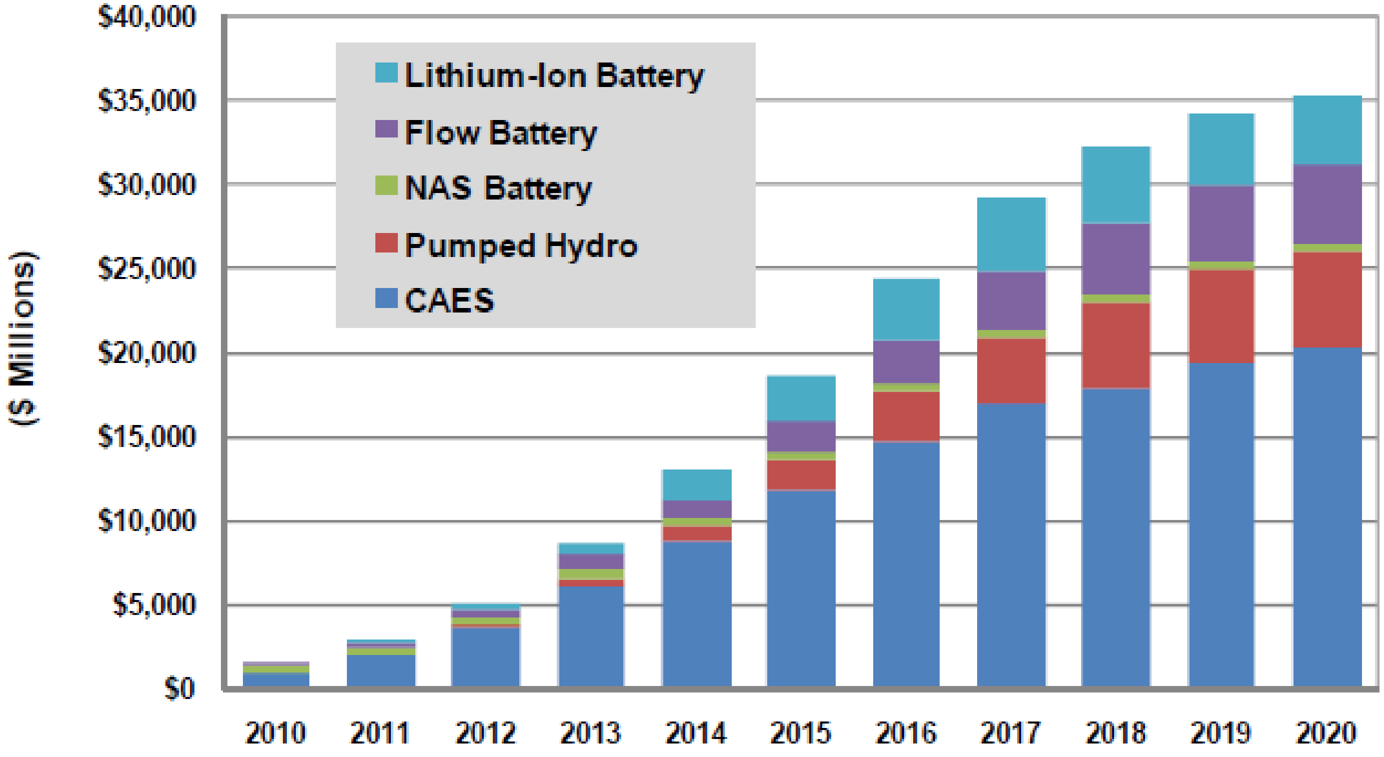


Source: Takeshita Report, 2008

- 5% penetration of PHEVs = $18B in annual revenue, for battery packs alone (assuming current estimates of $7500/pack)

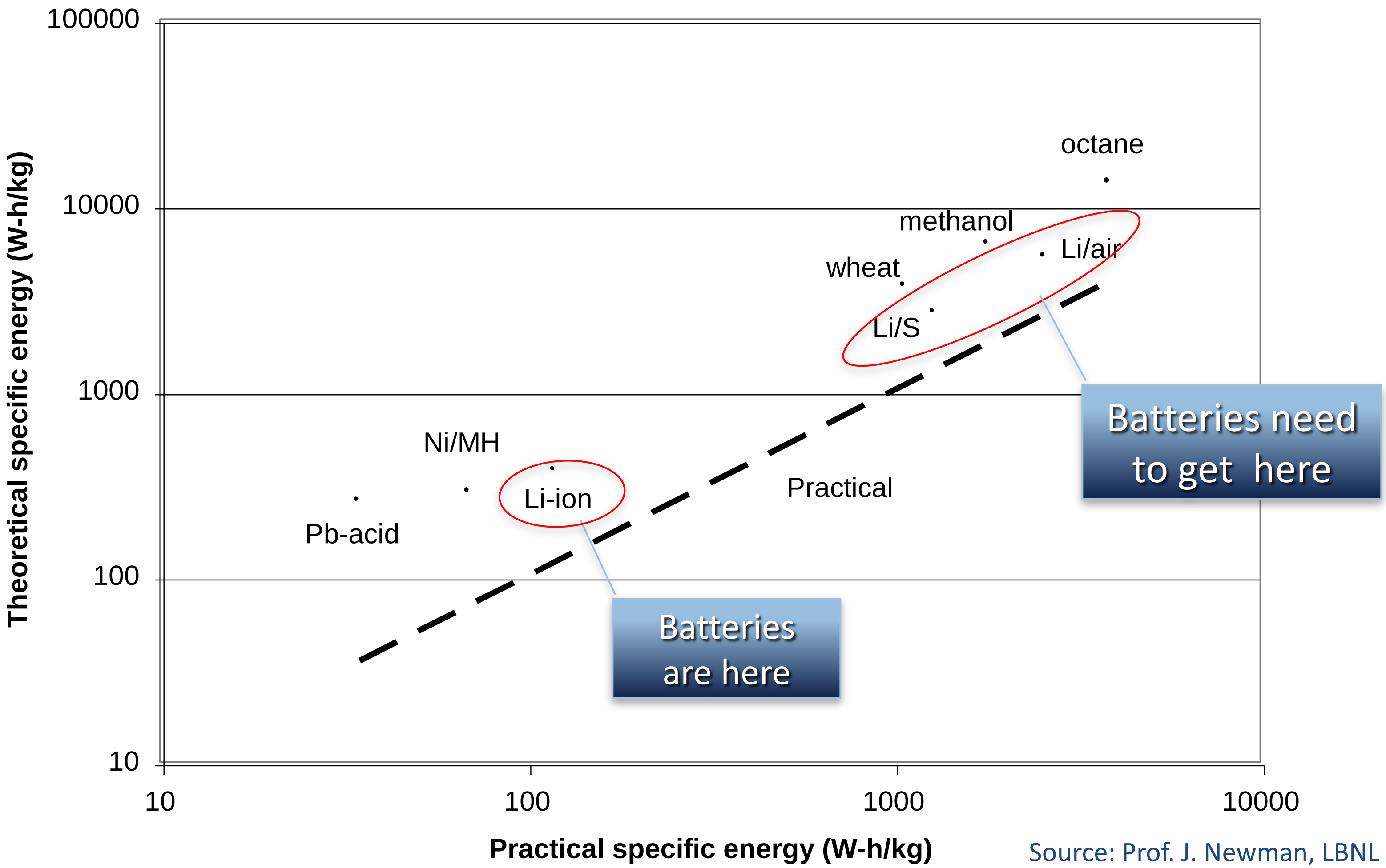
Economic Drivers are Enormous: **grid**

Chart 1.1 Installed Revenue Opportunity by ESG Technology, World Markets: 2010-2020



(Source: Pike Research)

We have interest in all non-aqueous battery technologies

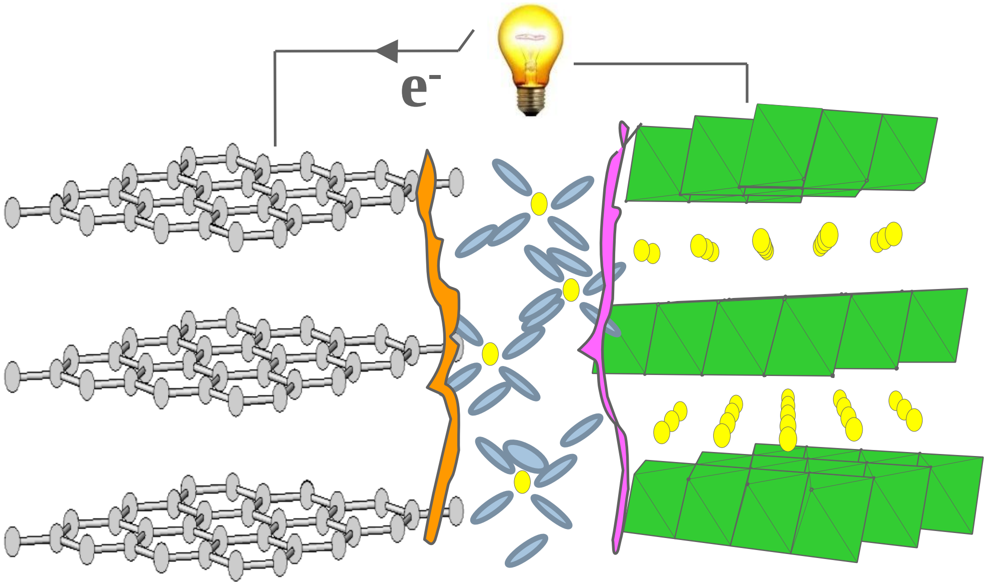


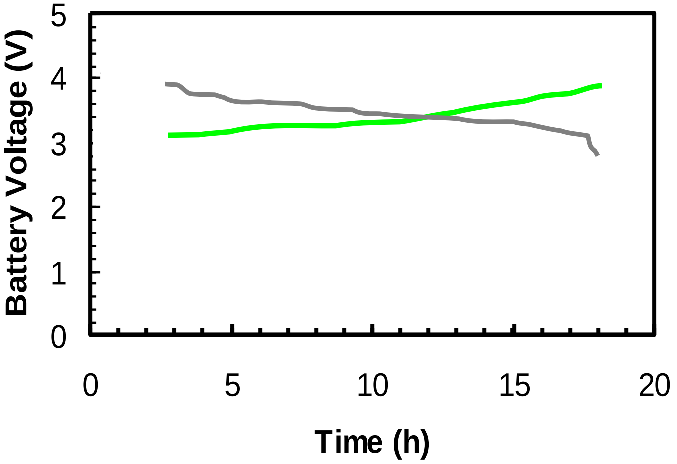
Batteries need to get here

Batteries are here

Source: Prof. J. Newman, LBNL

Schematic of a $Li_xC_6/Li_{1-x}CoO_2$ Li-Ion Cell Commercialized by Sony in 1991





