JCESR | JOINT CENTER FOR ENERGY STORAGE RESEARCH

Next Generation Energy Storage: Beyond Lithium Ion

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Outline

Today's revolution: lithium-ion → personal electronics

Tomorrow's revolution: beyond lithium-ion → transportation and electricity grid

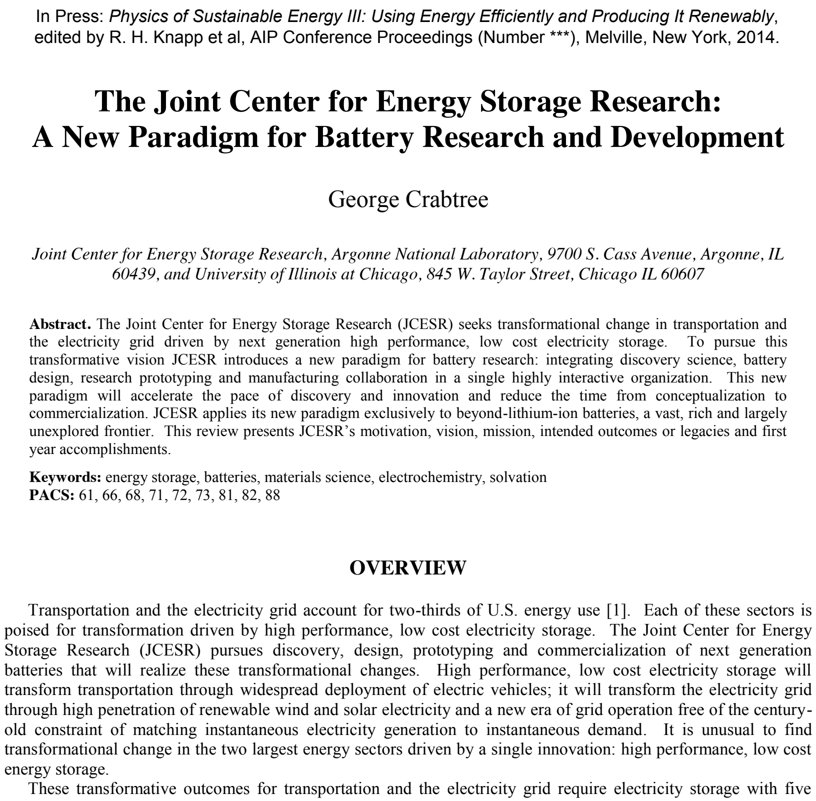
JCESR: a new paradigm for battery R&D

Promising technologies

How would life be different?

Argonne Training Program on Extreme Scale Computing
Pheasant Run, IL
August 4, 2015

Further Reading


In Press: *Physics of Sustainable Energy III: Using Energy Efficiently and Producing It Renewably*, edited by R. H. Knapp et al, AIP Conference Proceedings (Number ***), Melville, New York, 2014.

The Joint Center for Energy Storage Research: A New Paradigm for Battery Research and Development

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Abstract. The Joint Center for Energy Storage Research (JCESR) seeks transformational change in transportation and the electricity grid driven by next generation high performance, low cost electricity storage. To pursue this transformative vision JCESR introduces a new paradigm for battery research: integrating discovery science, battery design, research prototyping and manufacturing collaboration in a single highly interactive organization. This new paradigm will accelerate the pace of discovery and innovation and reduce the time from conceptualization to commercialization. JCESR applies its new paradigm exclusively to beyond-lithium-ion batteries, a vast, rich and largely unexplored frontier. This review presents JCESR's motivation, vision, mission, intended outcomes or legacies and first year accomplishments.

Keywords: energy storage, batteries, materials science, electrochemistry, solvation
PACS: 61, 66, 68, 71, 72, 73, 81, 82, 88

OVERVIEW

Transportation and the electricity grid account for two-thirds of U.S. energy use [1]. Each of these sectors is poised for transformation driven by high performance, low cost electricity storage. The Joint Center for Energy Storage Research (JCESR) pursues discovery, design, prototyping and commercialization of next generation batteries that will realize these transformational changes. High performance, low cost electricity storage will transform transportation through widespread deployment of electric vehicles; it will transform the electricity grid through high penetration of renewable wind and solar electricity and a new era of grid operation free of the century-old constraint of matching instantaneous electricity generation to instantaneous demand. It is unusual to find transformational change in the two largest energy sectors driven by a single innovation: high performance, low cost energy storage.

These transformative outcomes for transportation and the electricity grid require electricity storage with five

Review Article

https://anl.app.box.com/s/wixxv7f3mg9ev3t926rc

http://arxiv.org/abs/1411.7042

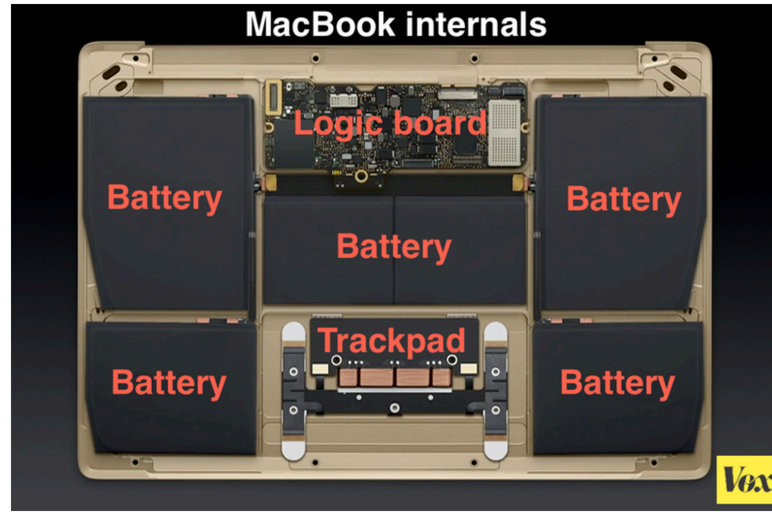
Webpage

http://www.jcesr.org/

This presentation:
https://anl.box.com/s/7vzrftvww6a6hzo9nka4o85uan3ffp84

Today

Lithium-ion batteries enabled
the personal electronics revolution



http://www.vox.com/2015/3/9/8178213/apple-macbook-all-batteries

Battery size and weight limits
the functionality of portable electronics

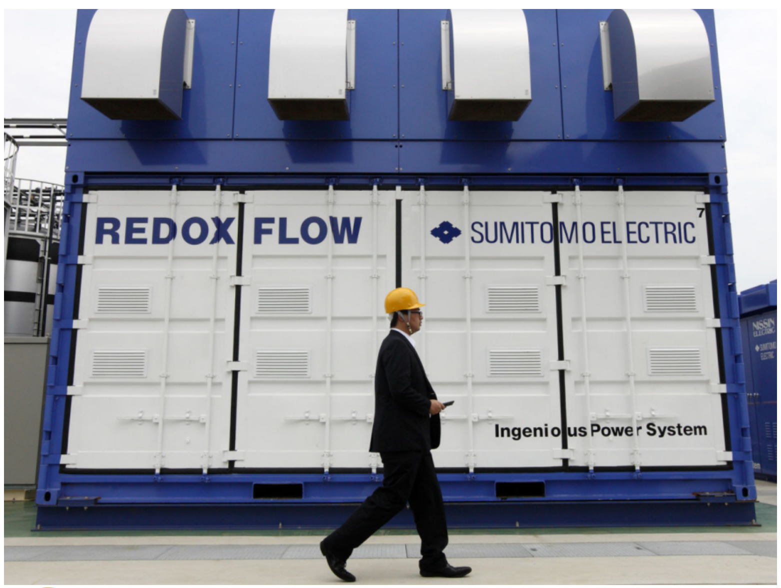
Tomorrow

$20K electric cars?

Displace gasoline cars

Replace foreign oil with domestic electricity

Reduce energy use and carbon emissions



Grid-scale electricity storage?

Enable widespread deployment of wind and solar

Enhance reliability, flexibility, resilience

Uncouple instantaneous generation from instantaneous demand

Next Generation Energy Storage Needed to Transform Transportation and the Grid

Two biggest energy uses and markets

Transportation 28%

Replace gasoline with electricity

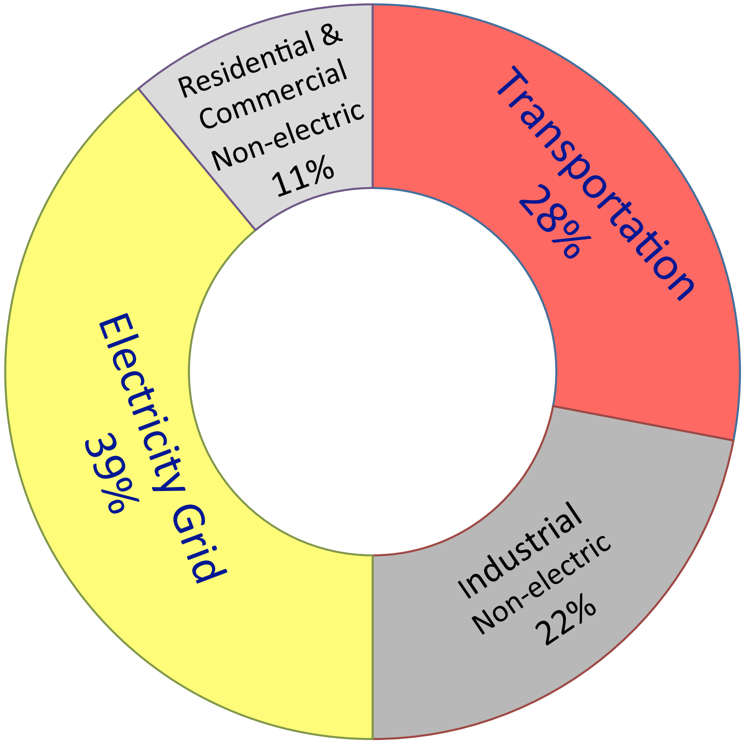
Electricity 39%

Uncouple instantaneous generation from instantaneous demand

Personal electronics < 2%

In energy terms, half the market for cars and the grid is ~10x personal electronics

