Joint Center for Energy Storage Research

JCESR: One Year Later

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Outline

Challenges: Transportation and Electricity Grid

Vision, Mission, Legacies

A New Paradigm

Highlights: solvation, trace water, Lithium-air batteries

Directions: solvation, metal anodes, novel prototypes, reaction pathways

Secretary of Energy Advisory Board
Argonne National Laboratory
June 20, 2014

Energy Storage Challenges

Two biggest energy uses poised for transformational change

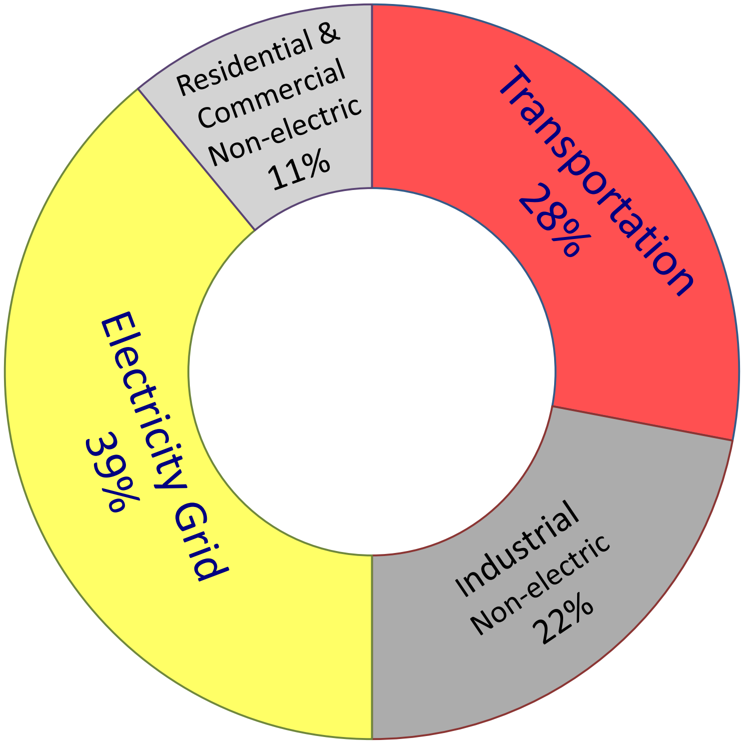
Transportation 28%

- *Foreign oil → domestic electricity*
- *Reduce energy use*
- *Reduce carbon emissions*

Electricity 39%

- *Coal → Gas → Wind and Solar*
- *Greater reliability, resiliency, flexibility*
- *Lower costs by deferring infrastructure*
- *Replace "just in time" with inventory*

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 Has Transformative Goals

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

Why So Aggressive?

- *Nothing less is transformative*
- *Next generation energy technology demands next generation electricity storage*
- *Open new horizons of performance and cost beyond lithium-ion*