Li_xC_6 (Anode)

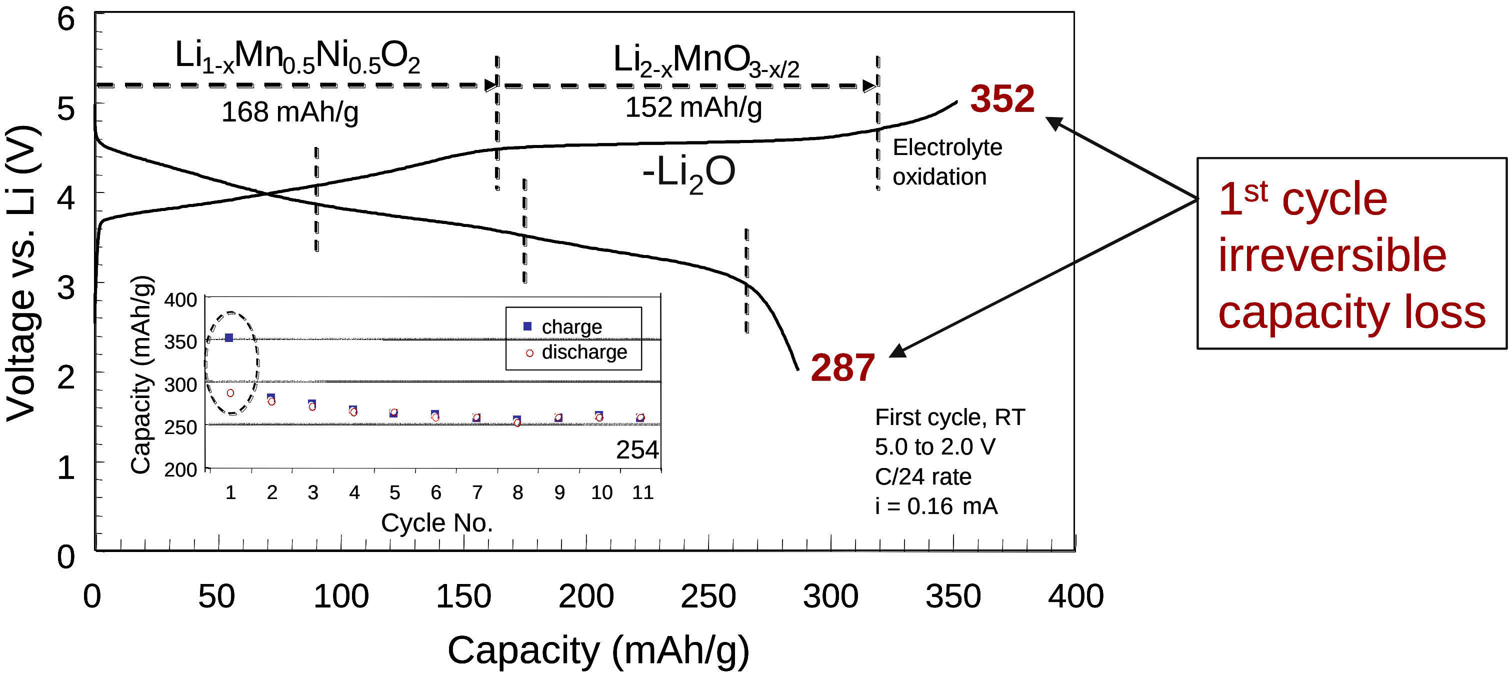
$LiCoO_2$ (Cathode)

- $$LiCoO_2 + 6C \underset{\text{discharge}}{\overset{\text{charge}}{\rightleftarrows}} Li_{1-x}CoO_2 + Li_xC_6$$

Graphite building block

x ~0.5 in practice (cathode limited)

Electrochemistry of a $Li/0.3Li_2MnO_3 \bullet 0.7LiMn_{0.5}Ni_{0.5}O_2$ Cell



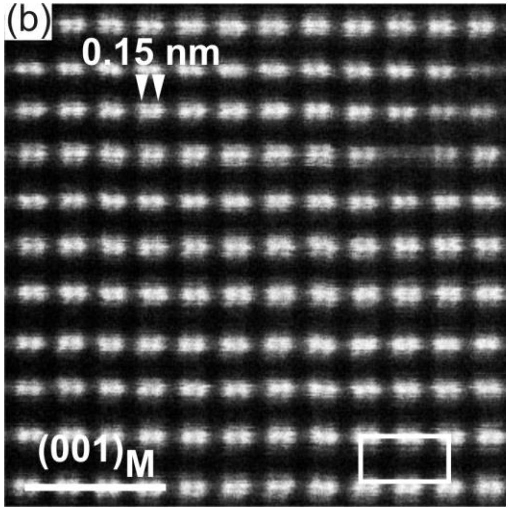
1st cycle irreversible capacity loss

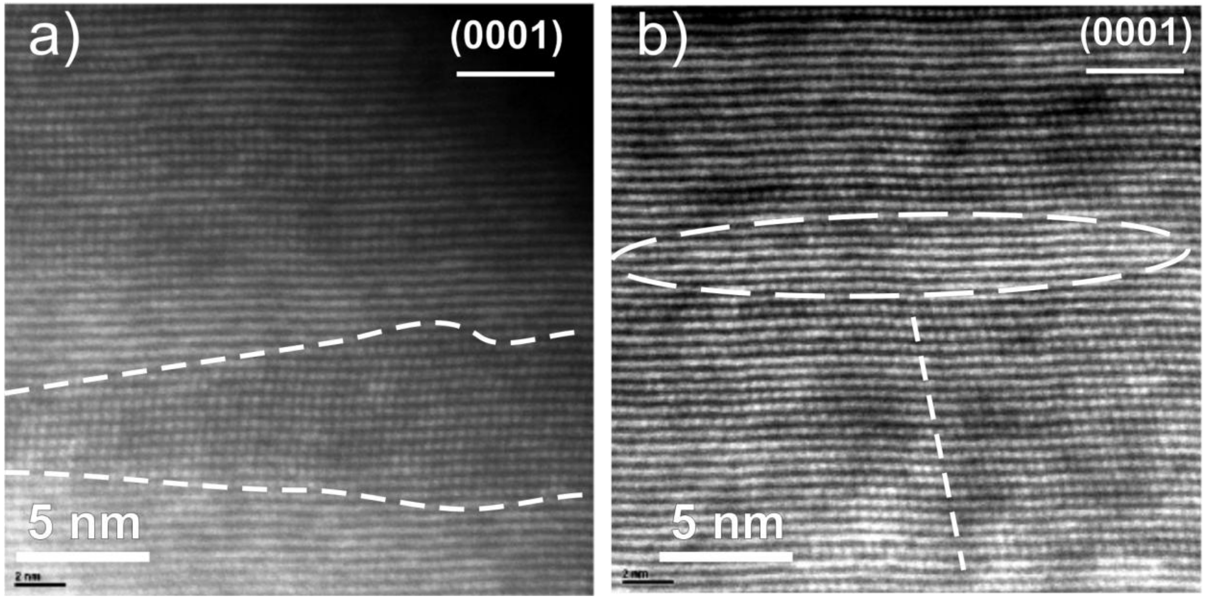
- Theoretical capacity of $LiMn_{0.5}Ni_{0.5}O_2$ Component: 184 mAh/g
- Theoretical capacity of Li_2MnO_3 Component: 158 mAh/g
- Theoretical charge capacity (total): 342 mAh/g
- Coulombic efficiency: 82% (1st cycle); >99% (10th cycle)
- Capacity (10th cycle): 254 mAh/g