Energy Demand



2013
EIA Monthly Energy Review Table 2.1
(May 2014)

The bottleneck for both transitions is inexpensive, high performance electrical energy storage

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JCESR: Beyond Lithium-ion Batteries for Cars and the Grid

TRANSPORTATION

$100/kWh

400 Wh/kg 400 Wh/L

800 W/kg 800 W/L

1000 cycles

80% DoD C/5

15 yr calendar life

EUCAR

GRID

$100/kWh

95% round-trip efficiency at C/5 rate

7000 cycles C/5

20 yr calendar life

Safety equivalent to a natural gas turbine

Vision

Transform transportation and the electricity grid with high performance, low cost energy storage

Mission

Deliver electrical energy storage with five times the energy density and one-fifth the cost of today's commercial batteries within five years

Legacies

- **A library of the fundamental science** of the materials and phenomena of energy storage at atomic and molecular levels
- **Two prototypes, one for transportation and one for the electricity grid**, that, when scaled up to manufacturing, have the potential to meet JCESR's transformative goals
- **A new paradigm for battery R&D** that integrates discovery science, battery design, research prototyping and manufacturing collaboration in a single highly interactive organization

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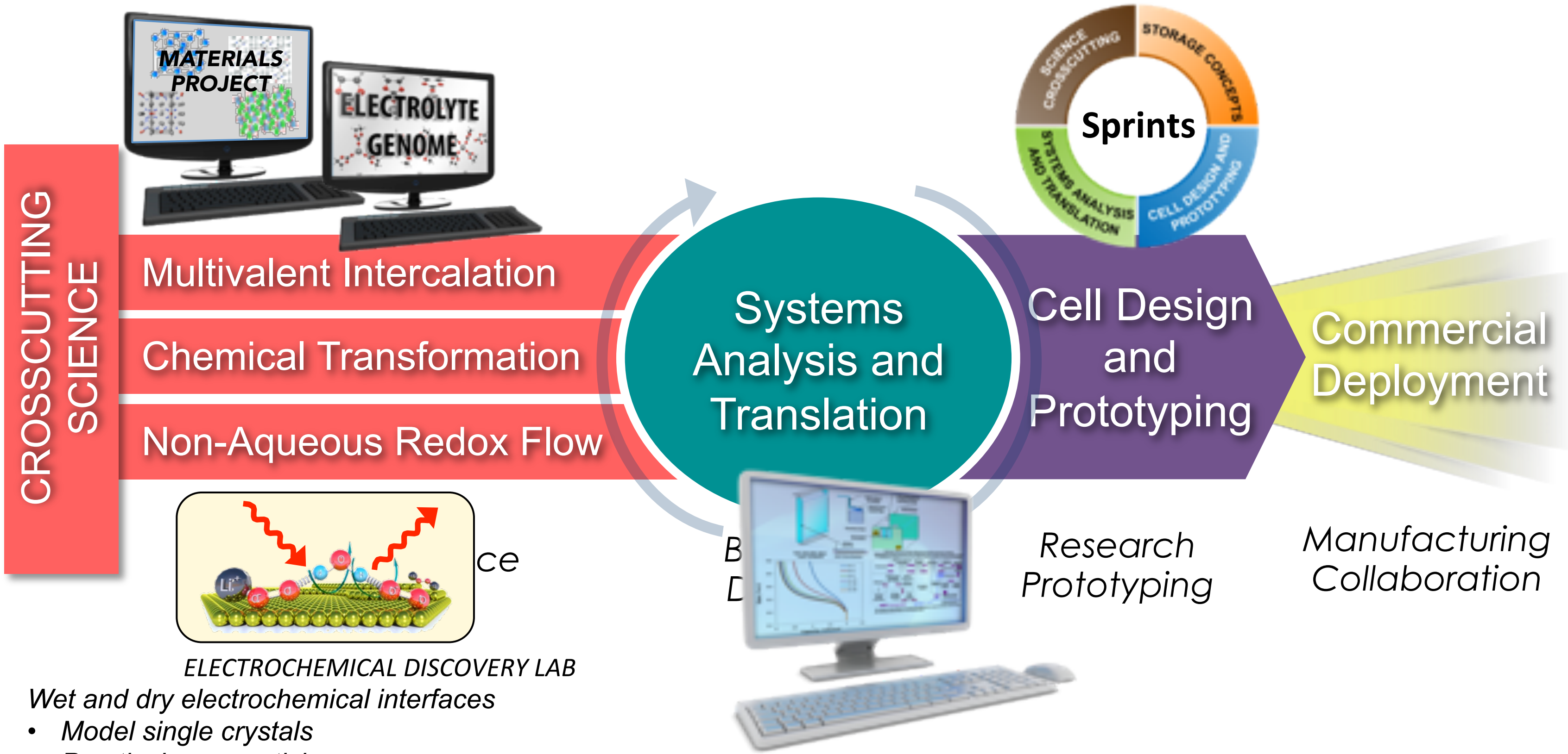
JCESR Creates a New Paradigm for Battery R&D



ELECTROCHEMICAL DISCOVERY LAB

Wet and dry electrochemical interfaces

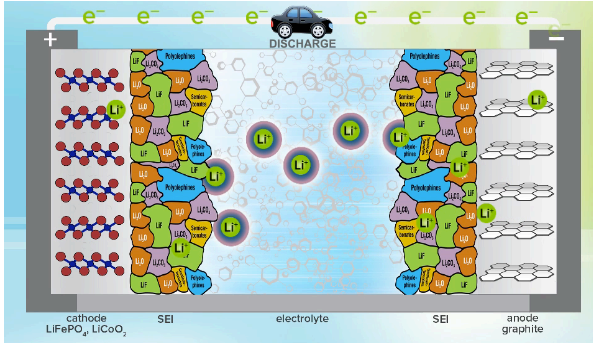
- *Model single crystals*
- *Practical nanoparticles*

TECHNO-ECONOMIC MODELING

"Building battery systems on the computer"

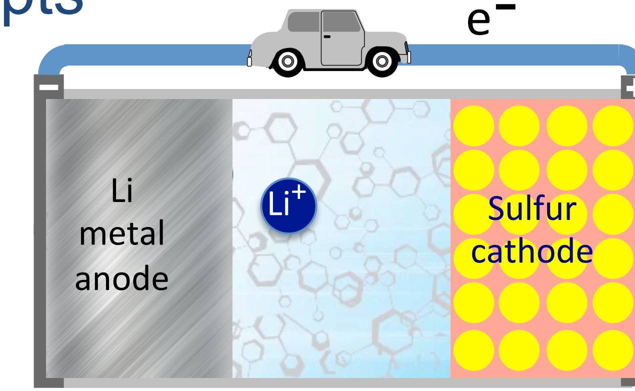
Lithium Ion Battery Technology

JCESR's Beyond Lithium-ion Concepts



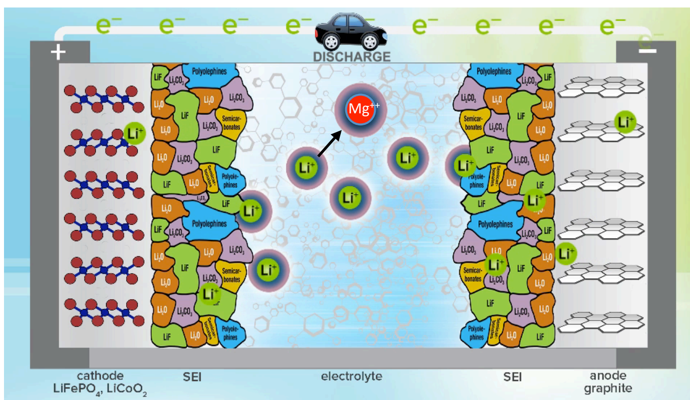
Lithium-ion "Rocking Chair"

Li^+ cycles between anode and cathode, storing and releasing energy



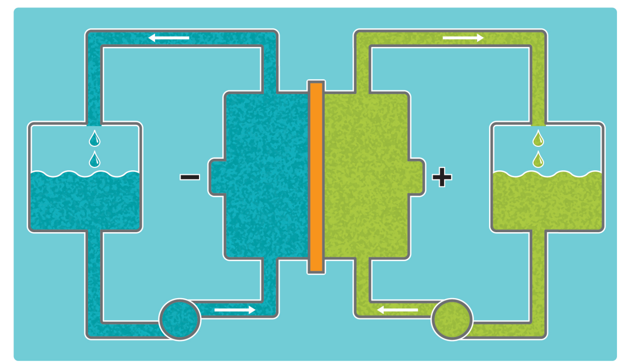
Chemical Transformation

Replace intercalation with high energy chemical reaction: Li-S, Li-O, Na-S, . . .