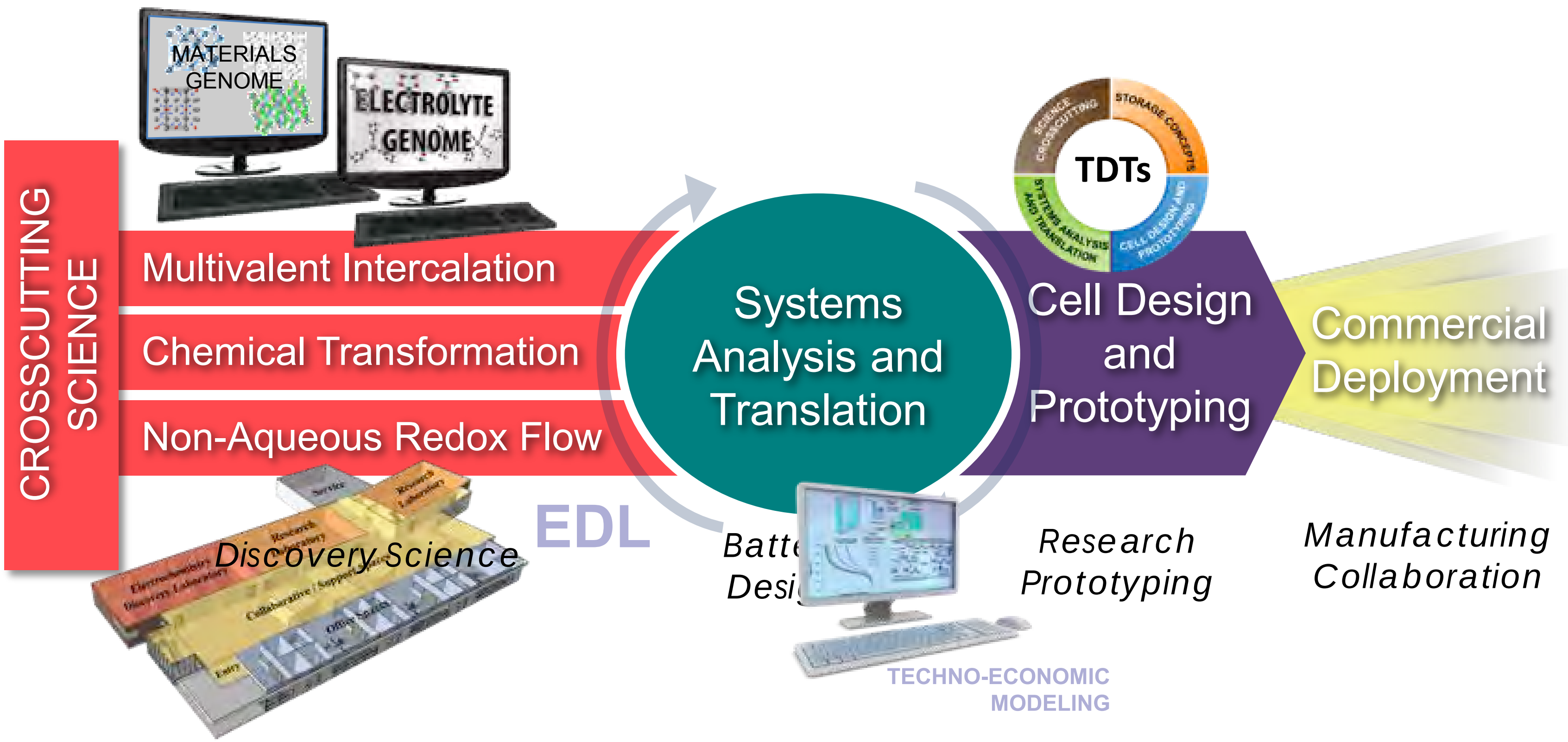
Lithium-ion – the best battery technology we have ever seen

- Increases energy density at 5%/yr
- Decreases cost at 8%/yr

. . . but cannot achieve transformative factors of five in cost and performance

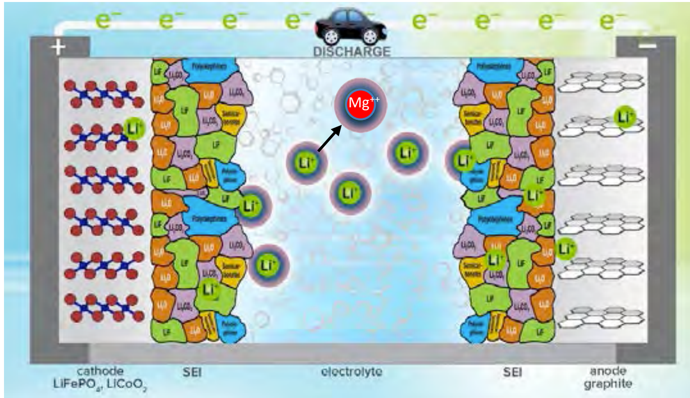
JCESR → beyond Lithium-ion

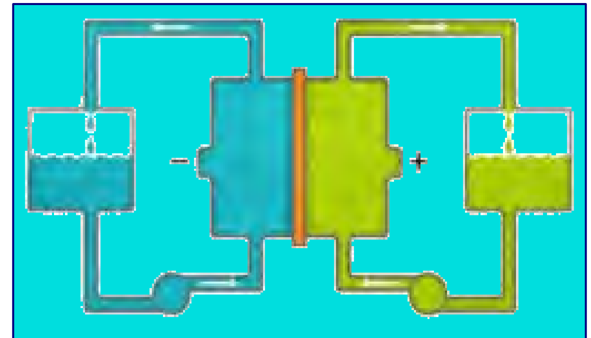
JCESR Creates a New Paradigm for Battery R&D



The JCESR Partner Team

JCESR's Beyond Lithium-ion Concepts





Yang, Zheng, Cui, Ener Env Sci 5, 1551 (2013)

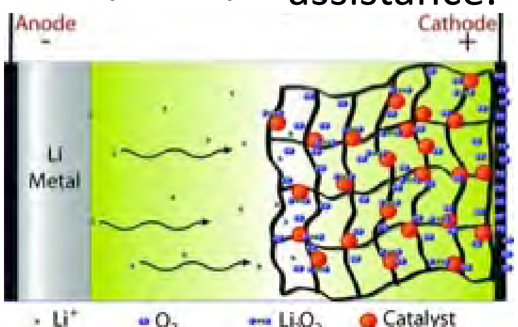
Multivalent Intercalation

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

Non-aqueous Redox Flow

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

please let us know if we can be of any assistance.



