Joint Center for Energy Storage Research

Beyond Lithium Ion Energy Storage

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Outline

Transforming transportation and electricity grid with electricity storage

JCESR: a new paradigm for battery R&D

Promising technologies

2015 Bay Area Battery Summit
Lawrence Berkeley National Laboratory
November 3, 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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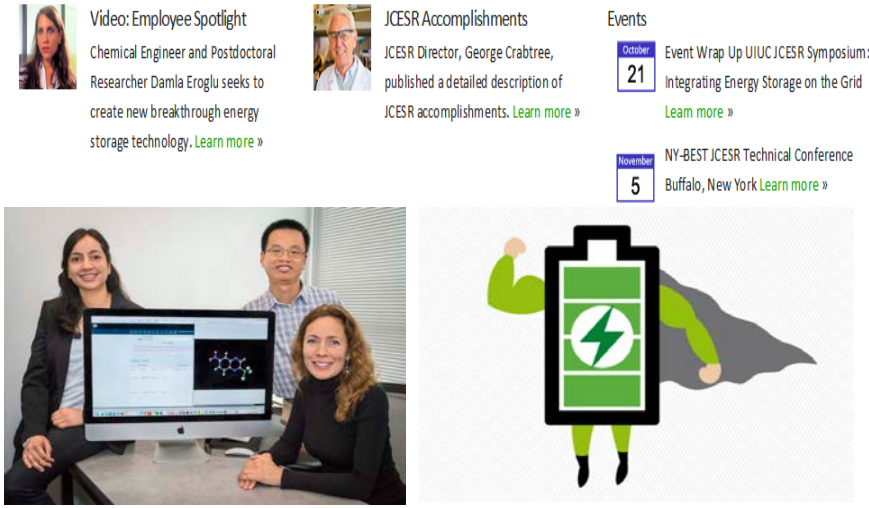
Abstract. The Joint Center for Energy Storage Research (JCESR) seeks transformational change in transportation and the electricity grid driven by next generation high performance, low cost electricity storage. To pursue this transformative vision JCESR introduces a new paradigm for battery research: 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

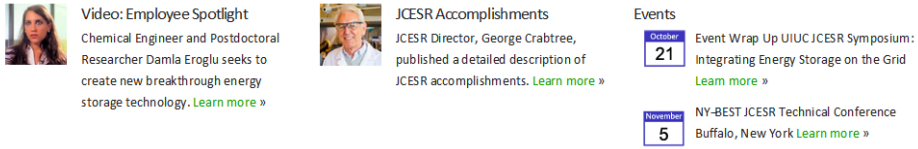
Transportation and the electricity grid account for two-thirds of U.S. energy use [1]. Each of these sectors is poised for transformation driven by high performance, low cost electricity storage. The Joint Center for Energy Storage Research (JCESR) pursues discovery, design, prototyping and commercialization 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



Electrolyte Genome Game-Changer

How computational screening of molecules at Berkeley Lab could accelerate electrolyte discovery.



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 enable
the personal electronics revolution

Forever changed the way we interact
with people and information

Tomorrow

$20K electric cars

Displace gasoline cars

Replace foreign oil with domestic electricity

Reduce energy use and carbon emissions

Grid-scale electricity storage

Widespread deployment of wind and solar

Enhance reliability, flexibility, resilience

Uncouple instantaneous generation from instantaneous demand

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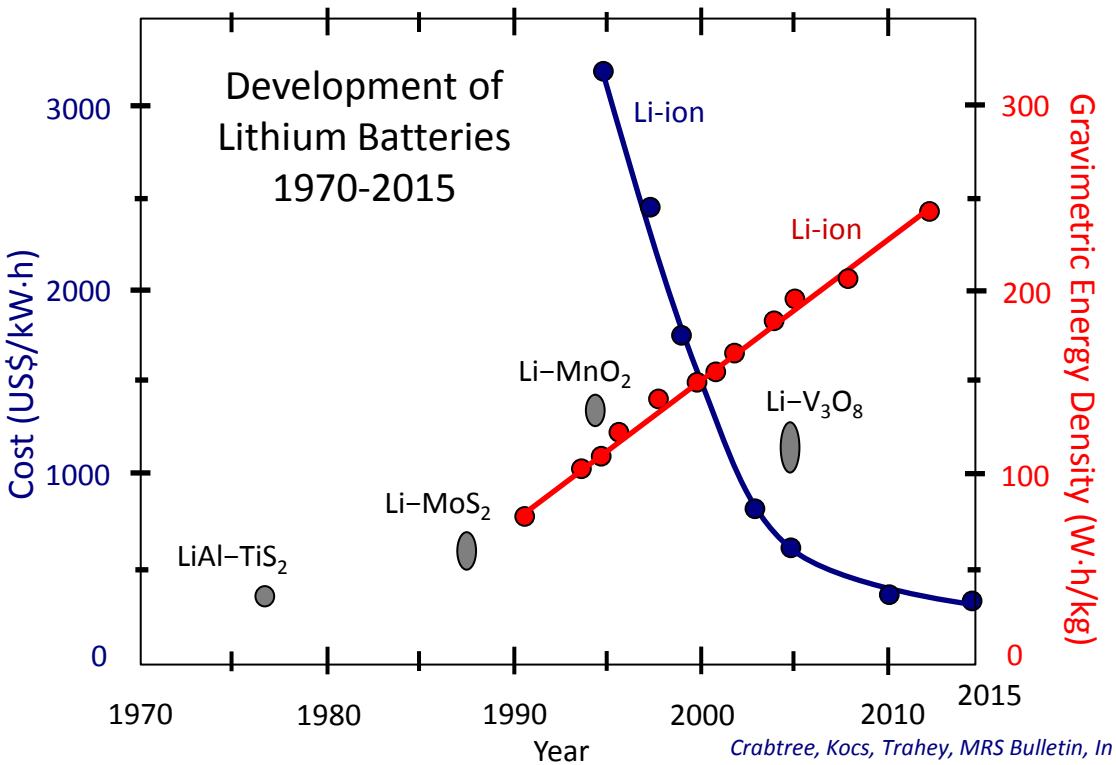
Lessons from Lithium-ion inform JCESR