Multivalent Intercalation

Replace monovalent Li^+ with di- or tri-valent ions: Mg^{++}, Ca^{++}, Al^{+++}, . . .
Double or triple capacity



Non-aqueous Redox Flow

Replace solid electrodes with liquid solutions or suspensions:
lower cost, higher capacity, greater flexibility

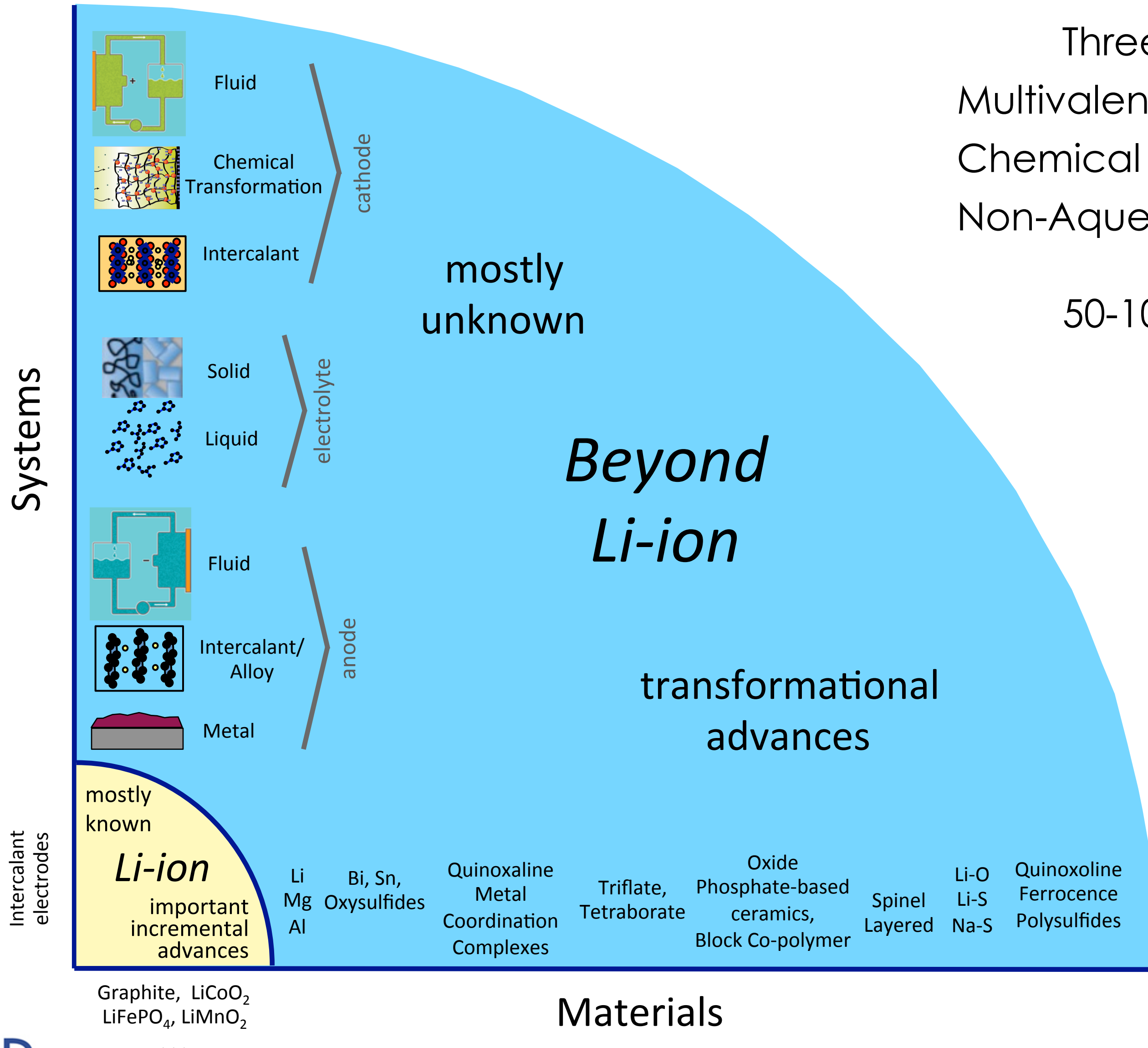
Three concepts

Multivalent Intercalation

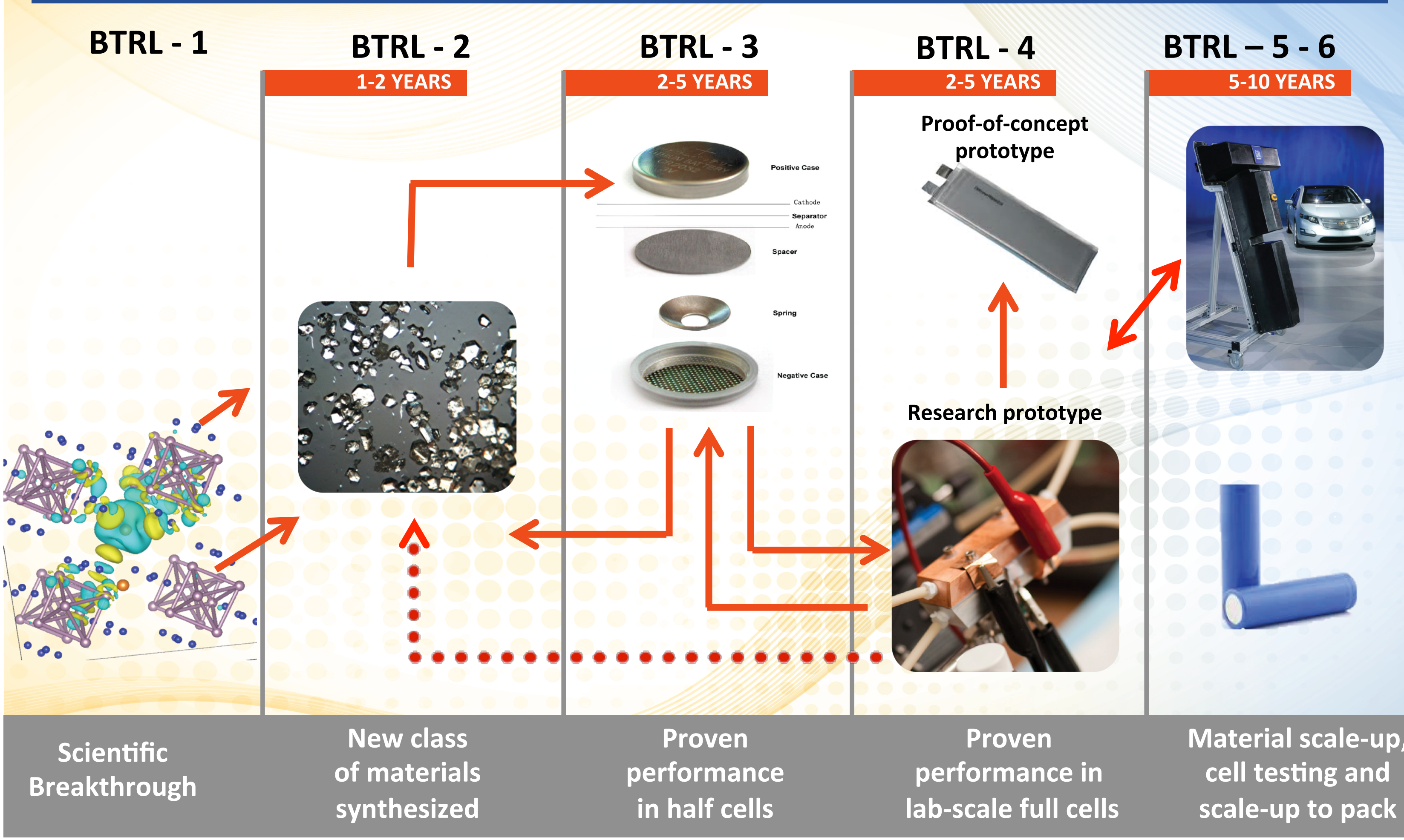
Chemical Transformation

Non-Aqueous Redox Flow

50-100 Batteries



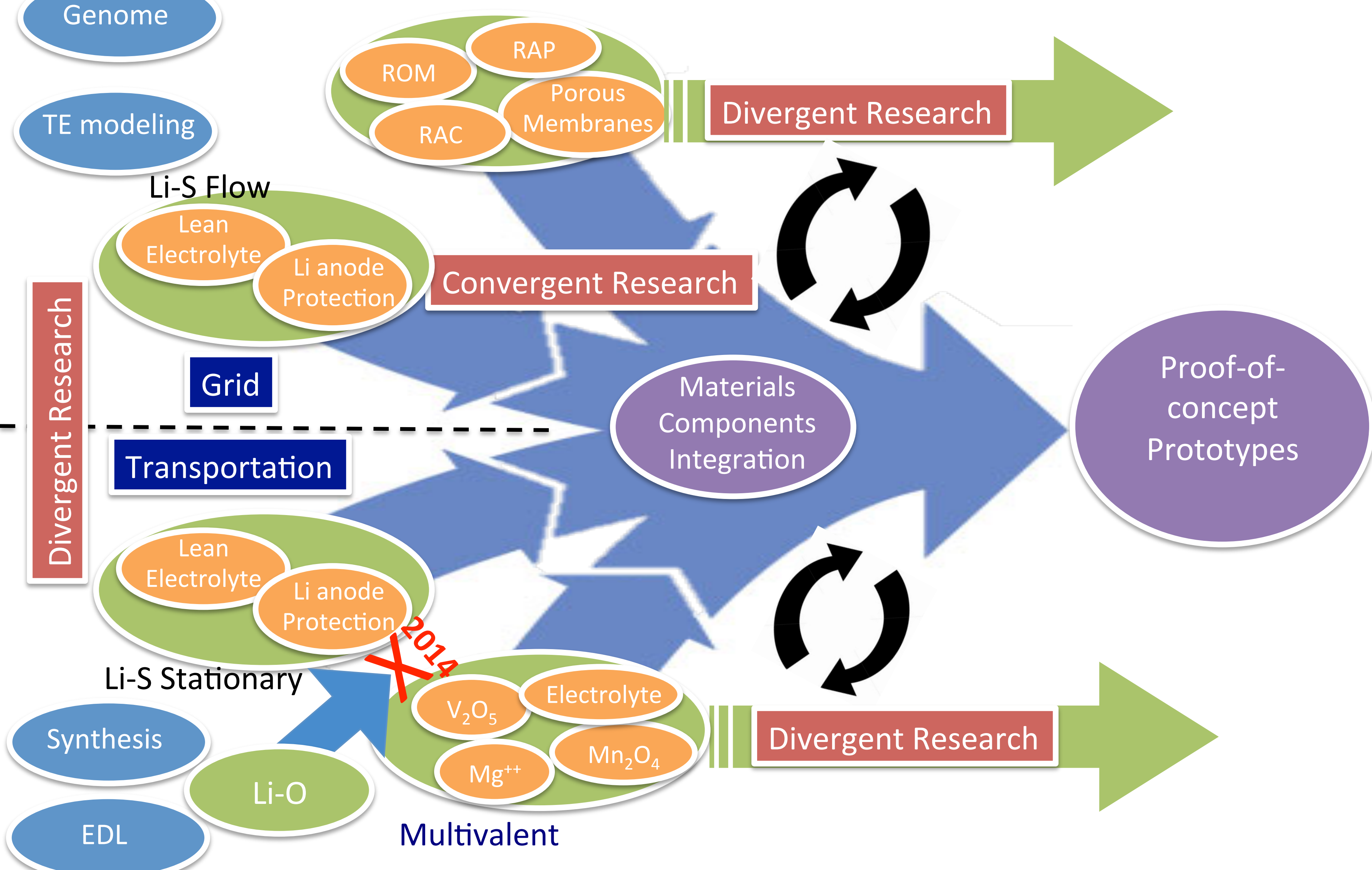
Battery Technology Readiness Level (BTRL)



Developed collaboratively with
JCI, NASA-Glenn, TARDEC

JCESR
"sweet spot"

Four Convergent Pathways Identified Oct 2014



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More on JCESR website
www.jcesr.org

Perspective

Vision: Transform transportation and electricity grid with high performance, low cost energy storage