Black, Adams, Nazar, Adv. Energy Mater 2, 801 (2012)

Chemical Transformation

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

Cross-cutting opportunity
Designer Organic Molecules

Tailored structure-function relationships
Redox couples, electrolytes, SEI . . .

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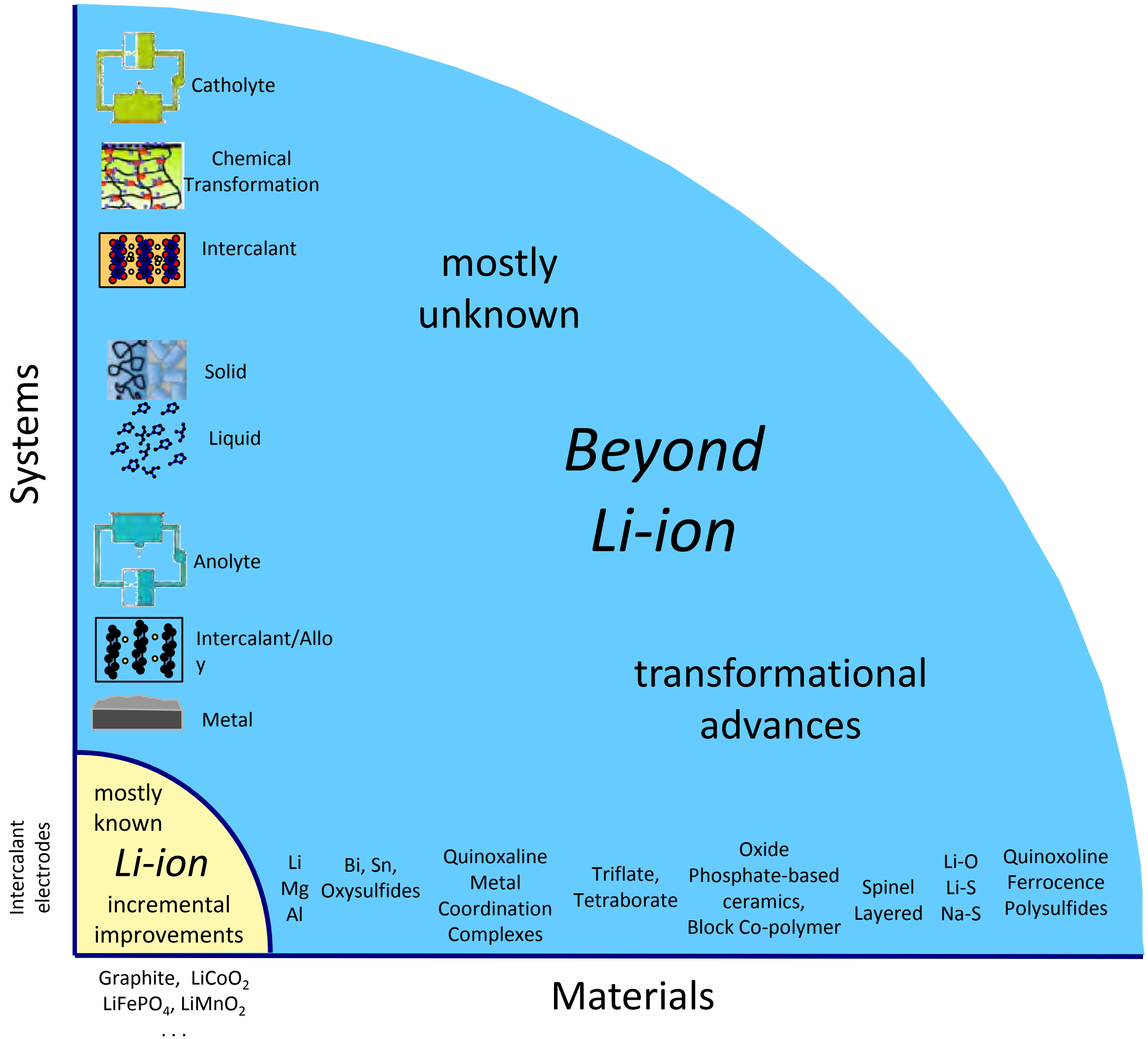
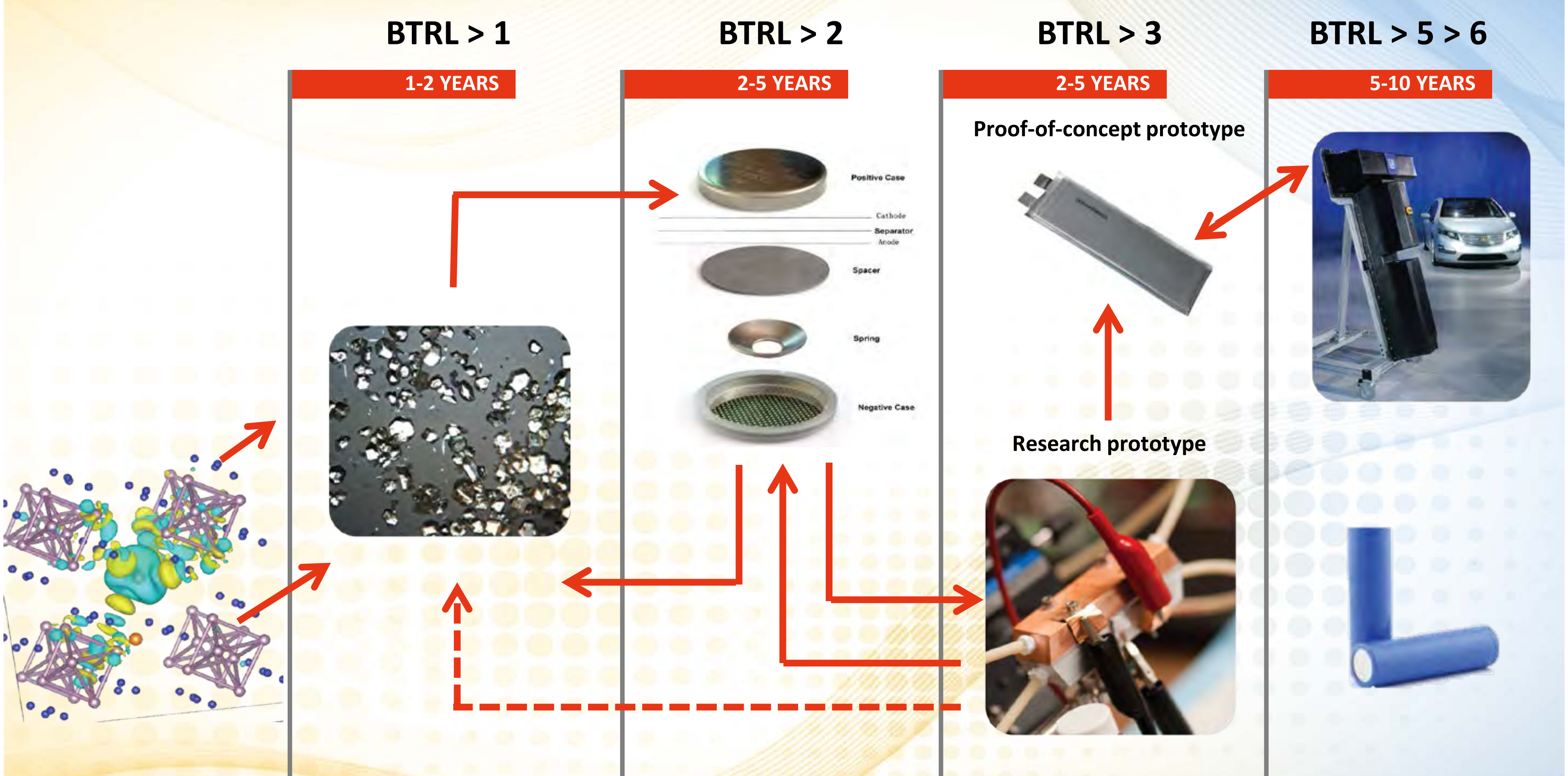
Beyond Lithium Ion Opportunity Space is Large, Unexplored and Rich