Crabtree, Kocs, Trahey, MRS Bulletin, In Press

1971
Conceptualization
Li metal anode
Intercalation cathode

1991
Commercialization
Carbon anode
Metal Oxide cathode

Steady
post-commercialization
improvement

20 year incubation period

Simple, elegant concepts
Complex interfering side effects

Many (most) ideas do not work

After 40 yeas of intense research, the "holy grail" of Lithium metal anodes still eludes us

Balance of

- targeted "convergent" outcomes
- back-up "divergent" alternatives

Many strategic pivots

A balance of convergent and divergent research

Transportation and Electricity Grid

Two biggest energy uses

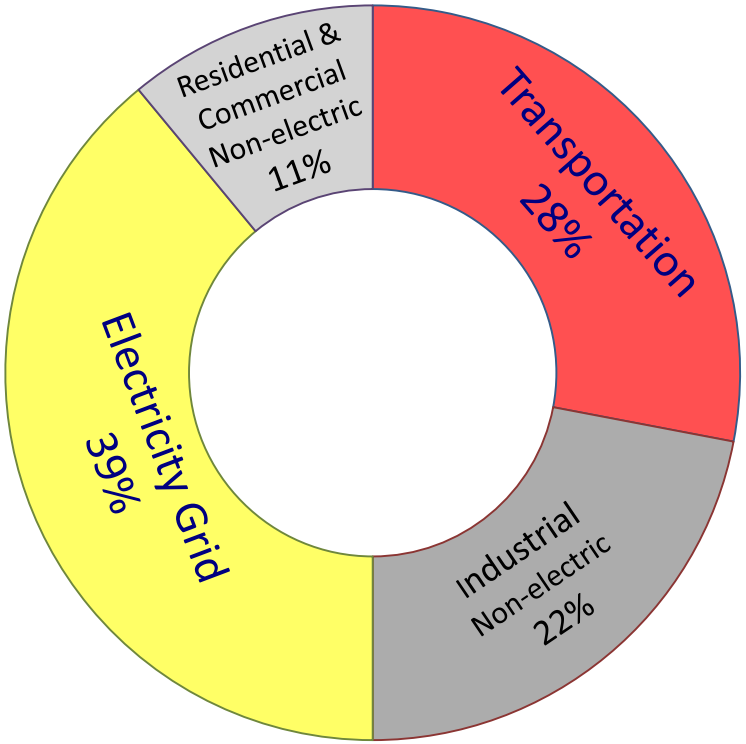
Transportation 28%

Electricity 39%

Personal electronics < 2%

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

US Energy Demand



2013

EIA Monthly Energy Review Table 2.1 (May 2014)

Widespread deployment of electric cars and storage on the grid requires inexpensive, high performance, next generation batteries

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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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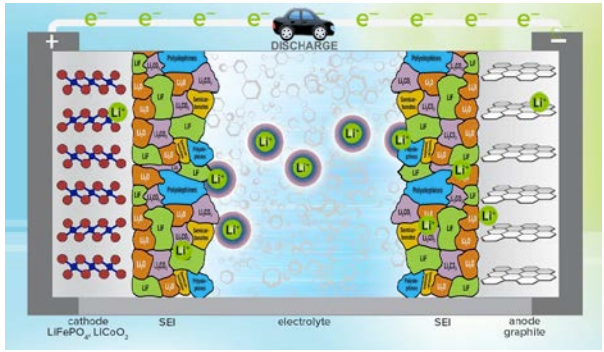
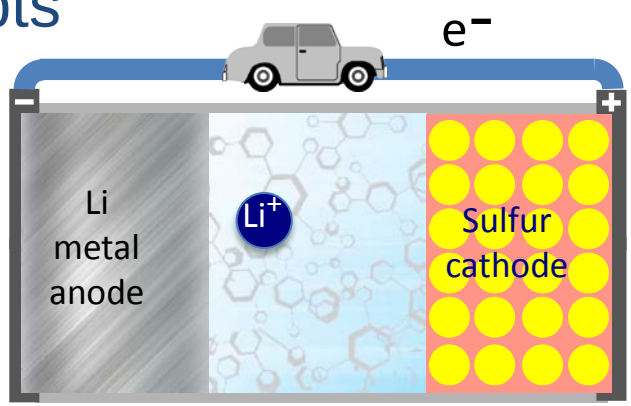
JCESR's Beyond Lithium-ion Concepts