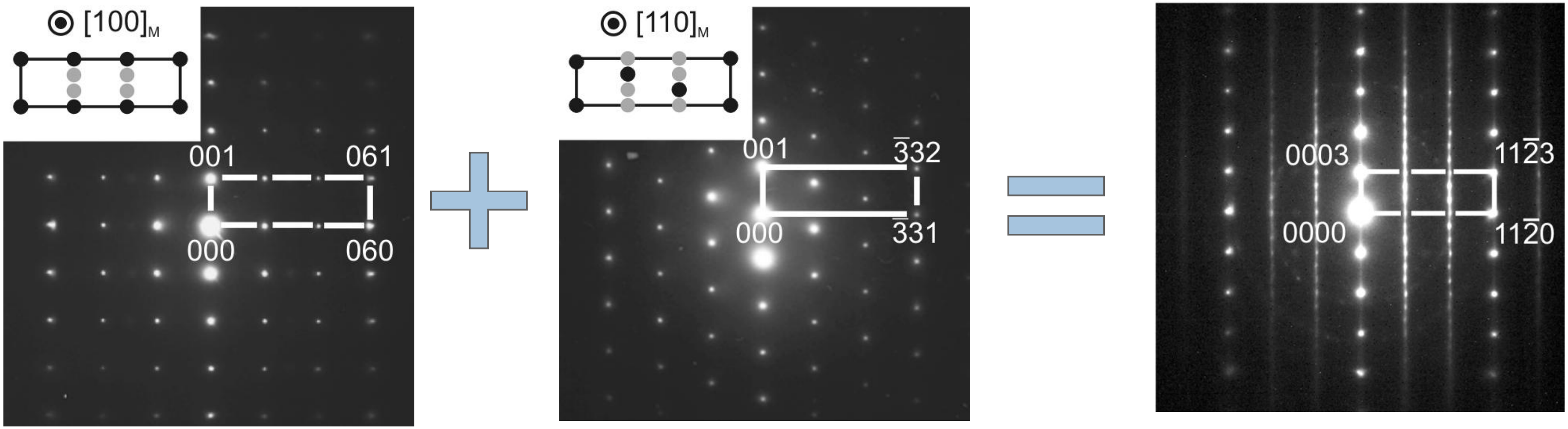
HAADF-STEM

$Li_{1.2}Co_{0.4}Mn_{0.4}O_2$

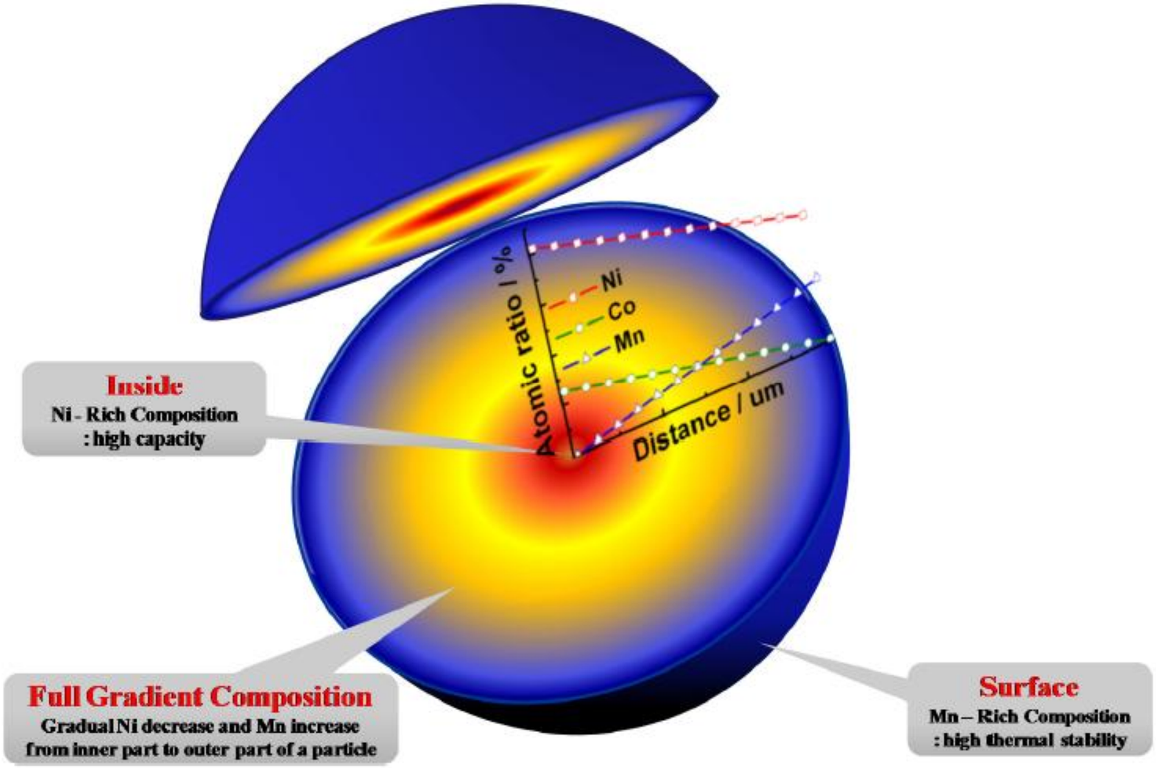
Li_2MnO_3







High Energy Continuous Gradient materials (FGM) with average composition $LiNi_{0.6}Co_{0.10}Mn_{0.30}O_2$



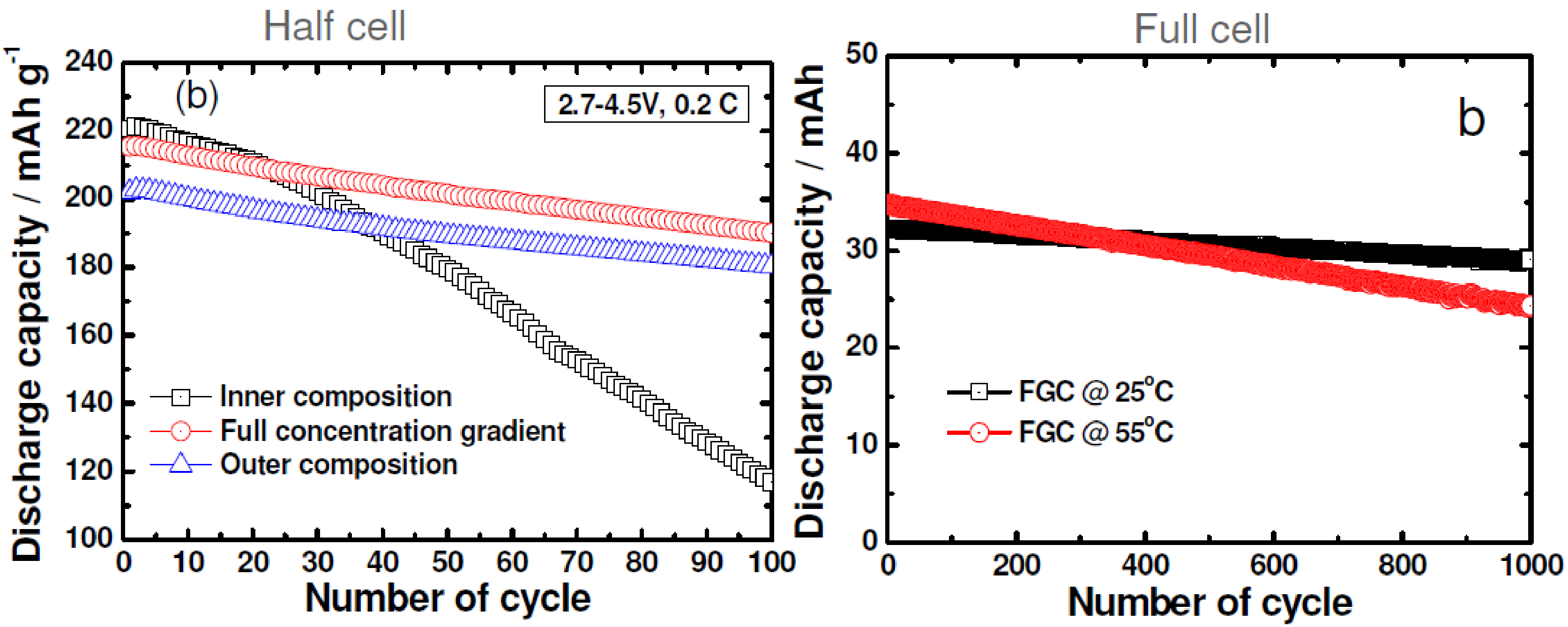
Inside
Ni - Rich Composition
: high capacity

Full Gradient Composition
Gradual Ni decrease and Mn increase from inner part to outer part of a particle

Surface
Mn – Rich Composition
: high thermal stability

Schematic diagram of the full concentration gradient lithium transition metal oxide particle with the nickel concentration decreasing from the center toward outer layer and the concentration of manganese increasing accordingly.

Half and Full Cell Cycling performance of High Energy Full Gradient materials (FGM) at 25 and 55°C

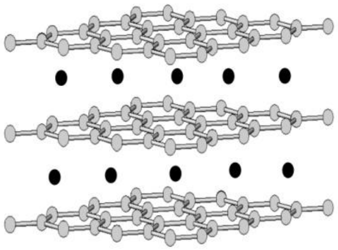


Full concentration gradient shows high capacity and very limited capacity fade after 1000 cycles at 55°C in a full cell, Electrolyte used is $LiPF_6$/EC:EMC with 1%VC

Li-Ion Batteries: Anode Materials

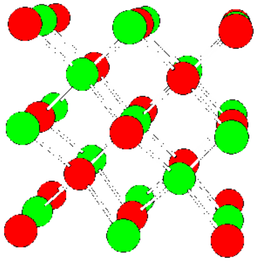
- Carbon
  - **Graphite:** <100 mV vs. Li^0
  - Moderate capacity (372 mAh/g)
  - Highly reactive, surface protection necessary

LiC_6



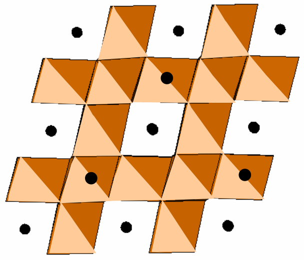
- Metals, Semi-metals and Intermetallic Compounds
  - Al, **Si,** CoSn, Cu_6Sn_5: <0.5 V vs. Li^0
  - High gravimetric/volumetric capacities (1000-4000 mAh/g)
  - Large volume expansion on reaction with lithium
  - Reactive, surface protection required
  - ***Greatest opportunity and challenge***

LiAl

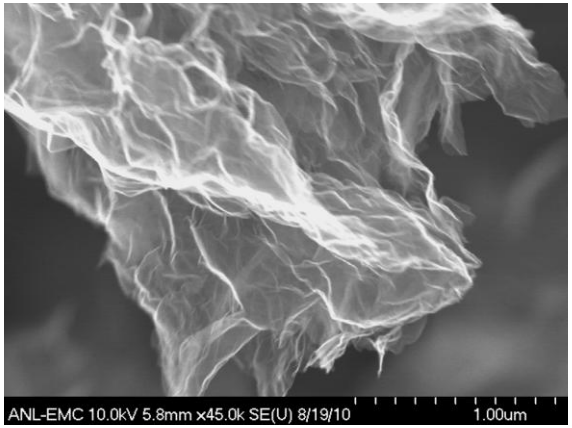


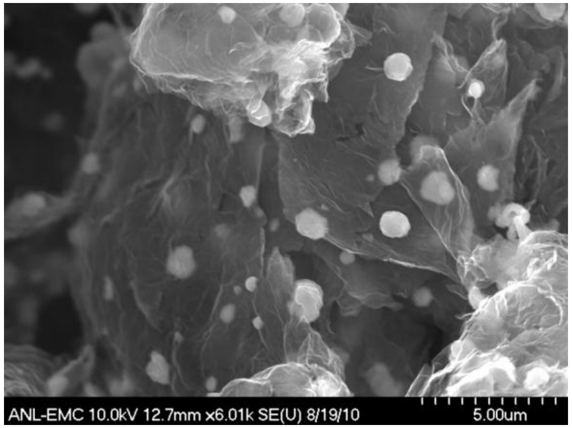
- Metal Oxides
  - **$Li_4Ti_5O_{12}$** ($Li[Li_{1/3}Ti_{5/3}]O_4$) Spinel: 1.5 V vs. Li^0
  - Low capacity (175 mAh/g)
  - Very high rate capability
  - Stable in nanoparticulate form