Battery Technology Readiness Level (BTRL)



Scientific Breakthrough	New class of materials synthesized	Proven performance in half cells	Proven performance in lab-scale full cells	Material scale-up, cell testing and scale-up to pack

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“sweet spot”

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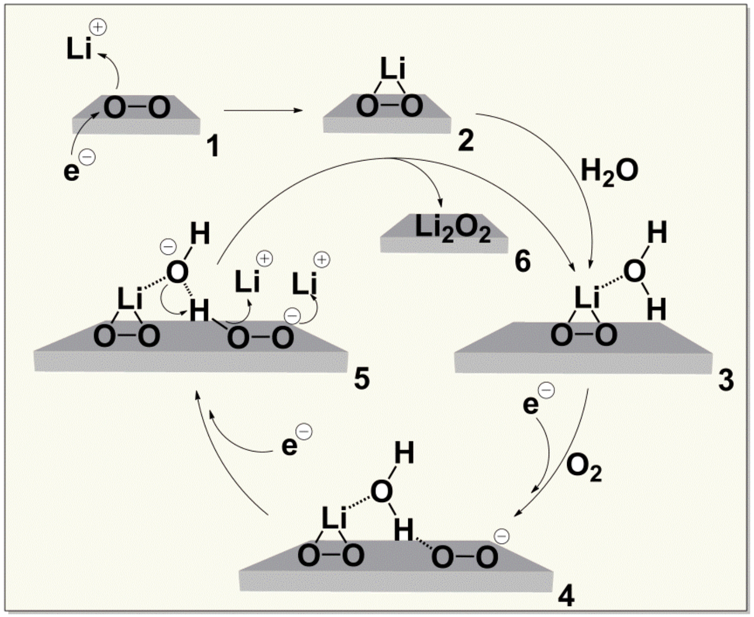
Trace Water Catalyzes Lithium Peroxide Electrochemistry



Reaction cycle for reduction of di-oxygen by lithium and water to lithium peroxide on single crystal gold surface.

Work performed at Argonne National Laboratory, Sandia National Laboratory, University of Illinois at Urbana-Champaign and Northwestern University

Performers: Jakub Jirkovsky, Ram Subbaraman, Dusan Strmcnik, Katharine Harrison, Charles Diesendruck, Rajeev Assary, Otakar Frank, Lukas Kobr, Gustav Wiberg, Bostjan Genorio, Vojislav Stamenkovic, Larry Curtiss, Jeffrey Moore, Kevin Zavadil, and Nenad Markovic

Submitted for publication 6-16-14

Scientific Achievement

Water at ppm levels catalyzes the conversion of lithium superoxide (Li-O_2) to lithium peroxide (Li_2O_2) by the reaction cycle shown. Because water is not consumed in the cycle, trace amounts leverage large effects.

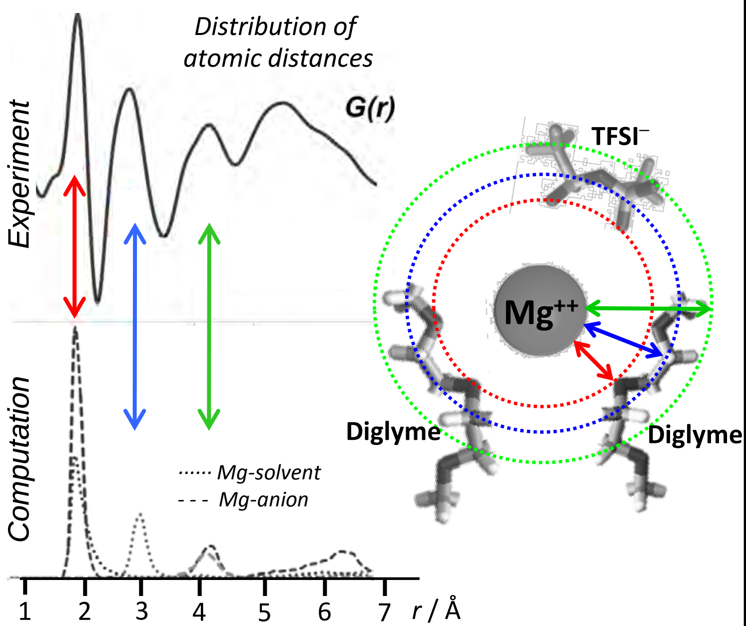
Significance and Impact

- **Trace water controls the rate and outcome of the discharge reaction in lithium-air batteries.**
- **Reversing the lithium peroxide reaction, a primary challenge for lithium-air batteries, requires understanding the role of trace water, an unexplored area.**
- **The strong polarity and active electrochemistry of trace water make it a likely player in many battery phenomena including solvation, the double layer, and redox behavior, all uncharted territory.**

Research Details

- **Novel procedure for elimination of water to <1 ppm from organic solvents, followed by controlled dilution**
- **The wet Electrochemical Discovery Laboratory (EDL) with exceptional purification and multi-modal Raman, FTIR, RRDE and AFM characterization enabled this research.**

Mg^{++} Solvation Shell in Electrolyte for Multivalent Batteries



Complementary pair/radial distribution functions G(r) from x-ray scattering (top) and molecular dynamics (bottom) define the solvation structure of Mg^{++} in a $Mg(TFSI)_2$/diglyme electrolyte (right). The presence of TFSI- in the first solvation shell indicates incomplete dissociation of the $Mg(TFSI)_2$ salt and partial compensation of the Mg^{++} charge.

