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ANNUAL UPDATE
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DIRECTOR'S MESSAGE
FIVE YEARS OF RESEARCH EXCELLENCE AND COUNTING

The Joint Center for Energy Storage Research (JCESR) recently reached an exciting and important milestone: completion of its initial five-year contract with the U.S. Department of Energy (DOE) and renewal for a planned five more years.

Five years is a fairly long time in our daily lives, but a short span for developing new, high performance technologies that could one day transform society. In its first five years, JCESR has many accomplishments in electrical energy storage to report, including 380 scientific publications and the formation of three start-ups. A select few accomplishments are summarized in this annual update.

First, a little history. The DOE established JCESR as an Energy Innovation Hub in late 2012. Led by DOE's Argonne National Laboratory, JCESR is a unique partnership of national laboratories, universities, and industrial firms with more than 150 scientists from many disciplines. Its founding mission was to develop next-generation energy storage technologies for beyond-lithium-ion batteries that would transform transportation and the electric grid the way lithium-ion batteries transformed personal electronics. From the start JCESR set aggressive and visionary stretch goals: achieve five times the energy density and one-fifth the cost of commercial lithium-ion batteries (as of 2012) within five years of startup.

George Crabtree
Director of the Joint Center for Energy Storage Research
Argonne National Laboratory

科学家们在伊利诺伊大学厄巴纳-香槟分校进行重要的JCESR研究作为可流动红oxmer科学主题的一部分。

科学家们在Argonne National Laboratory的Electrochemical Discovery Laboratory中合成并表征下一代电池材料的性质。

A Sandia Distinguished Member of Technical Staff deposits an electrode film for investigation as a cathode in a next-generation battery.

科学家们合成和表征下一代电池材料的性质在Electrochemical Discovery Laboratory at Argonne National Laboratory。
Throughout its first five years, JCESR research focused on four vastly different types of beyond-lithium-ion batteries.

**Multivalent battery.** The first type is the “multivalent” battery for transportation. This battery type replaces singly charged lithium with doubly charged magnesium, calcium, or zinc or triply charged aluminum as the working ion. This increased charge enables such batteries to store or release two or three times more energy per ion transfer on each charge or discharge cycle as compared to lithium-ion batteries. Coupled with a pure metal anode, these multivalent batteries are a candidate for a factor of five increase in energy density.

The challenge for multivalent batteries is discovering high energy cathodes, as none of the standard cathodes for lithium-ion batteries work with multivalent ions. JCESR demonstrated three new long-cycling multivalent batteries, based on doubly charged magnesium, calcium, and zinc working ions combined with different cathode materials. These demonstrations firmly establish the exciting future of multivalent batteries for next-generation applications.

JCESR broke new ground with the first comprehensive computational study of viable combinations of multivalent working ions with cathodes. This study simulated more than 1800 combinations of magnesium, calcium, zinc, and aluminum working ions with sulfide, phosphate, oxide, and fluoride cathodes. The resulting map of the multivalent battery landscape provided the first comprehensive account of multivalent materials performance, a significant advance for the battery community.

In the research on magnesium multivalent batteries and on solid electrolytes replacing the typical liquids, JCESR developed a new technique based on nuclear magnetic resonance imaging to measure the mobility of magnesium ions during charge and discharge. Our studies with this technique refuted an important tenet of pre-JCESR conventional wisdom—that the double charge of the magnesium ion severely limits its transport in the cathode and solid electrolyte. These new insights open the door to new horizons of innovation with multivalent batteries.

It is worth noting that in 2016, JCESR published nearly 25 percent of all scientific publications related to magnesium batteries, further illustrating its leadership position in the field.

**Flow battery.** Flow batteries replace solid electrodes with liquid solutions of energy-storing and energy-releasing molecules (“redox active”) and are promising for applications in the electric grid. Conventional flow batteries are based on a single molecule or ion such as vanadium ions, with restricted versatility and flexibility of behavior. JCESR’s new design of flow battery introduces the concept of redox-active macromolecules, which can be in the form of oligomers or polymers or colloids. The resulting “redoxmers” can consist of one to a billion active units ranging from nanometers to micrometers in size. Their major advantage is that they are highly versatile, with a wealth of pendant molecules that can be attached to the basic redox molecule to significantly improve key performance properties.

The new redoxmer configurations open a wide range of basic electrochemical phenomena with the potential to significantly improve flow battery performance. Further, we introduced a new methodology for the predictive design of redox-active organic molecules based on a form of machine learning. This methodology brings the emerging field of machine learning to bear on discovering and understanding new complex organic molecules and materials for flow batteries. Machine learning is a powerful new tool for materials exploration in battery research that promises to revolutionize the discovery of new materials.
In its first five years, JCESR promised to deliver two prototypes for beyond-lithium-ion batteries, one for transportation and one for the grid. We identified candidate battery materials and integrated them into a total of four prototypes: two for transportation and two for the grid. We came to within 20 percent of our manufacturing cost goal, and prototype testing demonstrated energy density increases of a factor of three, an impressive achievement in only five years.