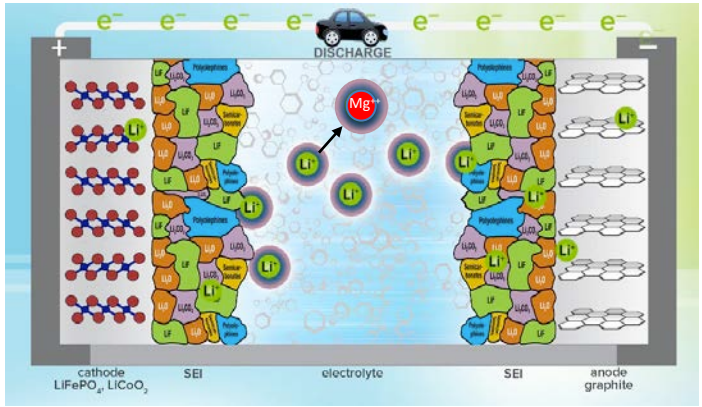
Lithium-ion "Rocking Chair"

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



Chemical Transformation

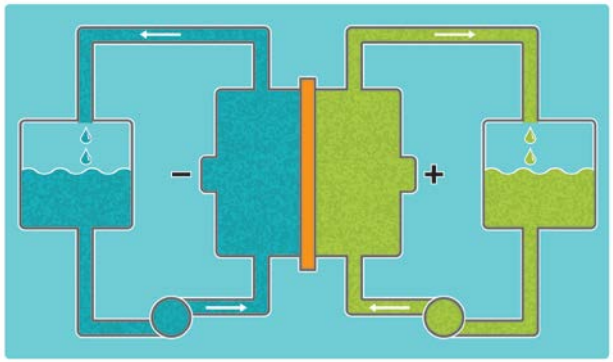
Replace intercalation with high energy chemical reaction: Li-S, Li-O, Na-S, . . .



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

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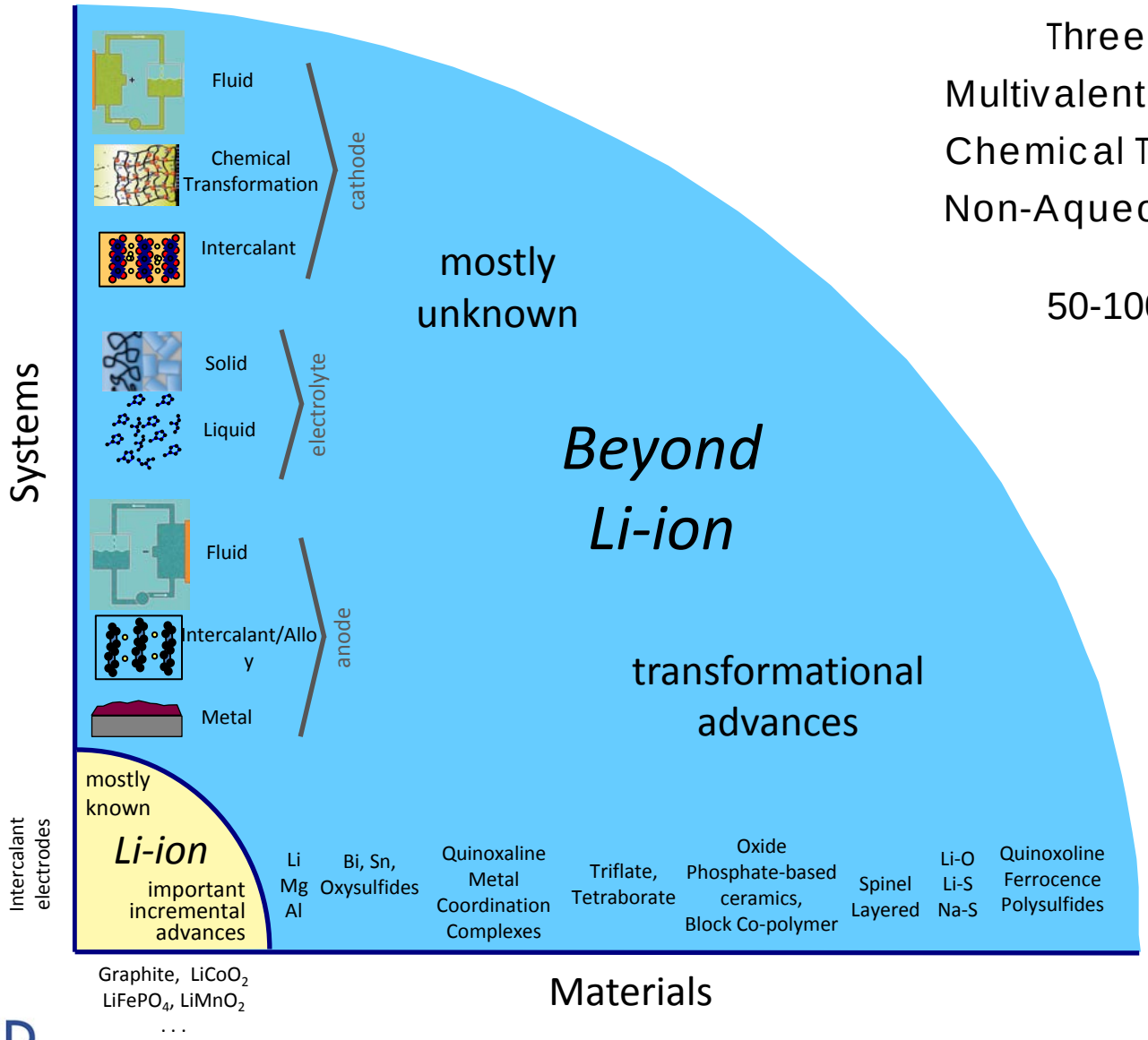
Argonne NATIONAL LABORATORY



