RESEARCH CORPORATION for SCIENCE ADVANCEMENT
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Scialog: Advanced Energy Storage

The purpose of Scialog initiatives is to accelerate fundamental science breakthroughs with applications to complex challenges of global concern.

Research Corporation for Science Advancement (RCSA) is launching a new Scialog initiative – *Advanced Energy Storage* (AES) – with a first meeting Nov. 2-5, 2017. Energy storage is critical for a wide variety of major societal challenges including transitioning to near zero emissions transportation and making the electrical power grid more compatible with renewable energy generation. There is tremendous need for fundamental discovery research in chemistry, materials science, engineering and related disciplines that will lead to new advanced batteries and capacitors with greater energy storage density, longer lifetimes, and which are cheaper, safer and easier to discharge and recharge.

Over the past 40 years, Li-ion battery technologies have progressed steadily, ultimately providing the current standard for portable storage with sufficient lifetimes (both per charge and per battery) for practical commercial success. Nonetheless, many non-ideal aspects of our reliance on current technologies remain, which is the inspiration behind Scialog AES – a program of search and discovery for truly transformative energy storage systems. Are we sufficiently exploring all of the chemical and physical systems which can be utilized for electrochemical energy storage? Are there new chemistries and materials which present unexplored opportunities as electrochemical energy storage components or systems? What breakthroughs or design parameters could be explored for a high risk, high reward technological transformation?

Scialog – Science and Dialog – provides grant support for teams of early-career academic scientists to seed novel projects, which are judged to be highly innovative, combining high-risk research with potentially high-reward outcomes.

Each Scialog initiative engages 50-60 Scialog Fellows, who are rising stars in a particular topical area. Initiatives bring together researchers from different communities across traditional disciplinary boundaries. Scialog initiatives are organized around annual meetings in which Scialog Fellows have the opportunity to develop interdisciplinary collaborations and identify bottlenecks and potential breakthroughs that may achieve transformative outcomes. At each conference significant time is devoted to breakout science discussions to explore novel ideas and strengthen communities of early career researchers. Scialog Fellows are challenged to form new collaborative teams and write proposals "on-the-spot" to provide seed funding for novel out-of-the-box research projects.

RCSA has run three Scialog initiatives – *Solar Energy Conversion*, *Molecules Come to Life* and *Time Domain Astrophysics*. The fourth initiative – *Advanced Energy Storage* – will begin in fall 2017. Scialog initiatives have garnered additional support of $2,255,000 from private foundations and federal agencies.

For the first three Scialog initiatives, over 125 Scialog Fellows have received awards totaling $8.3 million, of which $2.1 million has been provided by other private science foundations. Thirty completed awards in *Solar Energy Conversion* have yielded 224 papers acknowledging Scialog including 57 in journals with impact factors greater than 10. Additional related external funding is being generated at a five to one ratio of Scialog award funding. Analysis of the professional relationships formed at the conferences indicates that the Scialog process is effective for rapidly catalyzing collaborations among scientists previously unfamiliar with one another.

RCSA chose advanced energy storage (AES) as the next topic for Scialog because:

1. RCSA has enthusiastic support from highly distinguished scientists in the field.
2. Senior experts are in strong agreement on the importance and timeliness of the topic, are interested in participating, and can help focus the topic to areas in which a Scialog approach can make a significant difference.
3. We have identified and selected 60 early career rising stars as Scialog Fellows.

RCSA has so far consulted with the following experts in advanced energy storage who will serve as discussion facilitators at the Scialog AES meetings:

- **Héctor Abruña**, Cornell, RCSA awardee in 1982 and 1983, electrochemist studying batteries and fuel cells
- **Sarbajit Banerjee**, Texas A&M, Cottrell Scholar & Scialog Fellow for solar energy conversion, developing metal-organic syntheses for growth of metal oxide and oxyhalide nanocrystals
- **Richard Brutchey**, USC, Cottrell Scholar & Scialog Fellow for solar energy conversion, synthesizes complex oxide nanocrystals for energy storage
- **George Crabtree**, Argonne National Lab, Director of JCESR
- **Bruce Dunn**, UCLA, materials scientist noted for work on sol-gel derived materials, solid electrolytes, and battery electrode materials
- **Nancy Haegel**, Center Director of the Materials Science Center, National Renewable Energy Laboratory, RCSA awardee in 1994 and 1997.
- **Prashant Kamat**, Notre Dame, Editor-in-Chief ACS Energy Letters
- **Karl Mueller**, Pacific Northwest National Laboratory, Cottrell Scholar & Chief Science & Tech Officer at PNNL
- **Amy Prieto**, Colorado State, Scialog Fellow for solar energy conversion and founder, CEO & Chief Scientific Officer of Prieto Battery, which produces novel technology for lithium-ion batteries
- **Esther Takeuchi**, Stony Brook, inventor of the silver vanadium oxide battery that powers implantable cardiac defribrillators and holder of more than 145 U.S. patents
- **Yiying Wu**, Ohio State, Cottrell Scholar, ranked *#6* worldwide on the Times Higher Education list of "Top Materials Scientists of the Past Decade" and founder of KAir Battery
- **Stan Whittingham**, Binghamton, known for the discovery of intercalation electrodes

