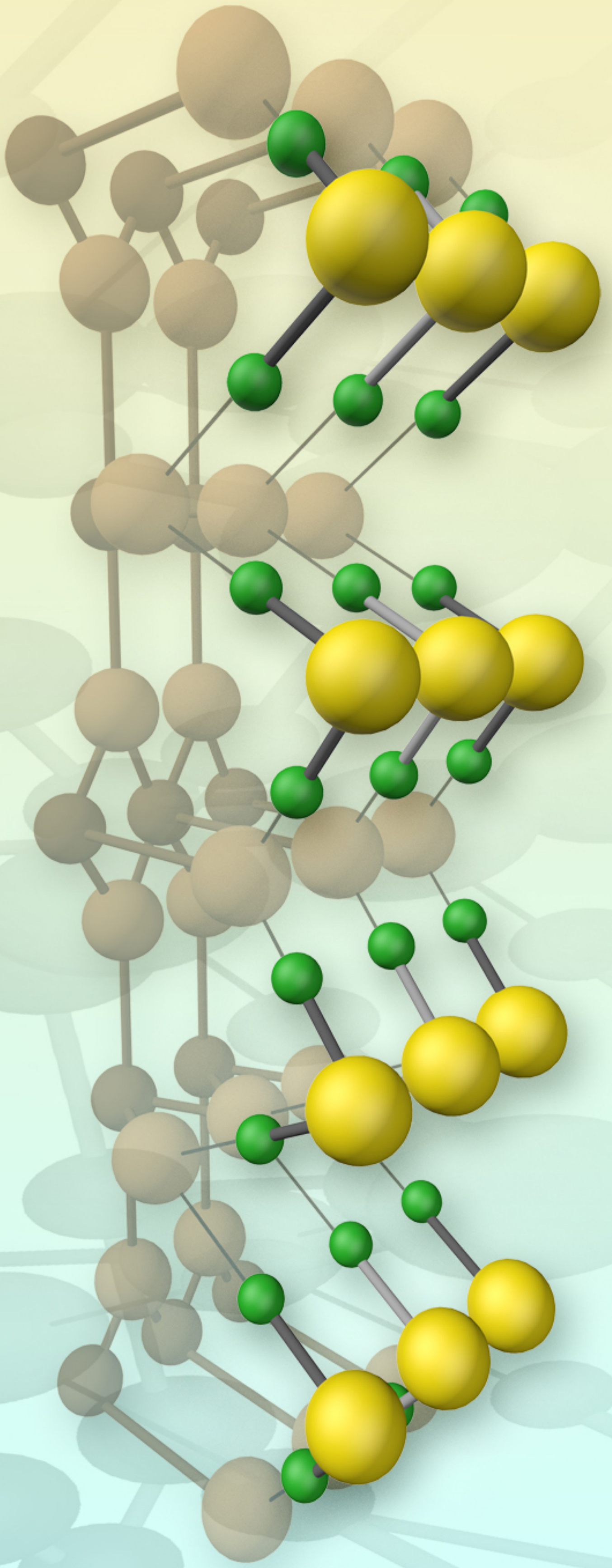

Basic Research Needs for Electrical Energy Storage

Report of the Basic Energy Sciences Workshop on Electrical Energy Storage

April 2-4, 2007

Office of Science
U.S. DEPARTMENT OF ENERGY

Office of Basic Energy Sciences
Serving the Present, Shaping the Future

CONTENTS

Page

EXECUTIVE SUMMARY OF THE DOE BASIC ENERGY SCIENCES WORKSHOP

BASIC RESEARCH NEEDS FOR ELECTRICAL ENERGY STORAGE

The projected doubling of world energy consumption within the next 50 years, coupled with the growing demand for low- or even zero-emission sources of energy, has brought increasing awareness of the need for efficient, clean, and renewable energy sources. Energy based on electricity that can be generated from renewable sources, such as solar or wind, offers enormous potential for meeting future energy demands. However, the use of electricity generated from these intermittent, renewable sources requires efficient electrical energy storage (EES). For commercial and residential grid applications, electricity must be reliably available 24 hours a day; even second-to-second fluctuations cause major disruptions with costs estimated to be tens of billions of dollars annually. Thus, for large-scale solar- or wind-based electrical generation to be practical, the development of new EES systems will be critical to meeting continuous energy demands and effectively leveling the cyclic nature of these energy sources. In addition, greatly improved EES systems are needed to progress from today’s hybrid electric vehicles to plug-in hybrids or all-electric vehicles. Improvements in EES reliability and safety are also needed to prevent premature, and sometimes catastrophic, device failure. Chemical energy storage devices (batteries) and electrochemical capacitors (ECs) are among the leading EES technologies today. Both are based on electrochemistry, and the fundamental difference between them is that batteries store energy in chemical reactants capable of generating charge, whereas electrochemical capacitors store energy directly as charge.