Mission: Deliver electrical energy storage with five times the energy density and one-fifth the cost

→ **Beyond lithium ion**

Legacies:

A library of the fundamental science of the materials and phenomena of energy storage at atomic and molecular levels

Two prototypes, one for transportation and one for the electricity grid, that, when scaled up to manufacturing, have the potential to meet JCESR's performance and cost goals

A new paradigm for battery R&D that integrates discovery science, battery design, research prototyping and manufacturing collaboration in a single highly interactive organization

- A bold new approach to battery R&D
- Accelerate the pace of discovery and innovation
- Bring the community to the beyond lithium-ion opportunity

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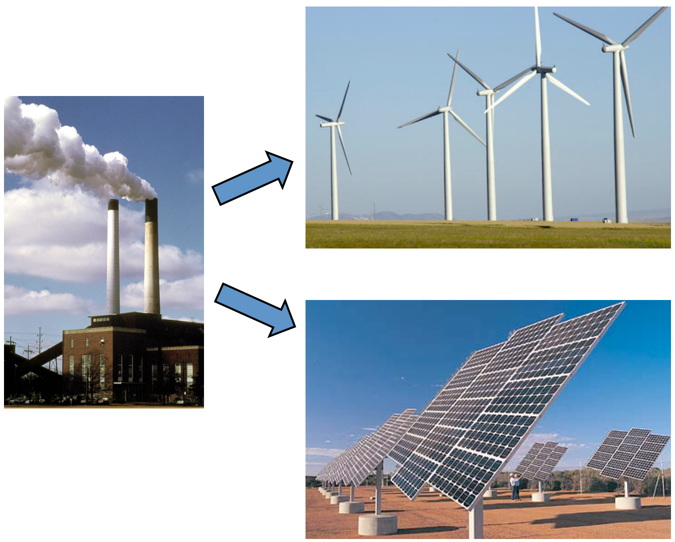
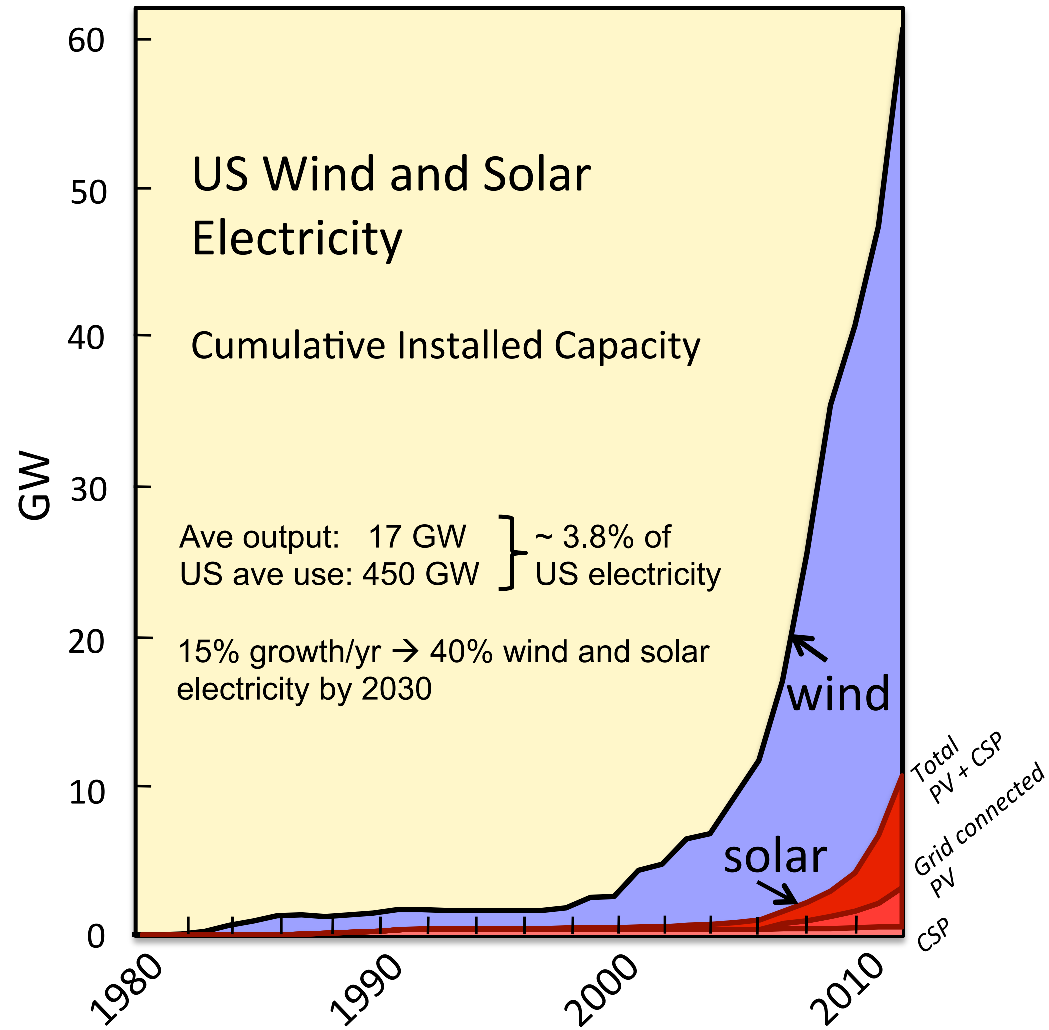
Argonne NATIONAL LABORATORY