Three concepts

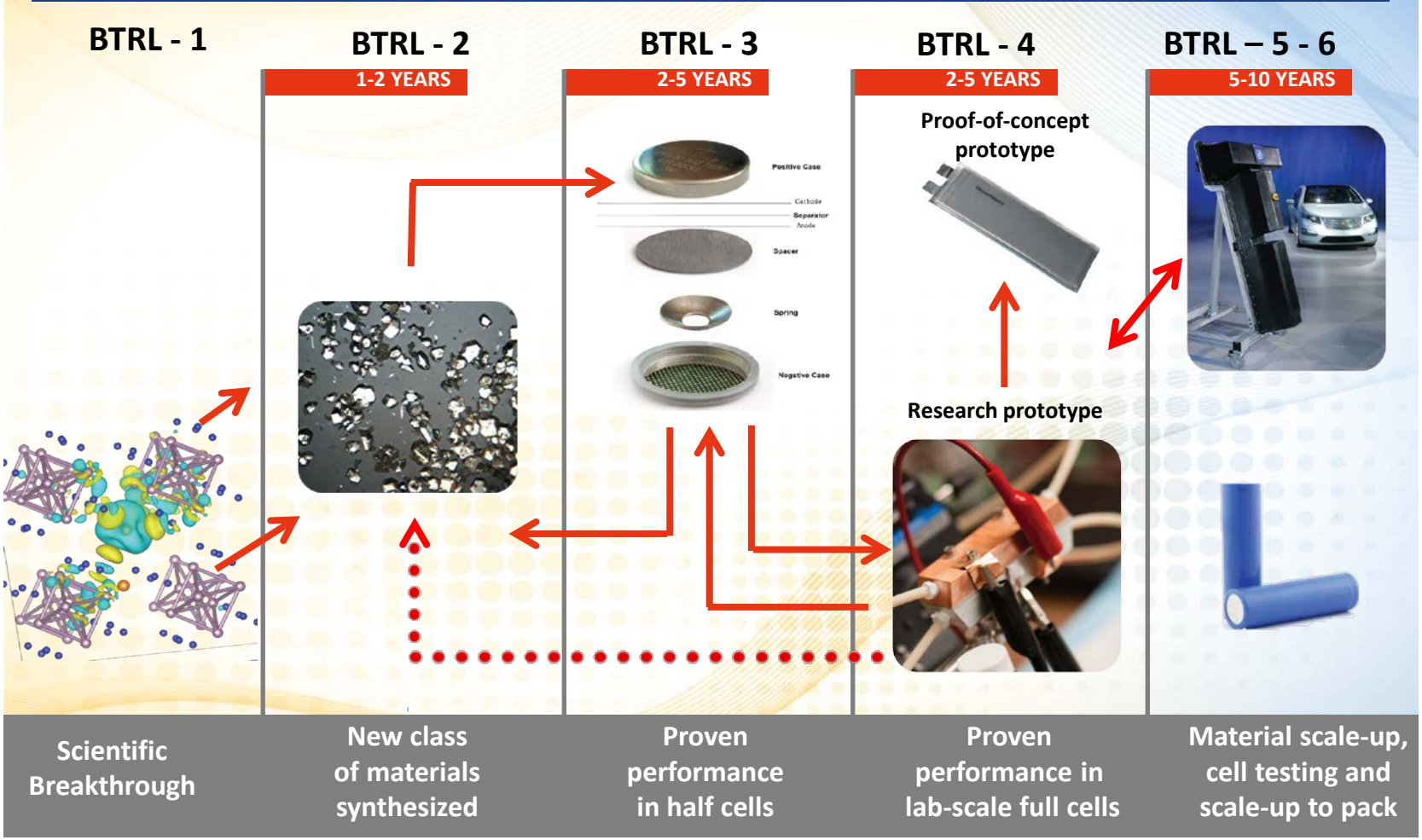
Multivalent Intercalation

Chemical Transformation

Non-Aqueous Redox Flow

50-100 Batteries

