Next Generation Electrical Energy Storage
Basic Research Needs (BRN) Workshop

Workshop held March 27-29, 2017
Workshop Chair: George Crabtree, Univ. of Illinois-Chicago/ANL
Co-Chairs: Gary Rubloff, University of Maryland
Esther Takeuchi, Stony Brook University/BNL

Report to the Basic Energy Sciences Advisory Committee

Esther Takeuchi
July 13, 2017
Fundamental breakthroughs in chemical & materials sciences are essential to transform the energy landscape

Estimated U.S. Energy Consumption in 2015: 97.5 Quads

Quad = 10^{15} BTU; 2007 consumption \approx 2015 consumption (~3.3 terawatts)

LLNL flowcharts available from https://flowcharts.llnl.gov
Basic Research Needs (BRN) Workshops
18 reports; 15 years; >2,000 participants from academia, industry, and DOE labs

BRN to Assure a Secure Energy Future BESAC (2002)
- BRN for Superconductivity (2006)
- BRN for Geosciences (2007)
- BRN for Clean and Efficient Combustion (2007)
- BRN for Catalysis for Energy Applications (2007)
- BRN for Materials under Extreme Environments (2007)
- BRN for Carbon Capture (2010)
- Computational Materials Science and Chemistry (2010)
- Science for Energy Technology (2010)
- BRN for Environmental Management (2016)
- BRN for Quantum Materials (2016)
- BRN on Synthesis Science for Energy Relevant Technology (2017)

https://science.energy.gov/bes/community-resources/reports/
Grid reliability and distributed power require innovative energy storage devices

- Enhancing grid resiliency in case of disruptive events and demand peaks
- Storage of large amounts of power
- Delivery of significant power rapidly

Transportation requires next generation batteries

- Providing higher energy and power densities, longer drive distance
- Longer lifetimes, faster recharge times
- Enabling greater communication and connection with information and guidance systems

Battery safety has emerged as cross-cutting research topic

Scientific tools for battery research have seen significant advancement
Given the transformative opportunity in 2017 and beyond to utilize electrical energy storage in diverse applications far beyond personal electronics, the workshop was designed to:

- Provide an assessment of the current status of electrical energy storage.
- Identify the highest priority basic science gaps and opportunities in our fundamental understanding.
- Define the new insights and innovations needed from basic research in materials science and chemistry to enable future scientific and technological advances for next-generation electrical energy storage.

Workshop held March 27-29, 2017 with 175 scientists representing theory, simulation, characterization, electrochemistry and synthesis in attendance.
NG-EES BRN: Plenary Speakers

**Electrical Energy Storage: Where have we come from and the scientific challenges still facing us?**
– M. Stan Whittingham, Binghamton University

**High-energy batteries: a systems perspective**
– Karen Thomas-Alyea, Samsung Research America

**Challenges for Solid State Batteries**
– Linda Nazar, University of Waterloo

**Nanoscience for Energy Storage: Success and Future Opportunity**
– Yi Cui, Stanford University

**Materials science for electrochemical storage: Achievements and new directions**
– Jean-Marie Tarascon, Collège de France
Six (6) panels discussed scientific challenges spanning existing and next generation electrochemical energy storage structures, the experimental and theoretical tools and techniques to explore them, and promising emerging architectures and approaches to achieve them.

- Pathways to simultaneous high energy and power
- Structure, interphases, and charge transfer at electrochemical interfaces
- In pursuit of long lifetime and reliability: Time-dependent phenomena at electrodes and electrolytes
- Discovery, synthesis and design strategies for materials, structures, and architectures
- Solid-state and semi-solid electrochemical energy storage
- Cross-cutting themes
NG-EES BRN: Panel Leadership

Panel 1: *Pathways to Simultaneous High Energy and Power* - Paul Braun, University of Illinois at Urbana-Champaign, and Jun Liu, Pacific Northwest National Laboratory

Panel 2: *Structure, Interphases, and Charge Transfer at Electrochemical Interfaces* - Lynden Archer, Cornell University, and David Prendergast, Lawrence Berkeley National Laboratory

Panel 3: *In pursuit of long lifetime and reliability: Time-dependent Phenomena at Electrodes and Electrolytes* - Shirley Meng, University of California-San Diego, and Jay Whitacre, Carnegie Mellon University

Panel 4: *Discovery, Synthesis, and Design Strategies for Materials, Structures, and Architectures* - Perla Balbuena, Texas A&M University, and Amy Prieto, Colorado State University

Panel 5: *Solid-State and Semi-Solid Electrochemical Energy Storage* - Nancy Dudney, Oak Ridge National Laboratory, and Jeff Sakamoto, University of Michigan

Panel 6: *Crosscutting Themes*: Yue Qi, Michigan State University, Eric Stach, Brookhaven National Laboratory, and Mike Toney, SLAC
• Each panel developed a list of critical research areas.
• On day 2, the research areas were evaluated and grouped into topics according to **five Priority Research Directions**.
• The panel leads and members joined the relevant Priority Research Direction (PRD) group.
• The PRD teams met to formulate the research approaches and thrust areas.
• Day 3, report out and writing of PRDs and Panel reports.
PRD1: Tune Functionality of Materials and Chemistries to Enable Holistic Design for Energy Storage

Holistic design of architectures and components
- Maximum performance with minimum complexity
- Consider full cell action and interaction at the outset

Multifunctional materials
- Many functions from one material
- May combine ion mobility and electronic conductivity
- Overcome paradigm of one material one function
**PRD1: Tune Functionality of Materials and Chemistries to Enable Holistic Design for Energy Storage**