The performance of current EES technologies falls well short of requirements for using electrical energy efficiently in transportation, commercial, and residential applications. For example, EES devices with substantially higher energy and power densities and faster recharge times are needed if all-electric/plug-in hybrid vehicles are to be deployed broadly as replacements for gasoline-powered vehicles. Although EES devices have been available for many decades, there are many fundamental gaps in understanding the atomic- and molecular-level processes that govern their operation, performance limitations, and failure. Fundamental research is critically needed to uncover the underlying principles that govern these complex and interrelated processes. With a full understanding of these processes, new concepts can be formulated for addressing present EES technology gaps and meeting future energy storage requirements. The Office of Basic Energy Sciences (BES) within the Department of Energy (DOE) Office of Science convened a workshop April 2–4, 2007, charged with identifying basic research needs and opportunities underlying batteries, capacitors, and related EES technologies, with a focus on new or emerging science challenges with potential for significant long-term impact on the efficient storage and release of electrical energy.

Prior to the workshop, BES worked closely with the DOE Office of Energy Efficiency and Renewable Energy and the DOE Office of Electricity Delivery and Energy Reliability to clearly define future requirements for EES from the perspective of applications relevant to transportation and electricity distribution, respectively, and to identify critical technology gaps. In addition, leaders in EES industrial and applied research laboratories were recruited to prepare a technology resource document, *Technology and Applied R&D Needs for Electrical Energy Storage*, which provided the groundwork for and served as a basis to inform the deliberation of basic research discussions for the workshop attendees. The invited workshop attendees, numbering more than 130, included representatives from universities, national laboratories, and industry, including a significant number of scientists from Japan and Europe. A plenary session at the beginning of the workshop captured the present state of the art in research and development and technology needs required for EES for the future. The workshop participants were asked to identify key priority research directions that hold particular promise for providing needed advances that will, in turn, revolutionize the performance of EES. Participants were divided between two panels focusing on the major types of EES, chemical energy storage and capacitive energy storage. A third panel focused on cross-cutting research that will be critical to achieving the technical breakthroughs required to meet future EES needs. A closing plenary session summarized the most urgent research needs that were identified for both chemical and capacitive energy storage. The research directions identified by the panelists are presented in this report in three sections corresponding to the findings of the three workshop panels.

The panel on chemical energy storage acknowledged that progressing to the higher energy and power densities required for future batteries will push materials to the edge of stability; yet these devices must be safe and reliable through thousands of rapid charge-discharge cycles. A major challenge for chemical energy storage is developing the ability to store more energy while maintaining stable electrode-electrolyte interfaces. The need to mitigate the volume and structural changes to the active electrode sites accompanying the charge-discharge cycle encourages exploration of nanoscale structures. Recent developments in nanostructured and multifunctional materials were singled out as having the potential to dramatically increase energy capacity and power densities. However, an understanding of nanoscale phenomena is needed to take full advantage of the unique chemistry and physics that can occur at the nanoscale. Further, there is an urgent need to develop a fundamental understanding of the interdependence of the electrolyte and electrode materials, especially with respect to controlling charge transfer from the electrode to the electrolyte. Combining the power of new computational capabilities and in situ analytical tools could open up entirely new avenues for designing novel multifunctional nanomaterials with the desired physical and chemical properties, leading to greatly enhanced performance.

The panel on capacitive storage recognized that, in general, ECs have higher power densities than batteries, as well as sub-second response times. However, energy storage densities are currently lower than they are for batteries and are insufficient for many applications. As with batteries, the need for higher energy densities requires new materials. Similarly, advances in electrolytes are needed to increase voltage and conductivity while ensuring stability. Understanding how materials store and transport charge at electrode-electrolyte interfaces is critically important and will require a fundamental understanding of charge transfer and transport mechanisms. The capability to synthesize nanostructured electrodes with tailored, high-surface-area architectures offers the potential for storing multiple charges at a single site, increasing charge density. The addition of surface functionalities could also contribute to high and reproducible charge storage capabilities, as well as rapid charge-discharge functions. The design of new materials with tailored architectures optimized for effective capacitive charge storage will be catalyzed by new computational and analytical tools that can provide the needed foundation for the rational design of these multifunctional materials. These tools will also provide the molecular-level insights required to establish the physical and chemical criteria for attaining higher voltages, higher ionic conductivity, and wide electrochemical and thermal stability in electrolytes.