Wind and Solar Electricity

✓ Stable climate

✓ Energy security





Viable technologies

on deployment path

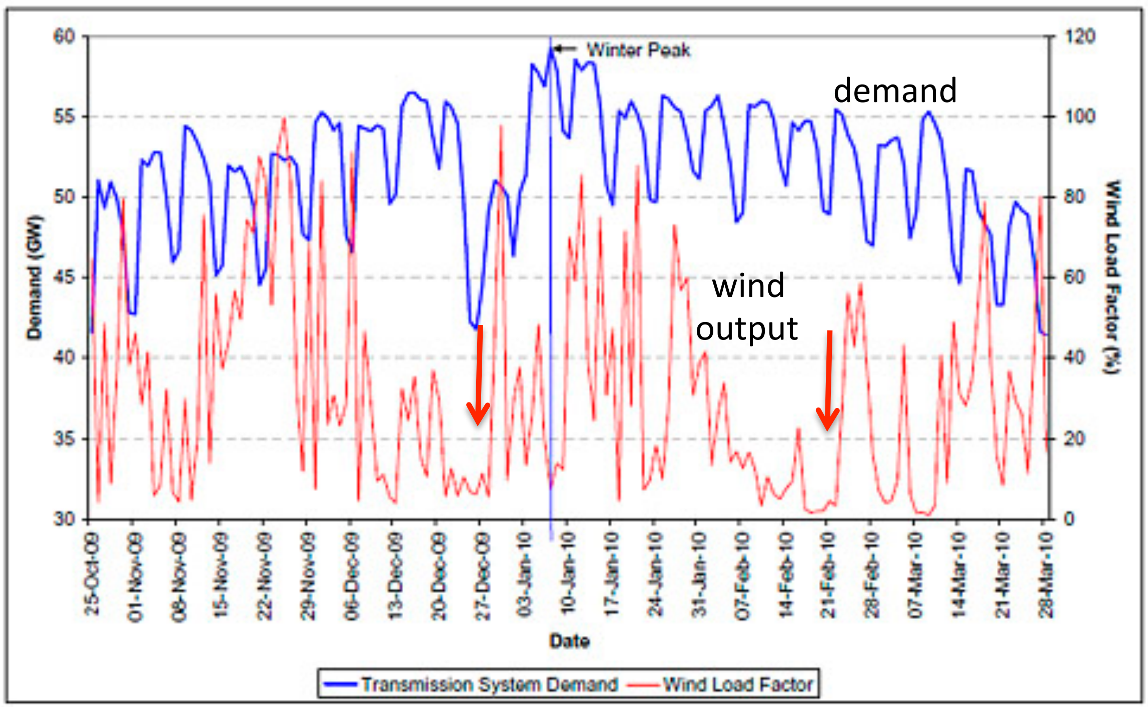
Remaining science challenges

improve efficiency

lower cost

Energy Storage Enables Variable Wind and Solar Generation

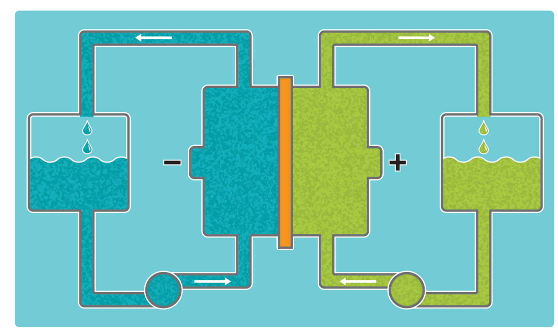
Figure A.30 – 2009/10 Daily Peak and Wind Generation



http://www.windbyte.co.uk/windpower.html

gas plant

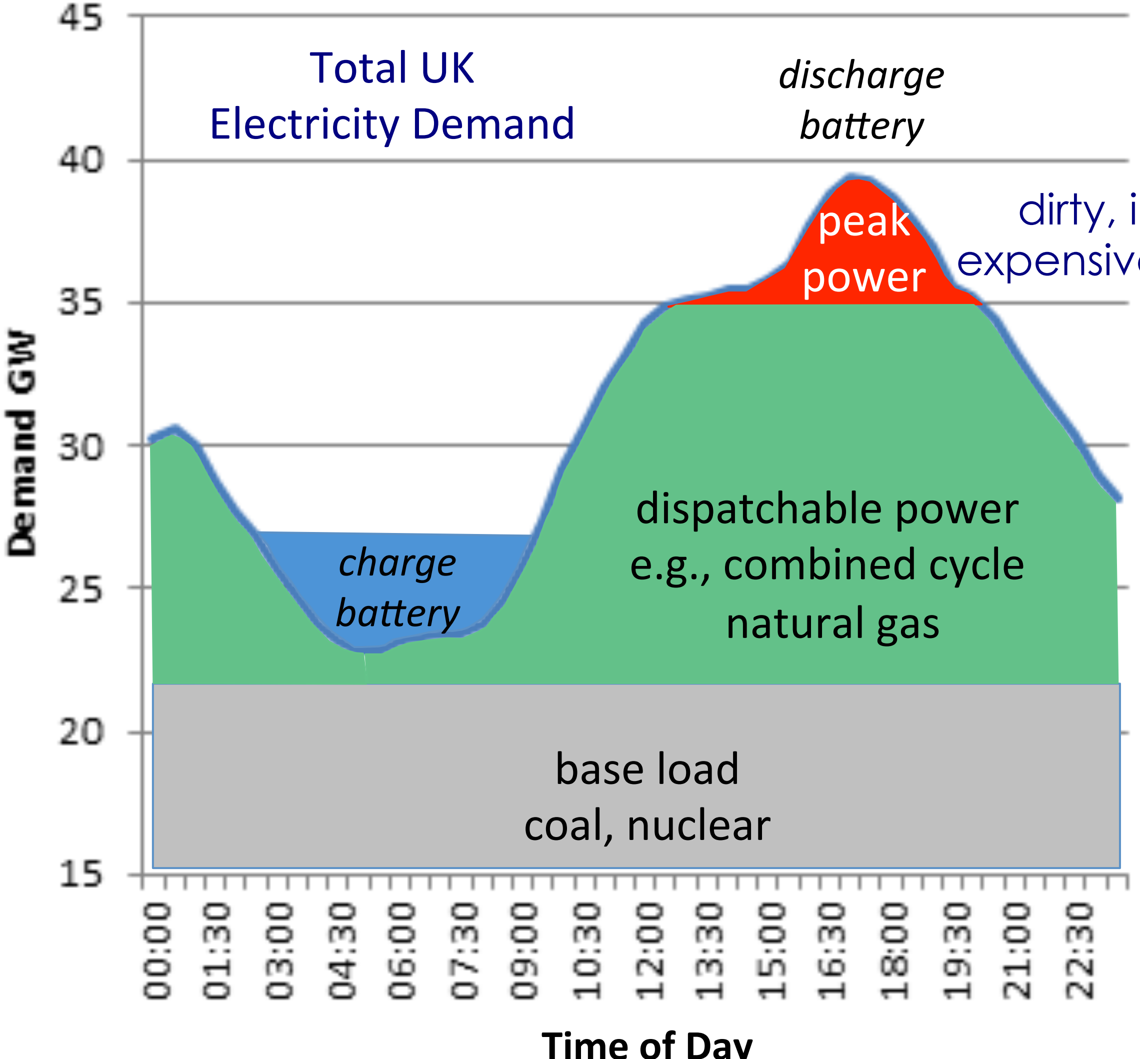
Back up the wind farm with



battery $ = 5x gas plant $

One or two calm days per month
Wind stronger at night
Wind does not follow diurnal pattern

Energy Storage Flatttens Generation Peaks and Valleys



dirty, inefficient, expensive generation → clean, efficient inexpensive generation

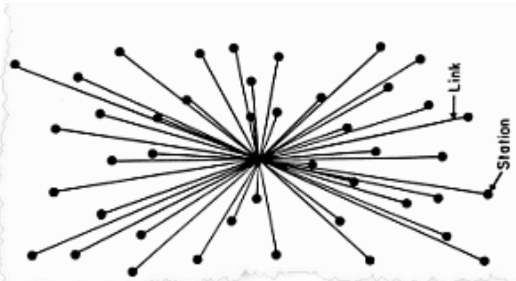
clean, efficient inexpensive generation

Tipping point

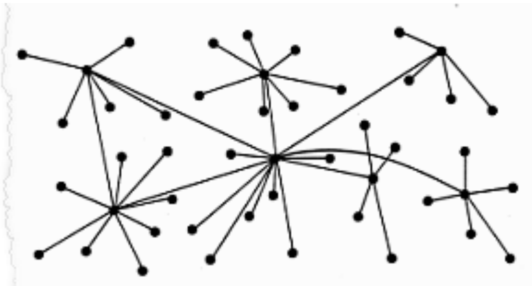
cost of batteries less than cost of peaker plant

Centralized, Decentralized or Distributed?

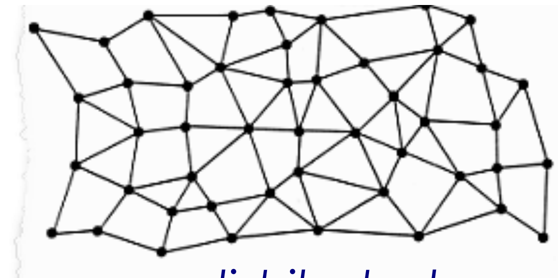
Electricity grid Internet Highways



centralized



decentralized



distributed

Until late 1960s

Central power plants

- expensive
- economies of scale
- unique
- unreliable

Electricity grid

- inexpensive
- reliable: most outages due central plants

1970s - 2000s

Central power plants

- inexpensive
- reliable
- fossil, nuclear, hydro
- environmental stigma

Electricity grid

- expensive
- regulatory challenge
- unreliable: most outages due to grid

2000s – 2015

Distributed wind and solar

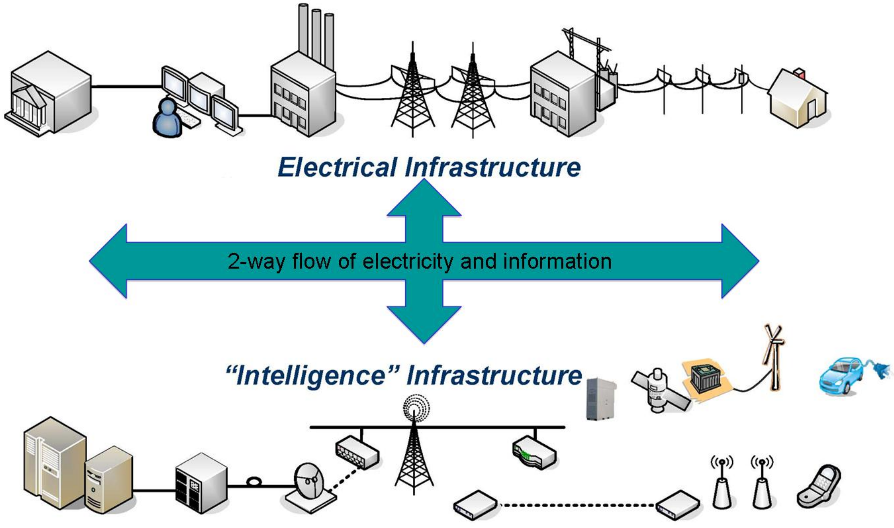
- *inexpensive*
- *robust*
- *mass produced*