These experts indicated that tremendous effort has already gone into battery and other energy storage research. However, they think much of this research has been focused on near term improvements and rapid commercialization of incremental advances. Large leaps forward almost certainly require new electrolytes and new solid and/or nanostructured materials for battery cathodes, anodes and membranes. New types of batteries such as lithium-sulfur, magnesium-ion, sodium-sulfur, lithium-air, as well as flow batteries, which have potential for very high storage capacity for long periods of time, are still early in development. Each of the experts think there are huge challenges remaining in fundamental research to achieve the needed understanding for advances in these and other promising energy storage technologies. These experts are also excited about using a Scialog approach to connect rising stars from several disciplines and encourage novel ideas for new lines of research.

Example discussion themes for AES

Multivalent Intercalation: The current Li-ion paradigm of battery technology is fundamentally constrained by the univalency of the Li-ion. A straightforward solution is to transition to multivalent ion chemistries. However, the intercalation and extraction of multivalent cations represents a formidable challenge and the repertoire of viable insertion hosts is rather slim. Elucidating design principles for multivalent cation insertion and realizing cathode materials that allow for high voltage as well as good reversibility has emerged as a critical imperative and will need synergistic collaborations between theorists and experimentalists. Electrolytes for multivalent cation insertion remain relatively unexplored. The development of electrolytes capable of high-voltage operation that allow for reversible plating/stripping of multivalent metals remains a fundamental challenge.

Rational and Mechanism-Driven Design of Cathode Materials and Electrolytes: Much of the development of cathode chemistries and architectures has been serendipitous and such a mode of discovery is now coming up against some fundamental limitations. Cation intercalation involves complex mass transport, charge transport, phase transition, and redox phenomena that often occur far from equilibrium. Electrolytes similarly form SEI (solid electrolyte interphase) layers with complex structure and charge/mass transport characteristics. The combination of state-of-the-art characterization methods and first-principles theory in conjunction with the design and synthesis of new materials is imperative for transformative advancements.

Multiscale Modeling Integrated with Experiments: While modeling at different scales has emerged as a useful screening method, complex phenomena are still not realistically captured by current methods and there is particularly a gap between first-principles density functional theory and mesoscale/continuum models. This discrepancy has not been adequately addressed and is the origin of the relatively low predictive value of modeling. Integration of experimental parameters and modeling across multiple scales is urgently needed for modeling to become an accurate predictive tool.

Lifetime/longevity is a critical issue in essentially all electrochemical energy storage systems. If a Li-ion battery could be cycled 100,000 times, the energy storage cost would be reduced dramatically. The fundamental degradation processes are not well understood in many cases. What role is there for fundamental science in tackling this issue? What methods can be used to understand the processes? Are there new chemistries to address degradation in various systems?

The fundamentals of electron transfer and catalysis at interfaces is central to energy conversion but, despite much study, relatively poorly understood. Most theories describing such processes are phenomenological. What can be gained by deeper understanding of the factors affecting interfacial electron transfer rates, especially for inner sphere, catalytic, processes? What is the role of theory and computation? What are good model systems? How might one apply new insight practically?

Spanning the capacitor/battery/fuel-cell continuum: There is a good argument that a continuum of energy storage devices will be needed to address the variety of practical needs. What role is there for creating new systems that bridge existing domains? For example pseudo-capacitor designs which use fast faradaic reactions (battery-like in nature) have been studied for decades, but there are not well-commercialized products. Are there new areas that can be developed? Can we design molecules that can be used as “reversible” fuels? Can flow batteries be designed with the energy density of solid batteries by using designed solid nanomaterials?

Mechanisms of ionic transport: The current state-of-the-art for positive electrodes in Li-ion batteries rely on $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$, $LiCoO_2$, or $LiMn_2O_4$. The common structural feature in these compounds is the presence of open channels that allow for easy movement of ions and, naively, may be expected to allow materials to be cycled with minimal change to the host framework. These channels typically result from a layered topology (as in $LiCoO_2$) or through a coherent network of empty interstices within a close-packed anionic lattice (as in $LiMn_2O_4$). While these oxides have found extensive commercial success, there are significant problems associated with the complex structural distortions and voltage losses that occur in these materials as they are cycled for extended periods of time. What are the mechanisms of ionic transport as identified by state-of-the-art characterization methods and computation, and how can we use this knowledge to inform the development of next-generation materials? Understanding the mechanism for ionic transport through densely packed solids is crucial to designing new materials that will allow the diffusion of larger ions that have the benefits of being less critical elements, having higher volumetric energy densities, and/or being safer by not exhibiting dendrite formation.

Advanced Experimental Methodologies: There are now a number of techniques that can provide information about batteries (and related systems) under operating (“operando”) conditions. These include X-ray based methods, TEM, “air-SEM” (Yes, Air!), NMR as well as other spectroscopic (IR, Raman) methods. Because of the very reactive nature of material interfaces in batteries and other energy storage technologies, use of in situ and operando methods is providing tremendous insights. Can these methods and other advanced experimental methodologies be pushed even further to make major advances in energy storage?