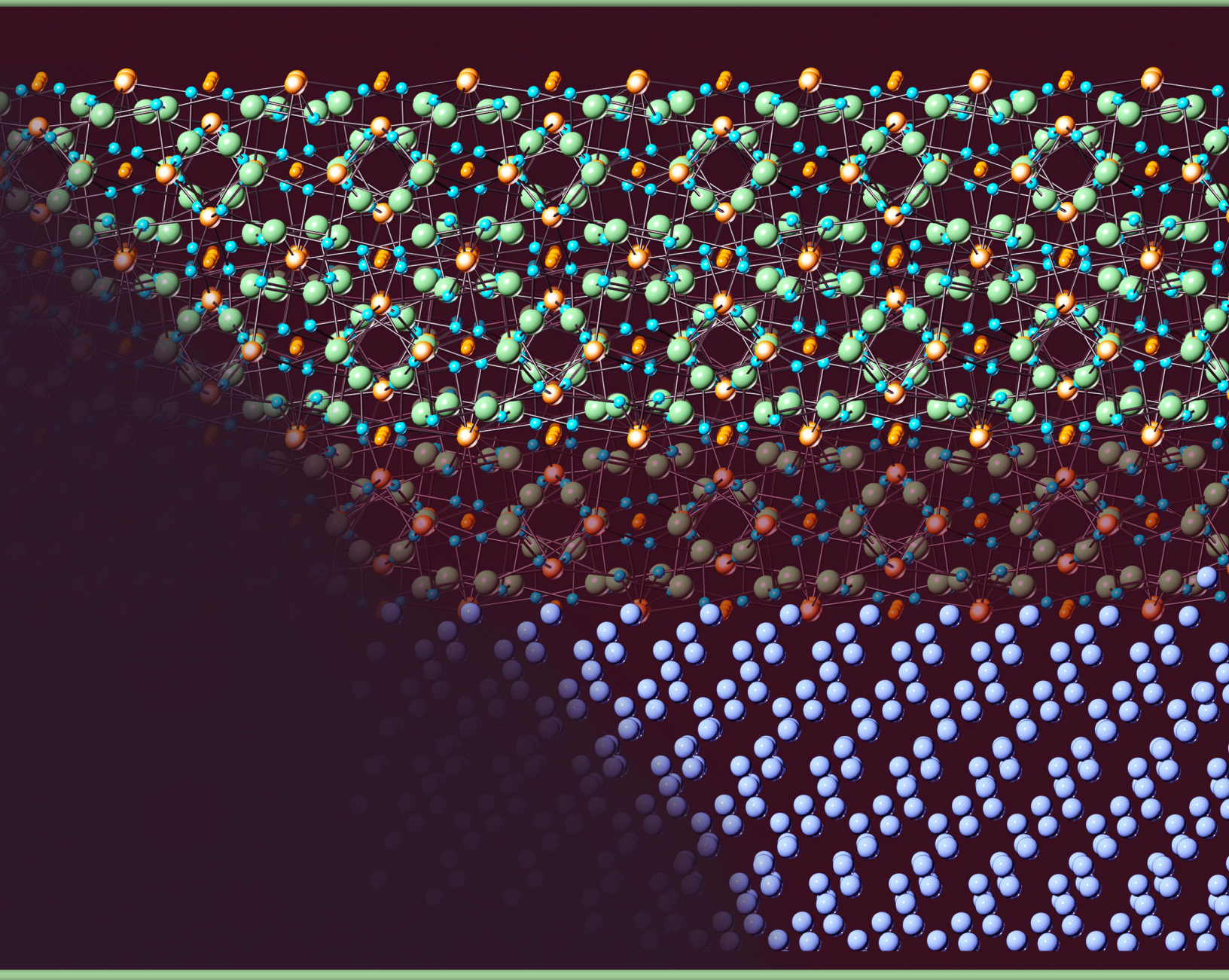
Basic Research Needs for

Next Generation Electrical Energy Storage



Electrical Energy Storage—*Discovery Science to Launch a Transformative Era of Energy Storage*

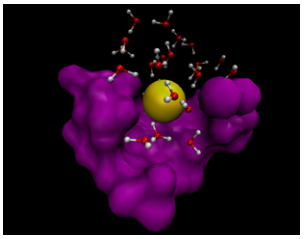
Electrical Energy Storage—Revolutionizing how we store and use energy…

Advances in how we store electricity have the potential to transform nearly every aspect of society, from transportation to communication to electricity delivery and domestic security. New energy storage systems will support the energy requirements for advanced technologies and strengthen critical infrastructure. This vision for the future can only be achieved through next-generation, high-performance batteries and related energy storage media that are safe, reliable, and affordable.

