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
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

- Transportation 28%
- Residential & Commercial Non-electric 11%
- Electricity Grid 39%
- Industrial Non-electric 22%

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

2013
EIA Monthly Energy Review Table 2.1
(May 2014)
JCESR Has Transformative Goals

**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 \(\rightarrow\) beyond Lithium-ion
JCESR Creates a New Paradigm for Battery R&D
The JCESR Partner Team

- Argonne National Laboratory
- Pacific Northwest National Laboratory
- SLAC National Accelerator Laboratory
- Sandia National Laboratories
- Johnson Controls
- Applied Materials
- Dow
- Northwestern University
- The University of Chicago
- Michigan University
- University of Illinois
- University of Illinois at Urbana-Champaign

May contain trade secrets or commercial or financial information that is privileged or confidential and exempt from public disclosure.
JCESR’s Beyond Lithium-ion Concepts

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

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

Non-aqueous Redox
Replace solid electrodes with liquid solutions or suspensions:
lower cost, higher capacity, greater flexibility.

Cross-cutting opportunity
Designer Organic Molecules
Tailored structure-function relationships
Redox couples, electrolytes, SEI . . .

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

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Beyond Lithium Ion Opportunity Space is Large, Unexplored and Rich

Beyond Li-ion

transformational advances

mostly unknown

Li-ion

incremental improvements

mostly known

Materials

Li, Mg, Al, Bi, Sn, Oxysulfides
Quinoxaline Metal Coordination Complexes
Triflate, Tetraborate
Oxide Phosphate-based ceramics, Block Co-polymer
Spinel Layered
Li-O, Li-S, Na-S
Quinoxoline Ferrocene Polysulfides

Systems

Catholyte
Chemical Transformation
Intercalant
Solid
Liquid
Anolyte
Intercalant/Alloy
Metal
Battery Technology Readiness Level (BTRL)

- **BTRL > 1**: 1-2 years
  - Scientific Breakthrough
  - New class of materials synthesized

- **BTRL > 2**: 2-5 years
  - Proven performance in half cells

- **BTRL > 3**: 2-5 years
  - Proven performance in lab-scale full cells
  - Material scale-up, cell testing and scale-up to pack

- **BTRL > 5 > 6**: 5-10 years
  - Proof-of-concept prototype
  - Research prototype

**JC ESR**
“sweet spot”
Trace Water Catalyzes Lithium Peroxide Electrochemistry

**Scientific Achievement**
Water at ppm levels catalyzes the conversion of lithium superoxide (Li-O₂) to lithium peroxide (Li₂O₂) 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\textsuperscript{++} Solvation Shell in Electrolyte for Multivalent Batteries

Scientific Achievement
- A new collaborative x-ray scattering and molecular dynamics simulation approach reveals the structure and energetics of Mg\textsuperscript{++} 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\textsuperscript{++} 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\textsuperscript{-} anions within the 1\textsuperscript{st} solvation shell indicates that the Mg(TFSI)\textsubscript{2} salt does not fully dissociate, with a less dynamic solvation structure than Li\textsuperscript{+}, 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

Scientific Achievement
- First comprehensive materials-to-system analysis of performance and manufacturing cost of Li-O₂ batteries
- Open (purifying O₂ from air) and closed (recycling pure O₂ within a pressure vessel) designs analyzed
- Compared against advanced Li-ion and beyond Li-ion designs

Significance and Impact
- Best case Li-O₂ 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\textsubscript{net} and 360V
- Materials - Gr: graphite; Si: advanced silicon composite; NMC333: metal oxide; LMRNMC: advanced metal oxide
- Li-O₂ closed system: cylindrical vessel contains high pressure oxygen gas similar to Ni/H₂ batteries used in satellites
- Li-O₂ open system: ambient air is compressed and purified to ppm levels of H₂O and CO₂

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

Quantifying the promise of Li-air batteries

Trace water catalyzes lithium peroxide electrochemistry
Jirkovský et al, submitted

Link to Private Sector
New IP
Infinite current collector
Industry-science collaboration
Six projects of interest to JCI
IP cross-license in negotiation
JCESR-US battery startup

Magnesium ion transportation prototype cycled

Additional highlights at www.jcesr.org
**Priority Research Areas**

**Solvation/desolvation**
structure and transfer dynamics

30-50 nm

Electrolyte

Solid-Electrolyte
Interphase

partially solvated ion at interface

fully solvated ion

In bulk electrolyte

Kang Xu ARL
Thackeray, ANL

**Metal Anodes**
Robust surfaces over multiple solution/deposition cycles

1 M solution of LiTFSI
in DME

1 M solution of LiTFSI
in tetraglyme

M solution of LiI in tetraglyme

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
**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
- Shorten the time from conception to commercialization