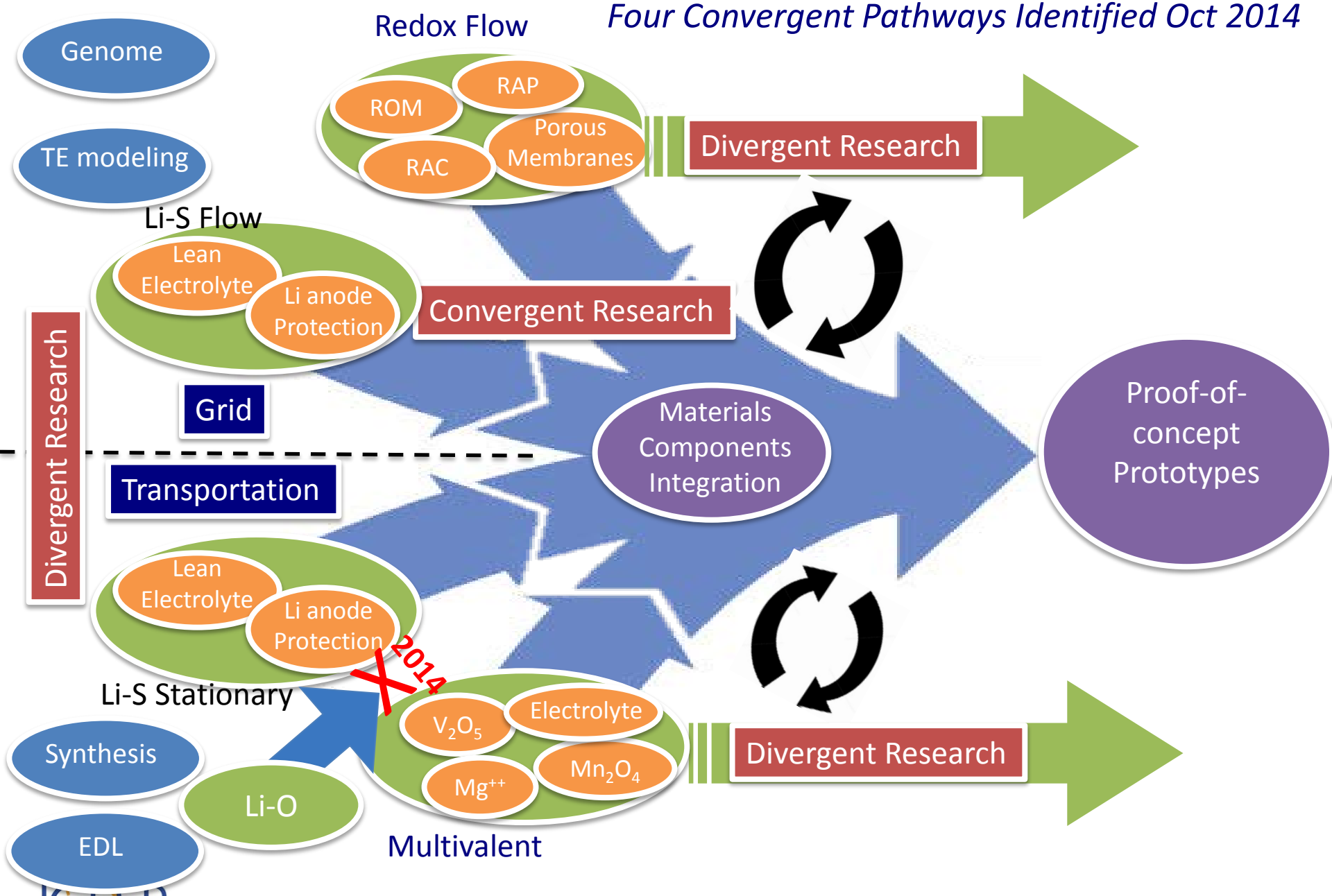
Battery Technology Readiness Level (BTRL)



Developed collaboratively with JCI, NASA-Glenn, TARDEC

JCESR "sweet spot"