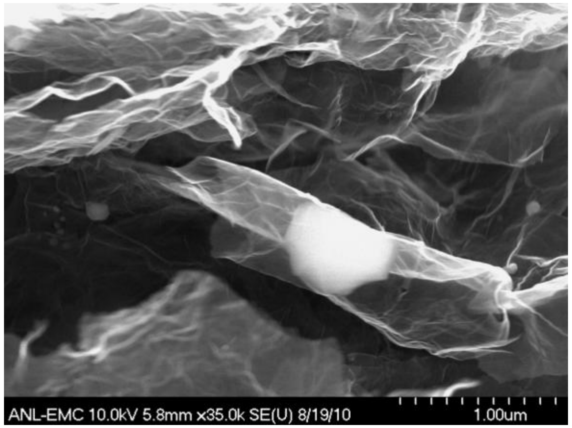
$Li_7Ti_5O_{12}$

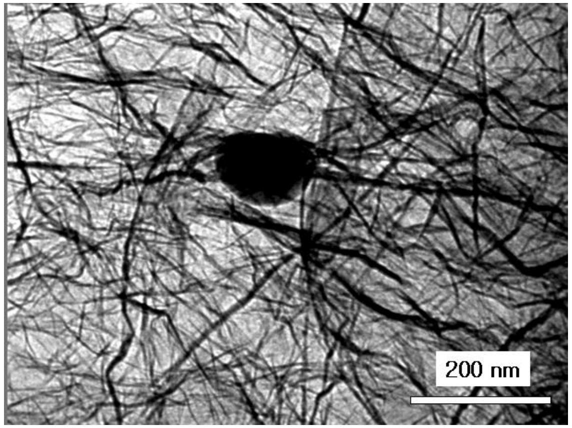


Si-Graphene composites prepared through Gas Phase Deposition



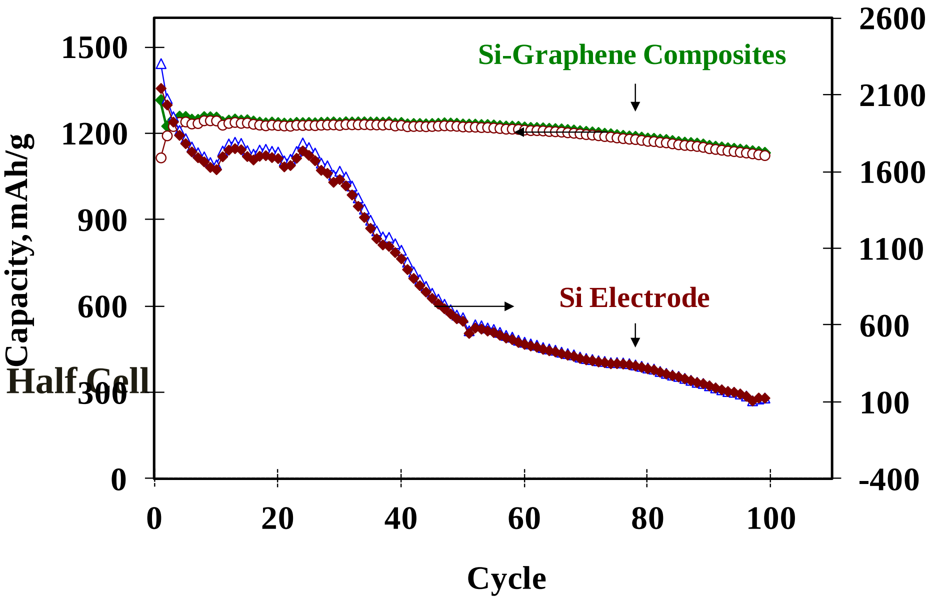


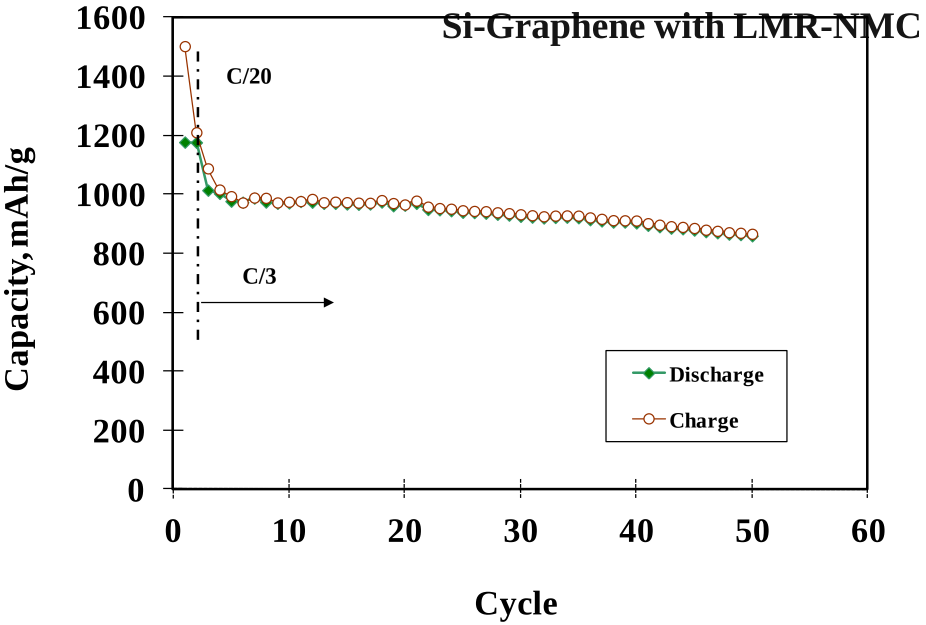




Silicon particles uniformly embedded inside graphene layers

Cell Data





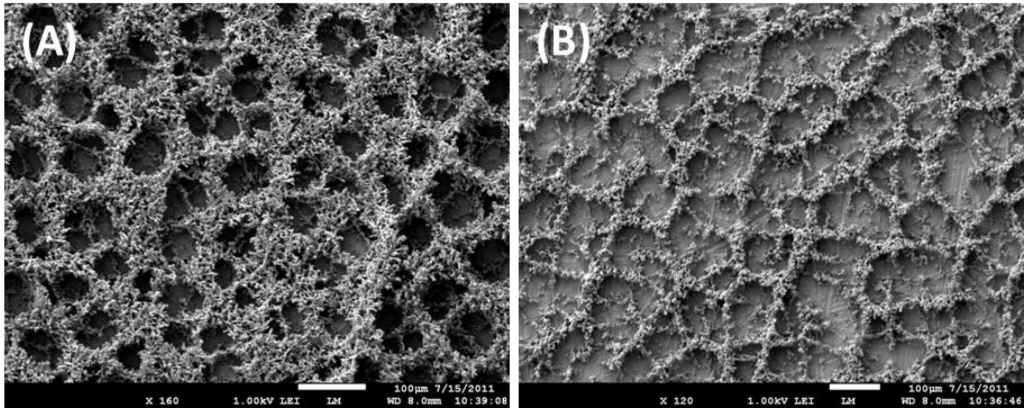
Si-Graphene possesses reversible capacity of 1100 mAh/g in 100 cycles

340 Wh/Kg energy density could be achieved by this chemistry*

*Based on Argonne's Battery Design Model

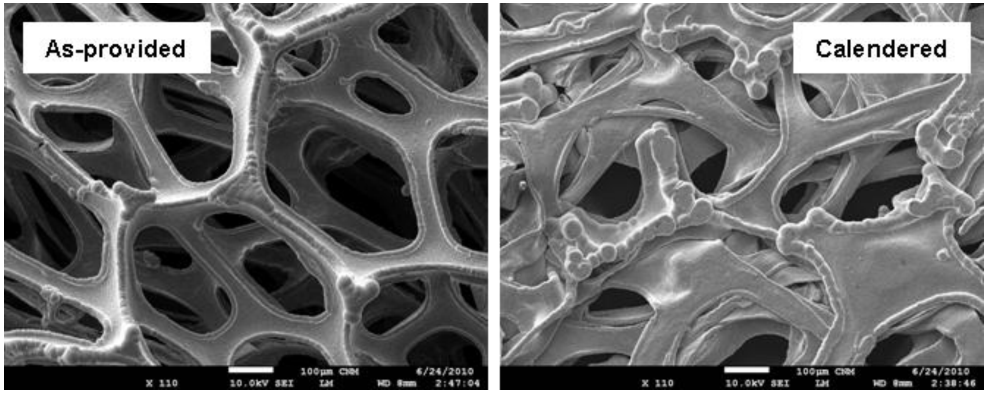
Silicon on 3-D Archtectures:

Substrates: Copper foam synthesis



(left) Electrodeposited Cu foams with same Sn deposition performed on each. (A) 1mM chloride concentration in Cu bath, (B) 4 mM chloride concentration in Cu bath

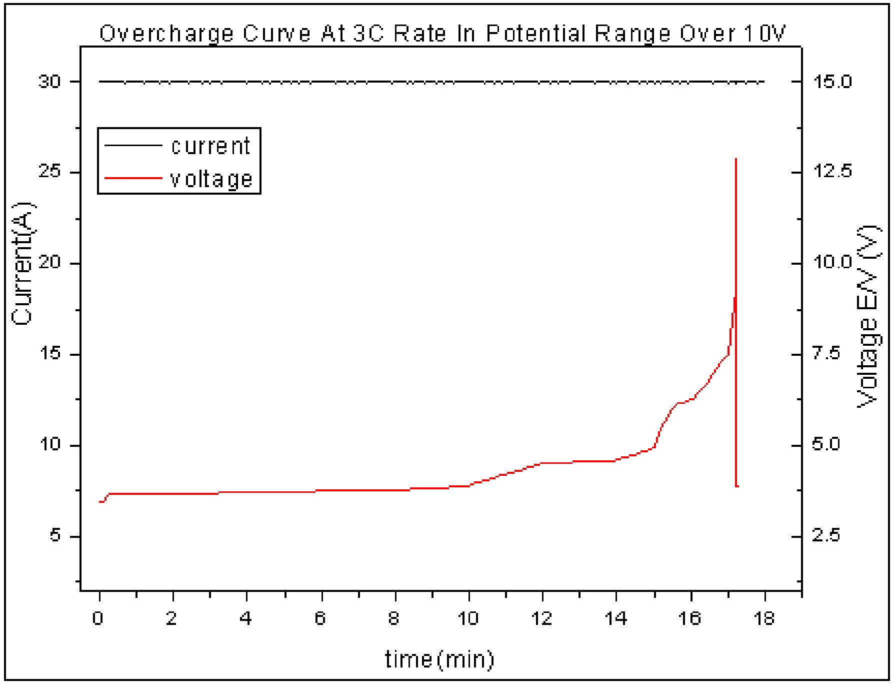
(right) Calendered commercial foams (CircuitFoil) before and after calendaring to 100 µm.