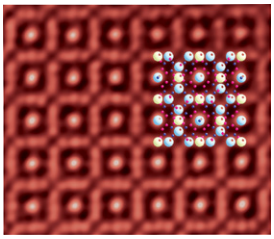
Energy can be stored in many forms, such as electrical, mechanical, thermal, and chemical, and then converted into electricity when needed. Batteries and related devices rely on *electrochemical* energy conversion. Unlike digital electronics that work by moving electrons through circuits, batteries move electrons, atoms, ions, and molecules through demanding chemical environments. The process can dramatically change the chemistry and structure of battery materials and limit their performance over time. Achieving greater efficiency, reliability, and resiliency in energy storage technologies requires a new level of understanding and control over the dynamics that govern electrochemical phenomena.

Science is poised to meet these challenges. Real-time nanoscale characterization of operating batteries will elucidate fundamental mechanisms of function and failure. Predictive computational simulations will move beyond the discovery of new materials and chemistries to unlock innovative system functionalities. Further, holistic approaches to the synthesis of materials, structures, and architectures will deliver new levels of electrochemical performance, enabling higher efficiency, extended lifetimes, and lower costs for energy storage devices. The integration of this knowledge promises a revolution in technologies and manufacturing processes for next-generation batteries.

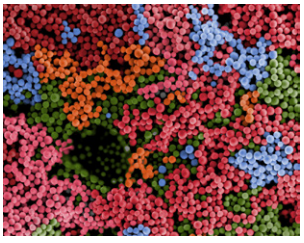
The report from a Basic Research Needs workshop held in 2017 identifies five priority research directions that will underpin the future capabilities of electrical energy storage. The full report will be available at https://science.energy.gov/bes/community-resources/reports/.



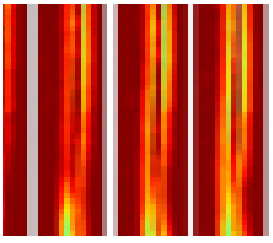
Computer modeling of ion movement in a membrane



Atomic resolution of a solid electrolyte



Combined imaging techniques track chemical changes



Neutron imaging of batteries in operation

Images courtesy of Pacific Northwest National Laboratory (left) and Oak Ridge National Laboratory (right).

Electrochemical energy storage devices such as batteries store and release electricity on demand. As negatively charged electrons move out of the battery, positively charged ions must move inside the battery through multiple chemical and material interfaces. Critical battery components in this process include electrodes, electrolytes, and separation membranes. Powerful new computational, imaging, and characterization tools are enabling scientists to understand this complex coupling of electronic and ionic transport at an unprecedented level of detail across multiple length and time scales. Integration of this new knowledge will enable the scientific design of innovative, complex materials and architectures for next-generation energy storage.

Priority Research Directions

- **Tune functionality of materials and chemistries to enable holistic design for energy storage**

  Key questions: *How can we understand the functionality of materials sufficiently to anticipate their behavior in electrochemical configurations? How can these insights inform the design of chemistries, materials, and structures for future energy storage?*

  Advances in synthesis, characterization, and computation will open new doors to control, balance, and integrate novel materials and chemistries, enabling innovative designs for electrochemical energy storage.

- **Link complex electronic, electrochemical, and physical phenomena across time and space**

  Key questions: *What modeling frameworks can express the spatiotemporal evolution of material-chemical systems, across varying spatial and temporal scales? How can models inform experimental strategies to provide insight on electrochemical phenomena?*

  Electrochemistry involves dynamic phenomena that vary during charging and discharging and are heterogeneous over space and time. Understanding the temporal evolution of spatially distributed properties in electrochemical systems will advance next-generation energy storage.

- **Control and exploit the complex interphase region formed at dynamic interfaces**

  Key questions: *Can we characterize the chemical and material reactions and behaviors that comprise dynamic interfaces? How can interfaces be designed and synthesized to enhance storage performance and/or mitigate degradation?*

  As batteries charge and discharge, ions are transferred across multiple phase boundaries. During this process, interfaces between electrodes and electrolytes and at membranes undergo significant changes as a result of spontaneous chemical and imposed electrochemical reactions, often leading to degradation. Scientific insights that guide design of interfaces, and associated interphases, can improve battery performance and extend lifetimes.

- **Revolutionize energy storage performance through innovative assemblies of matter**

  Key questions: *What strategies can we use to exploit high-capacity electrode materials and higher voltage electrolyte chemistries while ensuring reliable cycling? What approaches are needed to perform design, characterization, and simulation at the mesoscale?*

  A major opportunity for innovation lies in understanding how to design and assemble nanoscale materials and structures into mesoscale architectures. New approaches are crucial to effectively manage the mesoscale effects of complex pathways in electrochemical systems.