**Thrust 1: Simultaneous High Energy and High Power**

Concentric tube 3D battery
- Short transport lengths
- High surface area
- Large volume

**Thrust 2: Multifunctional Solid State Electrolytes**

Challenges:
- Low interfacial impedance
- Predictive interfacial simulation

- High ionic conductivity
- Low electronic conductivity
- Inhibit dendrite growth

**Thrust 3: New Battery Chemistries**

Multivalent electrode materials
- Challenge in adopting new multivalent materials is understanding of charge storage and transport mechanisms
- Focus on abundant and low cost elements

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*Chem. Mater., 2015, 27, 10, 3609*

*MRS Bull., 2011, 36, 523*

*Nat. Mater., 2017, 16, 572*
A comprehensive suite of multi-modal tools is needed to capture coupled electrochemical phenomena

- *in situ* observation
- Multiscale modeling

The opportunity is to characterize multiple coupled electro-chemical-mechanical phenomena over diverse time and length scales

Multiscale phenomena

X-Ray ptychography

Dendrite Growth

**Mobility and local strain**

**Bulk Solvation**

**Desolvation**

**Ionic Conduction**

**Intercalation**

**Cathode**

**Electrolyte**

**SEI**

**M. Toney, unpublished.**

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**Courtesy LLNL**

**PNAS, 2016, 113, 10779**
PRD 2—Link Complex Electronic, Electrochemical, and Physical Phenomena across Time and Space

Thrust 1: Create state-of-the-art modeling techniques and characterization tools

Models of coupled electro-chemical-mechanical battery phenomena

**References**

*Acc. Chem. Res., 2016, 49, 2363*

*JACS, 2011, 133, 14741*

*J. Phys. Chem. C, 2014, 118, 18362*


Thrust 2: Integrate computational and characterization tools

- **LiF**
  - Space charge mediated by LiF/Li$_2$CO$_3$ interfacial defects
- **Li$_2$CO$_3$**
- **LiF**
- **Li$_2$CO$_3$**

Computedionally-designed artificial SEI

**References**

*ACS Appl. Mater. Interfaces, 2016, 8, 5687*
PRD 3: Control and exploit the complex interphase region formed at dynamic interfaces

• Mechanical, chemical, electrical processes at interface evolve with emergent, different properties.
• Informed design of interfaces can produce beneficial interphases.

Targets
• Widen stability window of liquid electrolytes
• Understand, control electric potentials at solid state battery interfaces

Design, Synthesis and Characterization of Functional Interfaces
• Create relevant model systems for learning and theory validation
• New characterization methodologies
• Beneficial interphases from synthesized coatings, possibly with active or adaptive functionalities

E. J. Fuller and A. A. Talin, unpublished


Courtesy of ANL
PRD 3: Control and exploit the complex interphase region formed at dynamic interfaces

**Thrust 1. Unravelling interfacial complexity through in-situ and operando characterization and theory**
- Well-controlled model systems
- Intrusive interrogation of realistic and working systems
- Operando X-ray and neutron methods

**Thrust 2: Designing SEI for function**
- Understand ion transport in interphases
- Interphase design and controlled synthesis
- Self-healing to mitigate degradation

*Science, 2016, 353, 566
ACS Cent. Sci., 2017, 3, 5, 399*
PRD 4: Revolutionize energy storage performance through innovative assemblies of matter

- New architectures to reduce passive content and capacity fade
- Materials synthesis, processing, assembly from nano to meso
- Informed by hierarchical modeling/simulation and in-situ/ operando experimental results

Courtesy Wei Wang and Vijayakumar Murugesan, PNNL
PRD 4: Revolutionize energy storage performance through innovative assemblies of matter

**Thrust 1. Design and Synthesize New Mesoscale Architectures**
- Smart, multiscale architectural design
- Reverse design: synthesis to achieve multiple properties
- Architectures informed by experimental databases and machine learning

**Thrust 2: Develop New Concepts for Large-Scale Energy Storage and Conversion**
- Rethinking flow batteries
- Electrocatalytic chemical energy storage
- Manipulating solvation
- Membranes and interfaces tailored to new redox chemistries

*Solid State Ionics, 2004, 175, 243*
*Energy Environ. Sci., 2014, 7, 3307*
**PRD 5: Promote Self-healing and Eliminate Detrimental Chemistries to Extend Lifetime and Improve Safety**

- **Full understanding of the degradation pathways occurring during battery life**
  - when and where degradation events occur
  - how rapidly they advance
  - new approaches to slow or stop them and to design around them

- **Safer and more robust devices without sacrificing energy density or performance**
  - systematic and precise study
  - new tools and sensors
  - more sophisticated simulation

*J. Power Sources, 2017, 341, 373*
PRD 5: Promote Self-healing and Eliminate Detrimental Chemistries to Extend Lifetime and Improve Safety

**Thrust 1 – Multimodal in-situ experiments to quantify degradation and failure.**
- Identify key degradation and failure mechanisms.
- Determine roles of inhomogeneity and nonlinearities.
- Discover mitigation strategies.

**Thrust 2 – Multi-physics, multi-scale, predictive continuum models for degradation and failure**
- Use modeling and characterization in combination with representative and model systems.
- Develop and implement predictive multiscale models and continuum models.

*J. Electrochem. Soc., 2017, 164, A304*

*Nat. Comm., 2015, 6, 6924*
Current Status

- Brochure providing a high level summary of the workshop has been released.
- Workshop final report is in preparation.
- Content of report:
  - Priority research directions
  - Panel reports
  - Factual document