The porosity, thickness, and surface roughness of homemade foams is highly tunable. Commercial foams, however, offer the ease of reproducibility. More commercial vendors will be sought in order to have varying porosities.

Safety Issues: Overcharge Abuse and Preventions

Typical charging voltage profile of a lithium ion cell during overcharge.

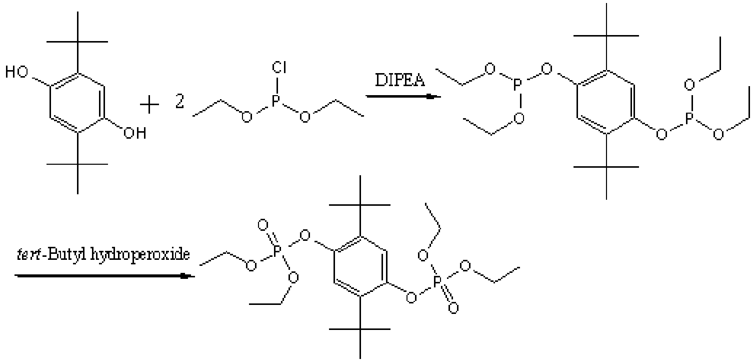


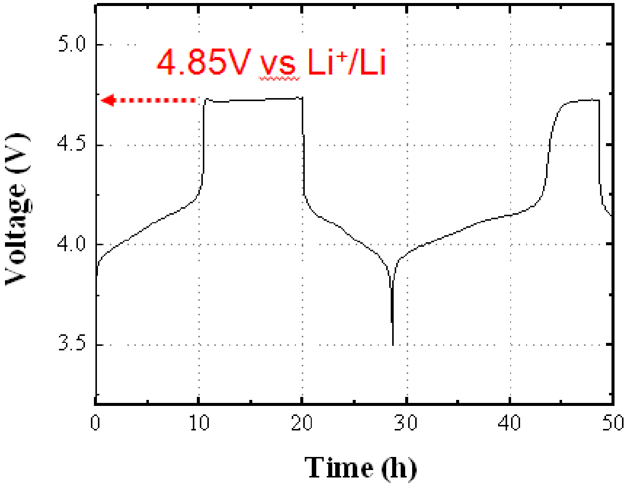
Overcharge Protection Methods:

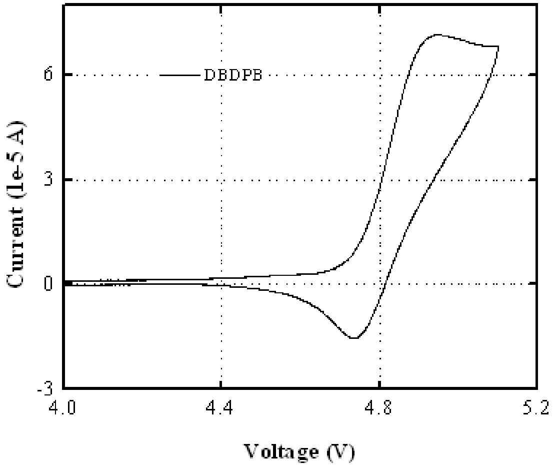
(1) Electronic circuit:
(2) Electrolyte Additives
  - redox shuttles
(3) Electroactive polymer

High Voltage Redox Shuttle for Protection of 5V Cathode

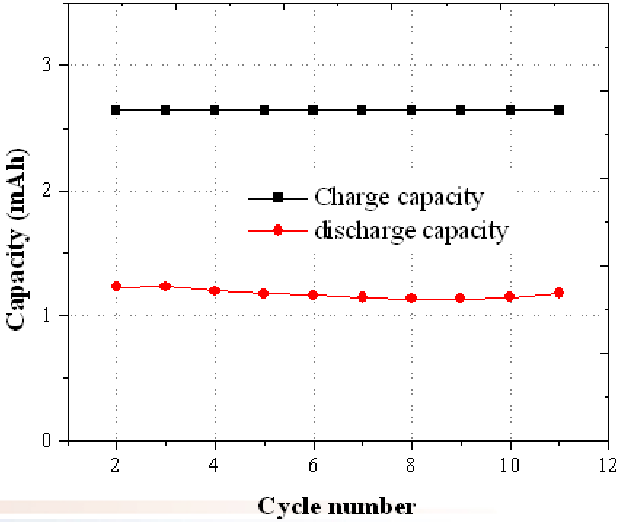
To Further Increase the Redox Potential-Synthesis Tailored for High Voltage (4.8-5.0V) Cathodes







Cyclic voltammetry in 1.2 M $LiPF_6$ in EC/EMC (3:7 by weight); Scan rate is 100mV/s.

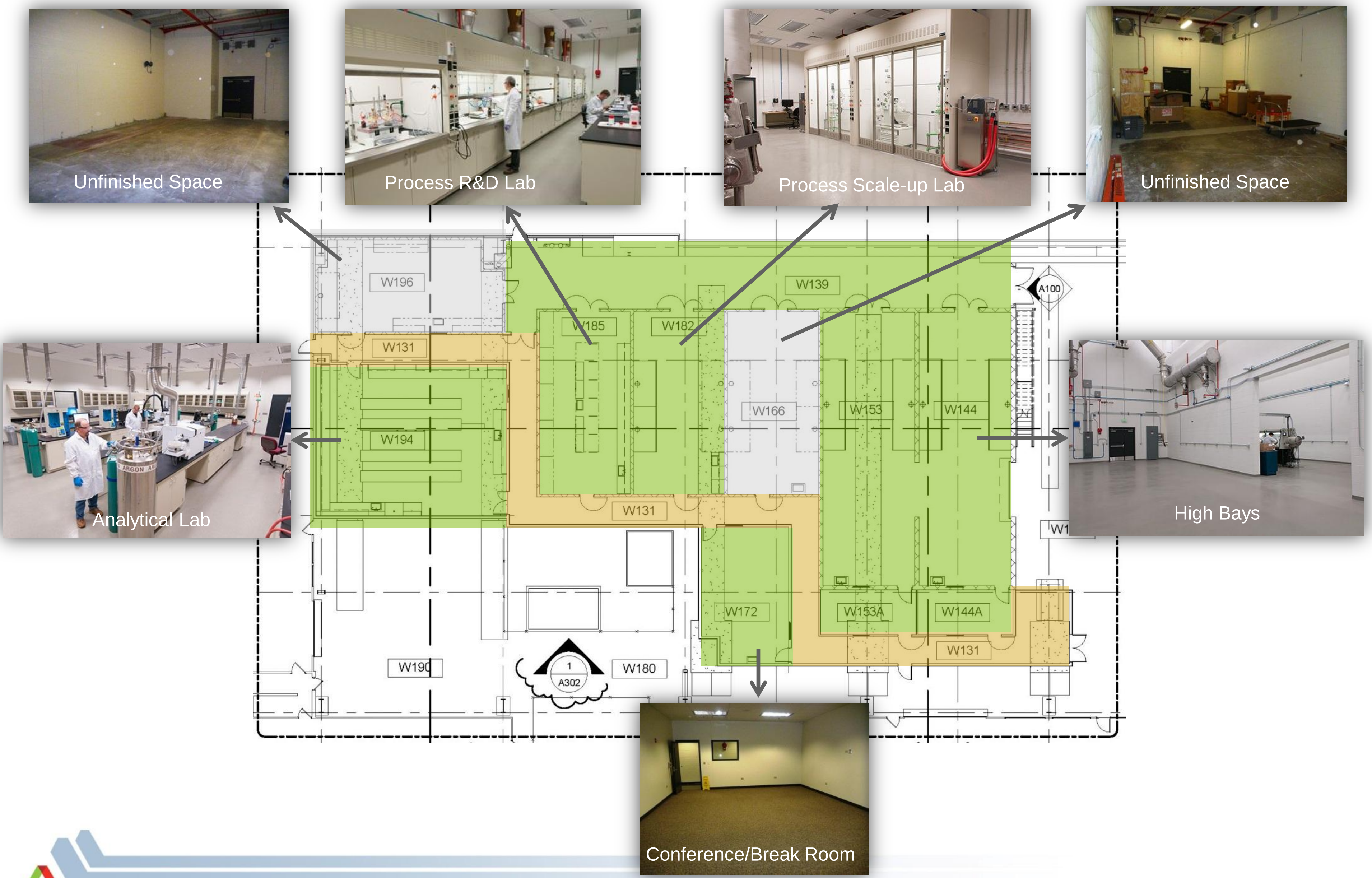


Battery Test & Evaluation Program (DOE-EERE Sponsored)

- ANL conducts independent performance and life evaluations of advanced battery technologies for DOE-EERE and the USABC.
  - Validate performance and life of contract deliverables (cells, modules, & batteries) on USABC contracts with industrial battery developers.
  - Benchmark testing of advanced battery technologies developed worldwide, to develop performance and life characteristics of these technologies under standardized test conditions.
  - Develop life prediction models, based on test data.
  - Conduct post-test analyses on cells, modules, or batteries to better understand life limiting mechanisms.