**Lithium-sulfur battery.** A fourth type of beyond-lithium-ion battery with immense potential is the lithium-sulfur system, which is based on strong chemical bonds between lithium metal and low-cost sulfur. JCESR developed a new cell design based on use of a “sparing solvation” electrolyte. This design prevents the intermediate reaction products of the lithium-sulfur reaction (the “polysulfides”) from dissolving in the electrolyte at the cathode and migrating to the anode and shorting out the battery. Sparing solvation not only increases battery life but also raises energy density.

JCESR introduced a second solution for preventing migration of dissolved molecules from cathode to anode and vice versa — a porous polymer membrane with nanometer size pores that blocks unwanted molecules on the basis of size. In a second advance, JCESR researchers lined the pores of the membrane with redox-active molecules that add charge discrimination to the pore size discrimination. This versatile membrane is effective not only against the polysulfide shuttle of lithium-sulfur batteries, but also against redoxmer crossover in JCESR’s new flow batteries.

**INNOVATIVE RESEARCH TOOLS EXPLOITED**

To expedite the above research, JCESR relied heavily upon four valuable new research tools. One is technoeconomic modelling of beyond-lithium-ion battery systems to evaluate their cost and performance before they are made. The second and third are the Materials Project and the Electrolyte Genome, two separate databases that enable simulation of crystalline cathodes and liquid organic electrolytes for designing the composition and structure of new battery materials. The fourth is state-of-the-art multimodal electrochemistry laboratories for synthesis and characterization of advanced battery materials and interfaces at atomic and molecular levels.

**PROTOTYPE PROGRESS**

JCESR’s third novel design is an aqueous flow battery with the lowest-cost rechargeable battery chemistry yet known. This chemistry combines an aqueous sulfur anode and air-breathing cathode with a water electrolyte. This unique concept, which has no parallel in the battery literature, addresses the emerging need for long duration energy storage.

JCESR transitioned one of its prototypes to a startup company, Form Energy, which is now pursuing commercialization of the battery concept, as described below.
THE NEXT FIVE YEARS OF JCESR

Our five-year effort led to the identification of the critical phenomena that control the behavior of next-generation batteries and the gaps in scientific knowledge that impede further development. With the renewal of JCESR in September 2018, this knowledge base is guiding our energy storage research as we redirect our mission toward uncovering the atomic-level origins of battery material behavior.

In its second five years, JCESR will turn from an emphasis on specific battery systems to transformative materials that will enable a diversity of batteries for a diversity of uses. JCESR will build these transformative materials from the bottom up, atom-by-atom and molecule-by-molecule, where every atom or molecule plays a prescribed role in producing desired overall materials behavior.

Such transformative materials can be mixed and matched to create a host of designer batteries tailored to a host of emerging applications, including resilient future electric grids, distributed energy management for customized electricity service, fast charging electric vehicles, and even regional electric flight.

We live in an energy storage moment, where batteries are expected to solve a variety of pressing and distinct societal challenges. JCESR will address this overarching challenge by laying the foundation for building transformative battery materials from the bottom up.

We eagerly anticipate the founding of even more frontier science spinoff companies as they mix and match JCESR transformative materials. Stay tuned for further developments.

JCESR-INSPIRED SPINOFFS

We live in the age of the high-tech startup company, and JCESR has spawned three: Blue Current, Sepion, and Form Energy. Blue Current is an offshoot of JCESR research on solid-state electrolytes, which would eliminate the flammability issue of organic liquid electrolytes. The JCESR development of the size-selective nanoporous polymer membrane gave birth to Sepion. Form Energy sprang out of the JCESR invention of the air-breathing aqueous sulfur battery, which can store weeks or months of energy. The cost for this battery could be as low as that of pumped hydroelectric storage, currently the dominant form of large-scale energy storage, but without its geographic limitations. Form Energy intends to leverage JCESR's cutting-edge air-breathing aqueous sulfur battery technology to meet the growing need for long-duration energy storage for the electric grid.

“Improvements in battery performance are paramount to the future of both transportation and the electric grid,” said DOE Under Secretary for Science Paul Dabbar during the JCESR renewal announcement at the InnovationXLab Energy Storage Summit held at SLAC National Accelerator Laboratory. “JCESR is one of our most important centers of discovery and innovation for electrical energy storage and will be critical in laying the scientific groundwork for the next generation of battery technology.”

David Danielson, Managing Director of Breakthrough Energy Ventures

“Breakthrough Energy Ventures chose Form Energy as one of its initial investments because the aqueous sulfur technology epitomizes innovations with great potential, developed through publicly-funded scientific research, which now require flexible, patient capital to realize its full societal impact. In this case, that impact is to provide reliable, affordable, zero-carbon electricity to the world.”