Work performed at Argonne National Laboratory (JCESR managing partner) and Lawrence Berkeley National Laboratory

Saul H. Lapidus, Nav Nidhi Rajput, Xiaohui Qu, Karena W. Chapman, Kristin A. Persson, Peter J. Chupas, *"Magnesium electrolytes for multivalent batteries: Solvation and energetics"*, Submitted for publication

Scientific Achievement

- A new collaborative x-ray scattering and molecular dynamics simulation approach reveals the structure and energetics of Mg^{++} ion solvation in a diglyme electrolyte.

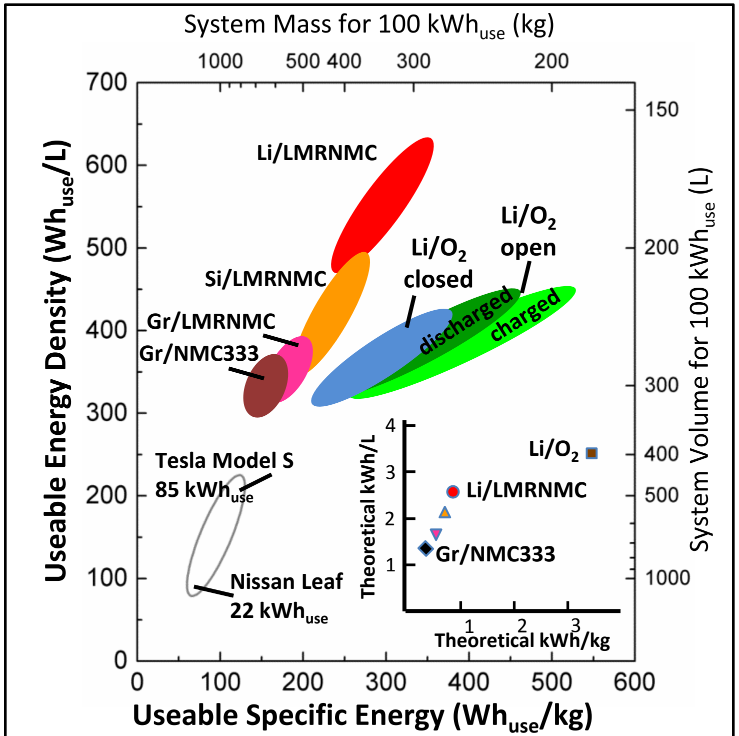
Significance and Impact

- Solvation of the working ion in an electrolyte mediates critical phenomena including ion mobility, chemical reactions, solubility and ion transfer to electrodes. Understanding solvation behavior at the atomic scale is essential for future multivalent battery development.
- A new experimental approach, multivariate analysis of the pair distribution function (PDF) derived from x-ray scattering, isolates the Mg^{++} solvation shell structure from the Mg-electrolyte mixture.
- Molecular dynamics simulations using parameters based on the experimental data interpret peaks in the PDF and provide high resolution, chemically-specific details not accessible experimentally.
- Location of $TFSI^-$ anions within the 1st solvation shell indicates that the $Mg(TFSI)_2$ salt does not fully dissociate, with a less dynamic solvation structure than Li^+, negatively affecting battery performance. Breaking strong Mg-anion pairs is a key design metric for future electrolytes.

Research Details

- X-ray total scattering and multivariate analysis of the pair distribution function performed at Argonne's Advanced Photon Source.
- Molecular dynamics simulations of solvation shell structures and energies carried out at Lawrence Berkeley National Laboratory

Quantifying the Promise of Lithium–Air Batteries for Electric Vehicles



Comparison of materials-to-systems analysis (main panel) and “active materials only” analysis (inset) of Li-O_2 batteries for electric vehicles

Work performed at Argonne National Laboratory (JCESR managing partner), Lawrence Berkeley National Laboratory and General Motors

Gallagher et al. “Quantifying the Promise of Lithium–Air Batteries for Electric Vehicles” *Energy & Environmental Science*, **2014**, DOI:10.1039/C3EE43870H

Scientific Achievement

- First comprehensive materials-to-system analysis of performance and manufacturing cost of Li-O_2 batteries
- Open (purifying O_2 from air) and closed (recycling pure O_2 within a pressure vessel) designs analyzed
- Compared against advanced Li-ion and beyond Li-ion designs