Electricity grid

- aging
- outmoded
- security target
- smart

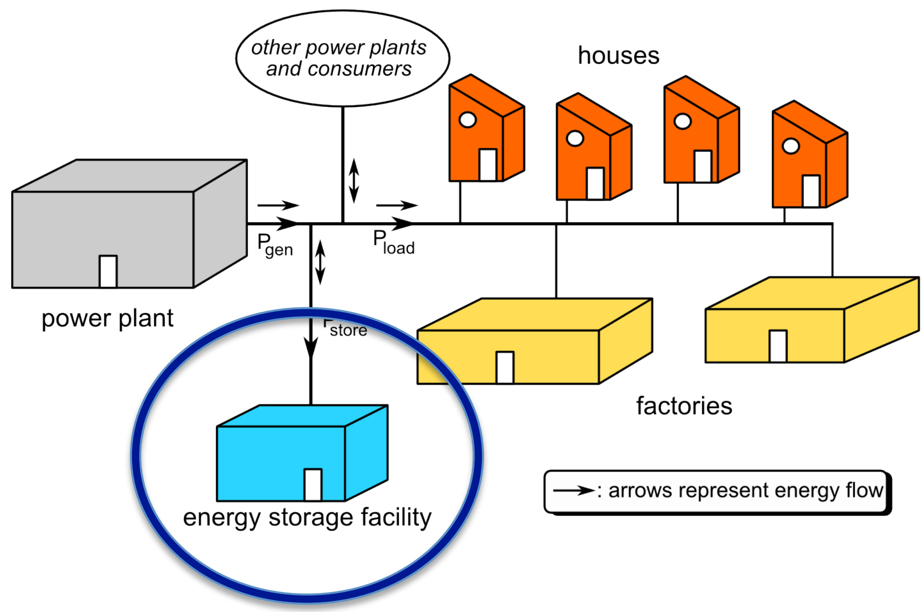
Economic, environmental, technological evolution favors distributed energy

Smart Grid: Two Way Information and Power Flows

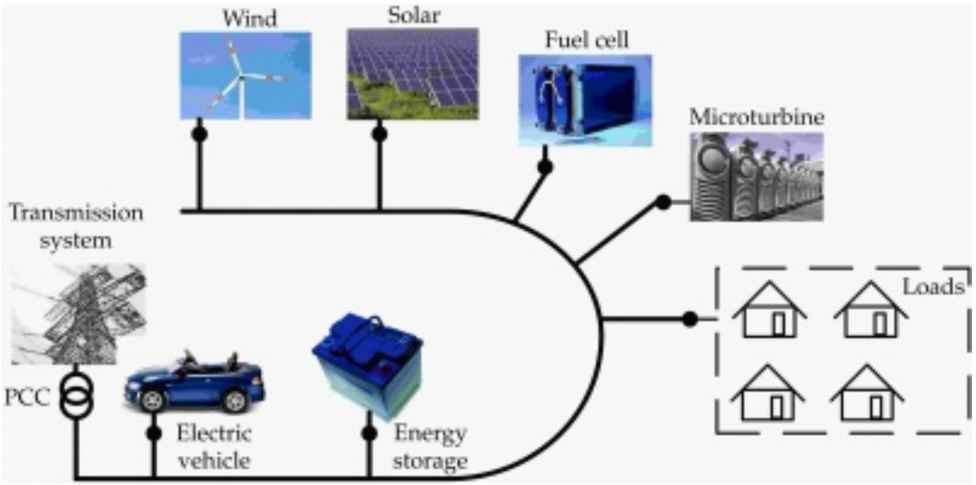


Energy Storage: Add a Third Dimension

Breaks the century old constraint to match instantaneous generation to instantaneous demand



Distributed Energy + Smart Grid + Energy Storage → Microgrid



Microgrid

Generation – Demand – Storage

- *Local energy management*
- *Renewable generation*
- *Co-generation: electricity+heating*
- *Short delivery distance*
- *Reduced dependence on grid*
- *Service profile tailored to customer*
- *"Personalized" energy*

Tailor service for customer

- *Residence*
- *Neighborhood*
- *Office buildings*
- *Shopping center*
- *Factory*
- *Campus*
- *Military base*

One size does not fit all

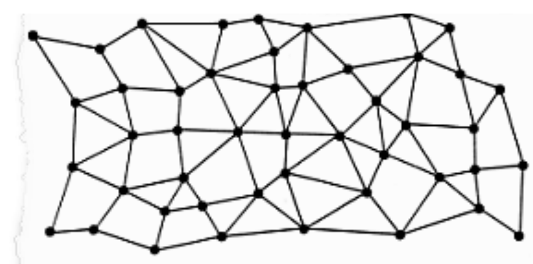
A DC Microgrid?

DC components

- *Solar panel*
- *Battery*
- *LED lighting*
- *Electronics*
- *Everything except motors*

Short delivery distance

Simplified, less expensive

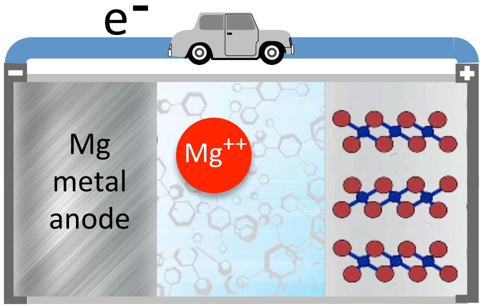


A network of interacting microgrids

Techno-economic Modeling

Transportation

Magnesium/Metal-Oxide

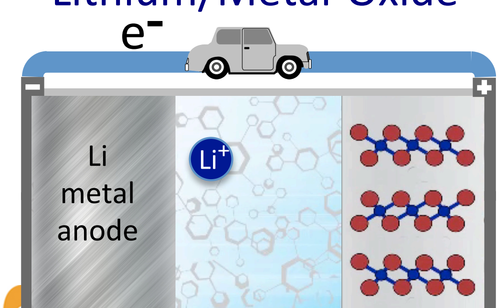


Metal oxide cathode

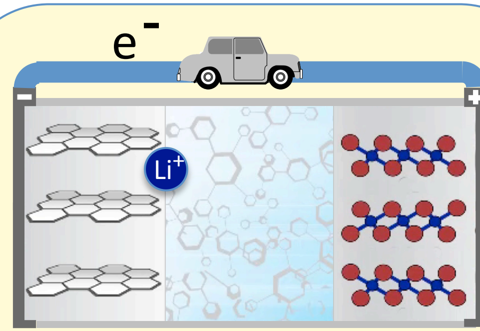
Lithium/Sulfur

Sulfur cathode

Lithium/Metal-Oxide



Metal oxide cathode



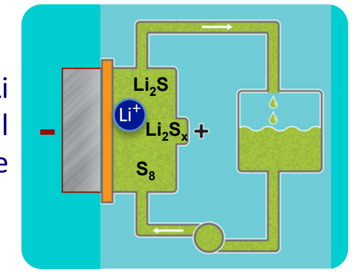
Graphite anode | Liquid organic electrolyte | Metal oxide cathode

Lithium-ion

Grid

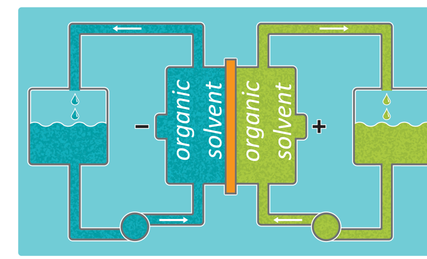
Polysulfide suspension semi-flow

Li metal anode



Non-aqueous redox flow

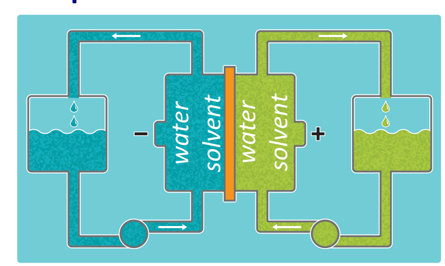
Various tailored molecules



System-to-materials performance and cost thresholds

Aqueous redox flow

Various tailored molecules



All have challenges that must be overcome to bridge the gap from today to $100/kWh