Four Convergent Pathways Identified Oct 2014



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Perspective

More on JCESR website
www.jcesr.org

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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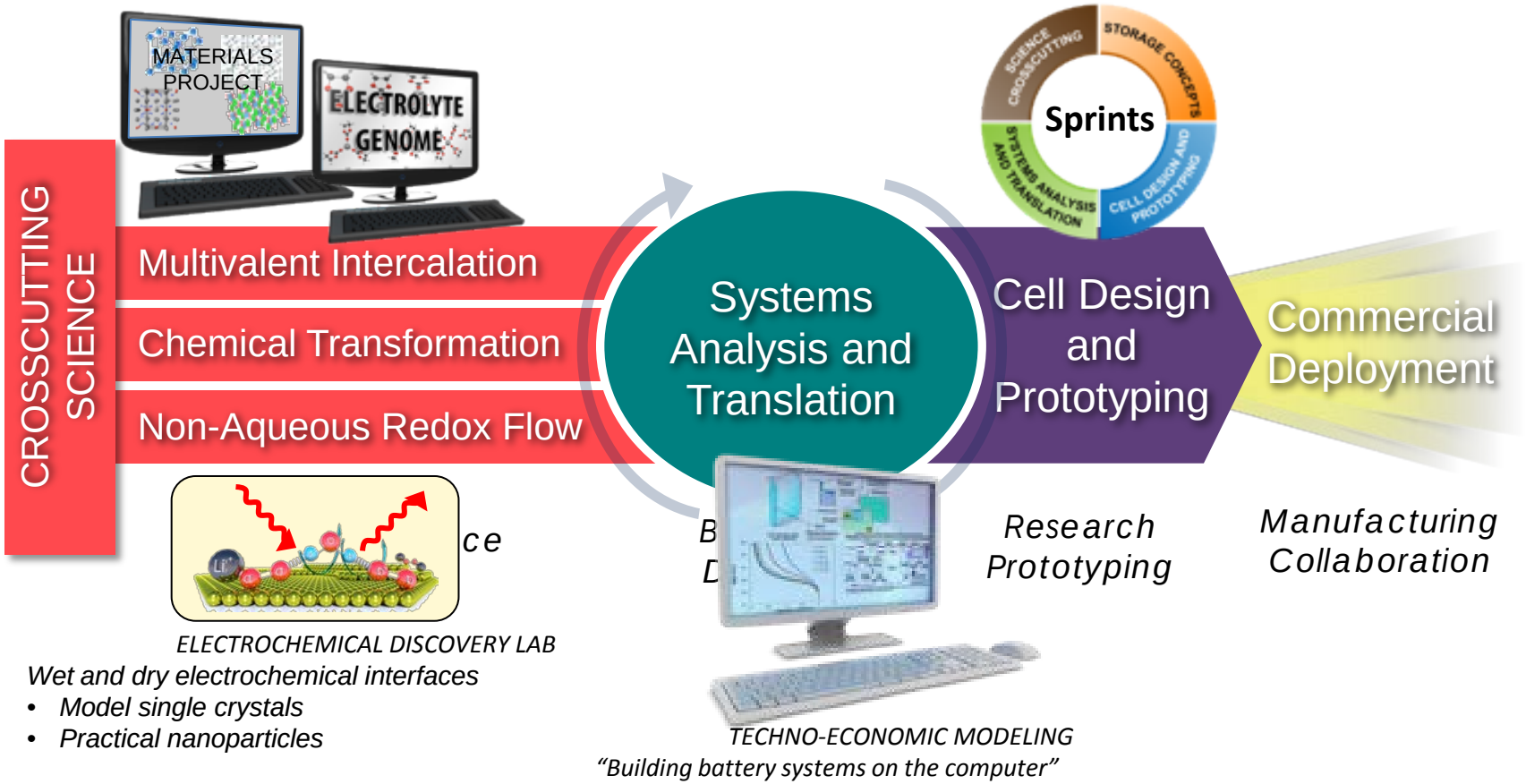
Supplemental Slides

May contain trade secrets or commercial or financial information that is privileged or confidential and exempt from public disclosure.