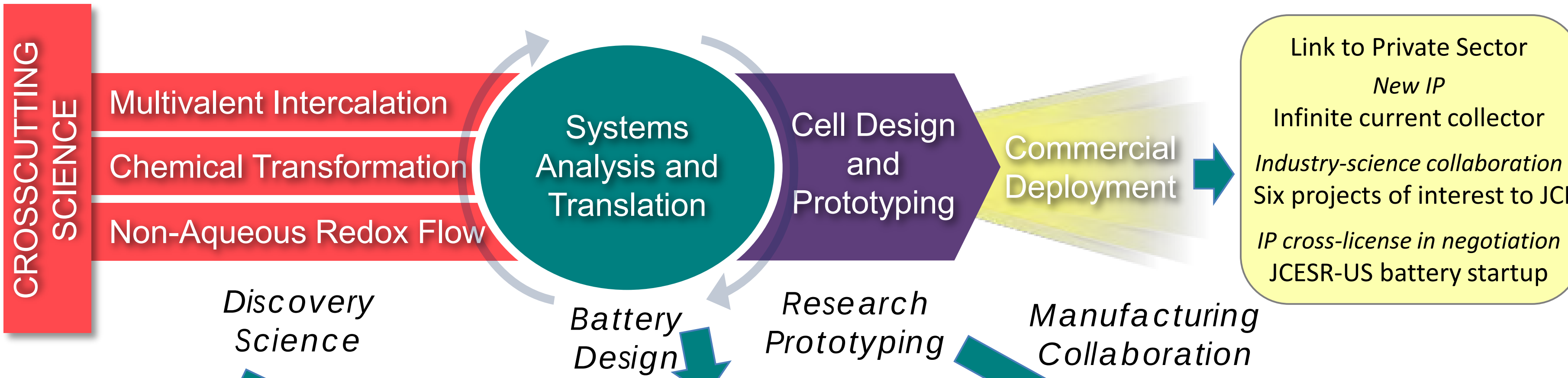
Significance and Impact

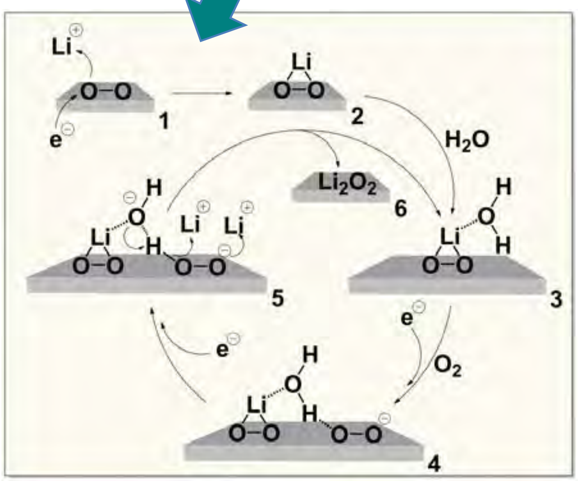
- Best case Li-O_2 systems achieve comparable cost and energy density to other more mature, lower-risk systems
- Lithium metal anode is a high-risk development critical to many high performance systems approaches
- Systems level analysis may contradict trends predicted from conventional “active materials only” analysis

Research Details

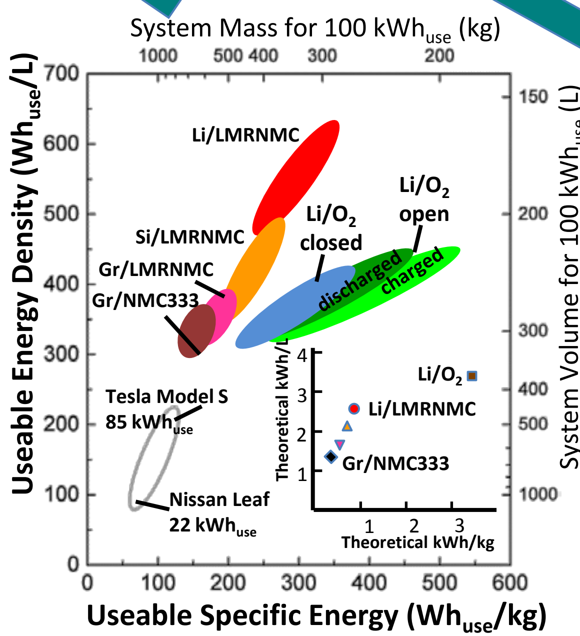
- Analysis for electric vehicle (EV) applications: 100 kWh, 80 kW$_{net}$ and 360V
- Materials - Gr: graphite; Si: advanced silicon composite; NMC333: metal oxide; LMRNMC: advanced metal oxide
- Li-O_2 closed system: cylindrical vessel contains high pressure oxygen gas similar to Ni/H_2 batteries used in satellites
- Li-O_2 open system: ambient air is compressed and purified to ppm levels of H_2O and CO_2

JCESR Achieves Across the Science-Manufacturing Spectrum





Trace water catalyzes lithium peroxide electrochemistry
Jirkovský et al, submitted



Quantifying the promise of Li-air batteries
Gallagher et al, Energy and Environmental Science (2014) DOI:10.1039/C3EE43870H

Magnesium ion transportation prototype cycled

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Additional highlights at www.jcesr.org