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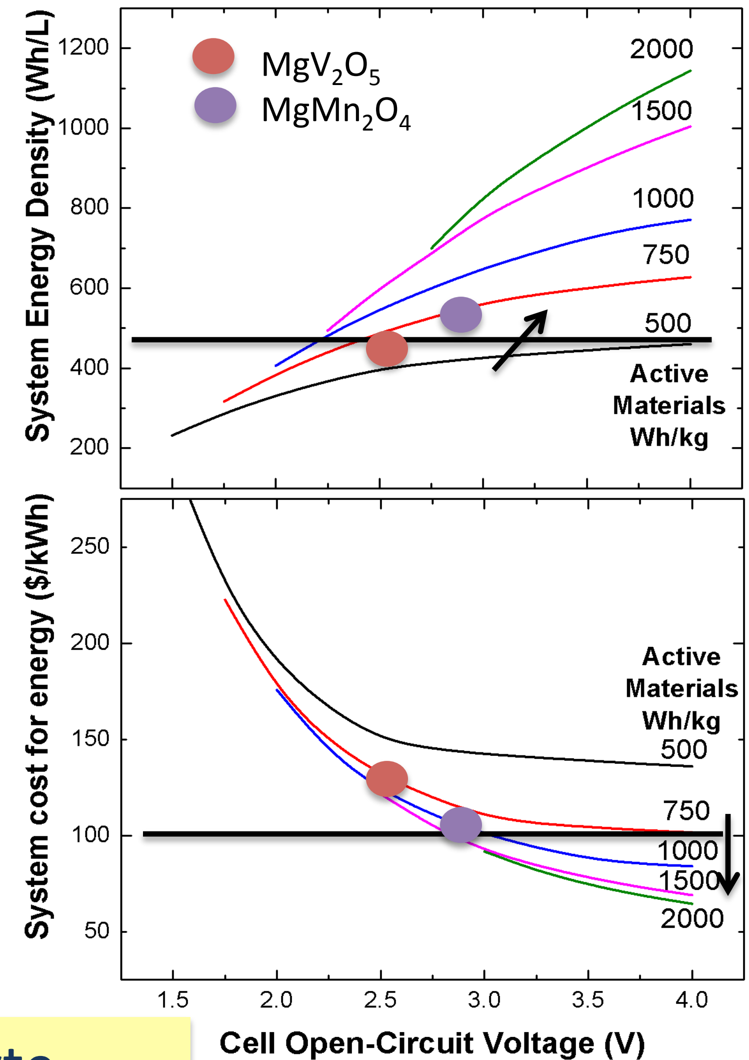
Multivalent Chemistries

- Metal anode is required
  - >99.9% coulombic efficiency
- Specific energy >800 Wh/kg
  - Cathode only value
  - Lower g/cm^3 requires higher Wh/kg target
- U_{ave} > 2.75 V
  - Lower voltages penalized by inactive materials



Key challenges

Functioning conventional electrolyte
High energy cathodes that enable transport

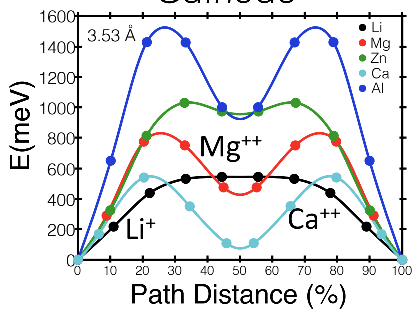
Transportation Energy Storage Arc

Multivalent-ion Intercalation

2014

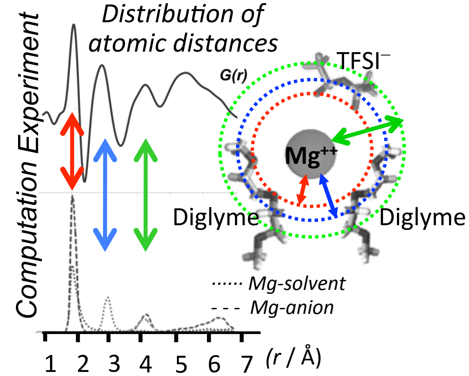
Cathodes

Mobility in Mn_2O_4 Cathode



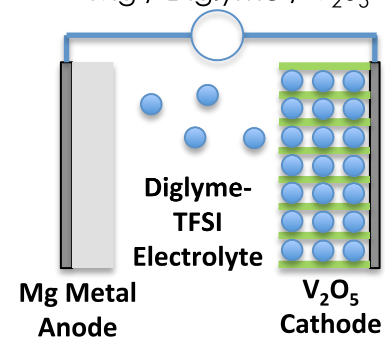
Electrolytes

Mg++ Solvation in Diglyme



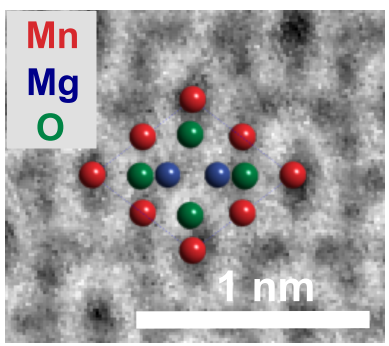
Battery System

Mg / Diglyme / V_2O_5



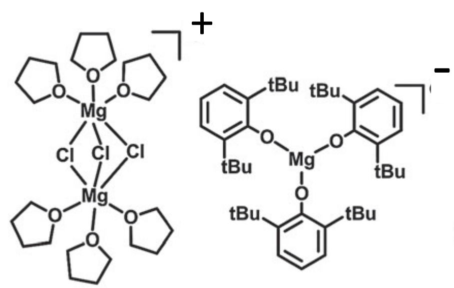
2015

New cathode: Mn_2O_4
Mg intercalation demonstrated



STEM, XRD, NMR, XAS, EDX
Kim et al, Adv Mater 27, 3377 (2015)

Electrolyte conditioning and structure → Mg stripping/deposition
Barile et al, J Phys Chem C 2014, 2015



Phenol-based All-Mg (DTBP)MgCl–$MgCl_2$
Pan et al Chem Comm 51, 6214 (2015)

Role of H_2O and solvent co-intercalation in V_2O_5
Gautam, Chem Mater 27, 3733 (2015)
Tepavcevik ACS Nano 2015

Sprints for

- *Ca++ in metal oxide*
  → *Prussian Blue*
- *Zn++ in metal oxide*
- *Mg++ in $MoO_{2.8}F_{0.2}$*
- Mg compatible Cl-free electrolytes

Battery Systems

Mg	Diglyme-TFSI (DTBP)MgCl-$MgCl_2$	V_2O_5 Mn_2O_4

Li-Sulfur Transportation and Grid Batteries

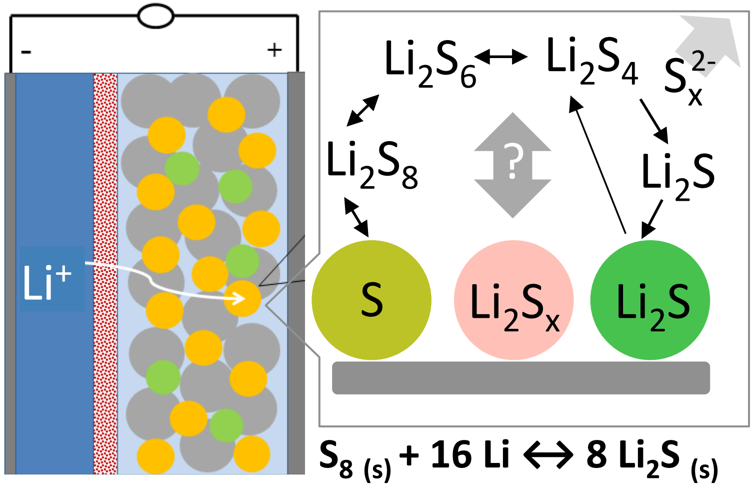
Appeal

- Very high theoretical specific energy (**2567 Wh/kg**)
- Sulfur: Naturally abundant, non-toxic, low cost

Challenges

- Instability of Li metal → Li/electrolyte depletion
- Polysulfide (PS) shuttle mechanism: self-discharge
- Insoluble S/Li_2S → Partial active material utilization

Common to Li-S Flow and Li-S Stationary



$S_{8\,(s)}$ + 16 Li ↔ 8 $Li_2S_{(s)}$

U = 2.2 V vs Li

JCESR Convergent Solutions

Cathodes that trap polysulfide's with PEO_6TFSI and other binders

Sparingly solvent electrolytes that do not solvate polysulfides: $LiTFSI(ACN)_2$:HFE

Protect Li anode with

Intrinsic SEIs from high concentration salts in conventional electrolytes: 4M LiFSI in DME

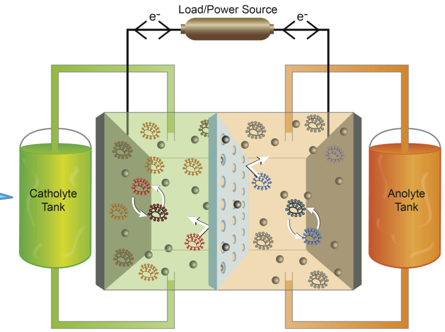
6000 cycles Qian et al, Nature Comm 6:6362 (2015)

ALD-deposited artificial membranes: $LiAlS_x$: high Li conductivity

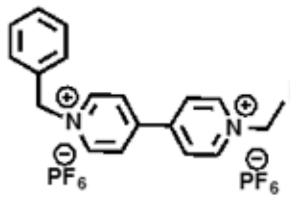
Composite polymer membranes: PFPE-diol + Li_2S-P_2S_5

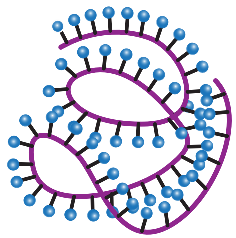
Flexible, high Li+ conductivity, 5V operating window, impervious to polysulfides