Argonne's Materials Engineering Research Facility

Argonne’s Materials Engineering Research Facility



Cell Fabrication Facility (CFF)


04/01/2010


04/01/2010

- The CFF was established by DOE-EERE, Vehicle Technologies Program, to fabricate commercial-grade sealed cells to facilitate the performance & life testing of promising advanced materials and cell chemistries developed on the ABR Program
  - Fabrication equipment housed in a new dry-room facility built for this purpose
  - Semi-automated equipment capable of coating, calendaring, & slitting electrodes; fabricating multi-electrode stacked pouch cells; & fabricating 18650 cylindrical cells
- ARRA funding used to procure cell formation, test, and characterization equipment

Battery Test Laboratory

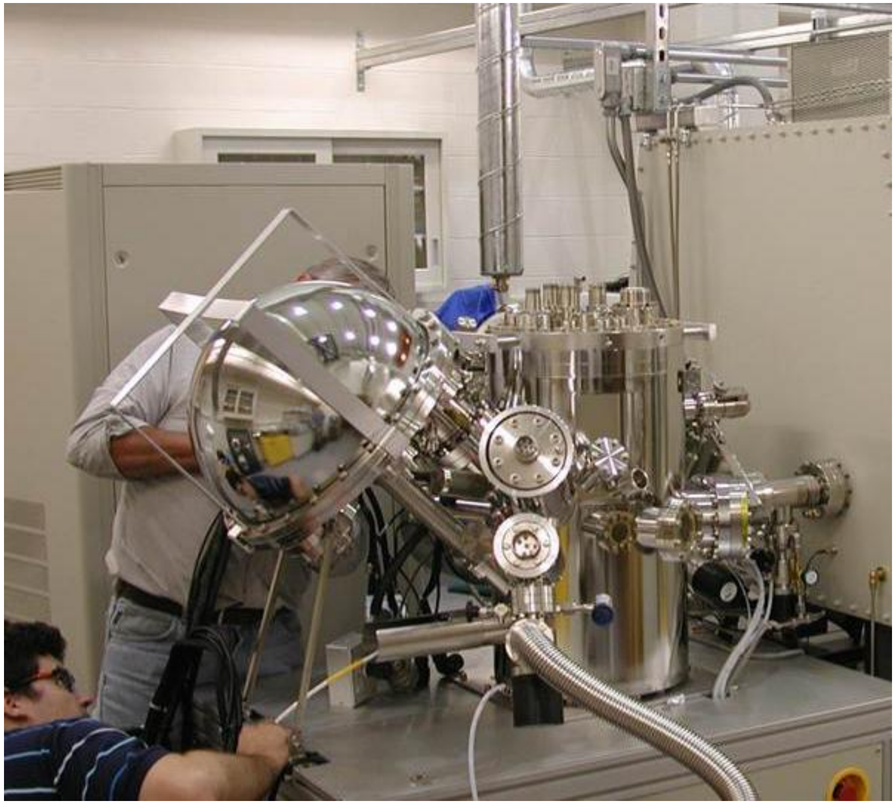
- New PC-based control & data acquisition system
- New software (PC compatible)
- New environmental chambers for testing cells and modules

Conduct independent performance & life tests:

- DOE/USABC deliverables
- Non-DOE supported technologies
- ABR Program cells

Utilize life test data to develop life prediction models for different technologies

New Post-Test Analysis Facility (PTF)



- Linked to & operated in a manner similar to the battery test facility
- ARRA funding was used to establish a new integrated post-test analysis facility incorporating a variety of teardown & diagnostic capabilities:

JOINT CENTER FOR ENERGY STORAGE RESEARCH: AN OVERVIEW

Jeff Chamberlain | JCESR Deputy Director

Messages

- Goals of JCESR
- JCESR Team
- JCESR’s approach to achieve the goals
  - What are we working on
  - How will we manage this

Start with the simple facts

- JCESR is a DOE Energy Innovation Hub, funded through the Basic Energy Sciences office of DOE, and led by Argonne National Laboratory

- Hubs are a bold initiative by DOE
  - Through science, focus on solving a single, societal problem
  - Integrated team effort
  - Rapid translation to societal impact

JCESR Targeted Outcomes

ACHIEVING GOALS FOR LASTING LEGACIES

- Transformational goals: 5-5-5
  - 5 times greater energy density → Beyond Li-ion
  - 1/5 cost
  - within 5 years
- Legacies
  - Pre-commercial prototypes for grid and transportation
  - Library of fundamental knowledge
    - Atomic and molecular understanding of battery phenomena
  - New paradigm of battery development
    - Science-based rational design
    - Systems-centric
    - End-to-end integration

The JCESR Team

5
National Laboratories

Argonne

Lawrence Berkeley

Sandia

Pacific Northwest

SLAC

5
Universities

University of Illinois at Chicago

University of Chicago

Northwestern University

University of Illinois at Urbana-Champaign

University of Michigan

4
Private Sector Partners

Dow

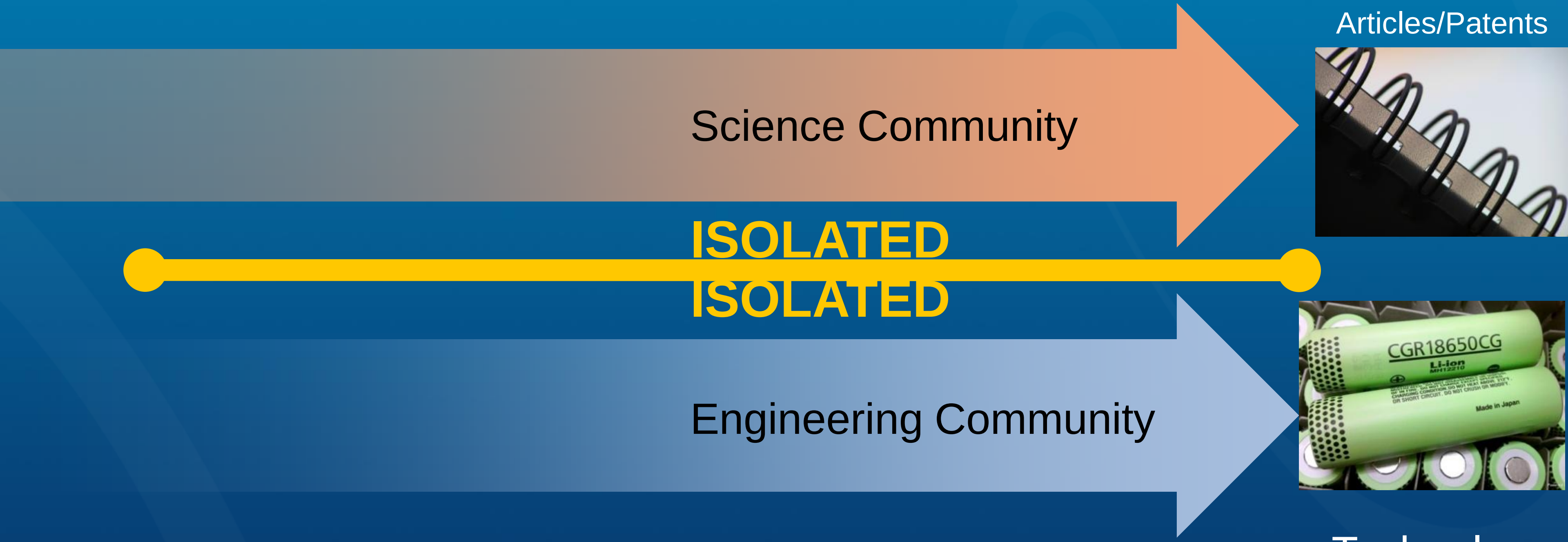
JCI

Applied Materials

Clean Energy Trust

Today’s Paradigm

Science
Journal
Articles/Patents



Science Community

ISOLATED

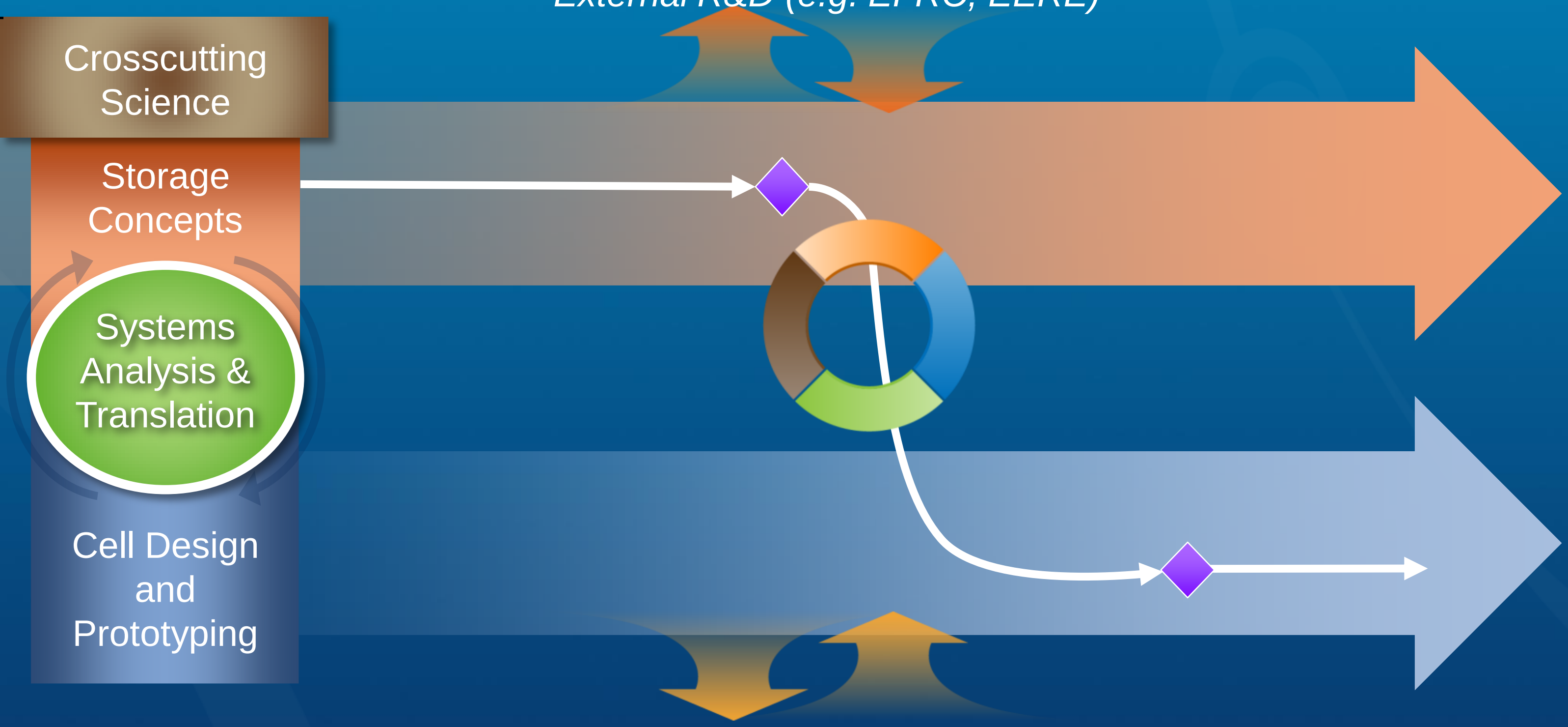
ISOLATED

Engineering Community

Technology
5% Improvement
per year

• Component-centric • Sequentially organized •
• Incremental improvement •

JCESR Paradigm



External R&D (e.g. EFRC, EERE)