JCESR Creates a New Paradigm for Battery R&D



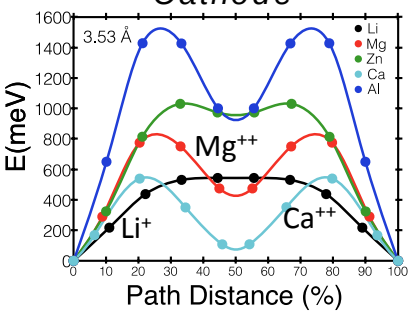
Transportation Energy Storage Arc

Multivalent-ion Intercalation

2014

Cathodes

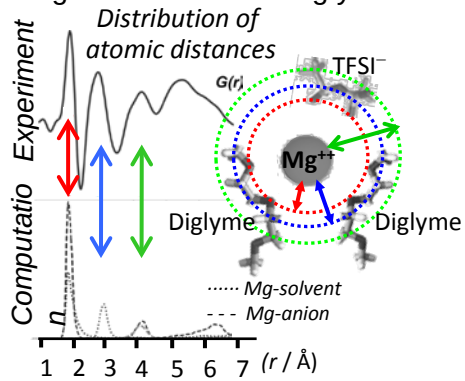
Mobility in Mn_2O_4 Cathode



Electrolytes

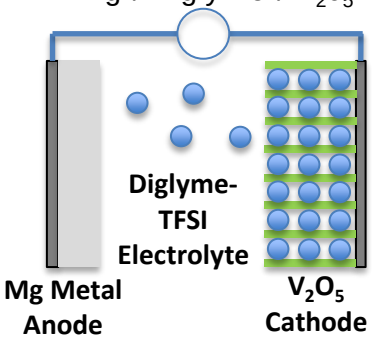
Mg++ Solvation in Diglyme

Distribution of atomic distances



Battery System

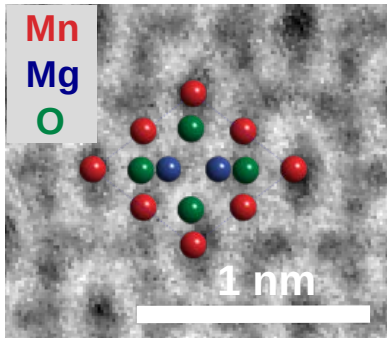
Mg / Diglyme / V_2O_5



2015

New cathode: Mn_2O_4

Mg intercalation demonstrated

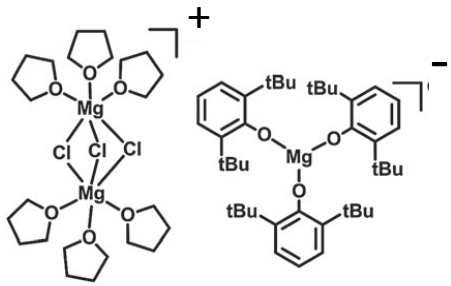


STEM, XRD, NMR, XAS, EDX

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

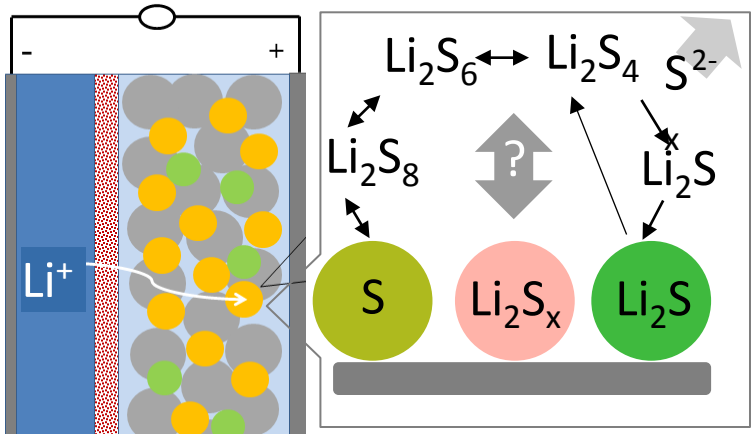
Li-Sulfur Transportation and Grid Batteries

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



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

U = 2.2 V vs Li

Common to Li-S Flow and Li-S Stationary

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

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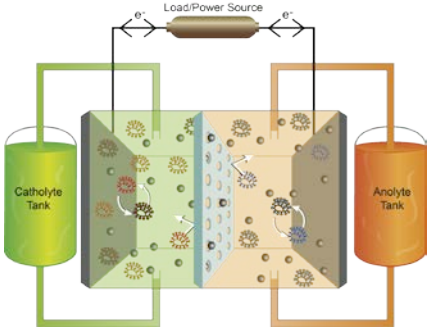
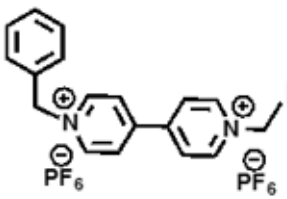
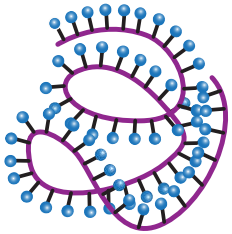
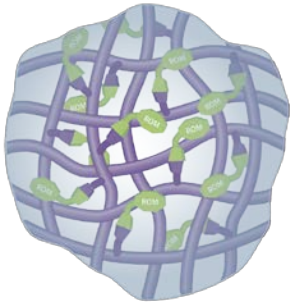
Toward a Non-aqueous Redox Flow Grid Battery