The third panel identified four cross-cutting research directions that were considered to be critical for meeting future technology needs in EES:

1. Advances in Characterization
2. Nanostructured Materials
3. Innovations in Electrolytes
4. Theory, Modeling, and Simulation

Exceptional insight into the physical and chemical phenomena that underlie the operation of energy storage devices can be afforded by a new generation of analytical tools. This information will catalyze the development of new materials and processes required for future EES systems. New in situ photon- and particle-based microscopic, spectroscopic, and scattering techniques with time resolution down to the femtosecond range and spatial resolution spanning the atomic and mesoscopic scales are needed to meet the challenge of developing future EES systems. These measurements are critical to achieving the ability to design EES systems rationally, including materials and novel architectures that exhibit optimal performance. This information will help identify the underlying reasons behind failure modes and afford directions for mitigating them.

The performance of energy storage systems is limited by the performance of the constituent materials—including active materials, conductors, and inert additives. Recent research suggests that synthetic control of material architectures (including pore size, structure, and composition; particle size and composition; and electrode structure down to nanoscale dimensions) could lead to transformational breakthroughs in key energy storage parameters such as capacity, power, charge-discharge rates, and lifetimes. Investigation of model systems of irreducible complexity will require the close coupling of theory and experiment in conjunction with well-defined structures to elucidate fundamental materials properties. Novel approaches are needed to develop multifunctional materials that are self-healing, self-regulating, failure-tolerant, impurity-sequestering, and sustainable. Advances in nanoscience offer particularly exciting possibilities for the development of revolutionary three-dimensional architectures that simultaneously optimize ion and electron transport and capacity.

The design of EES systems with long cycle lifetimes and high energy-storage capacities will require a fundamental understanding of charge transfer and transport processes. The interfaces of electrodes with electrolytes are astonishingly complex and dynamic. The dynamic structures of interfaces need to be characterized so that the paths of electrons and attendant trafficking of ions may be directed with exquisite fidelity. New capabilities are needed to “observe” the dynamic composition and structure at an electrode surface, in real time, during charge transport and transfer processes. With this underpinning knowledge, wholly new concepts in materials design can be developed for producing materials that are capable of storing higher energy densities and have long cycle lifetimes.

A characteristic common to chemical and capacitive energy storage devices is that the electrolyte transfers ions/charge between electrodes during charge and discharge cycles. An ideal electrolyte provides high conductivity over a broad temperature range, is chemically and electrochemically inert at the electrode, and is inherently safe. Too often the electrolyte is the weak link in the energy storage system, limiting both performance and reliability of EES. At present, the myriad interactions that occur in electrolyte systems—ion-ion, ion-solvent, and ion-electrode—are poorly understood. Fundamental research will provide the knowledge that will permit the formulation of novel designed electrolytes, such as ionic liquids and nanocomposite polymer electrolytes, that will enhance the performance and lifetimes of electrolytes.

Advances in fundamental theoretical methodologies and computer technologies provide an unparalleled opportunity for understanding the complexities of processes and materials needed to make the groundbreaking discoveries that will lead to the next generation of EES. Theory, modeling, and simulation can effectively complement experimental efforts and can provide insight into mechanisms, predict trends, identify new materials, and guide experiments. Large multiscale computations that integrate methods at different time and length scales have the potential to provide a fundamental understanding of processes such as phase transitions in electrode materials, ion transport in electrolytes, charge transfer at interfaces, and electronic transport in electrodes.

Revolutionary breakthroughs in EES have been singled out as perhaps the most crucial need for this nation’s secure energy future. The BES Workshop on Basic Research Needs for Electrical Energy Storage concluded that the breakthroughs required for tomorrow’s energy storage needs will not be realized with incremental evolutionary improvements in existing technologies. Rather, they will be realized only with fundamental research to understand the underlying processes involved in EES, which will in turn enable the development of novel EES concepts that incorporate revolutionary new materials and chemical processes. Recent advances have provided the ability to synthesize novel nanoscale materials with architectures tailored for specific performance; to characterize materials and dynamic chemical processes at the atomic and molecular level; and to simulate and predict structural and functional relationships using modern computational tools. Together, these new capabilities provide unprecedented potential for addressing technology and performance gaps in EES devices.