- **Promote self-healing and eliminate detrimental chemistries to extend lifetime and improve safety**

  Key questions: *What drives the key degradation and failure mechanisms? How can these, and possible mitigation strategies, be revealed through modeling and characterization of representative and model systems?*

  The heart of electrochemical energy storage—ion transport through materials and across interfaces—presents an exceptional challenge to chemical and mechanical stability, as well as safety. Transformational science can uncover degradation mechanisms and discover pathways to mitigate them.

Summary

The Priority Research Directions outline the scientific advances that will usher in a new era of electrochemical energy storage with significantly higher performance, lower cost, greater reliability, and increased safety. These advances and innovations for energy storage will find immediate impact in critical applications across many sectors—transportation, the electricity grid, communication, and security.

The scientific directions presented build on rich opportunities in the synthesis of complex materials and architectures with designed functionality, characterization of materials as they perform and chemistries as they evolve, and predictive computer simulation to discover new materials and functionalities prior to laboratory production and testing. This is a new trajectory for electrochemical science, linking materials, chemistry, and functionality across multiple time and length scales to create new horizons of efficiency, performance, and cost.

The convergence of knowledge, techniques, and ideas outlined in this report provides unprecedented opportunities to advance next-generation energy storage through an exciting, vibrant, and powerful scientific agenda.

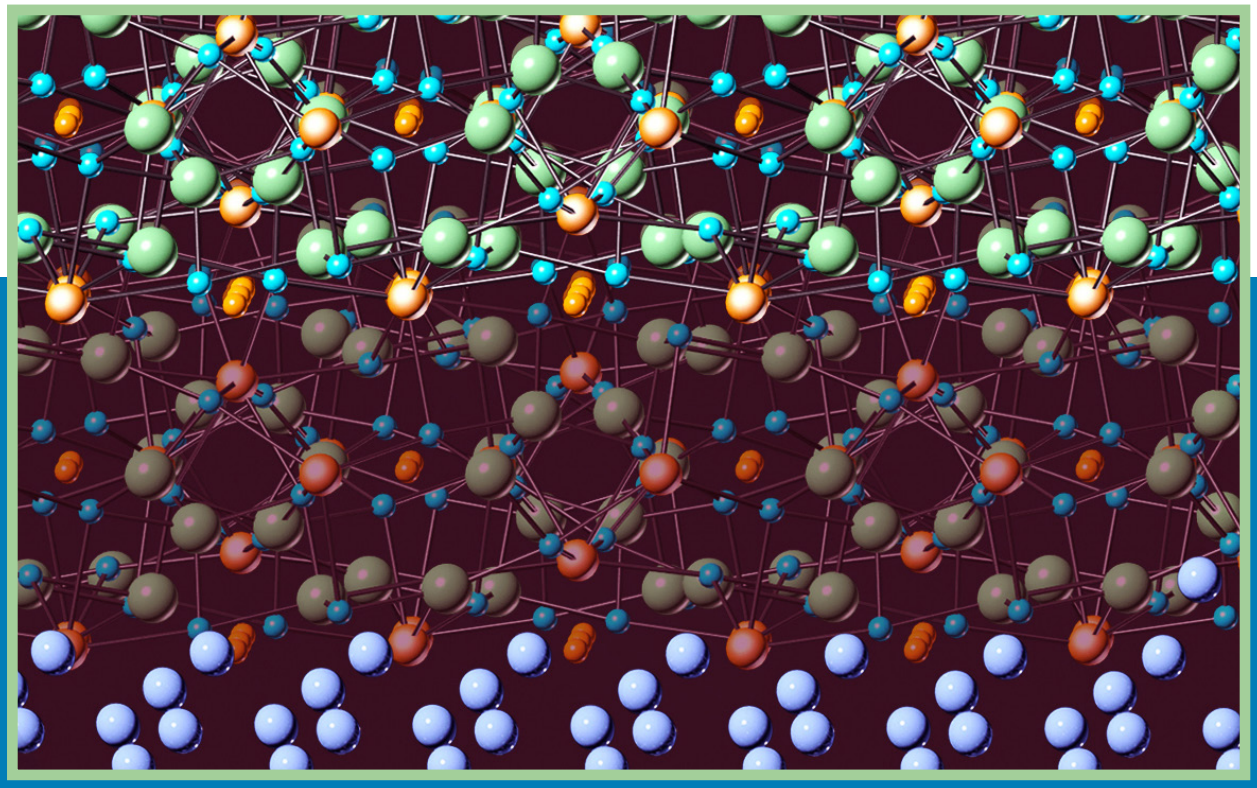


Image courtesy of Oak Ridge National Laboratory.

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