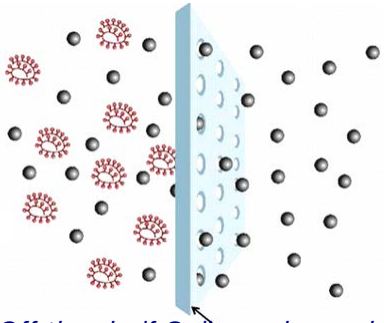


Three JCESR innovations









Off-the-shelf Cellguard membranes

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

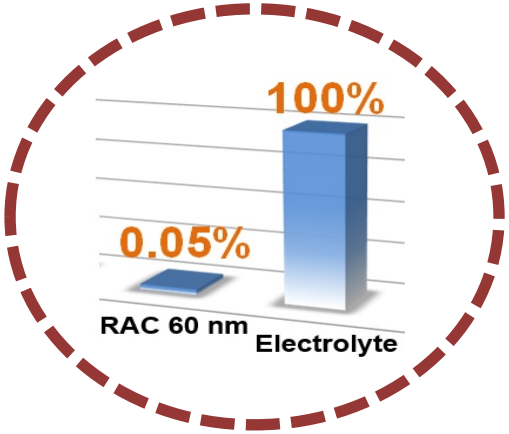
Selectively filter from non-active counterions by size

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

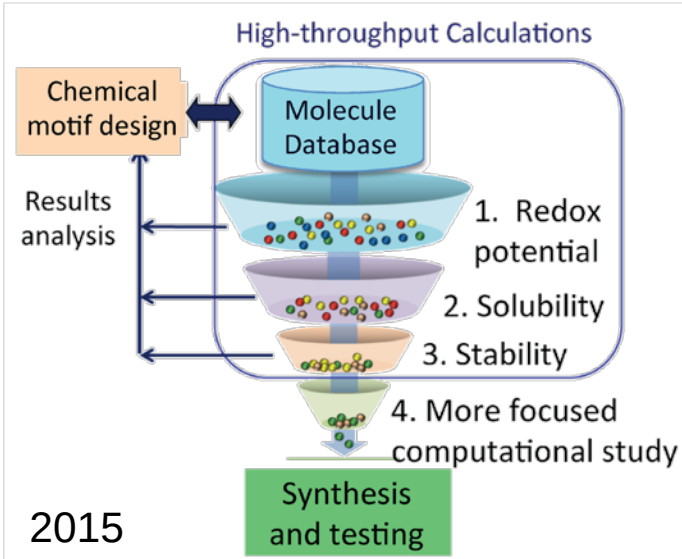


Challenge of mixing between energy storage tanks is solved

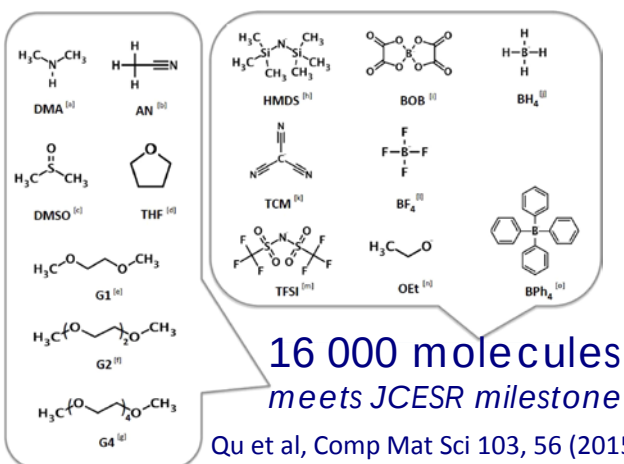
JCESR

Electrolyte Genome – Crosscutting Science

2014: 4 800 molecules



2015



16 000 molecules

meets JCESR milestone

Qu et al, Comp Mat Sci 103, 56 (2015)

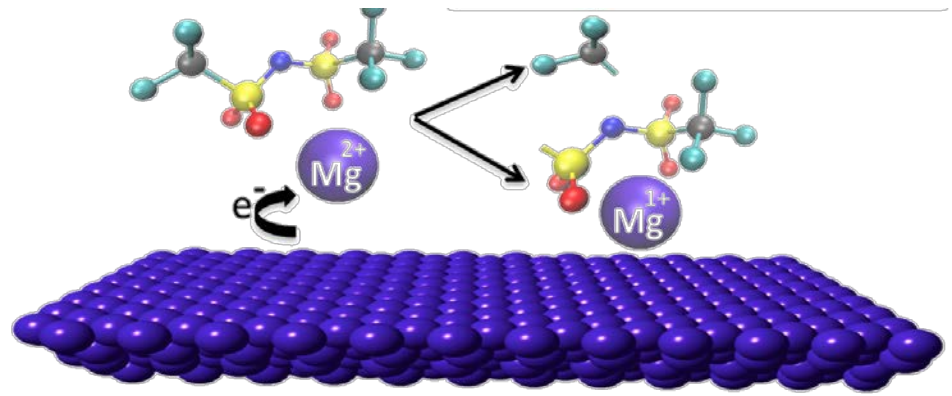
Cheng et al, J Phys Chem Lett 6, 283 (2014)

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)