Crosscutting Science

Storage Concepts

Systems Analysis & Translation

Cell Design and Prototyping

External Industry

Science

Library of Knowledge

Technology

5 Times Greater Energy Density

1/5 Cost

5 Years

• Science-based rational design • Parallel development •

• Systems-centric • End-to-end integration • Labs, Universities, Industry •

Multivalent Intercalation

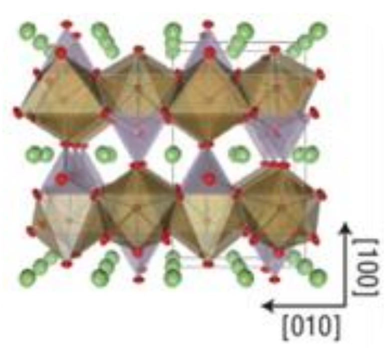
POTENTIAL TO DOUBLE CAPACITY OF CATHODE

Multivalent Intercalation

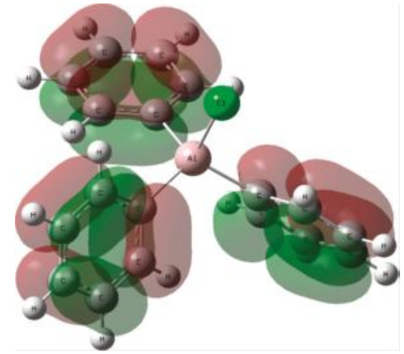
- Mobility in host structures
- Mobility across interfaces
- Stable and selective interfaces

Objectives

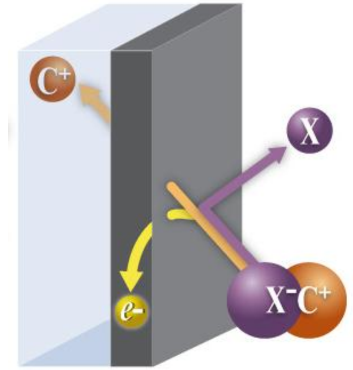
- Understand how highly charged cations move through solids, liquids and interfaces while under electrochemical control



Host Mobility



Ion/Solvent Interactions



Interfacial Transport

Combining multivalent cathode and reversible metal anode has potential to achieve 5x Li-ion energy density

Chemical Transformation

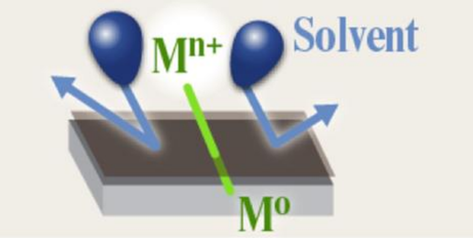
DRAMATICALLY HIGHER CAPACITY AND LOWER SYSTEM COSTS

Chemical Transformation

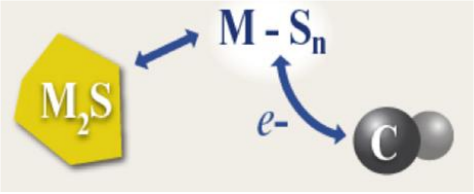
- Phase transformation and juxtaposition
- Functional electrolytes
- Stable and selective interfaces

Objectives

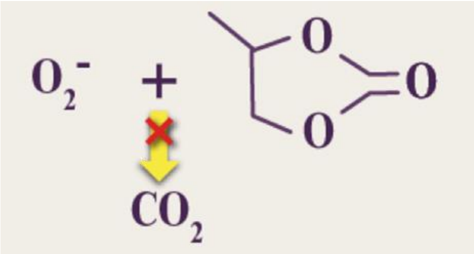
- Determine guiding principles and understand reaction pathways
- Design practical interfaces of increasing complexity
- Design new electrode materials, electrolytes, and architectures for highly reversible solid form reactions



Stable Selective Interfaces



Phase Transformation

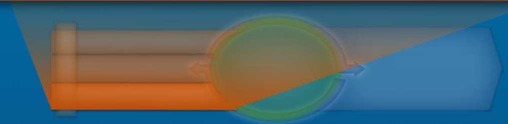


Functional Stable Electrolytes

Non-Aqueous Redox Flow

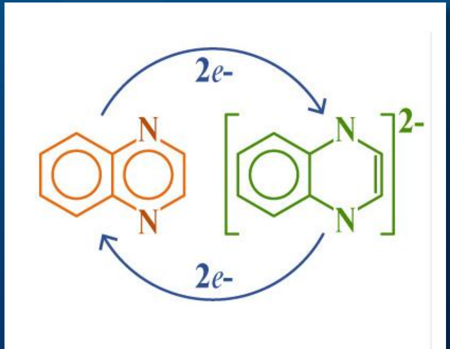
10X THE ENERGY DENSITY OF AQUEOUS FLOW BATTERIES AT 1/5 THE SYSTEM COST

Non-Aqueous Redox Flow
- Novel redox species
- Ionic mobility
- Interfacial transport
- Stable and selective membranes

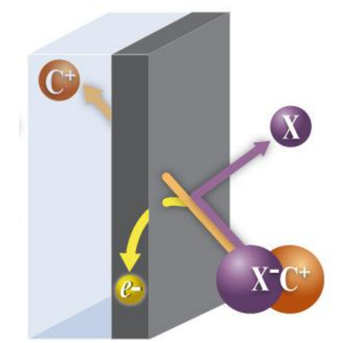


Objectives

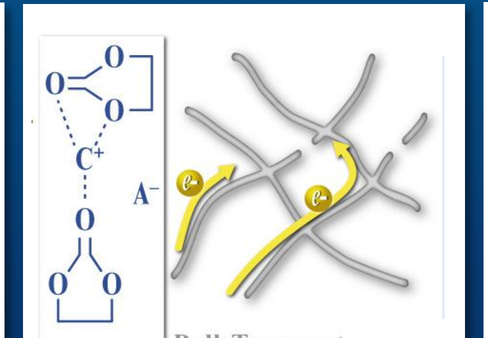
- Understand mechanisms of storage and charge transport
- Discover novel redox molecules, electrolytes, and membranes
- Design chemical systems and cells that maximize energy, power, and stability in long-term use



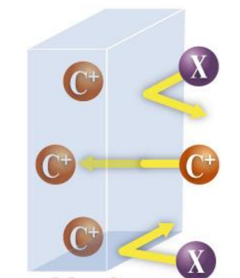
Novel Redox Species



Interfacial Transport



Bulk Transport



Membrane Selectivity/ Stability

Techno-Economic Modeling
BUILDING A BATTERY ON THE COMPUTER

Systems Analysis and Translation

Linking system level goals to materials level values

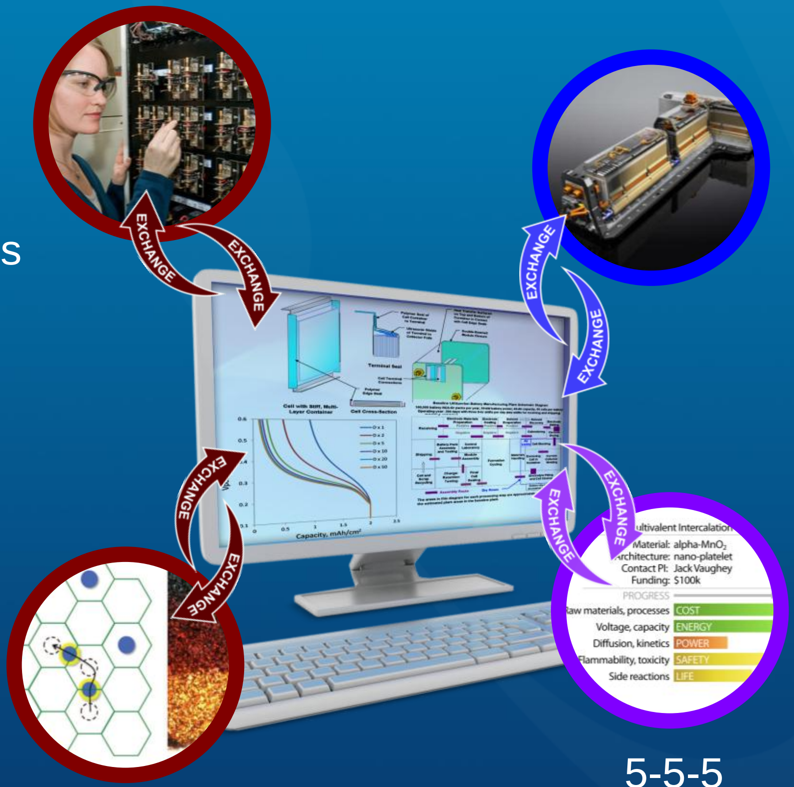
- What cell voltage, capacity, diffusion coefficient, ...etc… are needed to meet JCESR goals?