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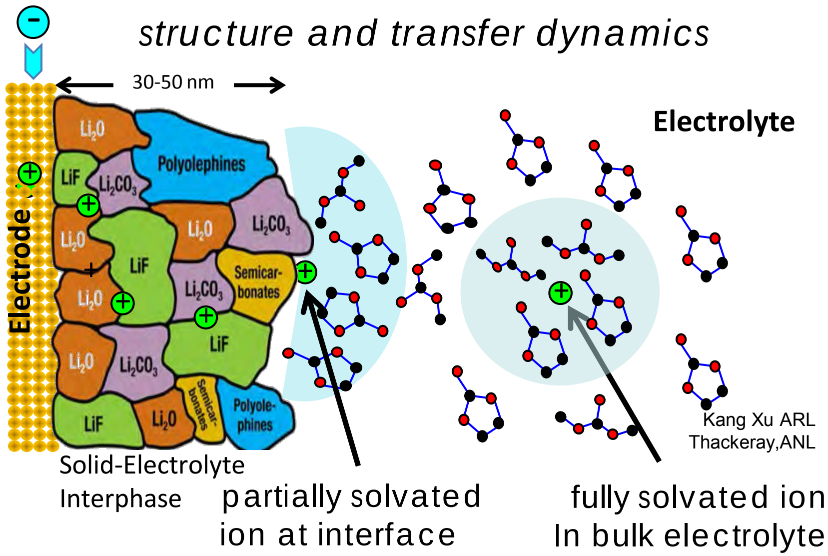
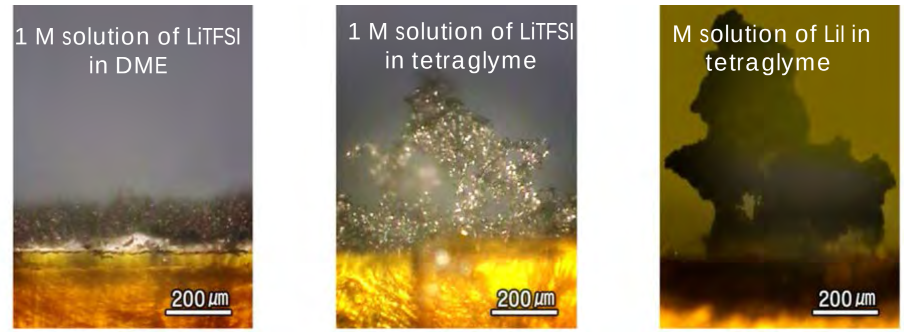
Priority Research Areas

Solvation/desolvation
structure and transfer dynamics



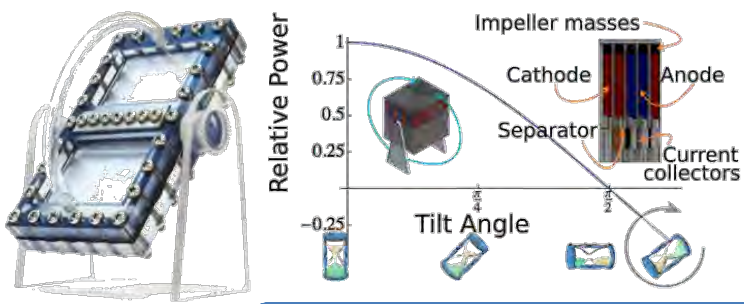
Metal Anodes
Robust surfaces over
multiple solution/deposition cycles



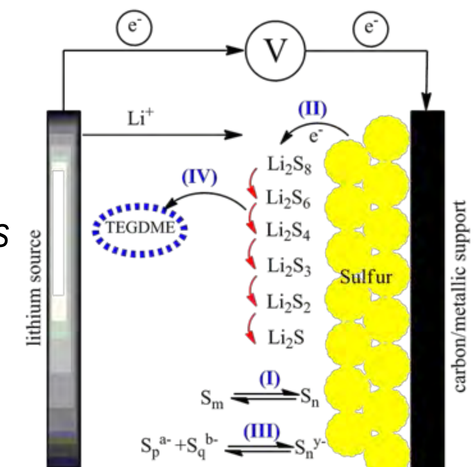
Solution/deposition dynamics, surface degradation, dendrite growth

Park et al, Nature Scientific Reports 4, Article number: 3815 doi:10.1038/srep03815

Novel Prototyping Concepts
Gravity Induced Flow Cell



Molecular Understanding
of Reaction Pathways
and Energetics
Lithium-Sulfur Batteries



Critical to battery science and technology strategies

Rich opportunities for in situ, time-resolved, multi-modal characterization, predictive theory and multiscale modeling

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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:

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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
- Shorten the time from conception to commercialization

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