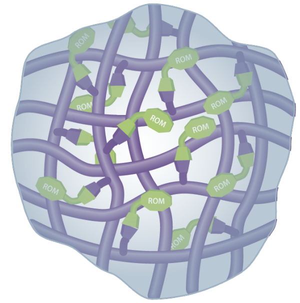
Toward a Non-aqueous Redox Flow Grid Battery



Three JCESR innovations







2013
Redox Organic Molecules (ROM)
< 1 nm

Design organic molecules

Active molecules

Solvent for active molecules

Salt: mobility

Rich design space

Largely unexplored

Electrolyte Genome

2014
Redox Active Polymers (RAP)
Few nm to sub-micron

Create long chain of active molecules

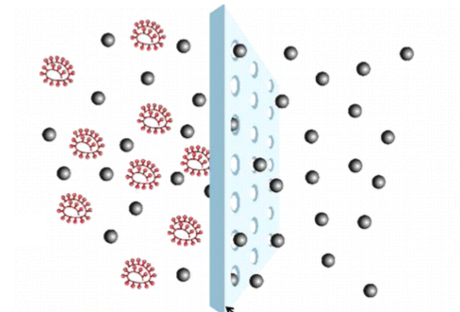
Selectively filter from non-active counterions by size

Dense chain of active molecules

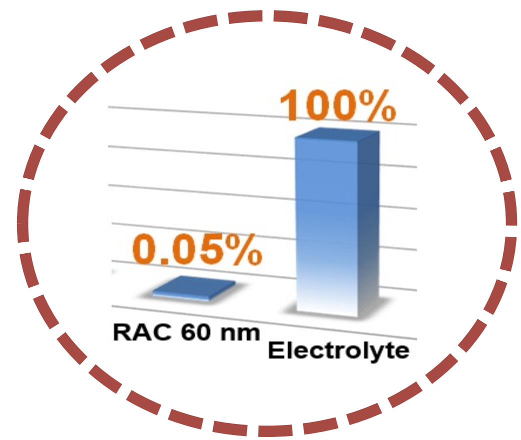
2015
Redox Active Colloids (RAC)
Microns and larger

Cross-link polymers to form large spherical colloids

Shape easier to control and filter



Off-the-shelf Celgard membranes

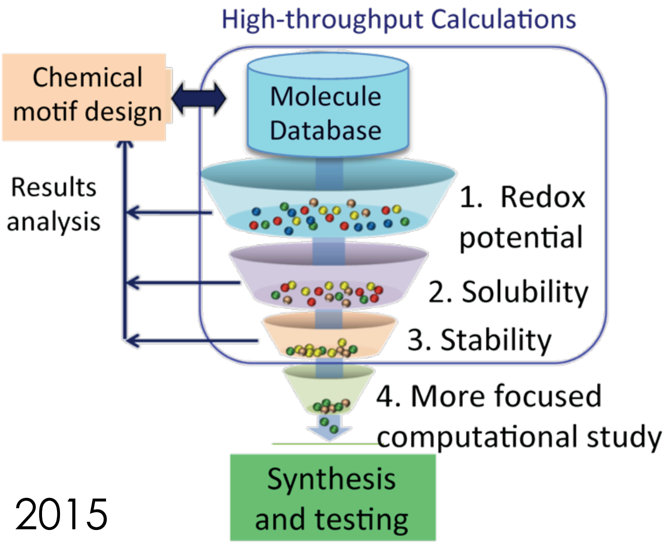


Challenge of mixing between energy storage tanks is solved

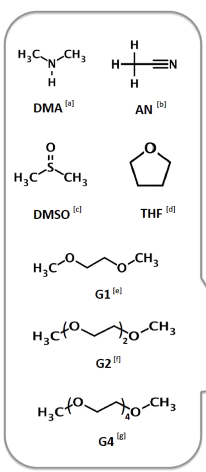
JCESR

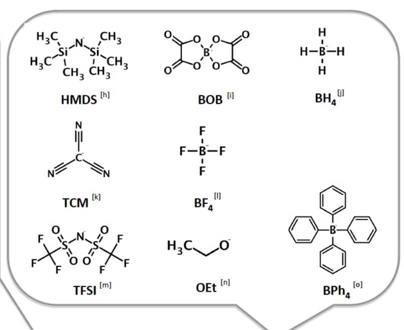
Electrolyte Genome – Crosscutting Science

2014: 4 800 molecules



2015





16 000 molecules

meets JCESR milestone

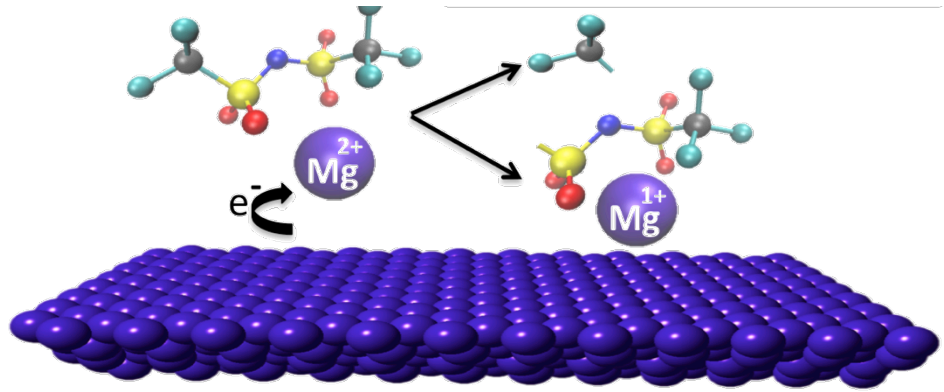
Qu et al, Comp Mat Sci 103, 56 (2015)
Cheng et al, J Phys Chem Lett 6, 283 (2014)

2015: Solvation and Interface Reactivity

Ion pairs are common in divalent solvation shells

Anions and solvents in divalent solvation shells are not stable at electrochemical interfaces

TFSI- and diglyme cleave on partial charge transfer



New opportunity

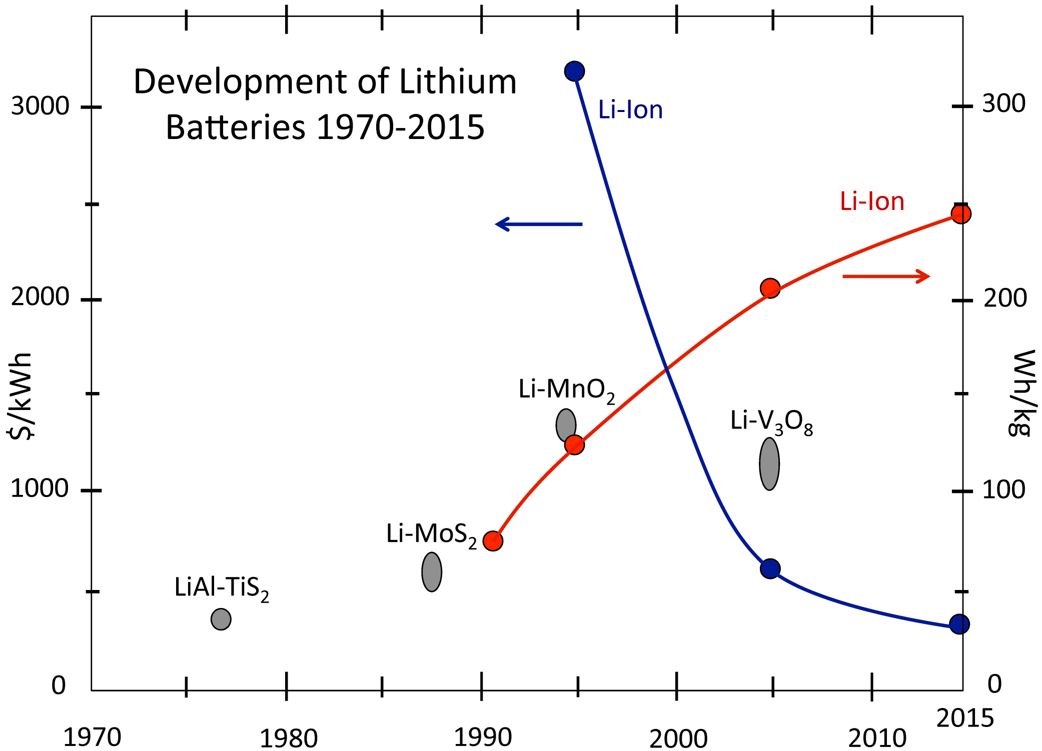
Design solvation shell as delivery vehicle for metal anode stripping and plating

Crosscutting theory – experiment program

Rajput et al JACS 134, 3411 (2015)

JCESR

Lessons from Lithium-ion inform JCESR



Crabtree, Kocs, Trahey, MRS Bulletin, Dec 2015

1971
Conceptualization
Li metal anode
Intercalation cathode

1991
Commercialization
Sony Lithium-ion

Steady but saturating
post-commercialization
discovery and development

20 year incubation period

Simple, elegant concepts, but . . .

Complex interfering side effects
Detrimental side chemical reactions
Incompatible materials

"Murphy's Law" worst case scenario

Many (most) ideas do not work
Many strategic pivots

Balance targeted outcomes
with back up alternatives

"Convergent" and "divergent" research

After 40 years, the "holy grail" of
Lithium metal anodes still eludes us

Nimble strategic pivots and
a balance of convergent and divergent research are essential