Directing research dollars to most promising approaches

- Informing JCESR leadership, assessing most promising candidates, creating new Translational Development Teams

Identifying and overcoming barriers to transformational advances

- Across all levels – materials, electrodes, cells, pack/stacks



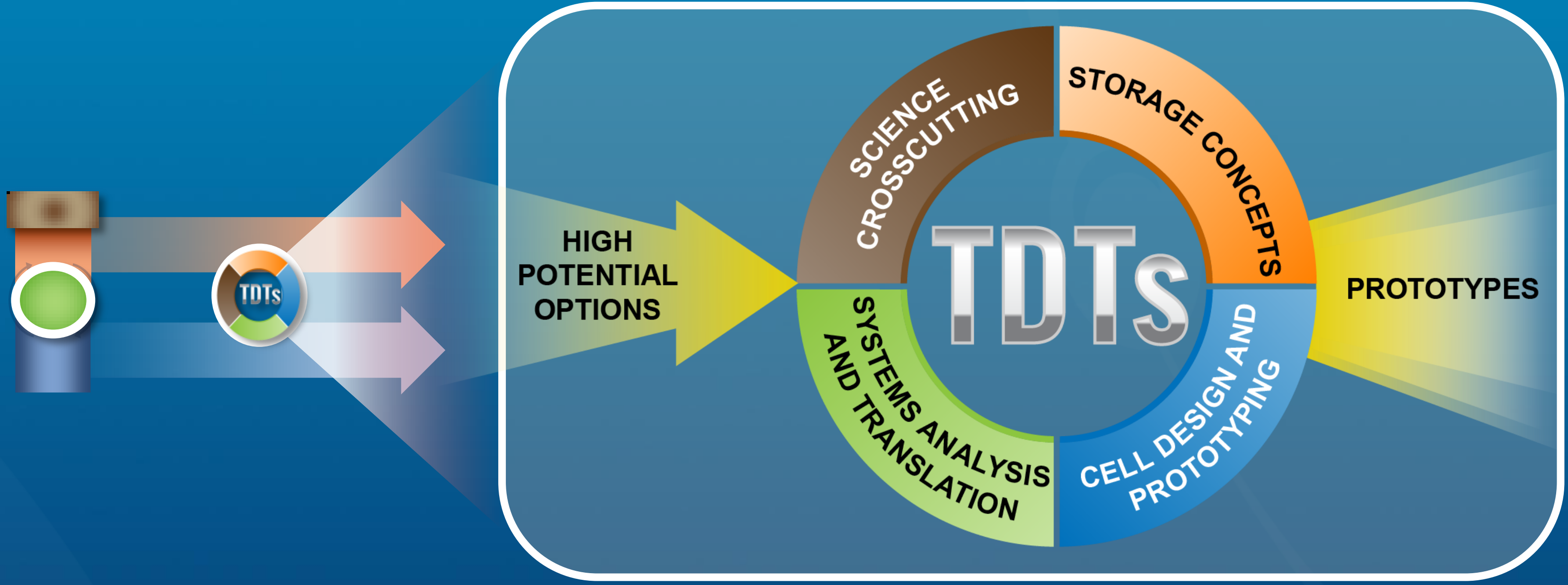
5-5-5

Diffusion
coefficient rate
constant
practical capacity
voltage

Technical performance
Manufacturing cost

Translational Development Teams

INTEGRATING SCIENCE WITH ENGINEERING



- We kickoff two TDTs to design and prototype cells
  - Grid
  - Transportation

JCESR Applies Several Mechanisms to Meet the 5-5-5

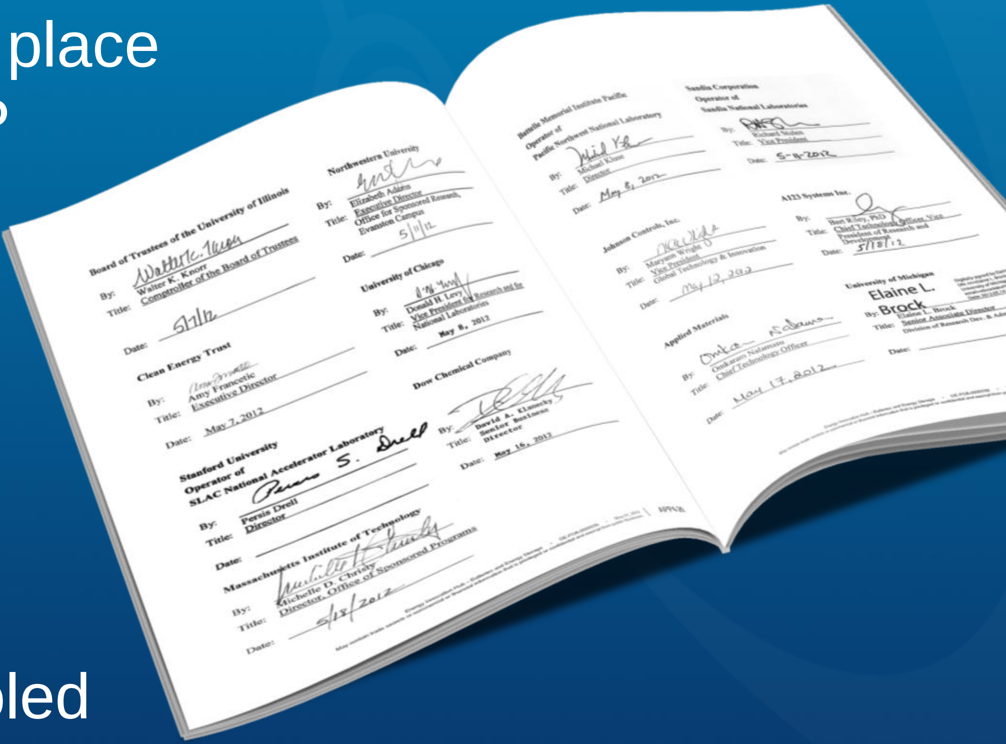
- RDD&D Spectrum
  - Systems Analysis and Translation
    - Techno-Economic Modeling
  - Translational Development Teams
  - Cell Design and Prototyping
- Intellectual Property Management
- Advisory groups
- Affiliates

RESULTS IN COMMON TEAM WORKING TO SHARED MISSION

IP Plan

FACILITATES OPEN COLLABORATION AND TRANSLATION TO MARKET

- Agreement signed and in place to operate under single IP Management Plan
- All foreground IP pooled, with centralized licensing
    - Allows industrial concerns to see a clear path to commercialization
    - One stop shopping
- Some Background IP pooled



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Elaine L. Brock
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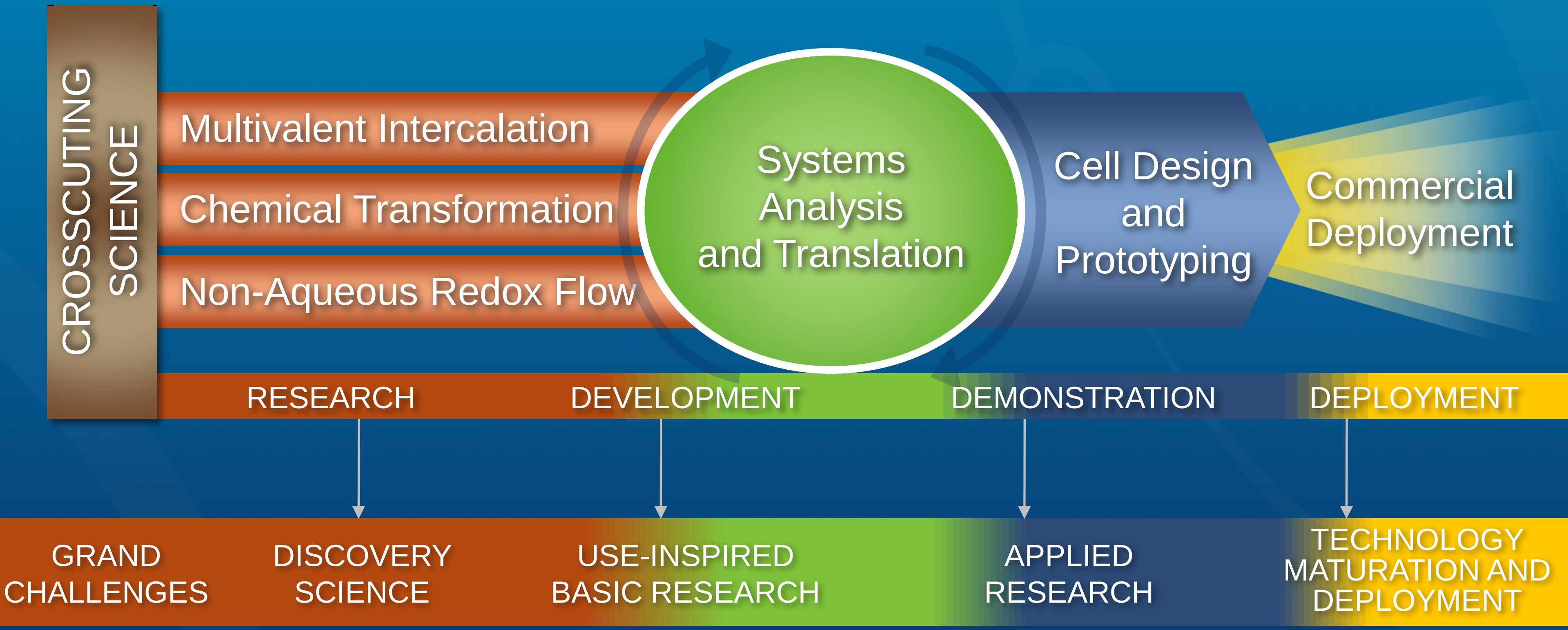
JCESR Integrates All Aspects of RDD&D



CROSSCUTTING SCIENCE

Multivalent Intercalation

Chemical Transformation

Non-Aqueous Redox Flow

Systems Analysis and Translation

Cell Design and Prototyping

Commercial Deployment

RESEARCH

DEVELOPMENT

DEMONSTRATION

DEPLOYMENT

GRAND CHALLENGES

DISCOVERY SCIENCE

USE-INSPIRED BASIC RESEARCH

APPLIED RESEARCH

TECHNOLOGY MATURATION AND DEPLOYMENT

Matches DOEs Discovery Deployment Spectrum

Questions?